Chemistry–A European Journal

Supporting Information

Highly Oxidized States of Phthalocyaninato Terbium(III) Multiple-Decker Complexes Showing Structural Deformations, Biradical Properties and Decreases in Magnetic Anisotropy

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Author Contributions

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M.D. Data curation: Equal; Formal analysis: Equal; Funding acquisition: Supporting; Investigation: Equal; Visualization: Equal; Writing - Original Draft: Equal; Writing - Review & Editing: Equal; equal contributions to the first-first author: Lead
M.A. Formal analysis: Supporting; Methodology for isolation of oxidized complexes: Equal
K.K. Funding acquisition: Equal; Project administration: Equal; Resources: Supporting; Supervision: Equal
Y.K. Funding acquisition: Supporting; Natural orbital analyses: Lead
L.C. Advice and validation of CASSCF calculations: Equal
L.U. Advice and validation of CASSCF calculations: Equal
M.M. Funding acquisition: Supporting; Project administration: Supporting; Supervision: Supporting
W.W. Resources: Supporting; Supervision: Supporting
B.B. Writing - Original Draft: Supporting; Writing - Review & Editing: Supporting
M.E. Funding acquisition: Equal; Project administration: Equal; Resources: Equal; Supervision: Equal; Validation: Equal
J.V. Conceptualization: Supporting; Funding acquisition: Equal; Project administration: Equal; Supervision: Equal; Validation: Equal
M.Y. Conceptualization: Lead; Funding acquisition: Lead; Project administration: Equal; Resources: Lead; Supervision: Equal; Validation: Equal.

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1. Experimental Section

4-tert-Butyltoluene and phenoxathiin were purchased from Tokyo Chemical Industry and Kanto Chemical, respectively. 1 M antimony pentachloride in CH_2Cl_2 was purchased from Sigma-Aldrich. The deuterated solvent CD_2Cl_2 (Sigma-Aldrich, 99.9% deuteration) was dried with conventional methods (3 Å molecular sieves) and degassed before use. All other reagents including the solvent used for column chromatography were purchased from FUJIFILM Wako Pure Chemical Corporation. All reagents were used without further purification. The obPc ligand, $\mathbf{[3]^0}$, $\mathbf{[4]^0}$ and $\mathbf{[5]^0}$ were synthesized according to literature methods[1-2], using reagents purchased from Wako chemicals.

Synthesis for phenoxathiin hexachloroantimonate Ox·$SbCl_6$

To a 30 mL Schlenk flask, phenoxathiin (1.0 g, 5.0 mmol) and dried CH_2Cl_2 (10 mL) were added in a flow of N_2 gas. Addition of 1 M $SbCl_5/CH_2Cl_2$ solution (6 mL, 6 mmol) gave a blue solid. The solvent was removed, the blue solid was washed three times with of CH_2Cl_2 (20 mL) and dried in vacuum (yield: 83%, 2.22 g). Elemental analysis calculated (%) for $C_{12}H_8SOSbCl_6$: C 26.95, H 1.51, N 0.00; found: C 27.02, H 1.60, N 0.00.

Chemical synthesis for $[3]^{2+}$

$\mathbf{[3]^0}$ (44 mg, 0.012 mmol), Ox·$SbCl_6$ (16 mg, 0.030 mmol) and toluene (2 mL) were added to a 10 mL screw vial and mixed using ultrasonication. The resulting oily compound was stored at ca. 20 °C for 1 week, affording the crystalline sample of $\mathbf{[3]^{2+}}$ (yield: 88%, 46 mg). Elemental analysis calculated (%) for $C_{192}H_{240}N_{24}O_{24}Tb_2Sb_2Cl_{12}$: C 54.20, H 5.69, N 7.90; found: C 54.13, H 5.63, N 7.76.

Chemical synthesis for $[4]^{2+}$

$\mathbf{[4]^0}$ (5.04 mg, 1.1 mmol) and Ox·$SbCl_6$ (1.15 mg, 2.2 mmol) were mixed in 1,1,2,2-tetrachloroethane (TCE) (0.5 mL) by ultrasonication. Slow diffusion of excess 4-tert-butyltoluene (TBT) to the solution for ca. 1 week gave the crystalline sample of $\mathbf{[4]^{2+}}$ (yield: 78%, 4.5 mg). Elemental analysis calculated (%) for $\mathbf{[4]^{2+}}$ containing 0.5 equivalents of TCE $C_{257}H_{321}N_{32}O_{32}Tb_2CdSb_2Cl_{14}$: C 55.71, H 5.84, N 8.09; found: C 55.63, H 5.81, N 8.01.

Chemical synthesis for $[4]^{4+}$

$\mathbf{[4]^0}$ (5.78 mg, 1.21 mmol) and Ox·$SbCl_6$ (2.89 mg, 5.4 mmol) were mixed in TCE (0.5 mL) by ultrasonication. Slow diffusion of excess TBT to the solution during ca. 1 week gave the crystalline sample of $\mathbf{[4]^{4+}}$ (yield: 84%,6.2 mg). Elemental analysis calculated (%) for $\mathbf{[4]^{4+}}$ containing 0.2 equivalent of TBT $C_{262.6}H_{329.6}N_{32}O_{32}Tb_2CdSb_4Cl_{24}$: C 50.75, H 5.35, N 7.21; found: C 50.53, H 5.16, N 6.91.

Chemical synthesis for $[5]^{4+}$

$\mathbf{[5]^0}$ (5.77 mg, 0.96 mmol) and Ox·$SbCl_6$ (2.29 mg, 4.3 mmol) were mixed in TCE (0.5 mL) by ultrasonication. Slow diffusion of excess benzene to the solution over ca. 1 week gave the crystalline sample of $\mathbf{[5]^{4+}}$ (yield: 82%, 5.8 mg). This sample spontaneously melts after drying because of the remaining 1,1,2,2-TCE. For collection of samples, we replaced the mother liquor with pure benzene by centrifuging and exchanging the solvent. Elemental analysis calculated (%) for $C_{320}H_{400}N_{40}O_{40}Tb_2Cd_2Sb_4Cl_{24}$: C 52.45, H 5.50, N 7.65; found: C 52.26, H 5.44, N 7.53.

Measurement and Calculation Details

Bulk electrolysis was conducted using a Metrohm Autolab PGSTAT101 and an ALS Model 2325 Bi-potentiostat with the Ag/Ag^+ reference eletrode, platinum working electrode and platinum reference electrode separated by vycor bridge under N_2 atmosphere. UV-Vis-NIR absorption spectra were acquired using an Agilent Cary 5000 UV-Vis-NIR and a SHIMADZU UV-3100PC in a quartz cell with a path length of 1 mm at room temperature.

For electrochemical UV-Vis-NIR measurements, the reaction solution of the bulk electrolysis was transferred to a sealed quartz cell using a Hamilton syringe. NMR spectra were recorded at a magnetic field of 9.4 T with a Bruker Avance II instrument equipped with a BBO probehead and at a magnetic field of 14.09 T with a Bruker Avance III instrument equipped with a cryo-probehead. SXRD measurements were performed using a Rigaku Varimax with Saturn724+ with CrysAlisPro 3.9[3] and a Rigaku VariMax with RAPID II with RAPID AUTO. Initial structures were obtained using SHELXT (2014/7) and refined with SHELXL (2014/7)[4] combined with Yadokari-XG[5]. Powder X-ray diffraction pattern was acquired by Rigaku RINT-2000 with a glass capillary. Magnetic measurements were performed on Quantum Design SQUID magnetometers MPMS2, MPMS-XL and MPMS3. Details about the DFT and *ab initio* ligand field calculations are given in section 4 and 5, respectively.

2. SQUID Measurements

2.1. Triple-Deckers **[3]**

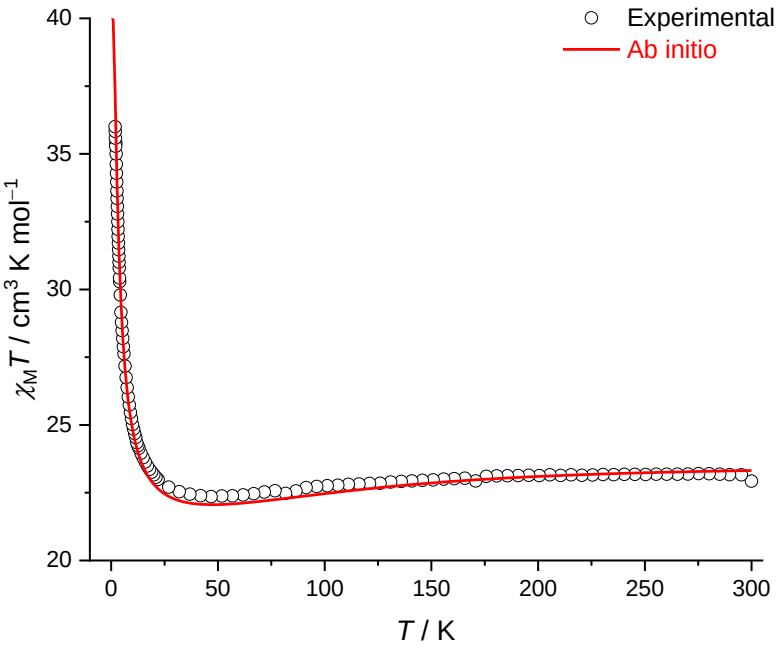

Fig. S1. $\chi_M T$ vs T plots for **[3]^0** at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio caculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure.

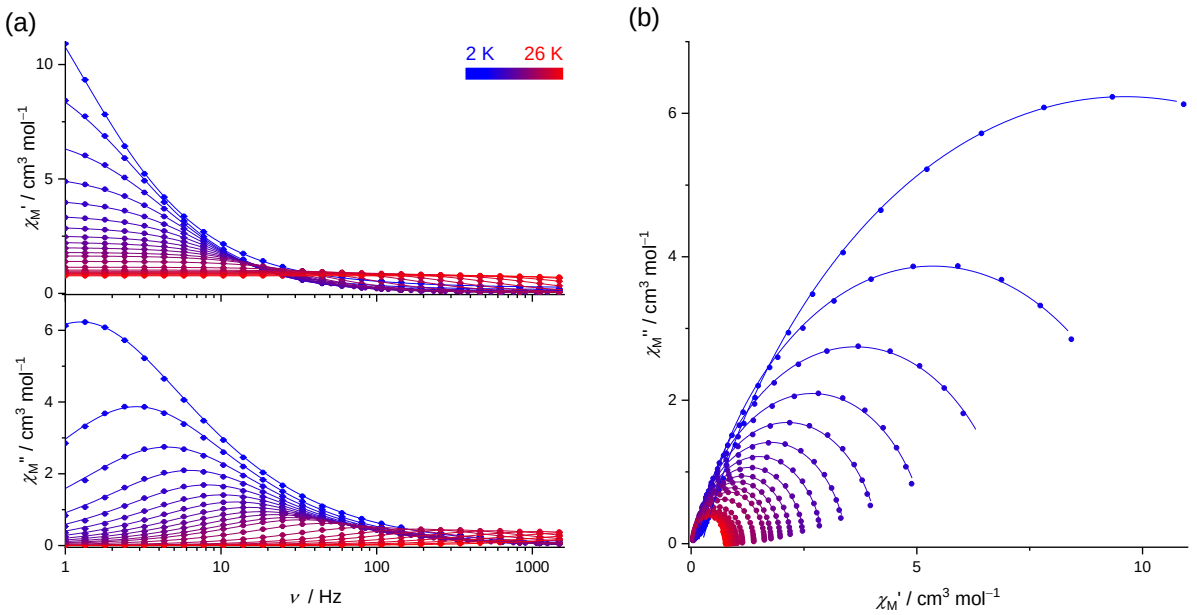

Fig. S2. (a) AC magnetic susceptibilities and (b) Argand plots of **[3]^{0}** at 0 Oe. Solid curves represent the fit using generalized Debye model equations.

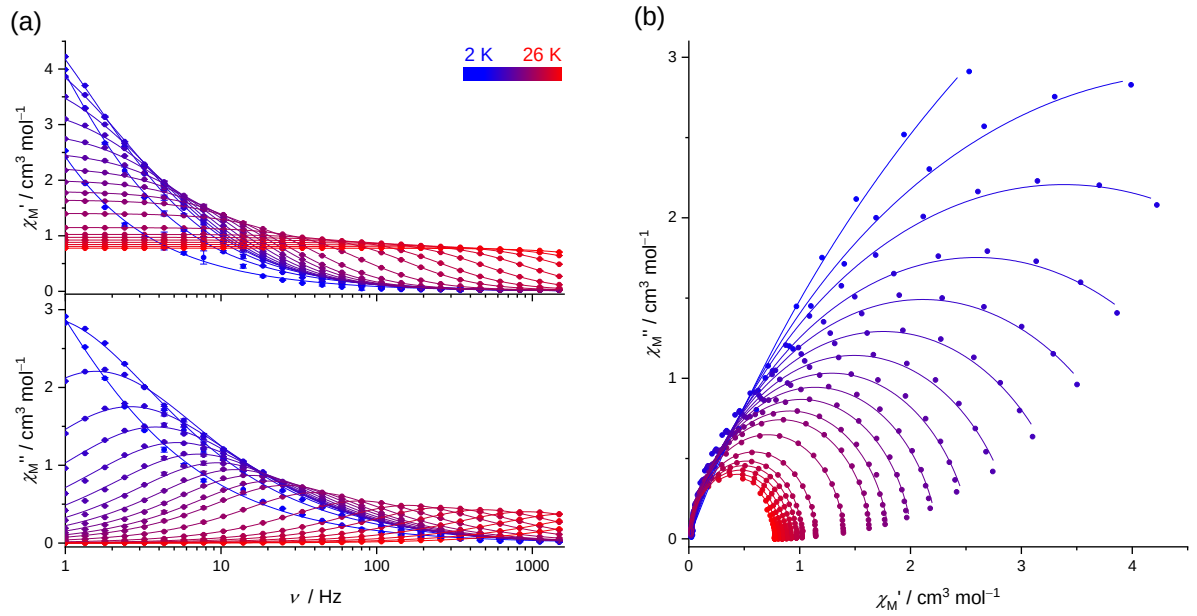

Fig. S3. (a) AC magnetic susceptibilities and (b) Argand plots of **[3]^{0}** at 2 kOe. Solid curves represent the fit using generalized Debye model equations.

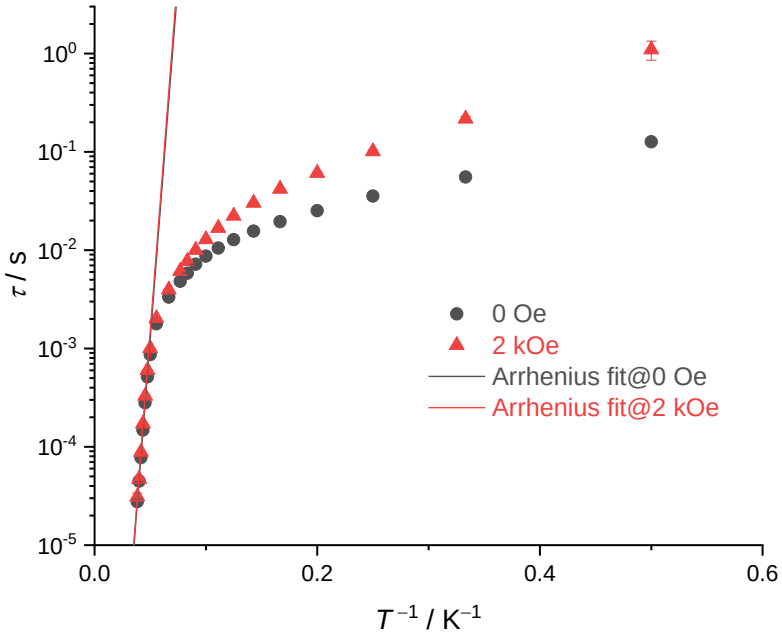

Fig. S4. (a) Arrhenius plots for **[3]^0** with and without a dc magnetic field. Solid lines represent Arrhenius fits using $\Delta E = 231(3)$ cm^{-1} and $\tau_0 = 8(2) \times 10^{-11}$ s at 0 Oe and $\Delta E = 233(5)$ cm^{-1} and $\tau_0 = 8(2) \times 10^{-11}$ s at 2 kOe.

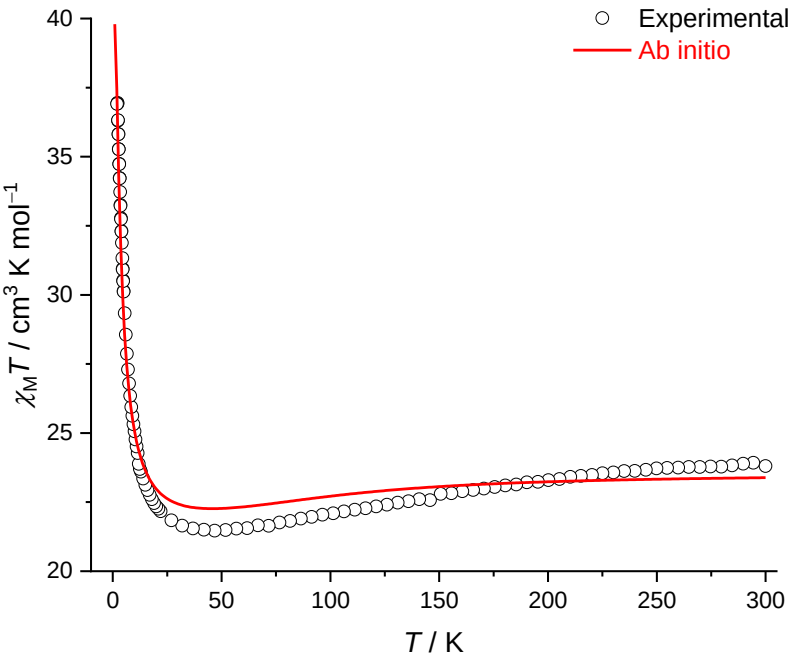

Fig. S5. $\chi_M T$ vs T plots for **[3]**$^{2+}$ at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio calculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure.

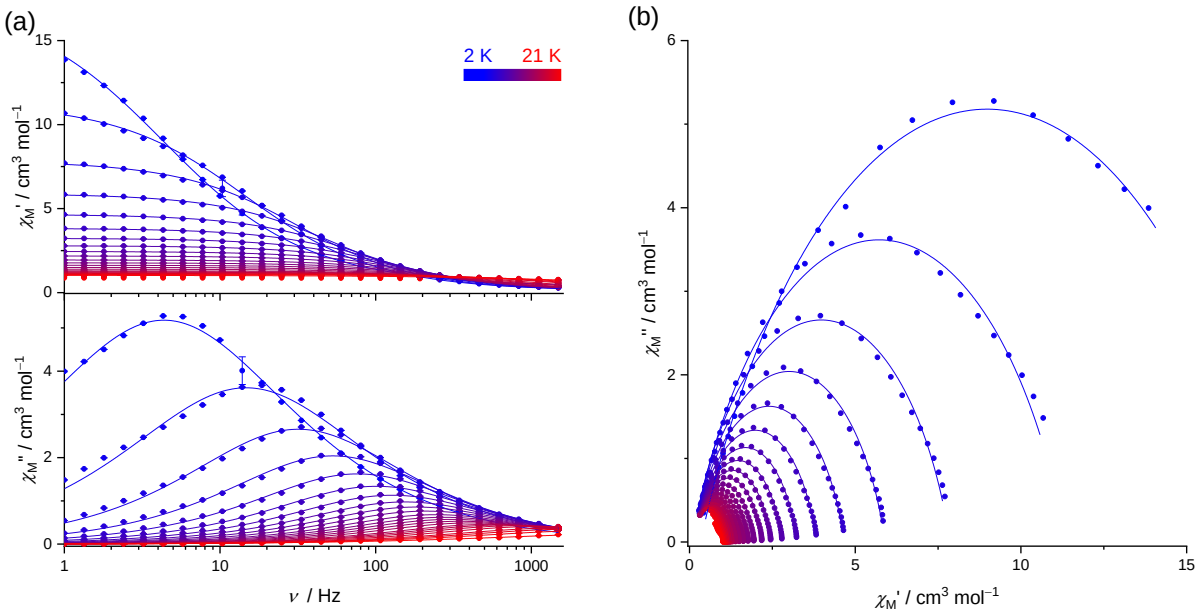

Fig. S6. (a) AC magnetic susceptibilities and (b) Argand plots of **[3]**$^{2+}$ at 0 Oe. Solid curves represent the fit using generalized Debye model equations.

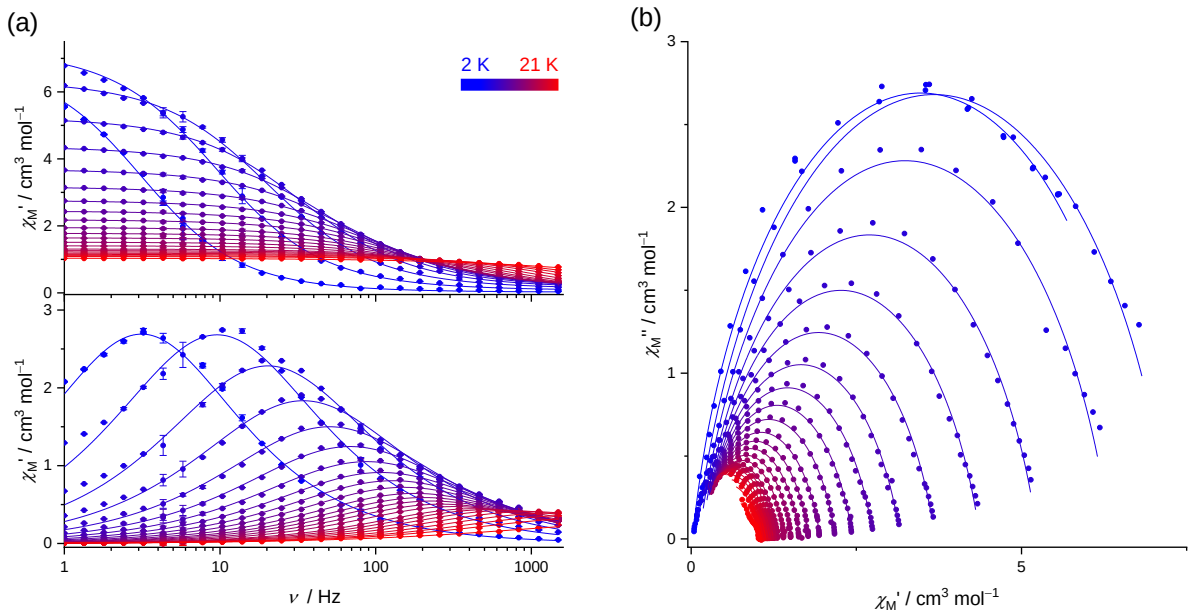

Fig. S7. (a) AC magnetic susceptibilities and (b) Argand plots of **[3]**$^{2+}$ at 2 kOe. Solid curves represent the fit using generalized Debye model equations.

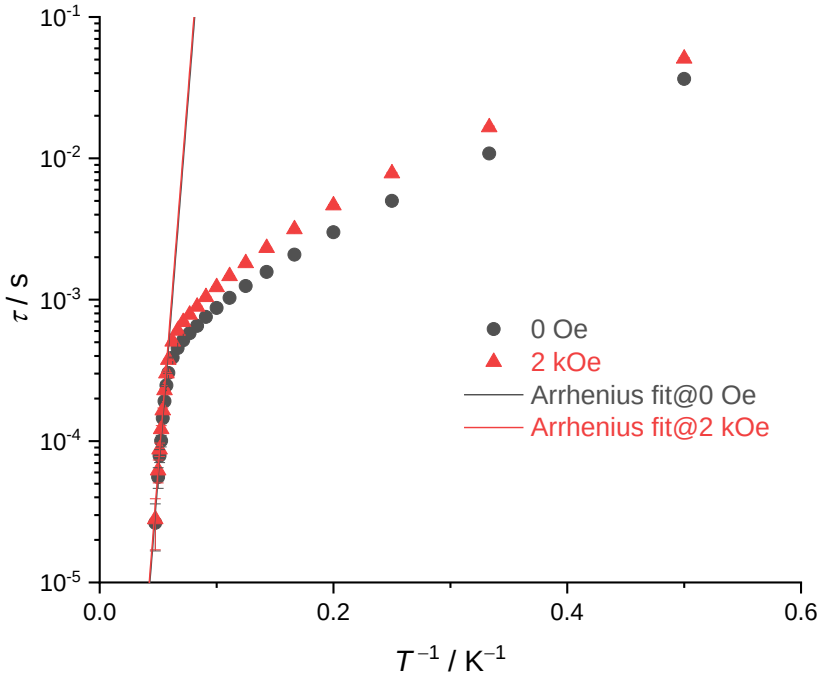

Fig. S8. (a) Arrhenius plots for **[3]**$^{2+}$ with and without a dc magnetic field. Two kinds of τ are shown since **[3]**$^{2+}$ shows dual magnetic relaxations at 0 Oe. Solid line represent the Arrhenius fit using ΔE = 167(7) cm^{-1} and τ_0 = 3(2) × 10^{-10} s at 0 Oe and ΔE = 167(9) cm^{-1} and τ_0 = 4(3) × 10^{-10} s at 2 kOe.

2.2. Quadruple-Deckers **[4]**

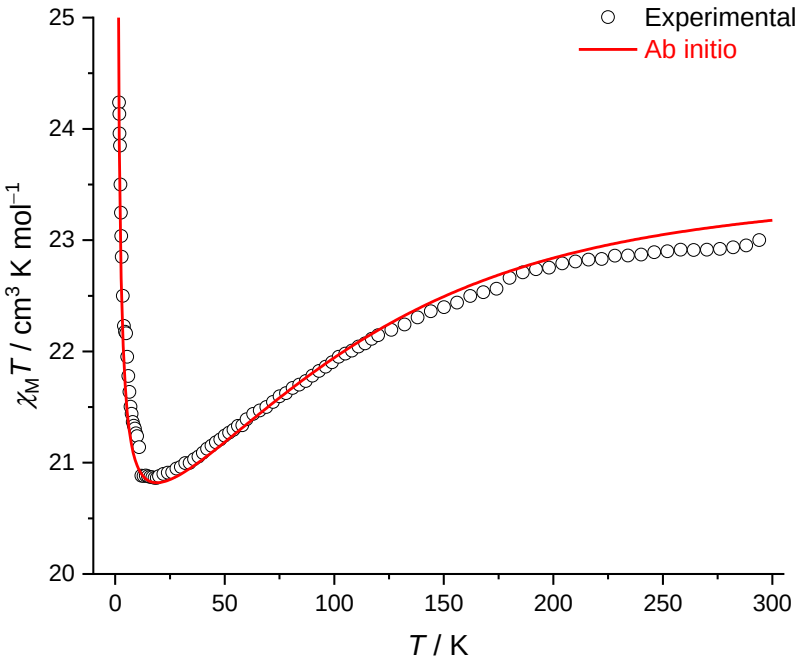

Fig. S9. $\chi_M T$ vs T plots for **[4]^0** at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio calculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure.

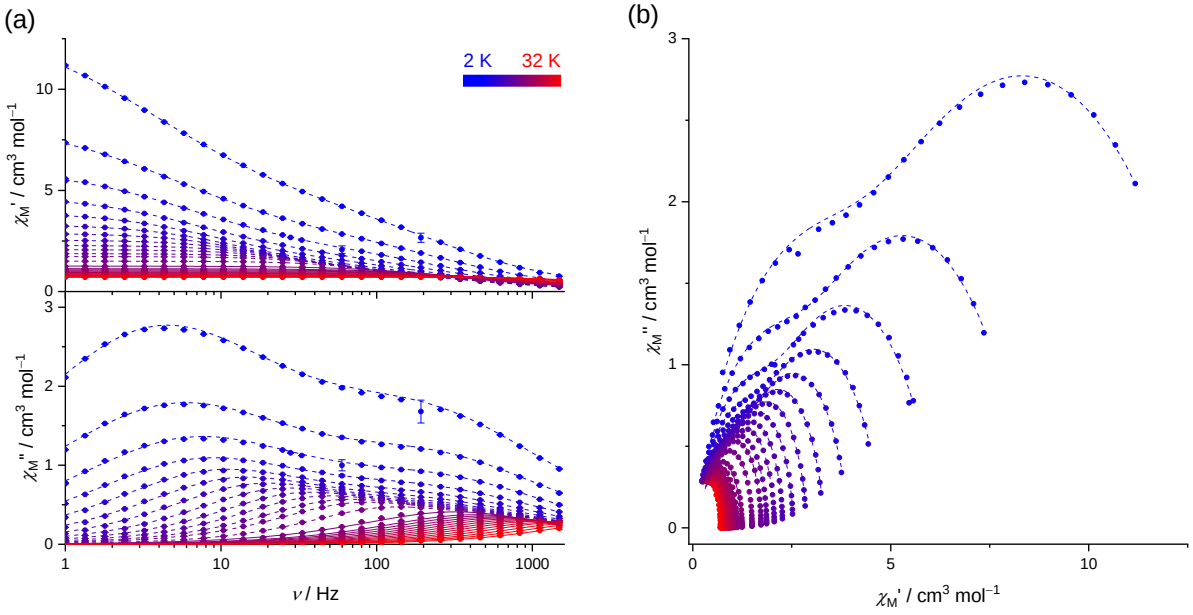

Fig. S10. (a) AC magnetic susceptibilities and (b) Argand plots of **[4]^0** at 0 Oe. Solid curves and dashed curves represent the fit using generalized and extended Debye model equations respectively.

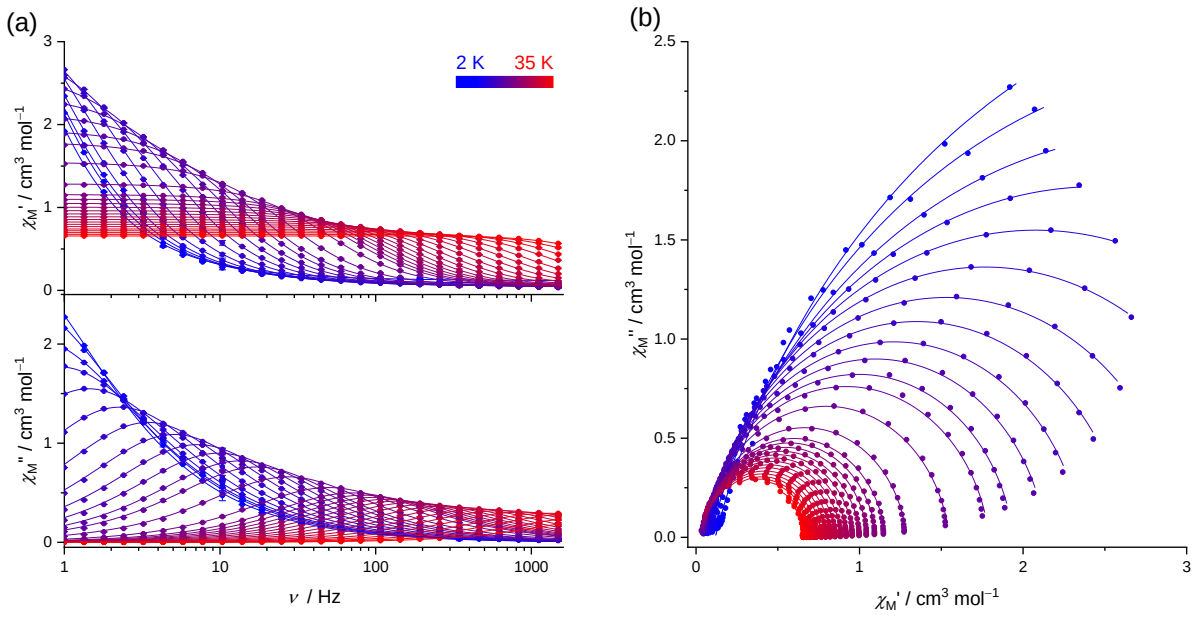

Fig. S11. (a) AC magnetic susceptibilities and (b) Argand plots of **[4]^0** at 2 kOe. Solid curves represent the fit using generalized Debye model equations.

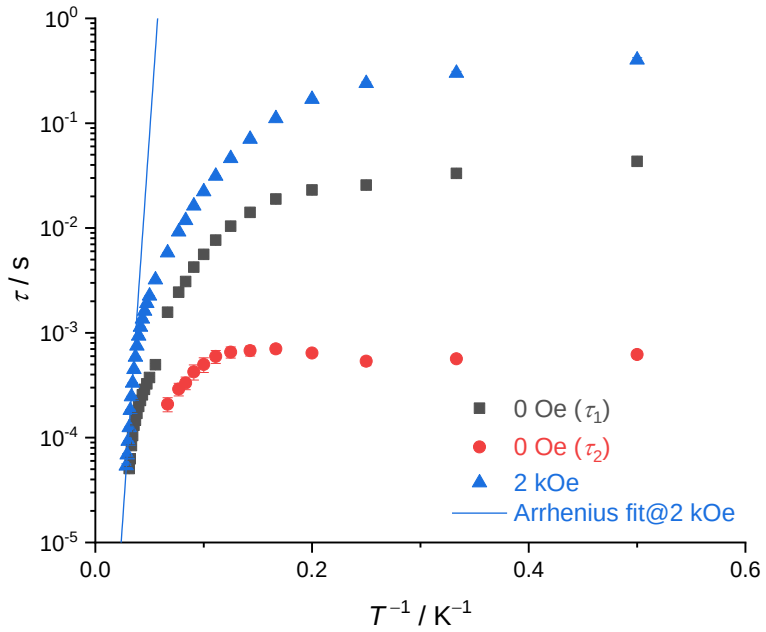

Fig. S12. (a) Arrhenius plots for **[4]^0** with and without a dc magnetic field. Two kinds of τ are shown since **[4]^0** shows dual magnetic relaxations at 0 Oe. Solid line represent the Arrhenius fit at 2 kOe using $\Delta E = 237(6)$ cm^{-1} and $\tau_0 = 3.0(8) \times 10^{-9}$ s.

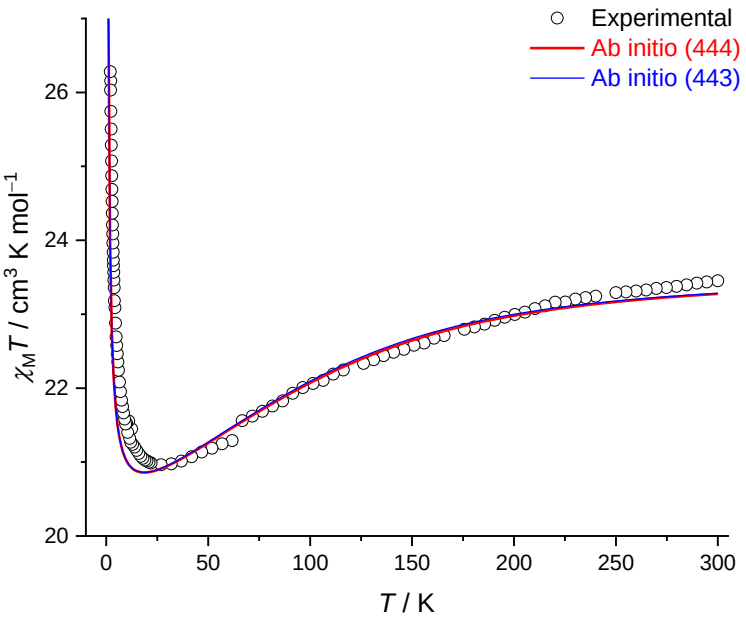

Fig. S13. $\chi_M T$ vs T plots for **[4]**$^{2+}$ at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio calculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure. The contribution of the biradical was not included in the calculations.

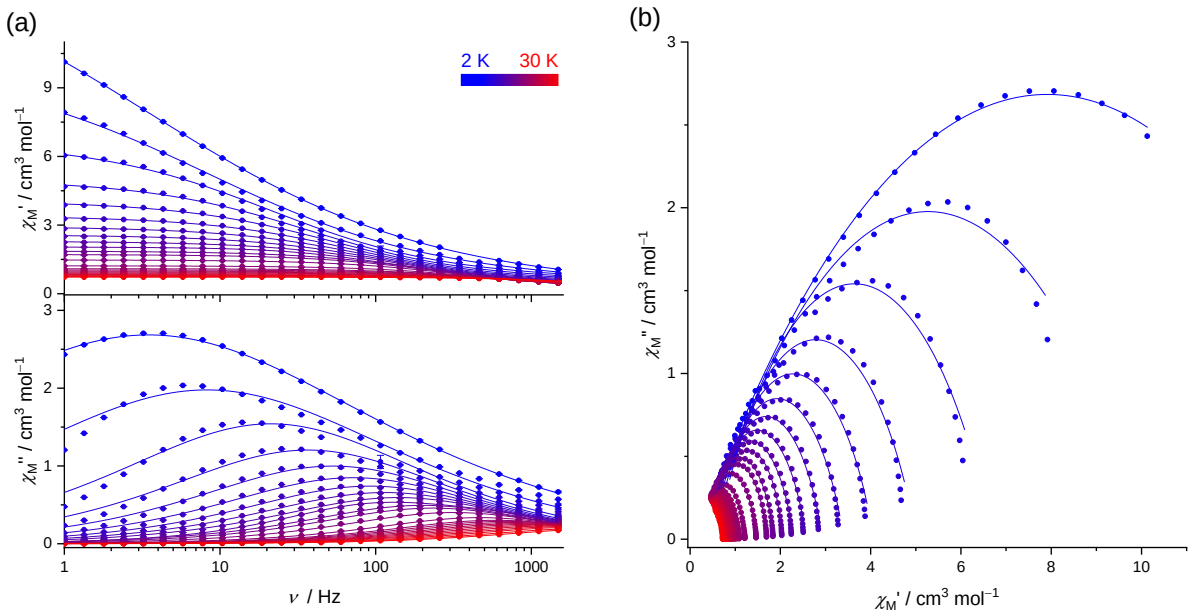

Fig. S14. (a) AC magnetic susceptibilities and (b) Argand plots of **[4]**$^{2+}$ at 0 Oe. Solid curves and dashed curves represent the fit using generalized and extended Debye model equations, respectively.

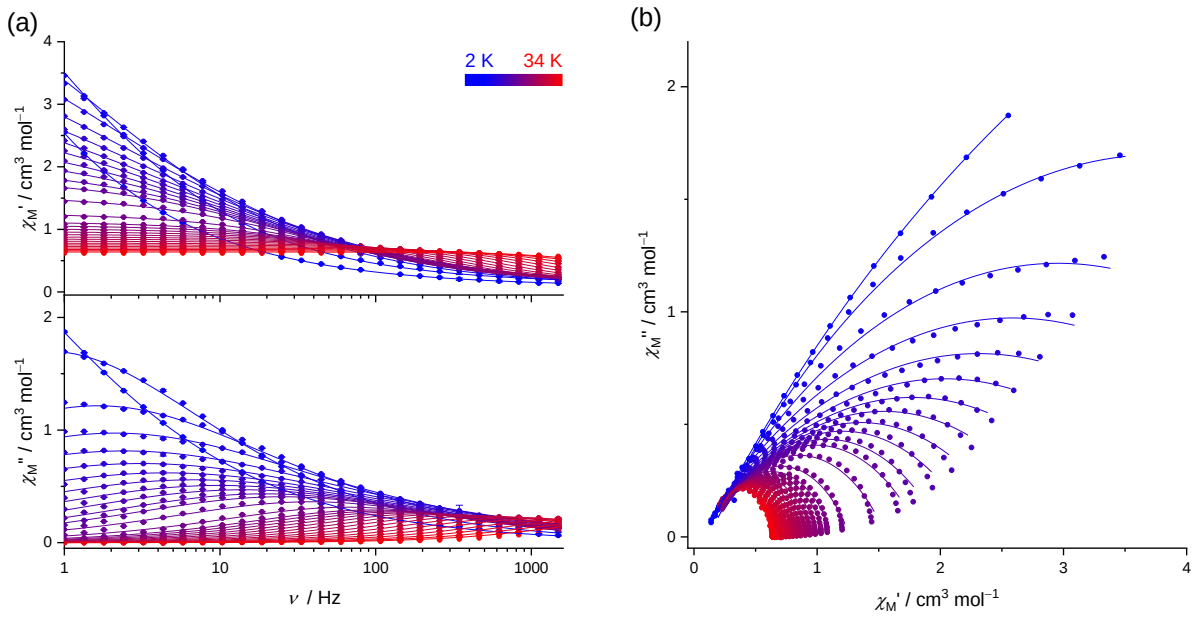

Fig. S15. (a) AC magnetic susceptibilities and (b) Argand plots of **[4]**$^{2+}$ at 2 kOe. Solid curves represent the fit using generalized Debye model equations.

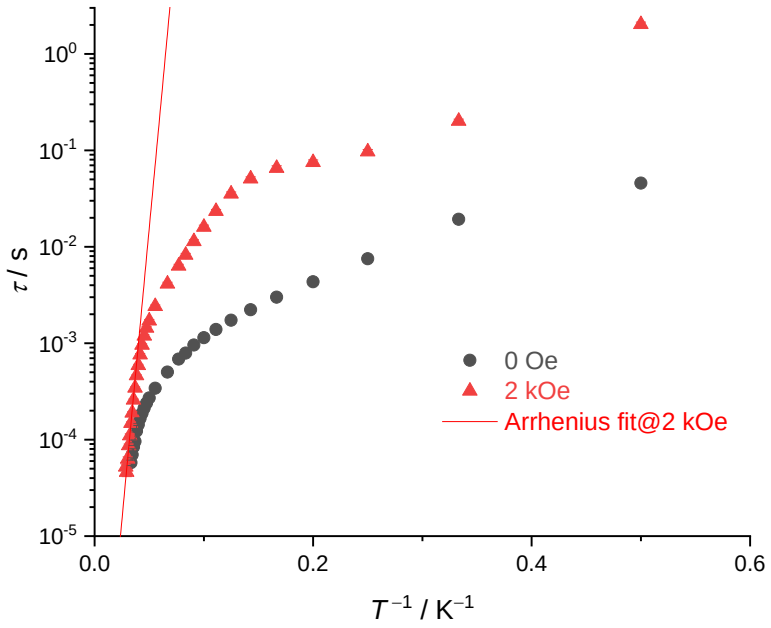

Fig. S16. (a) Arrhenius plots for **[4]**$^{2+}$ with and without a dc magnetic field. Solid line represent the Arrhenius fit at 2 kOe using ΔE = 194(9) cm^{-1} and τ_0 = 1.4(6) × 10^{-9} s.

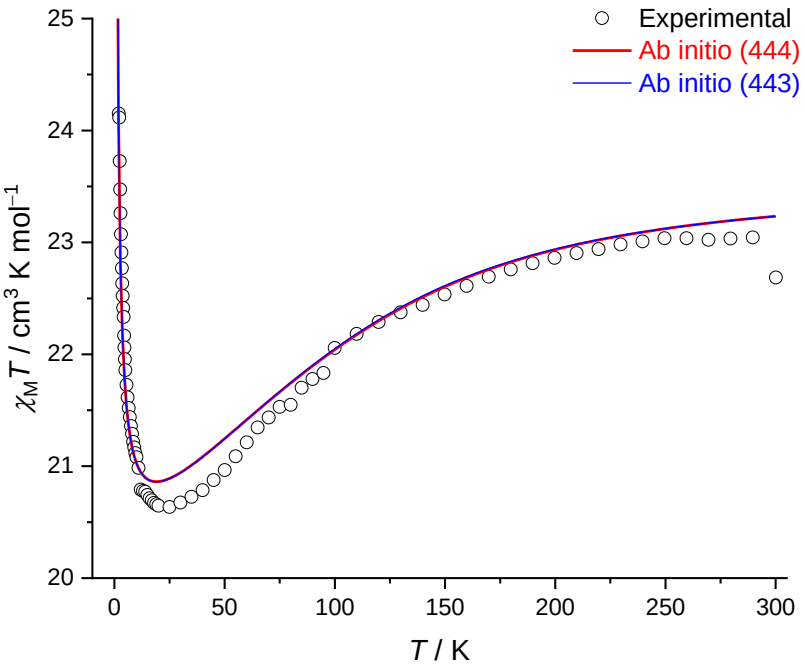

Fig. S17. $\chi_M T$ vs T plots for **[4]**$^{4+}$ at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio calculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure.

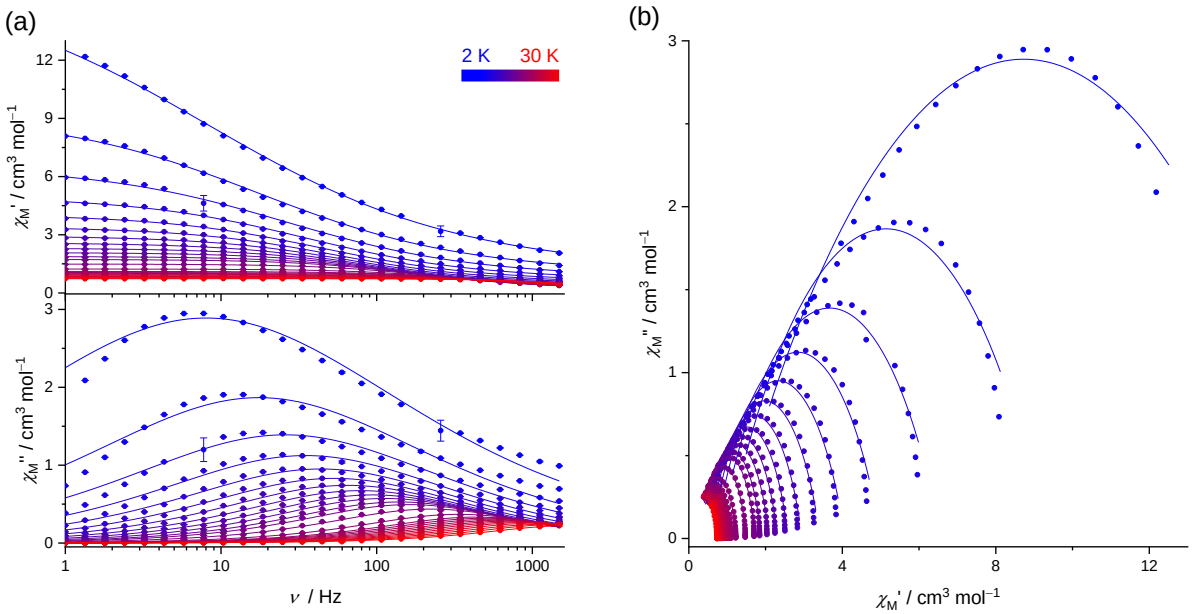

Fig. S18. (a) AC magnetic susceptibilities and (b) Argand plots of **[4]**$^{4+}$ at 0 Oe. Solid curves and dashed curves represent the fit using generalized and extended Debye model equations, respectively.

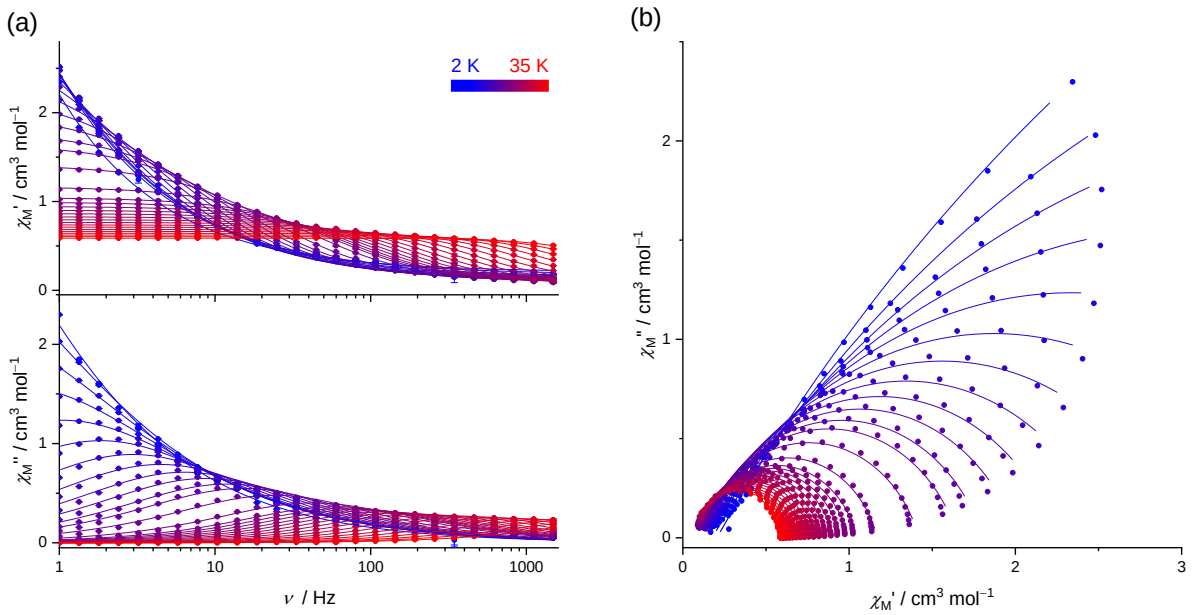

Fig. S19. (a) AC magnetic susceptibilities and (b) Argand plots of **[4]**$^{4+}$ at 2 kOe. Solid curves and dashed curves represent the fit using generalized and extended Debye model equations, respectively.

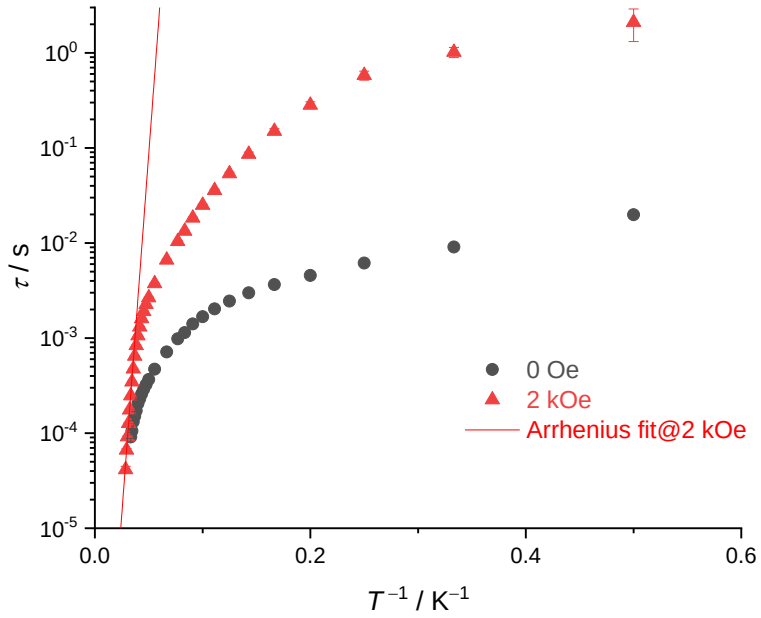

Fig. S20. (a) Arrhenius plots for **[4]**$^{4+}$ with and without dc magnetic field. Solid line represents the Arrhenius fit at 2 kOe using $\Delta E = 242(11)$ cm^{-1} and $\tau_0 = 2(1) \times 10^{-9}$ s.

2.3. Quintuple-Deckers **[5]**

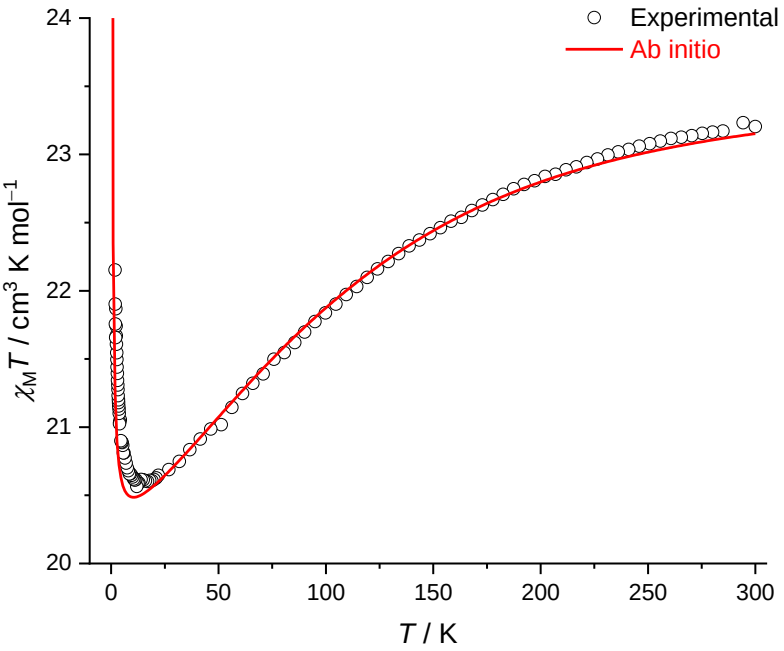

Fig. S21. $\chi_M T$ vs T plots for **[5]^0** at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio calculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure.

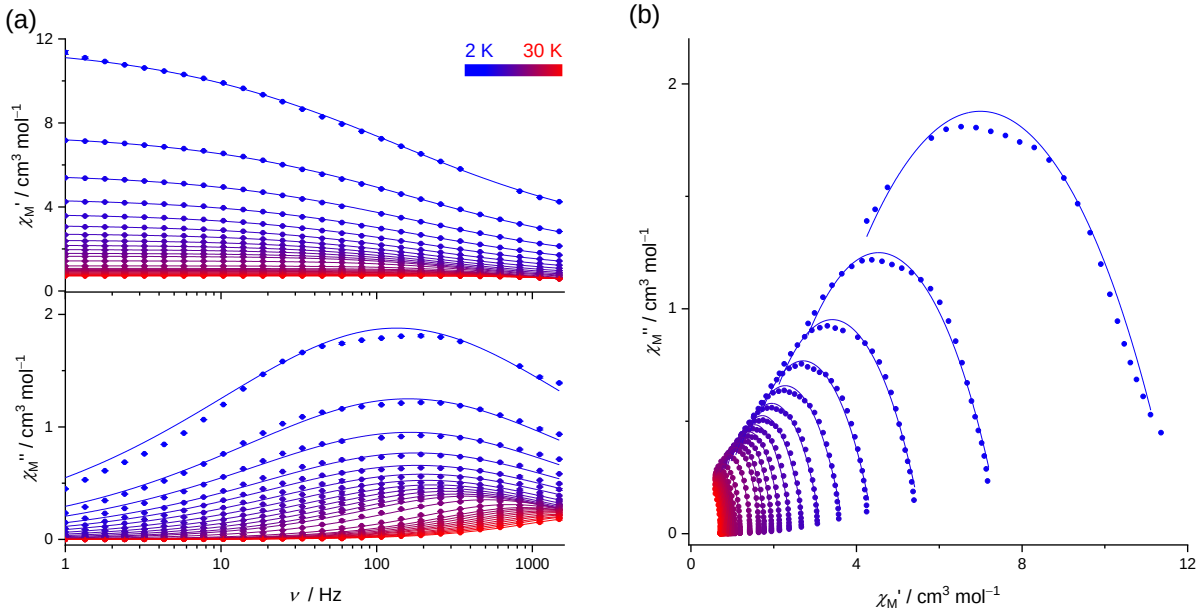

Fig. S22. (a) AC magnetic susceptibilities and (b) Argand plots of **[5]^0** at 0 Oe. Solid curves represent the fit using generalized Debye model equations.

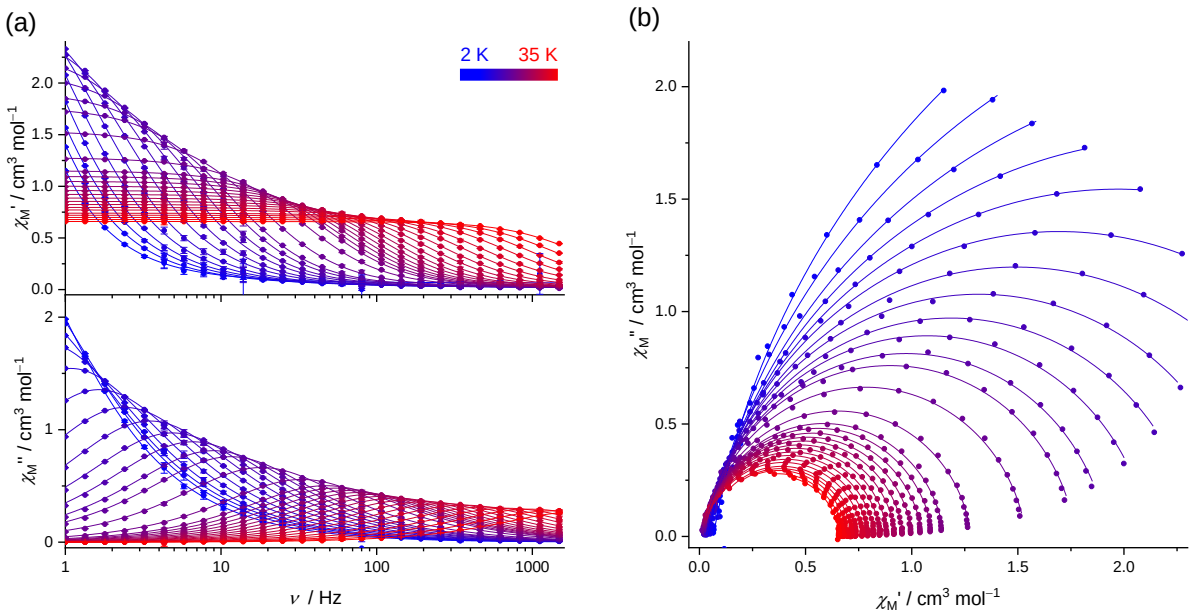

Fig. S23. (a) AC magnetic susceptibilities and (b) Argand plots of **[5]^0** at 2 kOe. Solid curves represent the fit using generalized Debye model equations.

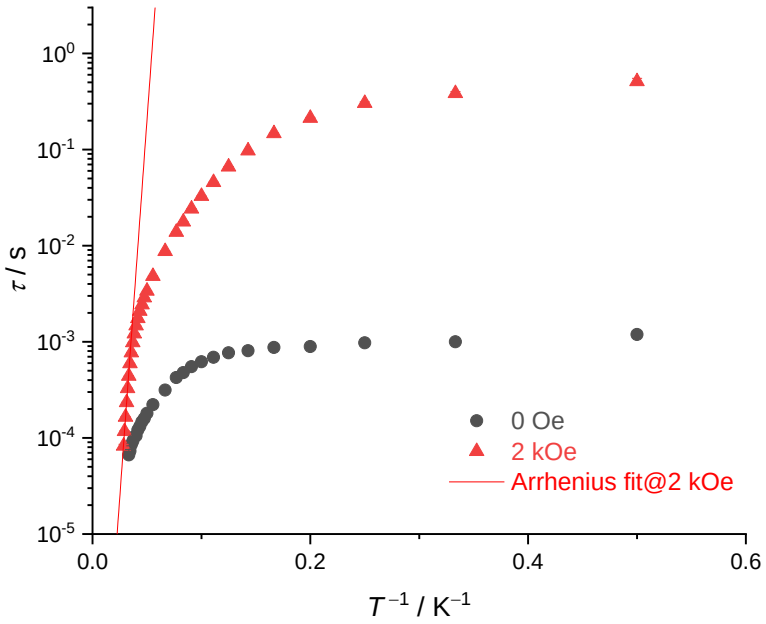

Fig. S24. (a) Arrhenius plots for **[5]^0** with and without dc magnetic field. Two kinds of τ are shown since **[5]^0** shows dual magnetic relaxations at 0 Oe. Solid line represent the Arrhenius fit at 2 kOe using $\Delta E = 251(6)$ cm^{-1} and $\tau_0 = 2.9(7) \times 10^{-9}$ s.

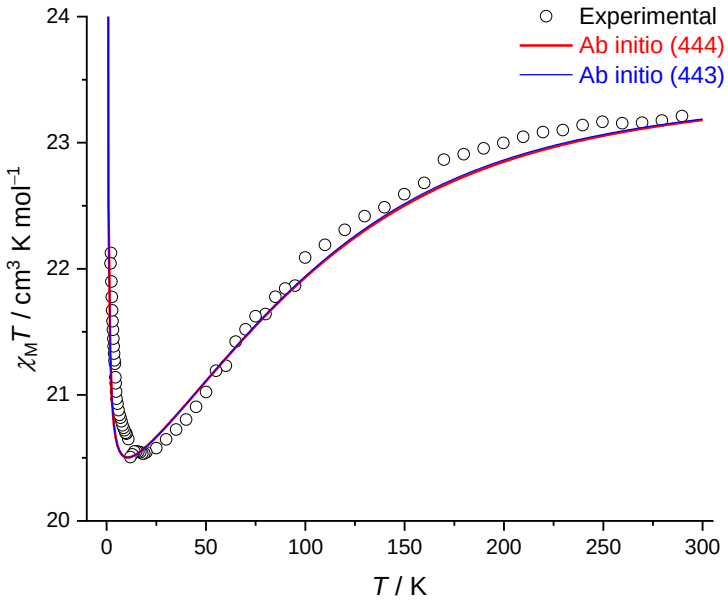

Fig. S25. $\chi_M T$ vs T plots for **[5]**$^{4+}$ at 1 kOe dc field. Intramolecular magnetic dipole-dipole interactions between Tb(III) ions were taken into account in ab initio calculations by using the poly_aniso[6-7] module with the position of Tb(III) ions in the crystal structure.

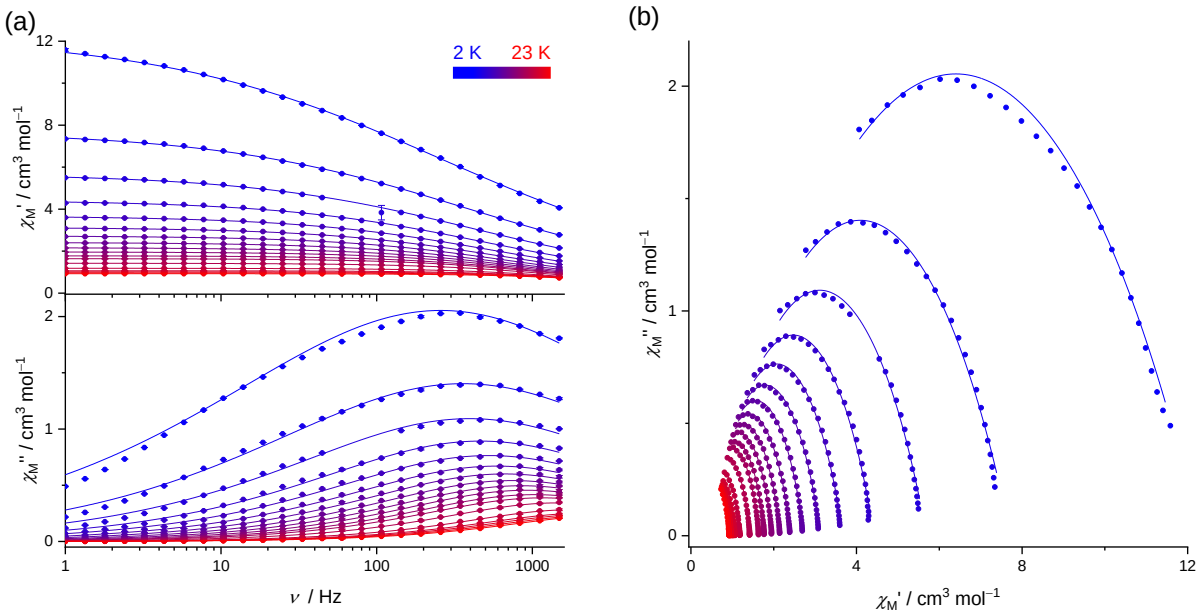

Fig. S26. (a) AC magnetic susceptibilities and (b) Argand plots of **[5]**$^{4+}$ at 0 Oe. Solid curves represent the fit using generalized Debye model equations.

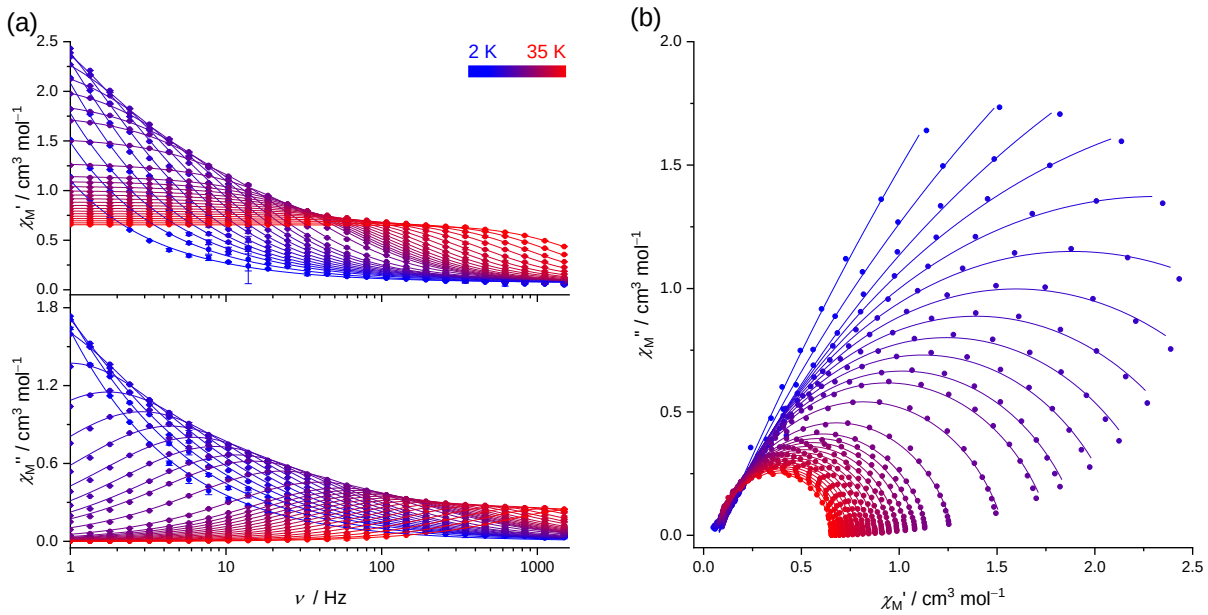

Fig. S27. (a) AC magnetic susceptibilities and (b) Argand plots of **[5]**$^{4+}$ at 2 kOe. Solid curves represent the fit using generalized Debye model equations.

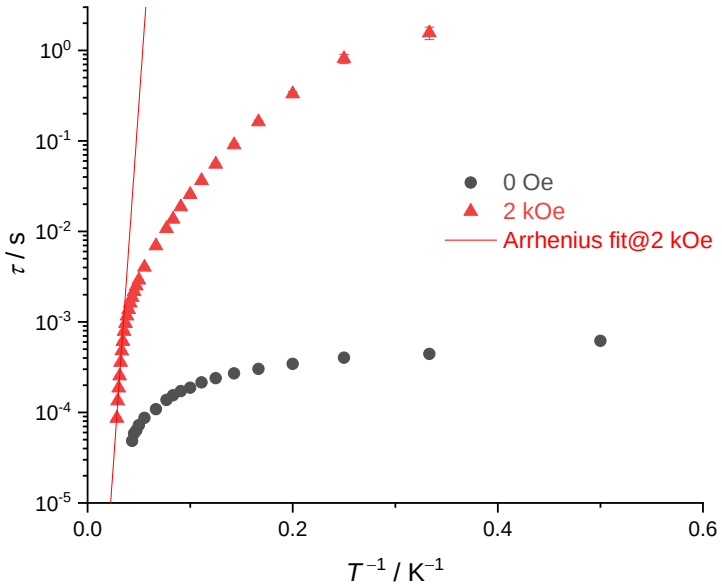

Fig. S28. (a) Arrhenius plots for **[5]**$^{4+}$ with and without a dc magnetic field. Two kinds of τ are shown since **[5]**$^{4+}$ shows dual magnetic relaxations at 0 Oe. Solid line represents the Arrhenius fit at 2 kOe using ΔE = 256(13) cm^{-1} and $\tau_0 = 2.5(15) \times 10^{-9}$ s.

3. NMR Measurements

3.1. General Information

NMR spectra were recorded at a magnetic field of 9.4 T with a Bruker Avance II instrument equipped with a BBO probehead (for variable temperature ^{1}H measurements) and at a magnetic field of 14.09 T with a Bruker Avance III instrument equipped with a cryo-probehead. Solvent resonances were taken as references for all ^{1}H and ^{13}C NMR spectra.[8] For variable temperature measurements, temperature calibration was done using the method of Berger *et al*.[9] Samples were prepared in an inert gas atmosphere (in a glovebox with either argon or nitrogen gas) and stored in Teflon-sealed NMR tubes (with "J. Young" valves).

^{1}H NMR measurements for Y(III) analogues of the multiple-decker complexes were acquired at a magnetic field of 9.4 T with a JEOL AL400 at room temperature (ca. 24 °C). The recorded signals were used as the dorb values for simulation of chemical shift of Tb(III) multiple-decker complexes.

The position of the signals was calculated using eq. 2, eq. 3 and the geometry parameters (r and θ) of the optimized structures.

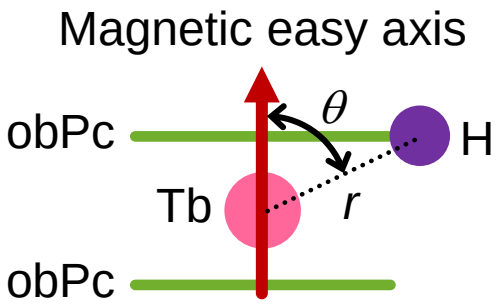

Fig. S29. Schematic representation of the r and the θ values.

3.2. Complex **[3]^{0}**

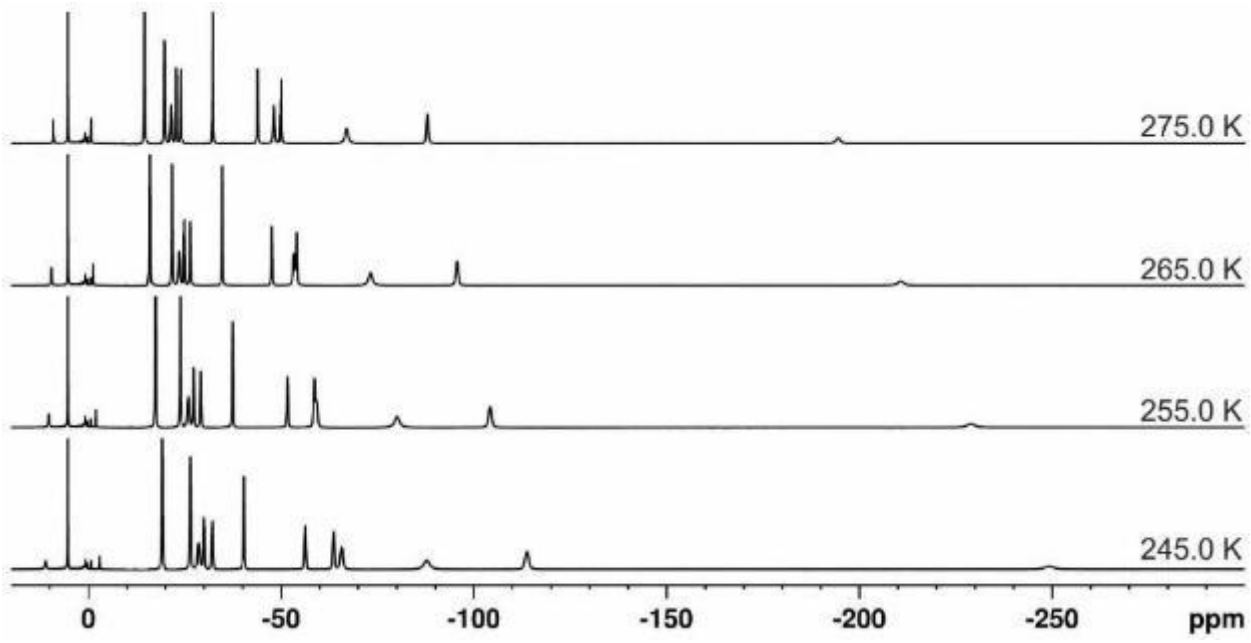

Fig. S30. Variable-temperature ^{1}H NMR spectra of complex **[3]^{0}** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 285.0 K.

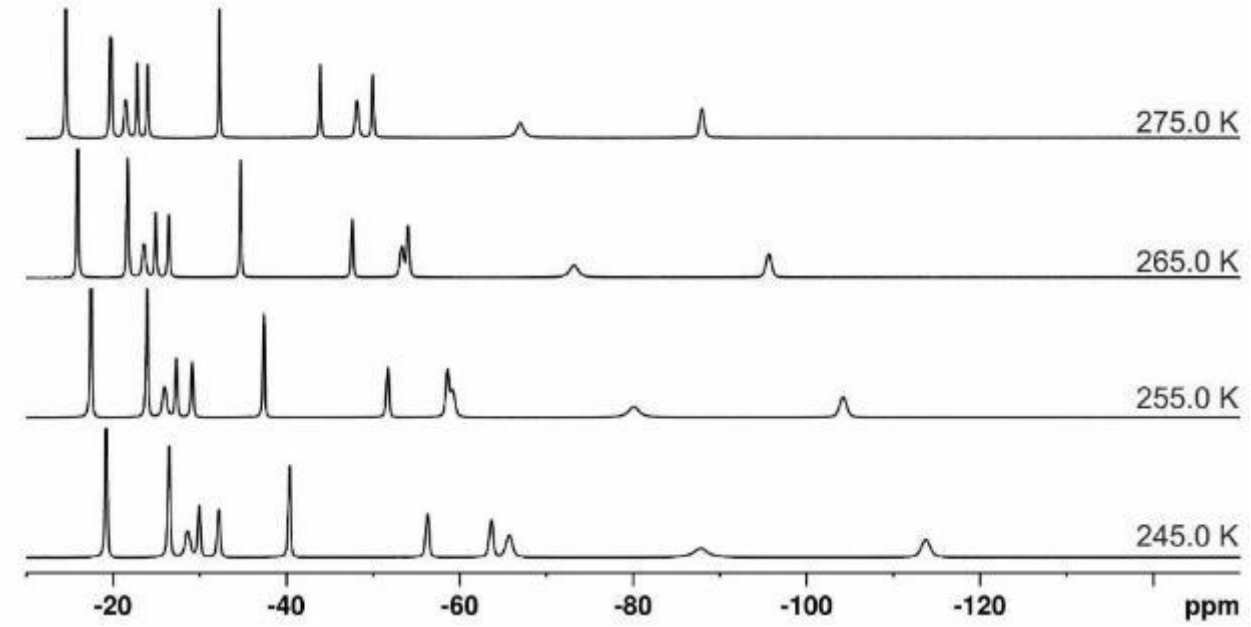

Fig. S31. Variable-temperature ^{1}H NMR spectra of complex **[3]^{0}** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 285.0 K. Expanded from -15 ppm to -150 ppm.

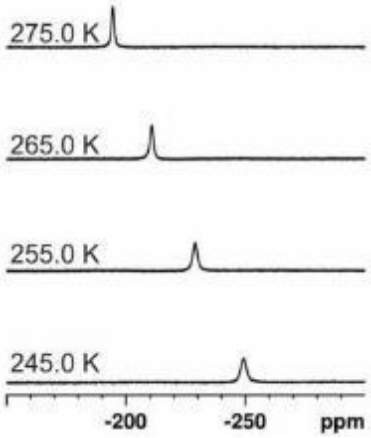

Fig. S32. Variable-temperature ^{1}H NMR spectra of complex **[3]^{0}** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 285.0 K. Expanded from -150 ppm to -300 ppm.

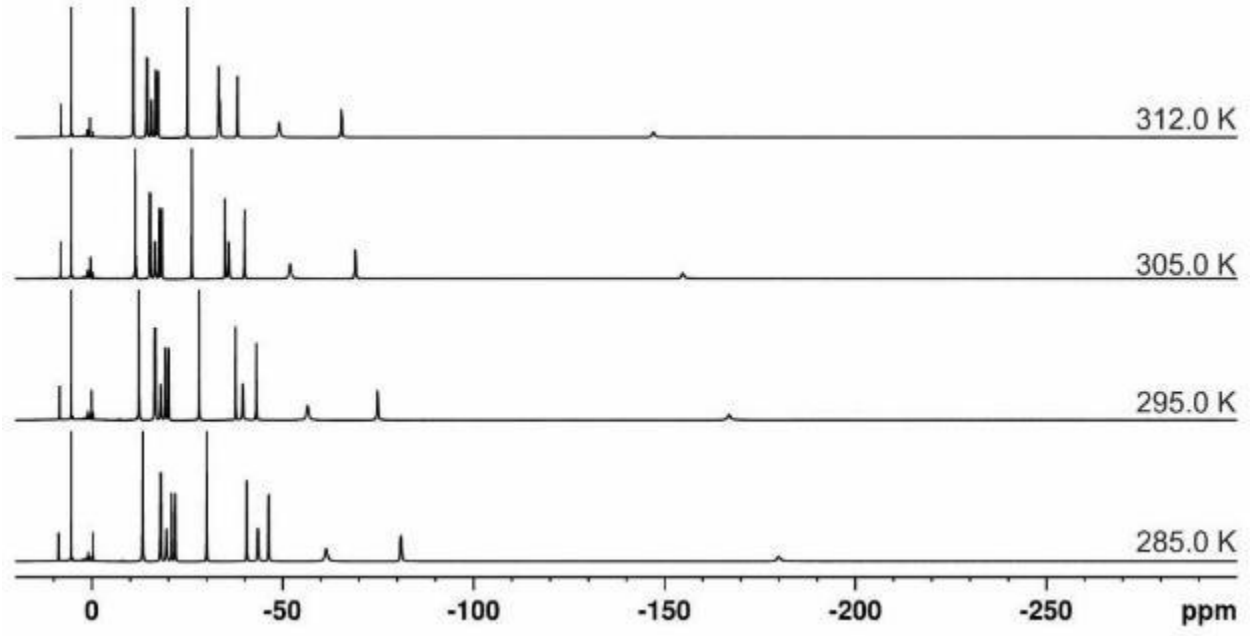

Fig. S33. Variable-temperature ^{1}H NMR spectra of complex **[3]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

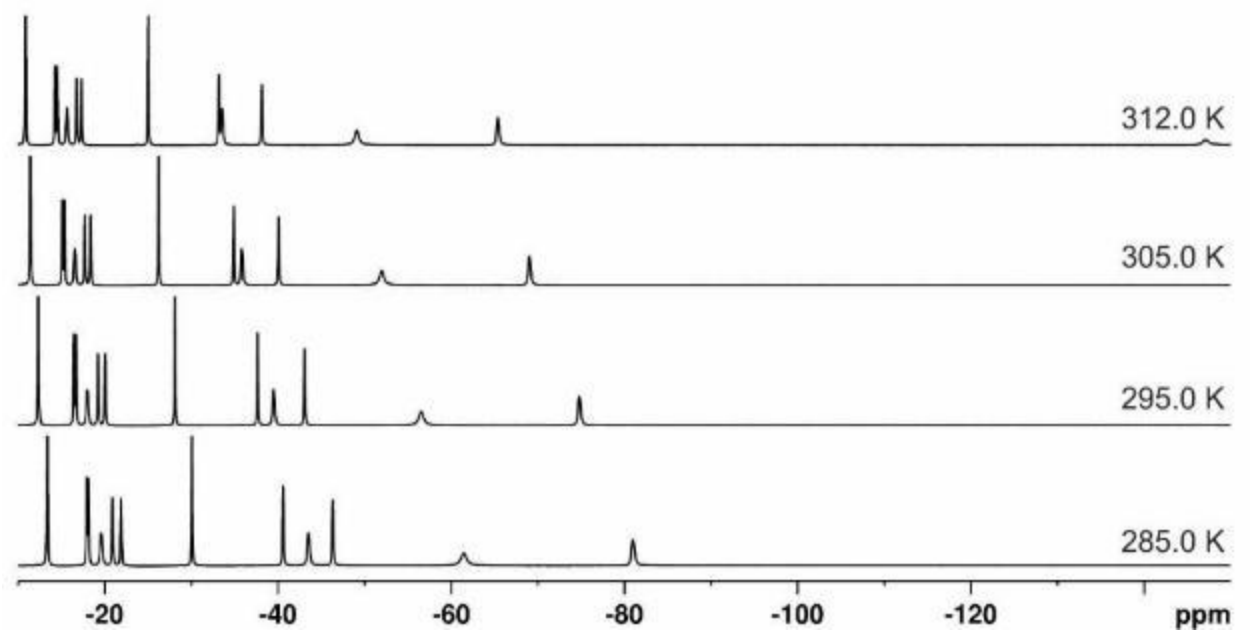

Fig. S34. Variable-temperature ^{1}H NMR spectra of complex **[3]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expanded from -10 ppm to -150 ppm.

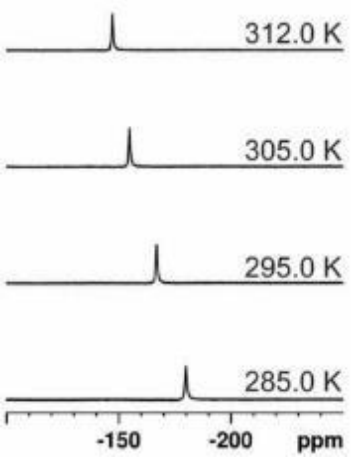

Fig. S35. Variable-temperature ^{1}H NMR spectra of complex **[3]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expanded from -100 ppm to -150 ppm.

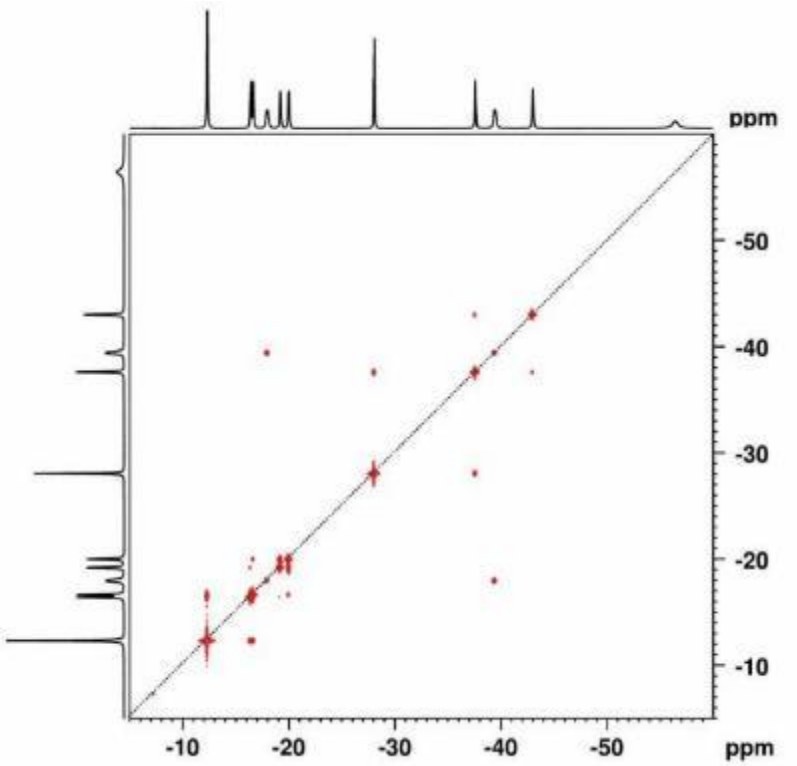

Fig. S36. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K.

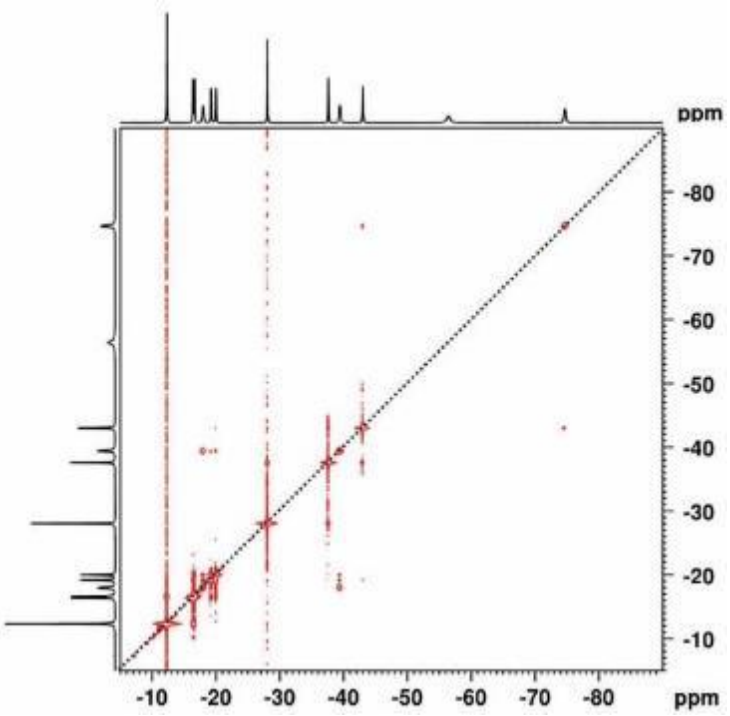

Fig. S37. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from -10 ppm to -90 ppm.

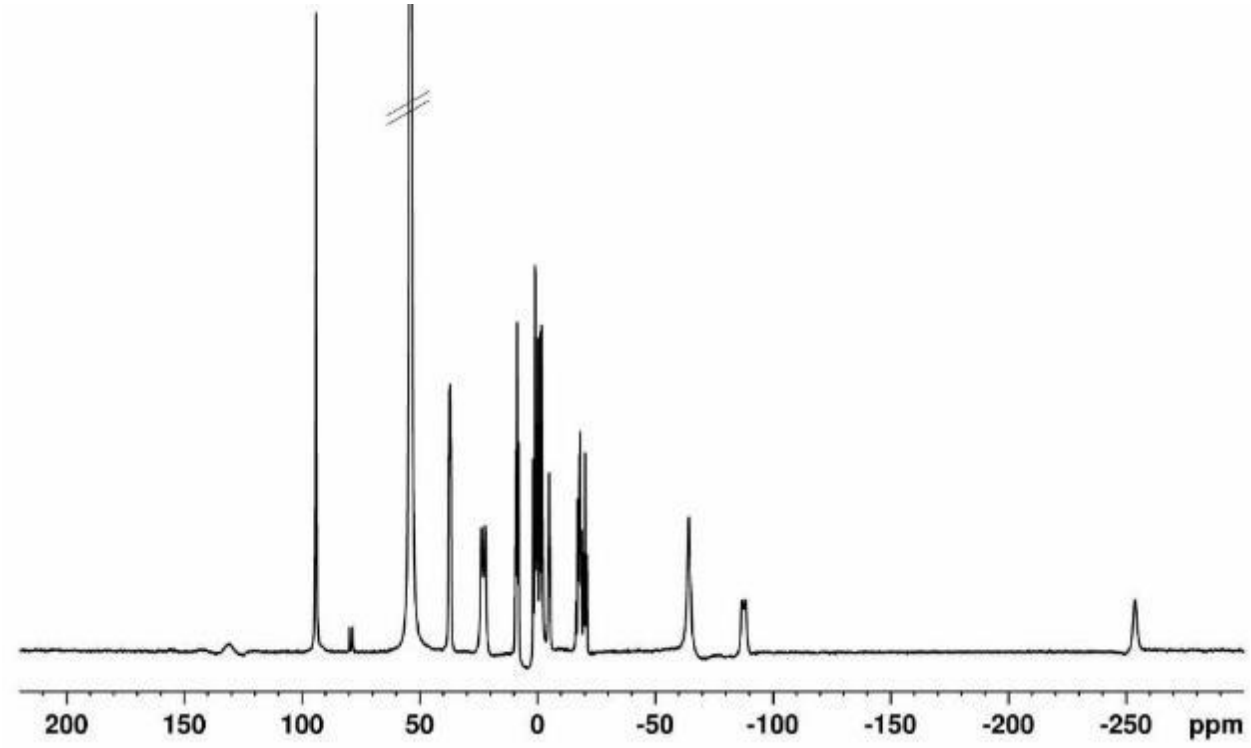

Fig. S38. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]^{0}** in CD_2Cl_2, recorded at 295.0 K.

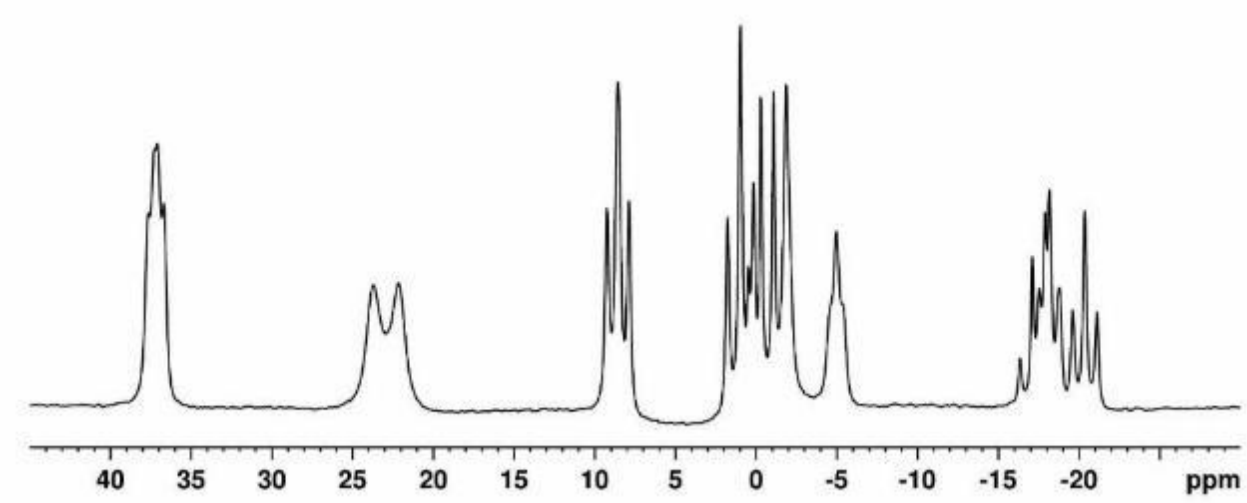

Fig. S39. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]^{0}** in CD_2Cl_2, recorded at 295.0 K. Expanded from +45 ppm to -30 ppm.

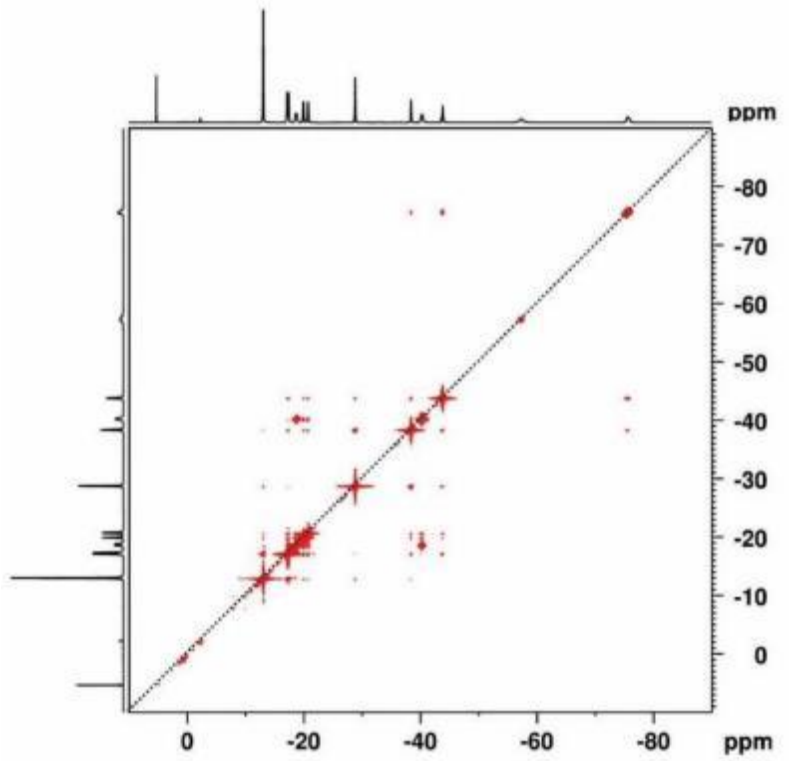

Fig. S40. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K. Expanded from +10 ppm to -90 ppm.

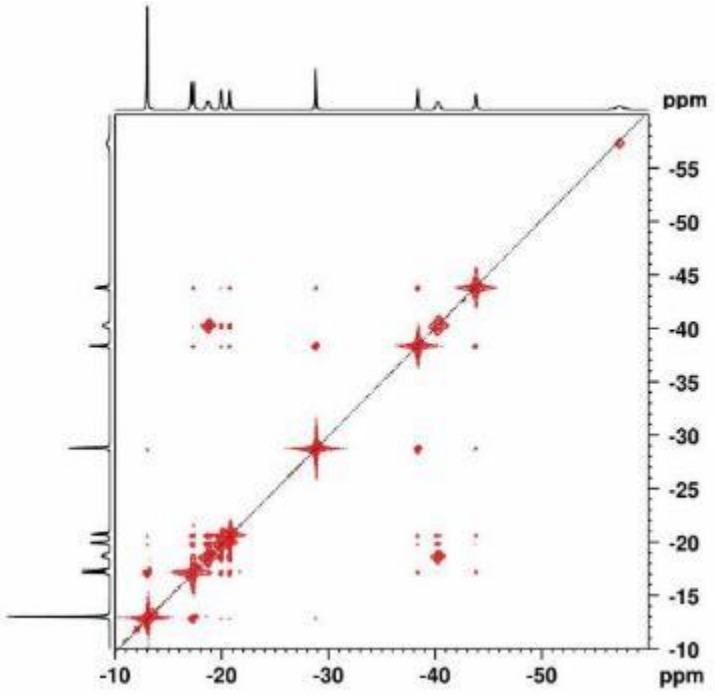

Fig. S41. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K.

Table S1. ^{1}H NMR experimental chemical shifts for **[3]^{0}** in CD_2Cl_2. Details about the assignment are given in our previous work[10]. No distinctions are made between diastereotopic protons within the same methylene group, as these are not relevant for the analysis in this work.

	T in K								Calculated@295 K			
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm											Integral
1: CH_{ar}i	-249.44	-228.95	-210.77	-194.49	-179.92	-166.95	-154.78	-147.17	-163.31	8.35	-154.96	1
2: CH_2αi	-113.79	-104.21	-95.63	-87.92	-80.99	-74.79	-69.05	-65.40	-76.59	4.88	-71.71	2
3: CH_{ar}o	-84.82	-80.10	-73.14	-66.99	-61.46	-56.54	-51.98	-49.10	-61.83	7.98	-53.85	2
4: CH_2βi	-65.70	-59.13	-53.33	-48.12	-43.52	-39.48	-35.83	-33.55	-41.02	2.55	-38.47	2
5: CH_2αo	-63.65	-58.60	-54.05	-49.97	-46.33	-43.09	-40.07	-38.16	-54.56	4.61	-49.95	2
6: CH_2γi	-56.30	-51.71	-47.60	-43.91	-40.61	-37.67	-34.93	-33.19	-38.76	2.20	-36.56	2
7: CH_3i	-40.38	-37.41	-34.72	-32.29	-30.09	-28.11	-26.24	-25.04	-23.28	1.53	-21.75	3
8: CH_2βo	-32.20	-29.13	-26.42	-24.00	-21.89	-20.04	-18.37	-17.33	-24.36	2.14	-22.22	2
9: CH_2βo	-29.94	-27.30	-24.93	-22.79	-20.90	-19.23	-17.71	-16.76	-24.36	2.14	-22.22	2
10: CH_2αo	-28.60	-25.92	-23.54	-21.43	-19.57	-17.97	-16.53	-15.64	-25.04	4.31	-20.73	2
11: CH_2γo	-26.47	-23.93	-21.70	-19.82	-18.15	-16.69	-15.37	-14.55	-24.90	1.82	-23.08	2
12: CH_2γo	-26.47	-23.93	-21.70	-19.66	-17.93	-16.45	-15.11	-14.28	-24.90	1.82	-23.08	2
13: CH_3o	-19.24	-17.48	-15.92	-14.56	-13.37	-12.34	-11.42	-10.85	-16.19	1.22	-14.97	6

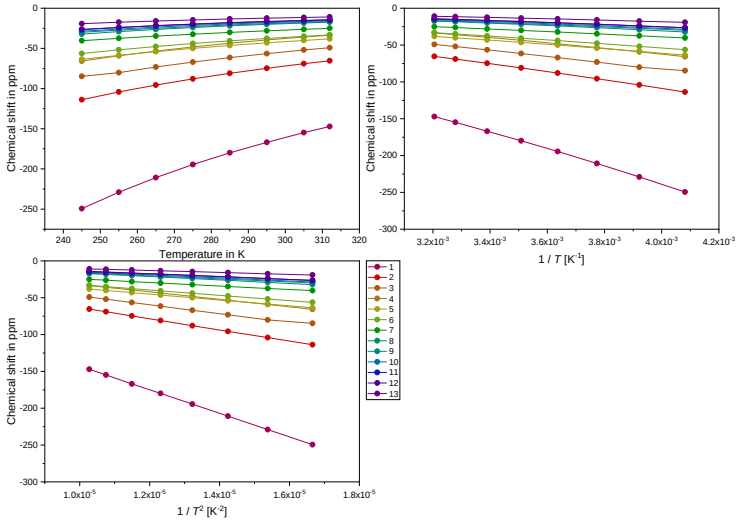

Fig. S42. Plot of the ^{1}H chemical shifts of **[3]^{0}** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S2. ^{13}C NMR chemical shifts of **[3]^{0}** and **[3]$^{2+}$** observed at 295.0 K in CD_2Cl_2. Assigment is based on previous work. [10]

		[3]^{0}	**[3]$^{+2}$**
Signal Nr.	Assignment	Chemical Shift [ppm]:	Chemical Shift [ppm]:
1	C_qi	-254.5	-206.1
2	CH_{ar}i	-88.2	-50.6
3	C_qo	-64.8	-62.5
4	CH_2γi	-20.8	-11.5
5	CH_2βi	-18.6	-8.3
6	CH_3i	-17.9	-11.9
7	CH_2αi	-5.4	10.6
8	C_{qo}i	-2.3	6.0
9	CH_3o	-1.1	4.7
10	CH_2γo	0.5	7.0
11	CH_2βo	8.2	15.1
12	CHaro	22.5	40.6
13	CH_2αo	36.7	47.0
14	C_{qo}o	93.6	104.9
(15)	C_Ni (?)	103.8	NA
(16)	C_No (?)	NA	NA

3.3. Complex **[3]**$^{+}$

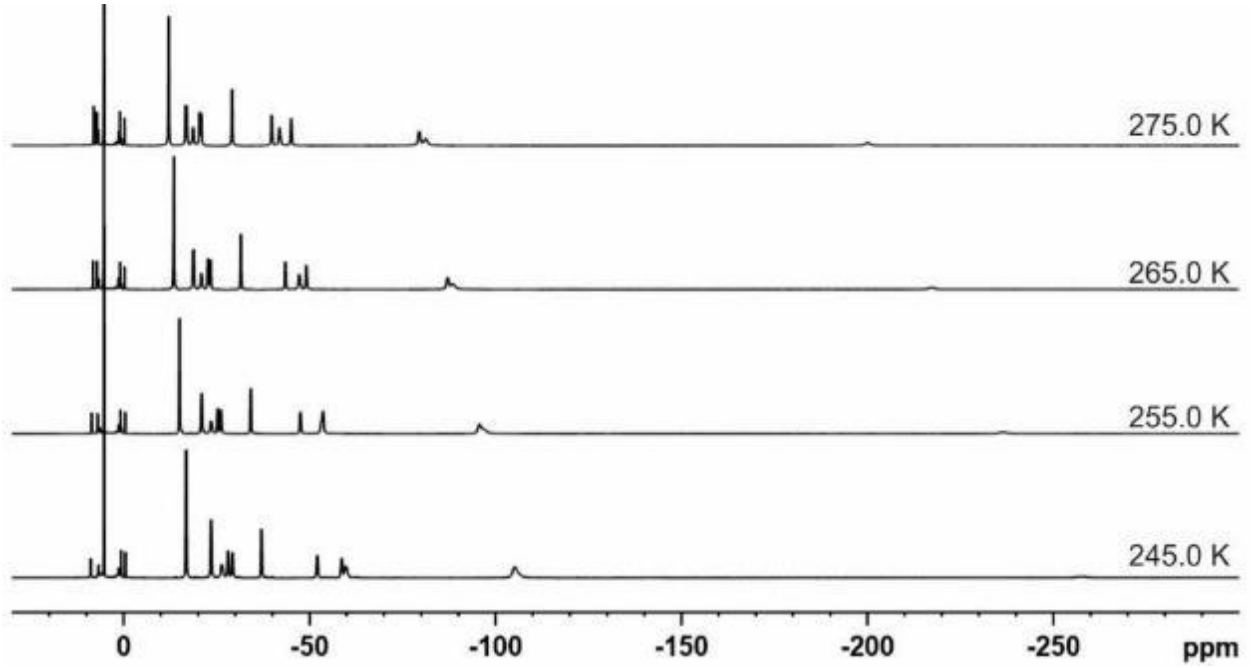

Fig. S43. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

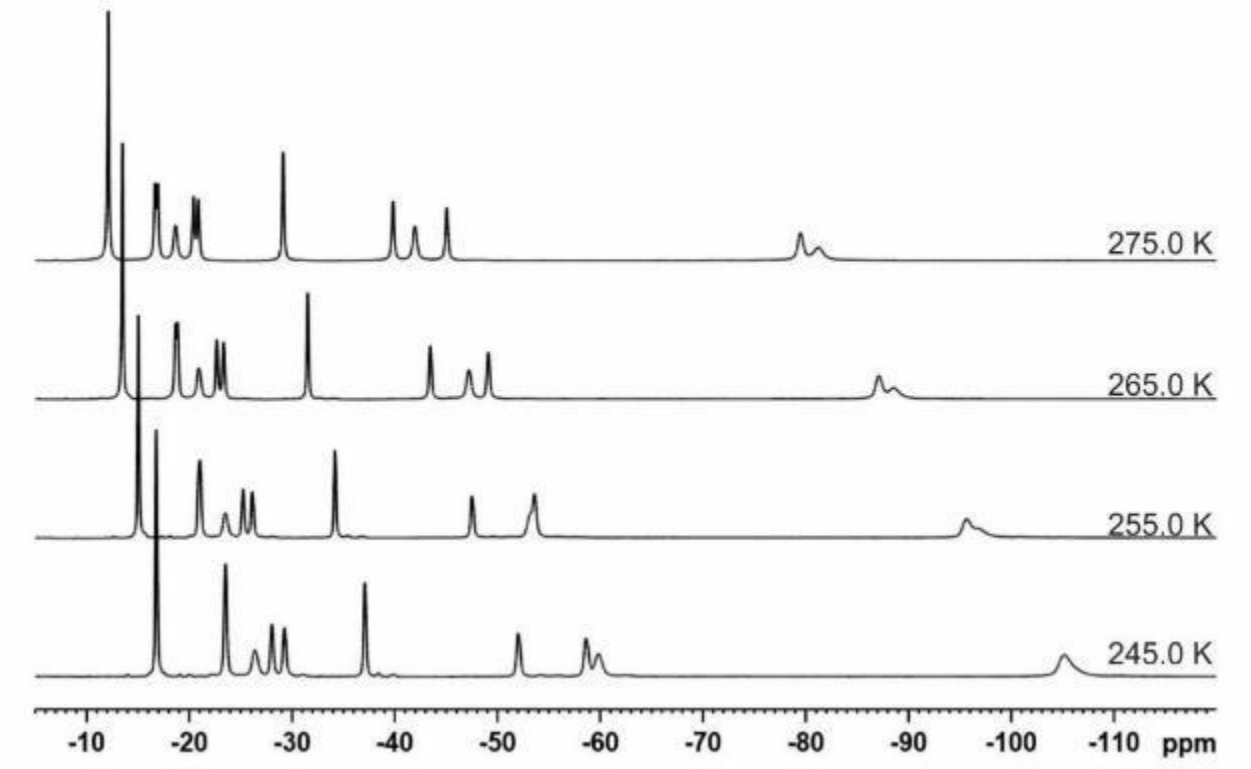

Fig. S44. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -5 ppm to -120 ppm.

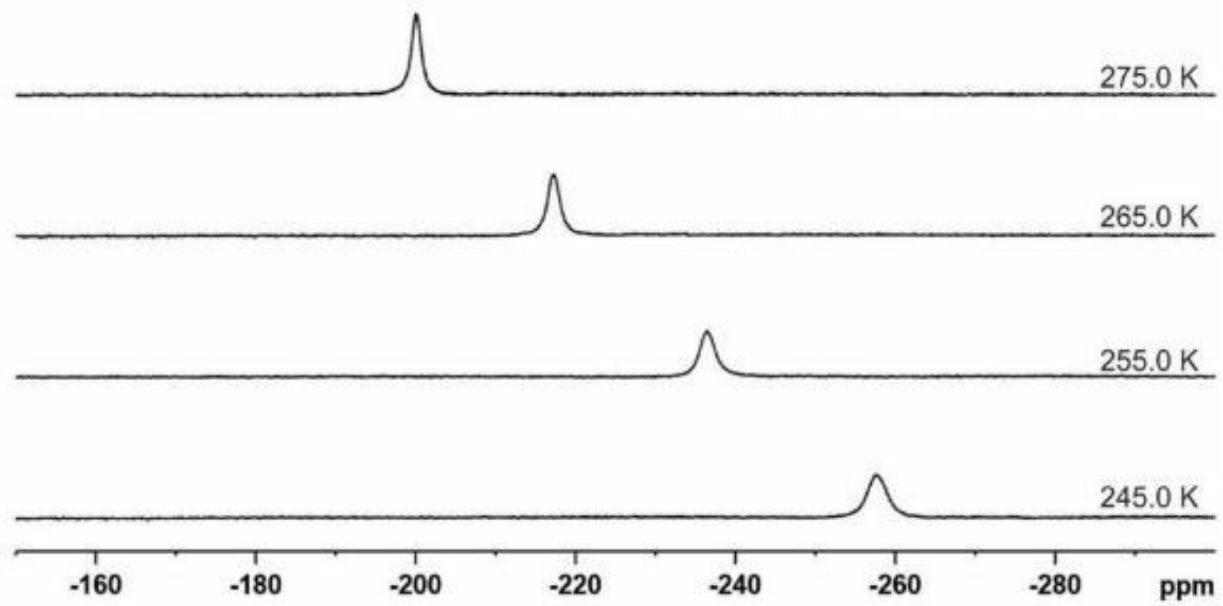

Fig. S45. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -150 ppm to -300 ppm.

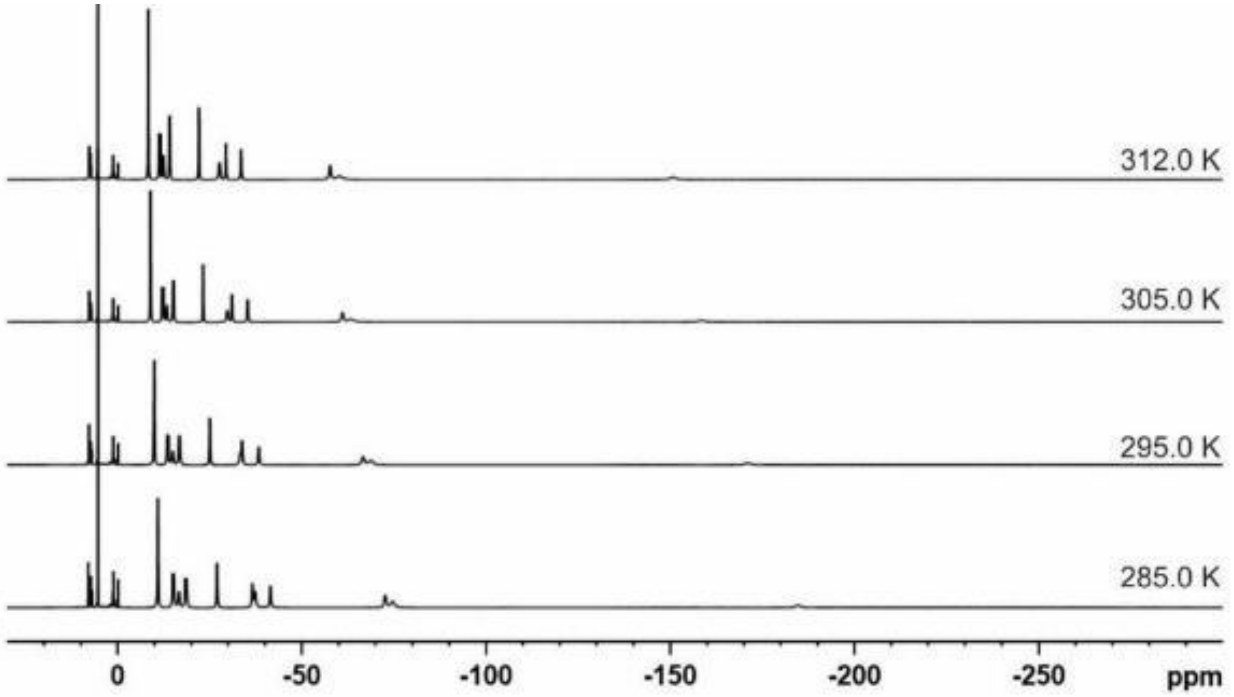

Fig. S46. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

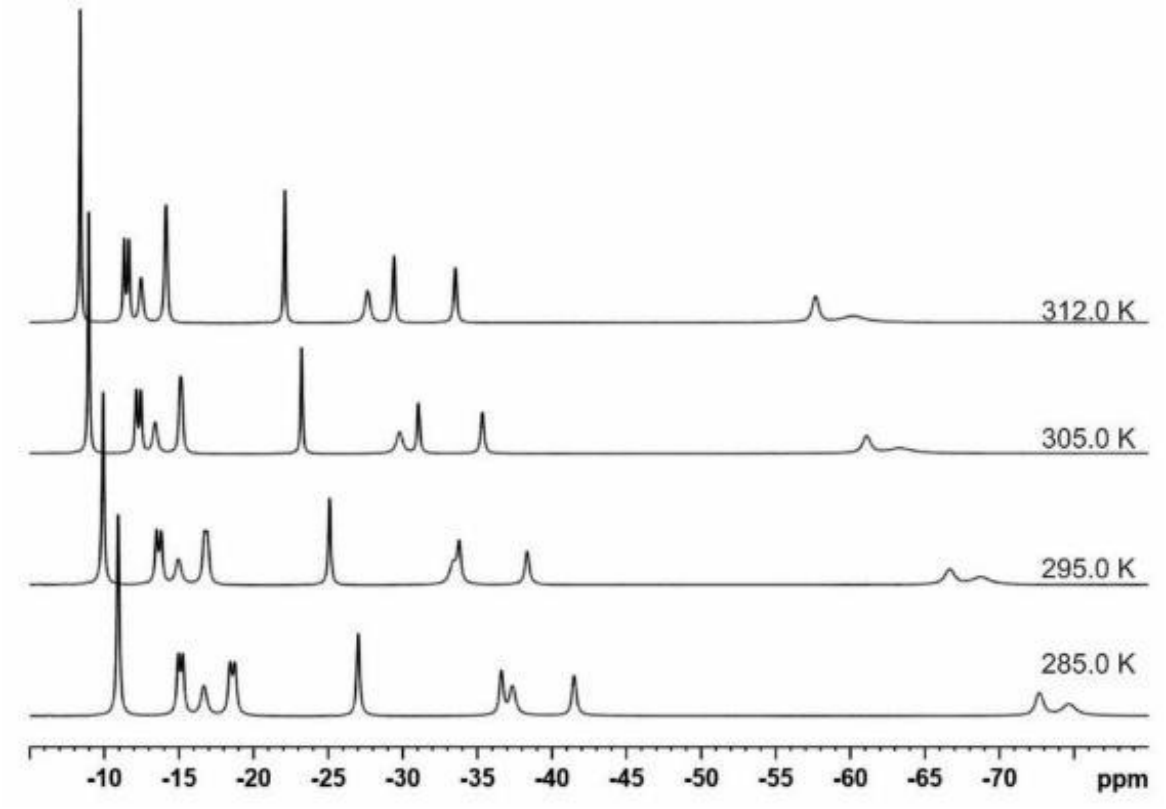

Fig. S47. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -90 ppm.

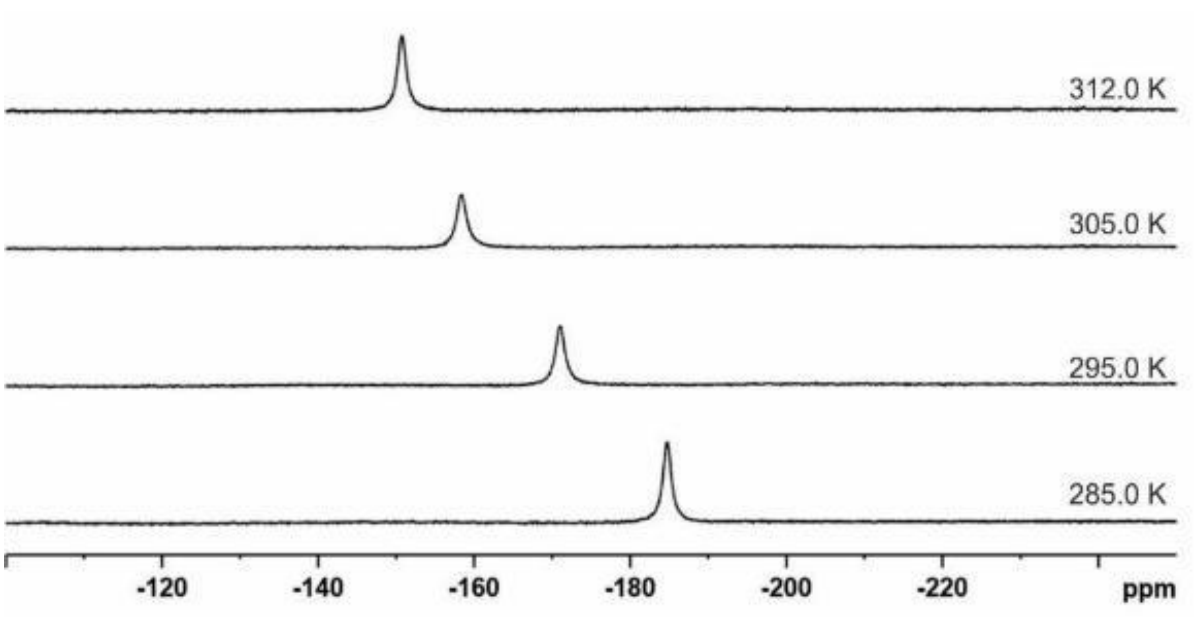

Fig. S48. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -100 ppm to -250 ppm.

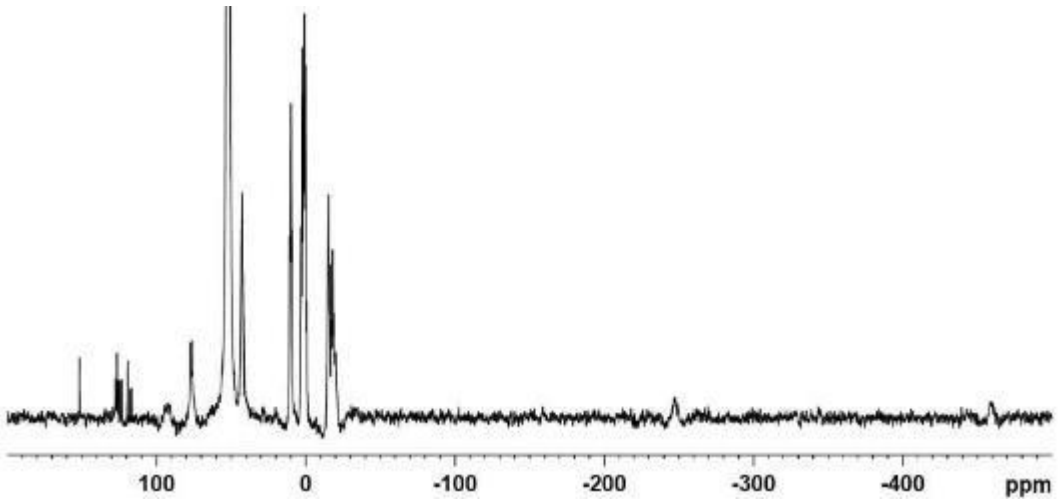

Fig. S49. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K.

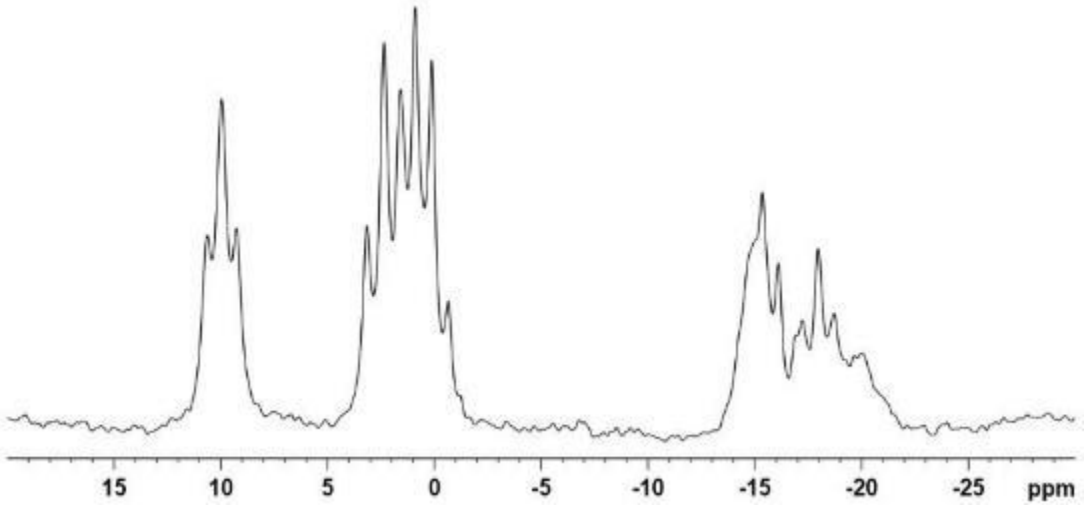

Fig. S50. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expanded from +20 ppm to -30 ppm.

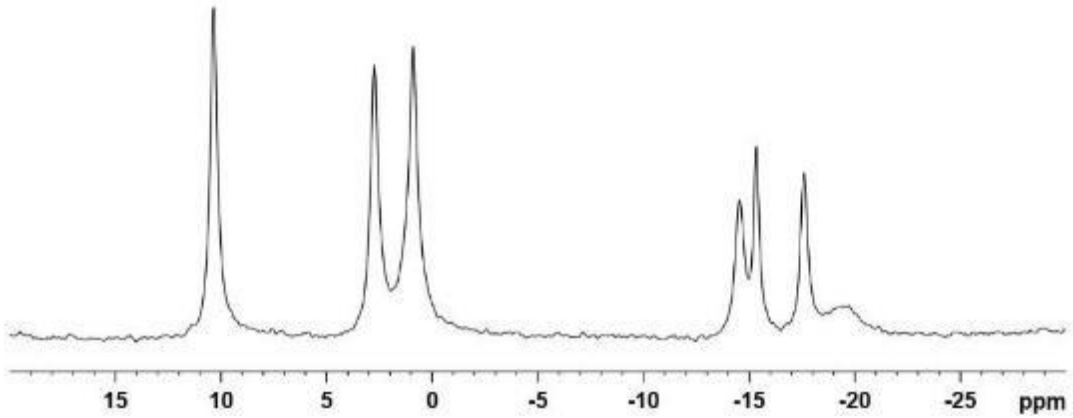

Fig. S51. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expanded from +20 ppm to -30 ppm.

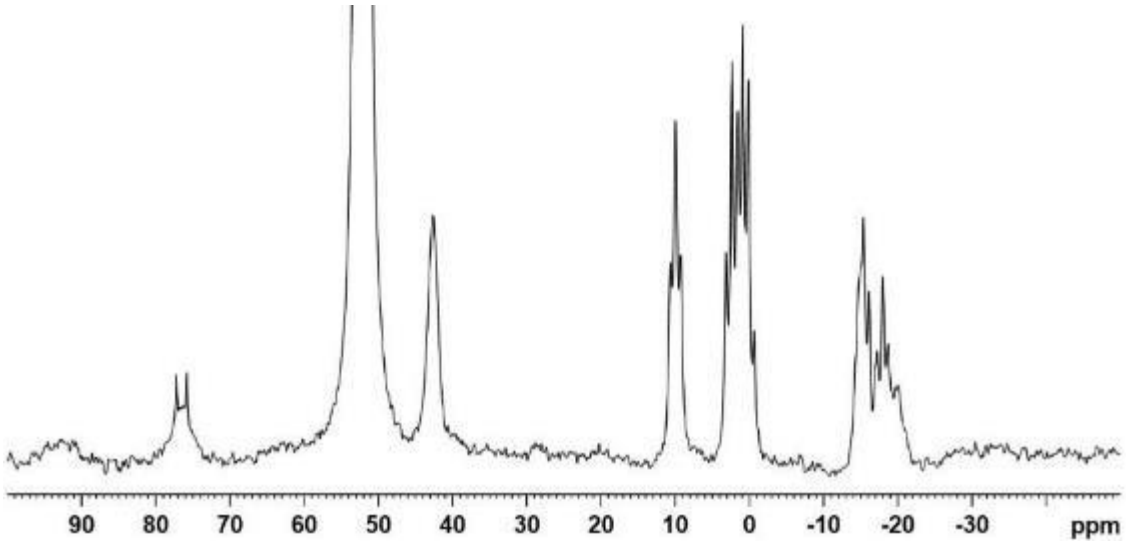

Fig. S52. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expanded from +100 ppm to -50 ppm.

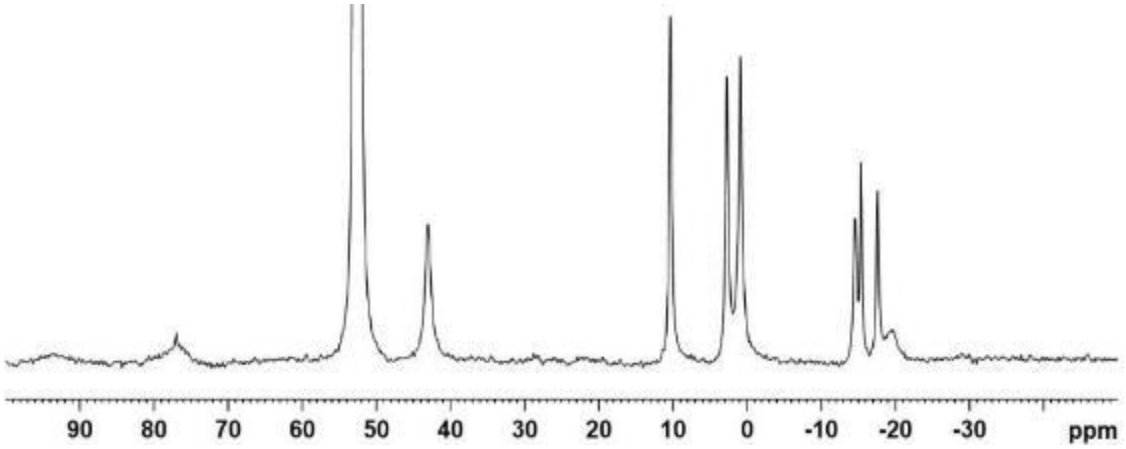

Fig. S53. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expanded from +100 ppm to -50 ppm.

Table S3. ^{1}H NMR experimental chemical shifts for **[3]**$^+$ in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}i$	-257.56	-236.47	-217.28	-200.08	-184.75	-171.03	-158.48	-150.72	-158.24	-20.34	8.35	-170.23	1
2: $CH_{ar}o$	-106.28	-96.51	-88.57	-81.25	-74.65	-68.78	-63.24	-60.28	-42.80	-25.13	7.98	-59.95	2
3: $CH_2\alpha i$	-105.22	-95.70	-87.15	-79.50	-72.68	-66.66	-61.10	-57.69	-73.31	-	4.64	-68.67	2
4: $CH_2\beta i$	-59.85	-53.59	-49.12	-45.08	-41.50	-38.36	-35.36	-33.54	-39.21	-	2.47	-36.74	2
5: $CH_2\gamma i$	-58.65	-53.22	-47.24	-41.99	-37.37	-33.79	-31.07	-29.43	-36.86	-	2.17	-34.69	2
6: $CH_2\alpha o$	-52.04	-47.54	-43.48	-39.85	-36.63	-33.41	-29.81	-27.66	-37.38	-	4.40	-32.98	2
7: CH_3i	-37.10	-34.20	-31.55	-29.16	-27.03	-25.11	-23.24	-22.11	-22.14	-	1.47	-20.67	3
8: $CH_2\beta o$	-29.29	-26.16	-23.37	-20.90	-18.75	-16.88	-15.12	-14.14	-14.81	-	2.13	-12.68	2
9: $CH_2\beta o$	-28.06	-25.25	-22.71	-20.43	-18.45	-16.74	-15.12	-14.14	-14.81	-	2.13	-12.68	2
10: $CH_2\alpha o$	-26.40	-23.52	-20.95	-18.66	-16.69	-14.98	-13.42	-12.48	-9.20	-	4.22	-4.98	2
11: $CH_2\gamma o$	-23.54	-23.52	-18.89	-16.95	-15.26	-13.82	-12.46	-11.66	-15.17	-	1.81	-13.36	2
12: $CH_2\gamma o$	-23.54	-21.04	-18.68	-16.69	-14.98	-13.52	-12.15	-11.35	-15.17	-	1.81	-13.36	2
13: CH_3o	-16.81	-15.06	-13.50	-12.13	-10.94	-9.92	-8.97	-8.40	-10.15	-	1.17	-8.98	6

[a]The δ_{orb} values of **[3]**^{0} were used. [a]The δ_{orb} values of **[3]**$^{2+}$ were used.

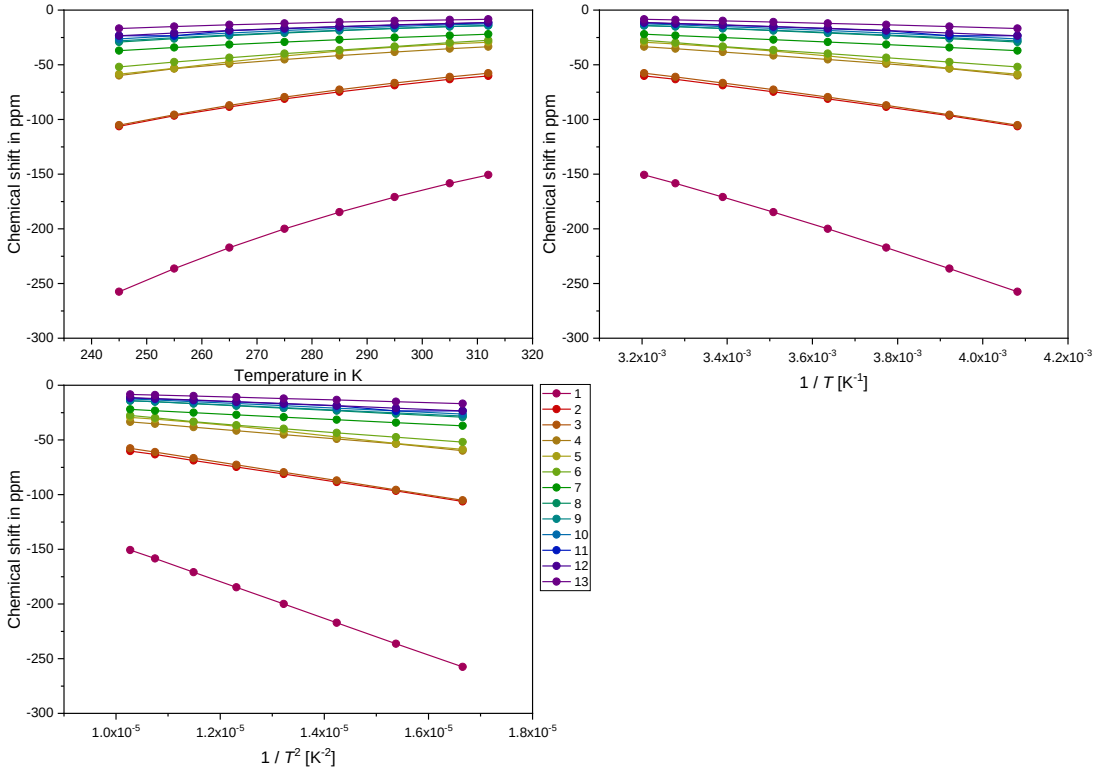

Fig. S54. Plot of the ^{1}H chemical shifts of **[3]**$^+$ in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S4. ^{13}C NMR chemical shifts of **[3]**$^{+}$ observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-458.7	s
2	-246.9	s
3	-19.8	s
4	-17.9	t
5	-15.3	t
6	-14.8	m
7	0.5	q
8	2.4	t
9	10.0	t
10	42.8	s
11	75.8	s
12	76.6	s
13	77.3	s
14	93.1	s

3.4. Complex **[3]**$^{2+}$

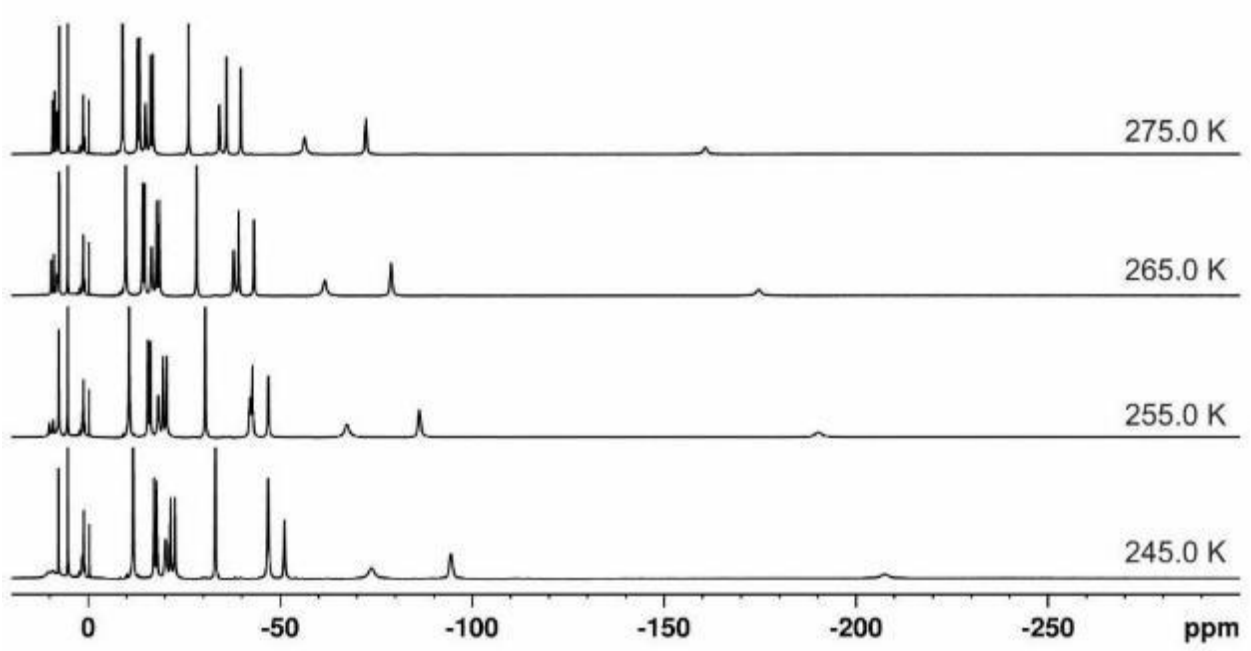

Fig. S55. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

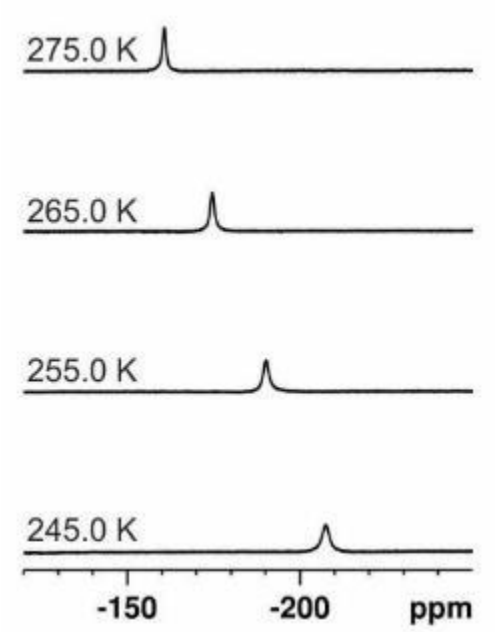

Fig. S56. Variable-temperature ^{1}H NMR spectra of complex $[\mathbf{3}]^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -100 ppm to -250 ppm.

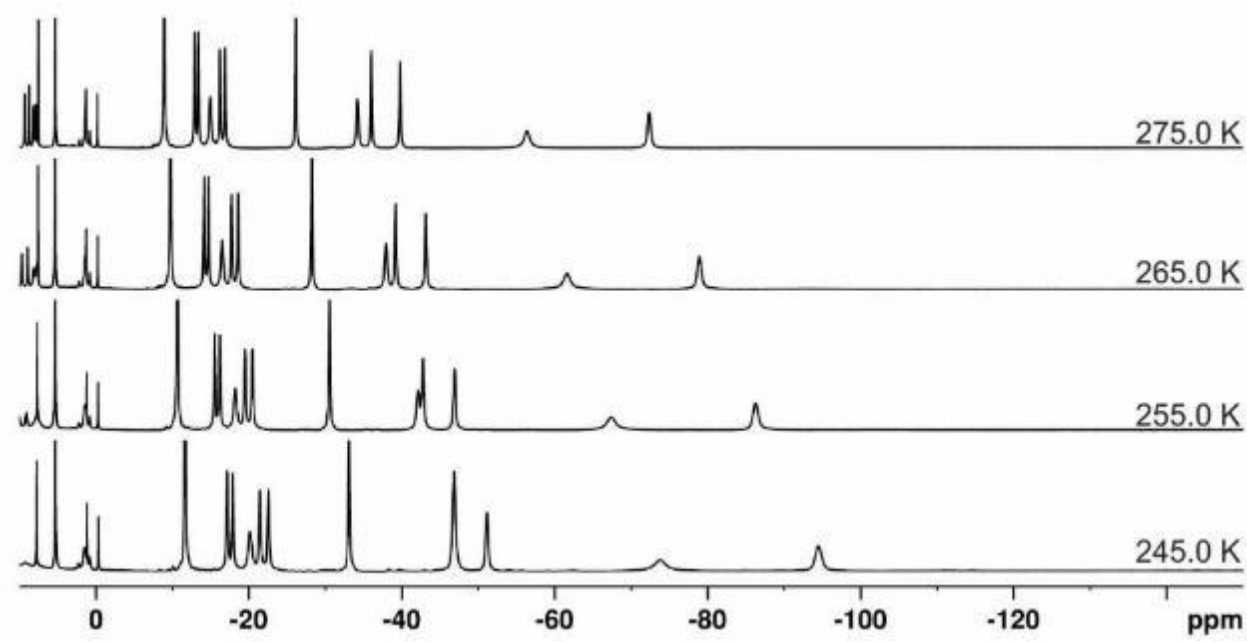

Fig. S57. Variable-temperature ^{1}H NMR spectra of complex $[\mathbf{3}]^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +10 ppm to -150 ppm.

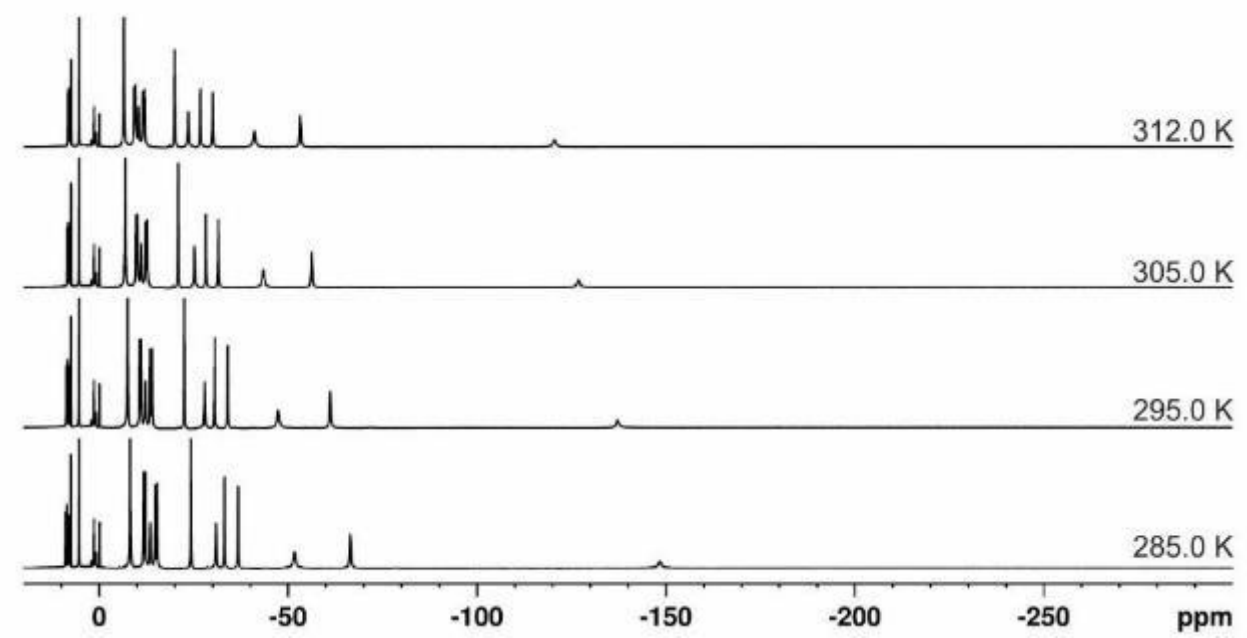

Fig. S58. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

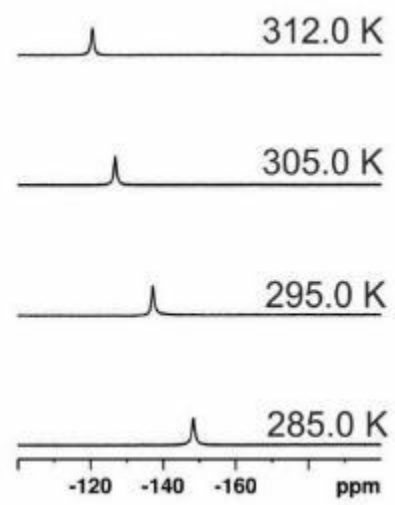

Fig. S59. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -100 ppm to -200 ppm.

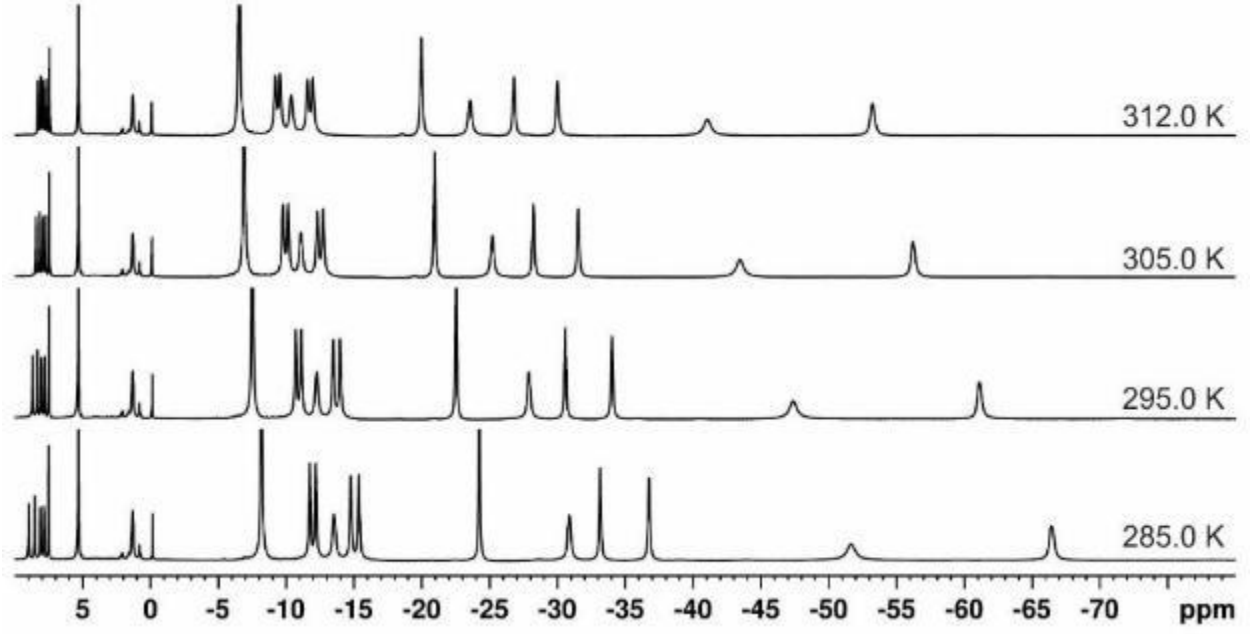

Fig. S60. Variable-temperature ^{1}H NMR spectra of complex $\mathbf{[3]^{2+}}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +10 ppm to -80 ppm.

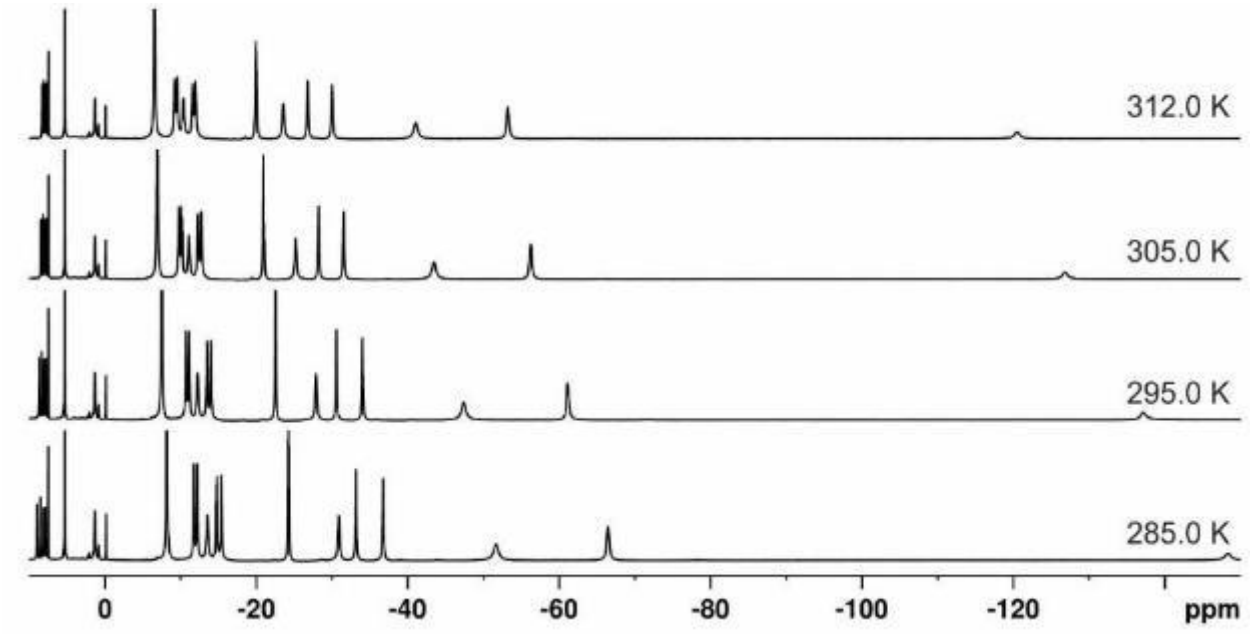

Fig. S61. Variable-temperature ^{1}H NMR spectra of complex $\mathbf{[3]^{2+}}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +10 ppm to -150 ppm.

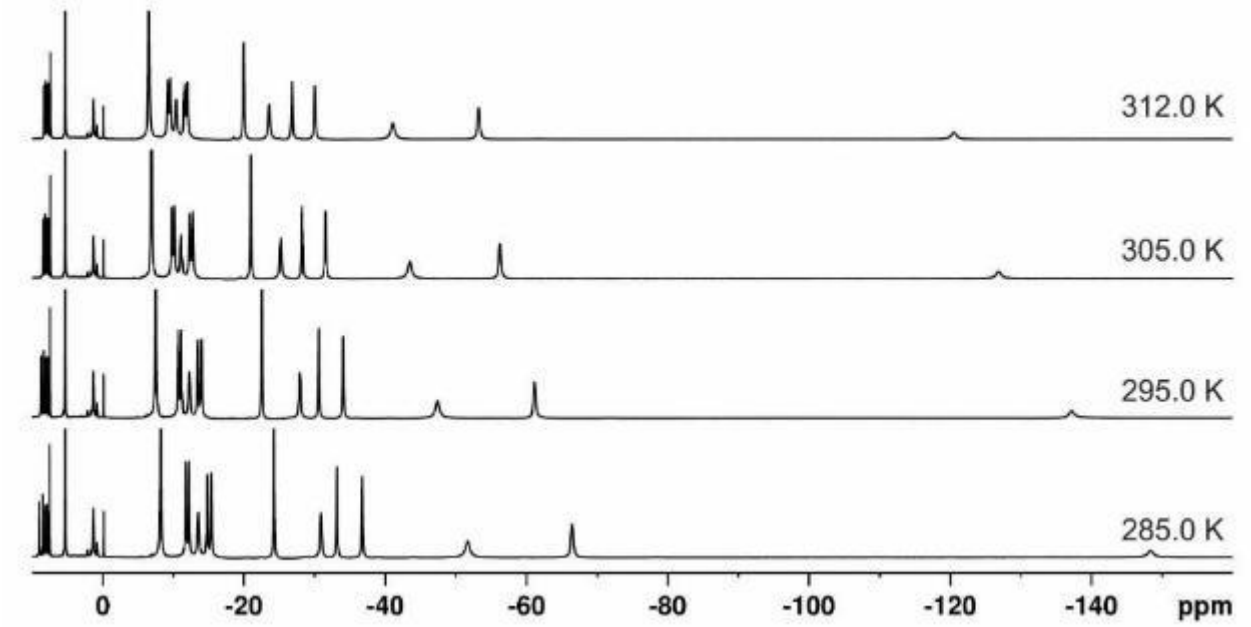

Fig. S62. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +10 ppm to -160 ppm.

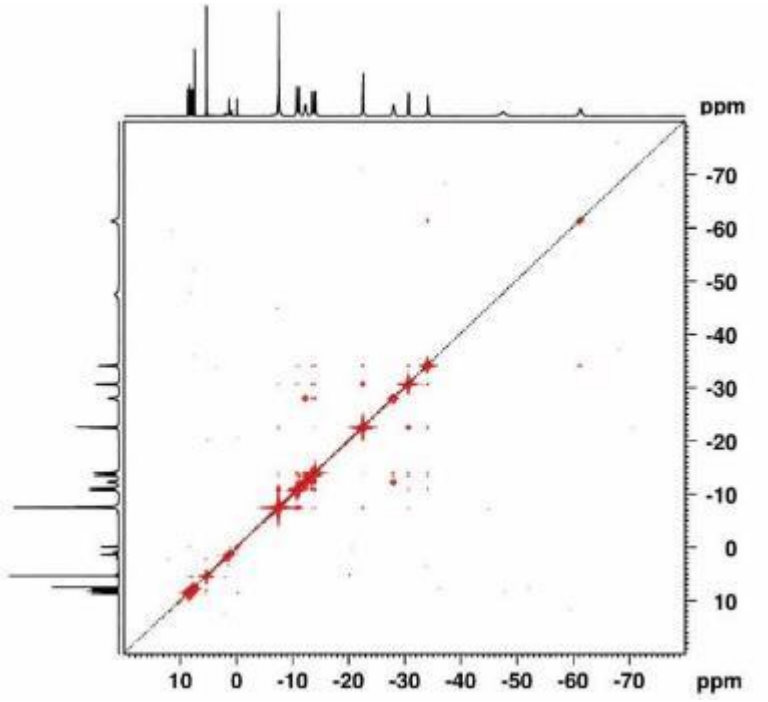

Fig. S63. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K.

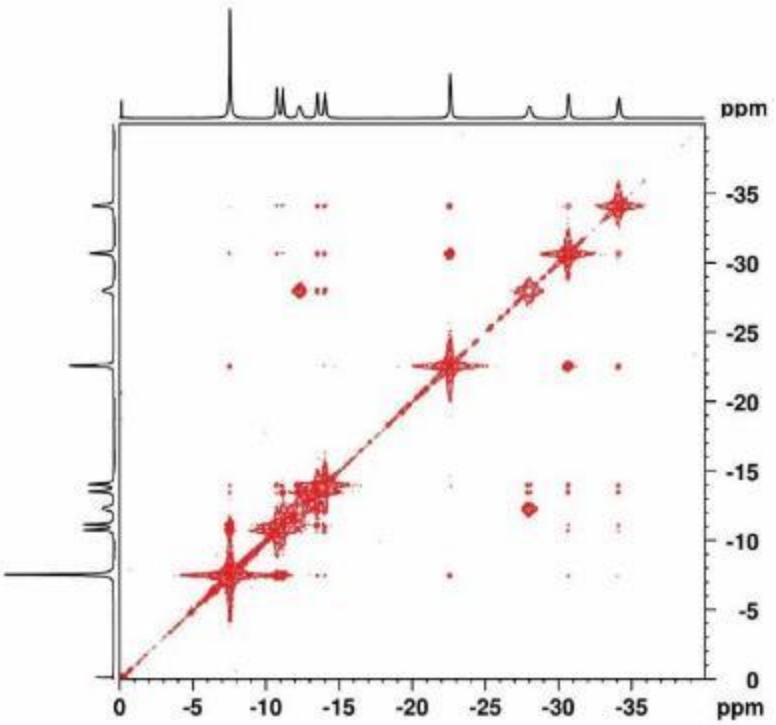

Fig. S64. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from 0 ppm to -40 ppm.

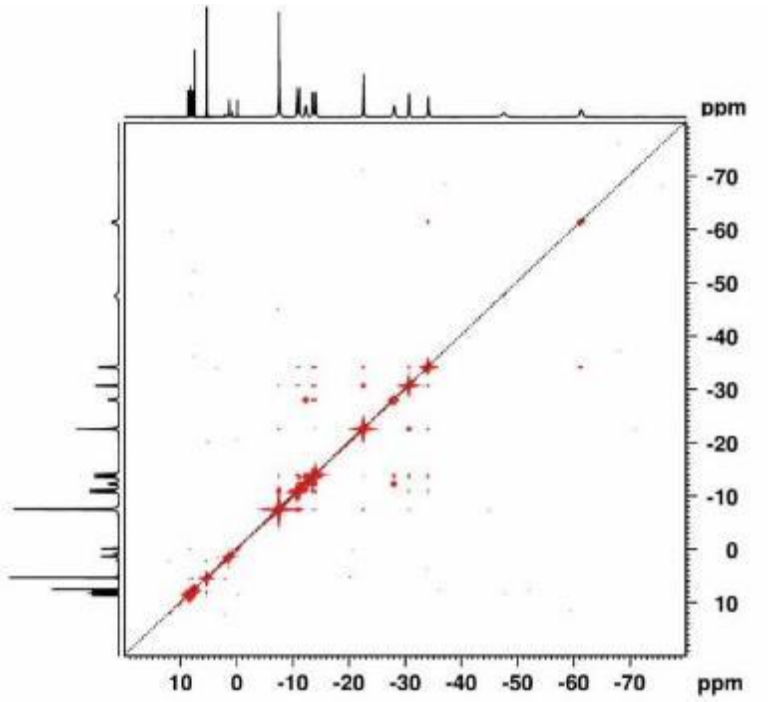

Fig. S65. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from +20 ppm to -80 ppm.

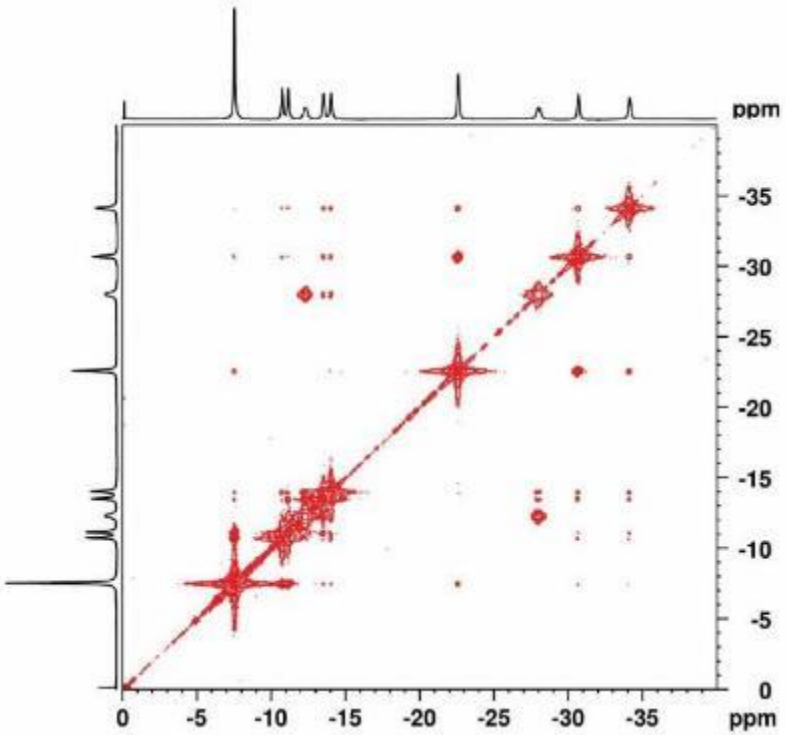

Fig. S66. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[3]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from 0 ppm to -40 ppm.

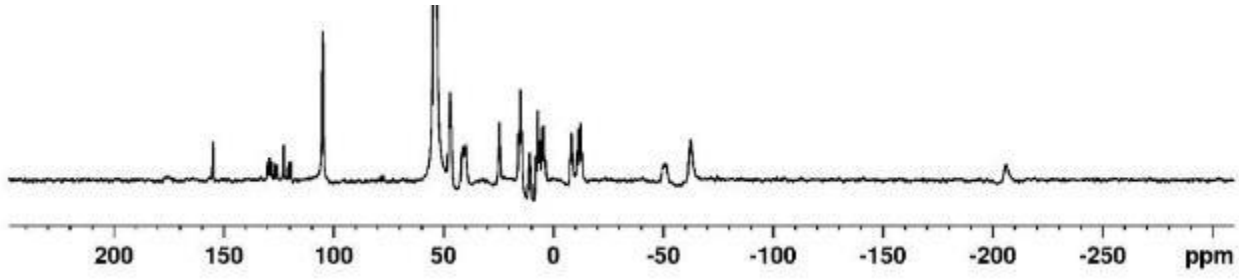

Fig. S67. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K.

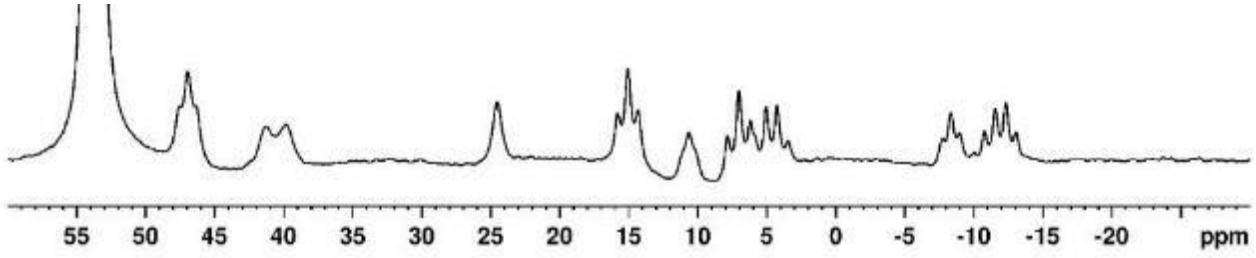

Fig. S68. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +60 ppm to -30 ppm.

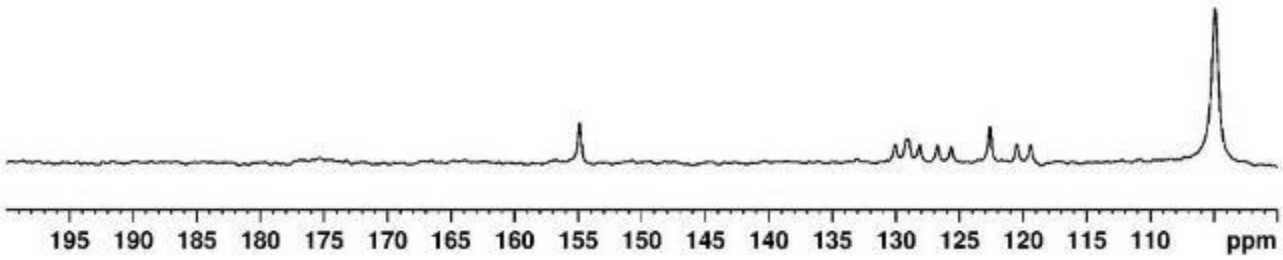

Fig. S69. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +200 ppm to +100 ppm.

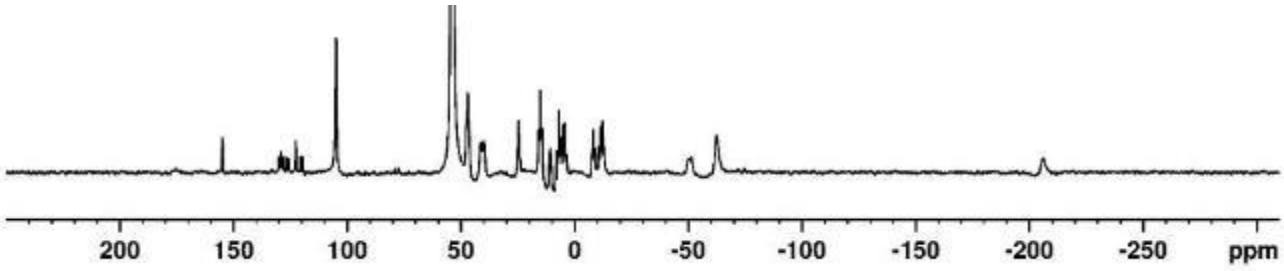

Fig. S70. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K.

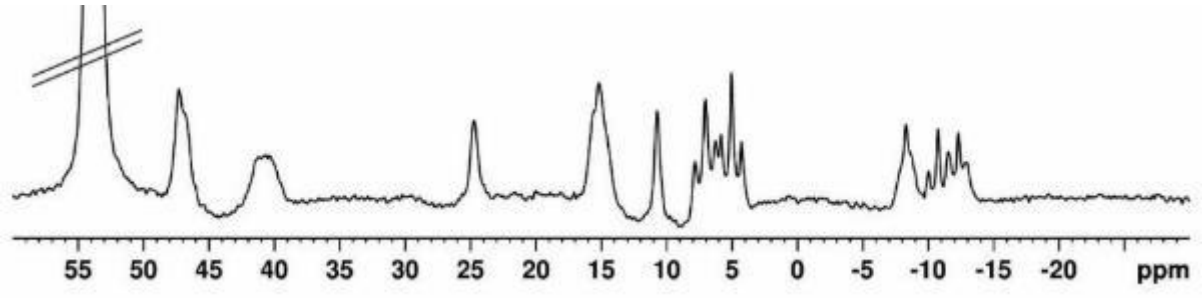

Fig. S71. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +60 ppm to -30 ppm.

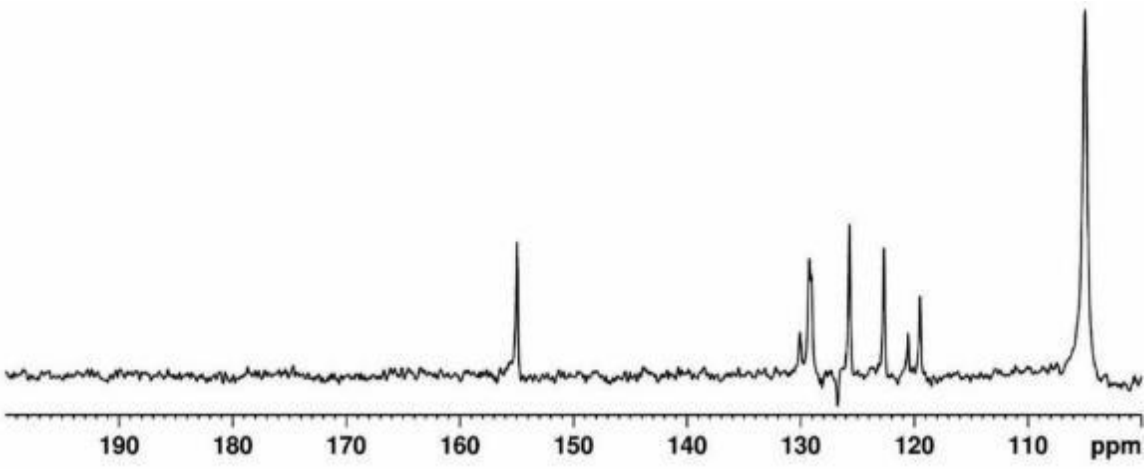

Fig. S72. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +200 ppm to +100 ppm.

Table S5. ^{1}H NMR experimental chemical shifts for **[3]$^{2+}$** in CD_2Cl_2. ^{13}C NMR shifts for this complex are tabulated above, together with those of the neutral triple-decker.

	T in K								Calculated@295 K			
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm											Integral
1: $CH_{ar}i$	-207.52	-190.16	-174.64	-160.78	-148.38	-137.15	-126.85	-120.51	-144.38	8.35	-136.03	1
2: $CH_2\alpha i$	-94.48	-86.24	-78.89	-72.32	-66.43	-61.10	-56.22	-53.23	-66.29	4.64	-61.65	2
3: $CH_{ar}o$	-73.74	-67.38	-61.57	-56.36	-51.66	-47.38	-43.45	-41.06	-41.46	7.98	-33.48	2
4: $CH_2\beta i$	-51.13	-46.90	-43.12	-39.76	-36.75	-34.03	-31.53	-30.01	-35.56	2.39	-33.17	2
5: $CH_2\gamma i$	-46.82	-42.79	-39.20	-36.01	-33.16	-30.59	-28.23	-26.80	-33.25	2.04	-31.21	2
6: $CH_2\alpha o$	-46.82	-42.13	-37.92	-34.19	-30.87	-27.89	-25.20	-23.56	-34.60	4.40	-30.20	2
7: CH_3i	-33.11	-30.54	-28.21	-26.13	-24.25	-22.53	-20.94	-19.97	-20.03	1.41	-18.62	3
8: $CH_2\beta o$	-22.54	-20.46	-18.58	-16.89	-15.36	-13.98	-12.73	-11.96	-13.74	2.04	-11.70	2
9: $CH_2\beta o$	-21.52	-19.50	-17.76	-16.19	-14.77	-13.47	-12.30	-11.58	-13.74	2.04	-11.70	2
10: $CH_2\alpha o$	-20.13	-18.22	-16.45	-14.93	-13.53	-12.25	-11.09	-10.38	-9.22	4.22	-5.00	2
11: $CH_2\gamma o$	-17.88	-16.20	-14.71	-13.38	-12.20	-11.12	-10.15	-9.56	-13.78	1.71	-12.07	2
12: $CH_2\gamma o$	-17.13	-15.56	-14.15	-12.89	-11.75	-10.71	-9.77	-9.20	-13.78	1.71	-12.07	2
13: CH_3o	-11.65	-10.64	-9.74	-8.93	-8.19	-7.51	-6.90	-6.53	-9.12	1.13	-7.99	6

[a]The δ_{orb} values of **[3]^{0}** were used.

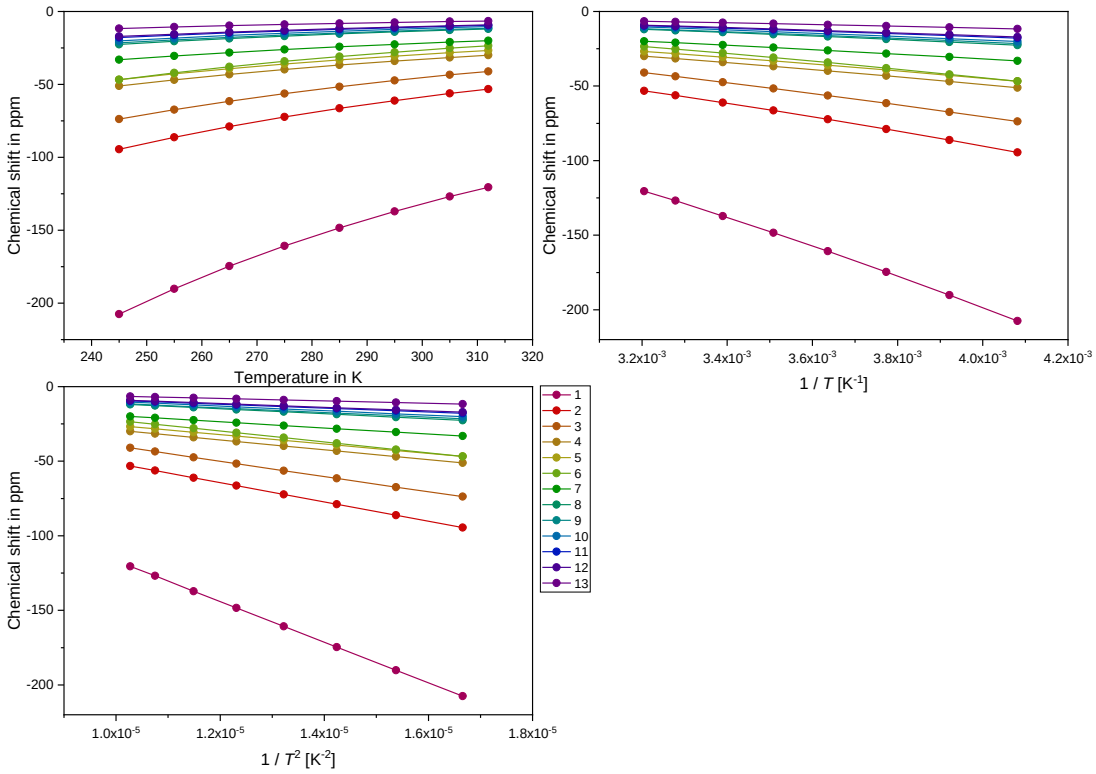

Fig. S73. Plot of the ^{1}H chemical shifts of **[3]$^{2+}$** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S6. ^{13}C NMR chemical shifts of **[3]$^{2+}$** observed at 295.0 K in CD_2Cl_2. Assignment based on spectra of **[3]^{0}** (see above).

Signal Nr.:	Assignment	Chemical Shift [ppm]:
1	C_qi	-206.1
2	CH_{ar}i	-50.6
3	C_qo	-62.5
4	CH_2γi	-11.5
5	CH_2βi	-8.3
6	CH_3i	-11.9
7	CH_2αi	10.6
8	C_{qo}i	6.0
9	CH_3o	4.7
10	CH_2γo	7.0
11	CH_2βo	15.1
12	CHaro	40.6
13	CH_2αo	47.0
14	C_{qo}o	104.9

3.5. Complex **[3]$^{3+}$**

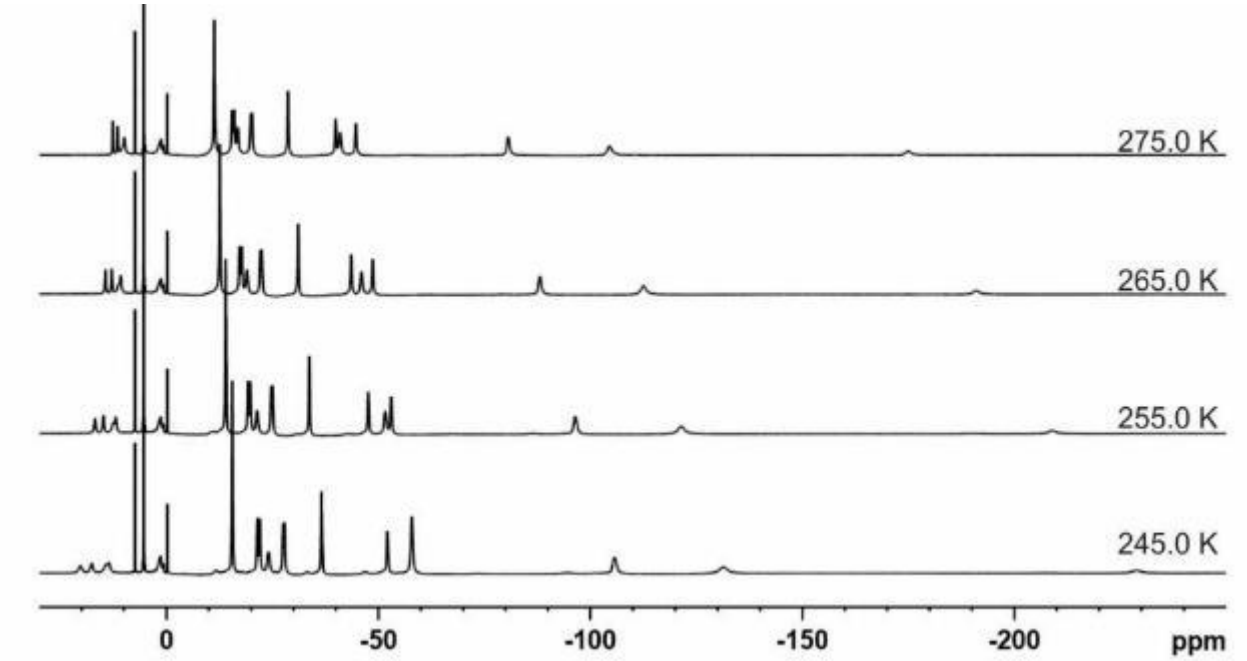

Fig. S74. Variable-temperature ^1H NMR spectra of complex **[3]$^{3+}$** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 285.0 K.

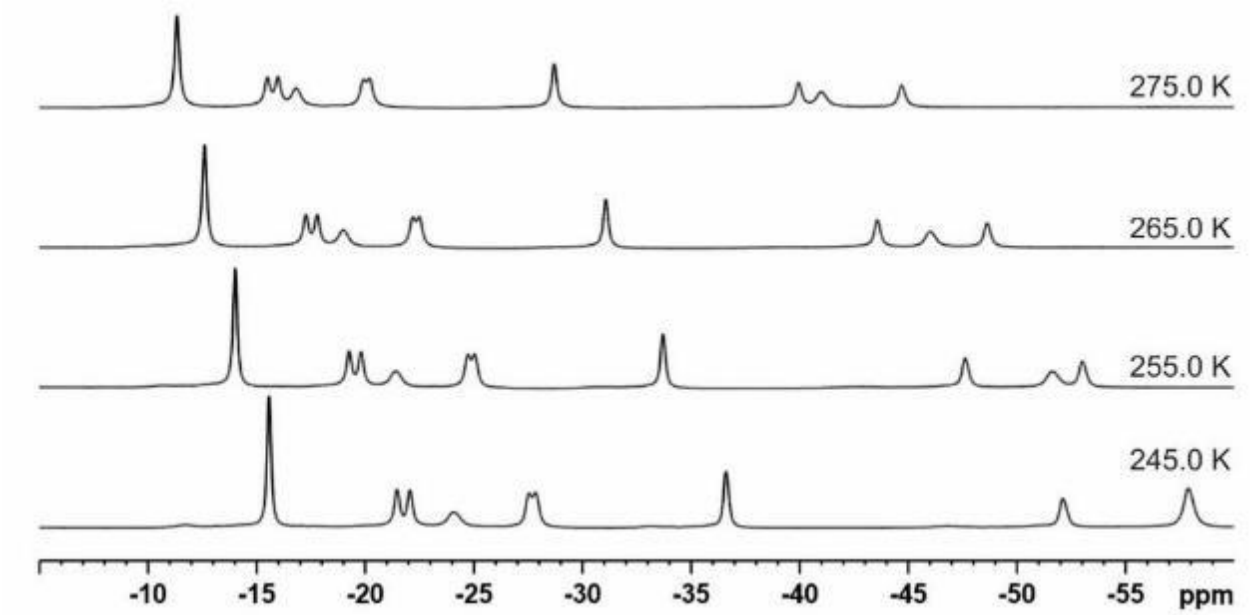

Fig. S75. Variable-temperature ^{1}H NMR spectra of complex $\mathbf{[3]^{3+}}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 285.0 K. Expansion from -5 ppm to -60 ppm.

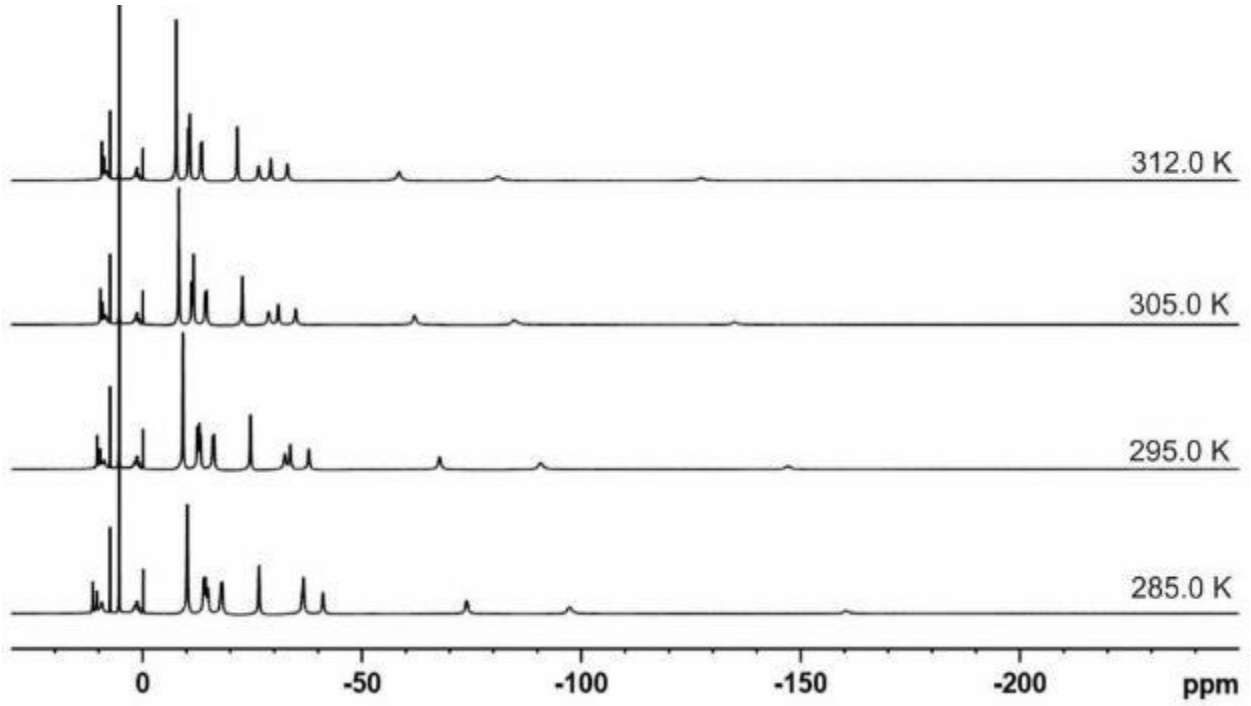

Fig. S76. Variable-temperature ^{1}H NMR spectra of complex $\mathbf{[3]^{3+}}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

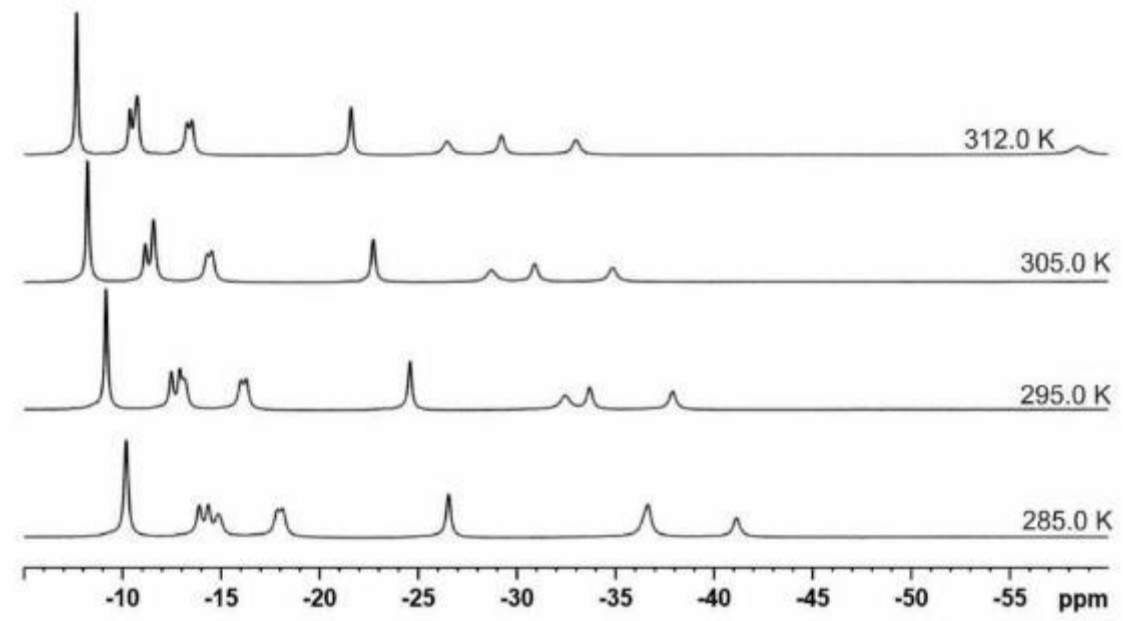

Fig. S77. Variable-temperature ^{1}H NMR spectra of complex **[3]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -5 ppm to -60 ppm.

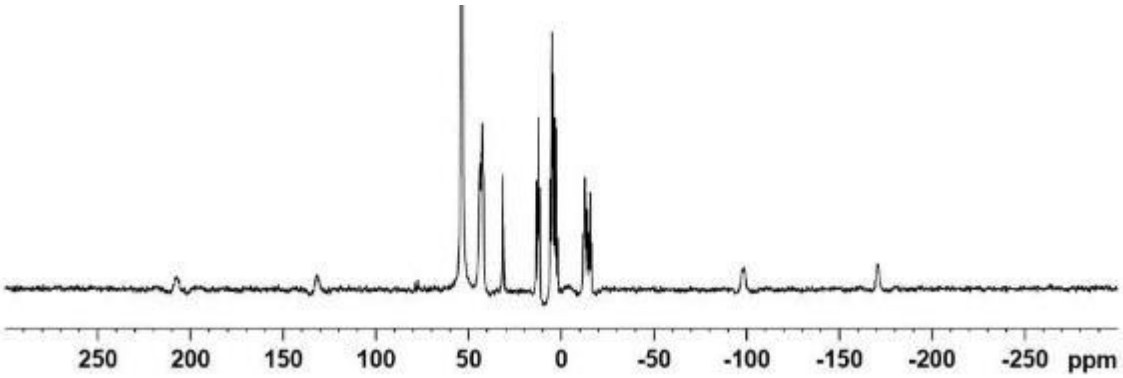

Fig. S78. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K.

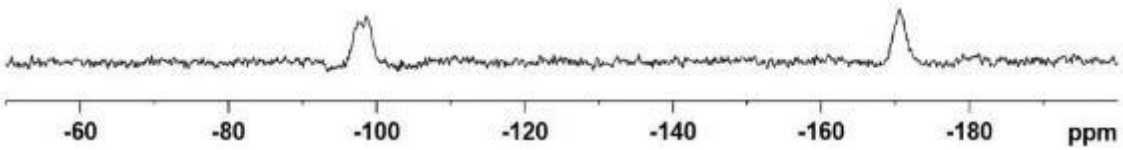

Fig. S79. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from -50 ppm to -200 ppm.

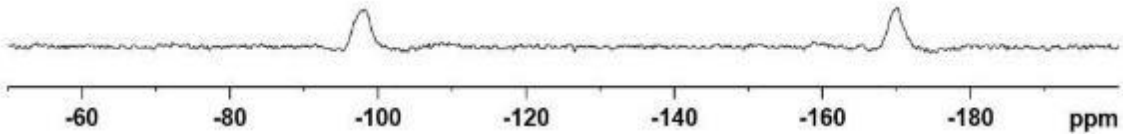

Fig. S80. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from -50 ppm to -200 ppm.

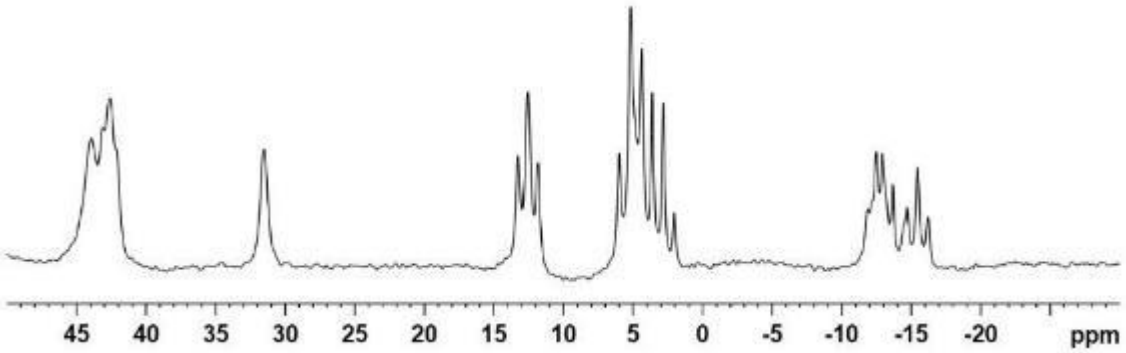

Fig. S81. ^{13}C NMR spectrum (^{1}H coupled) of complex **[3]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -30 ppm.

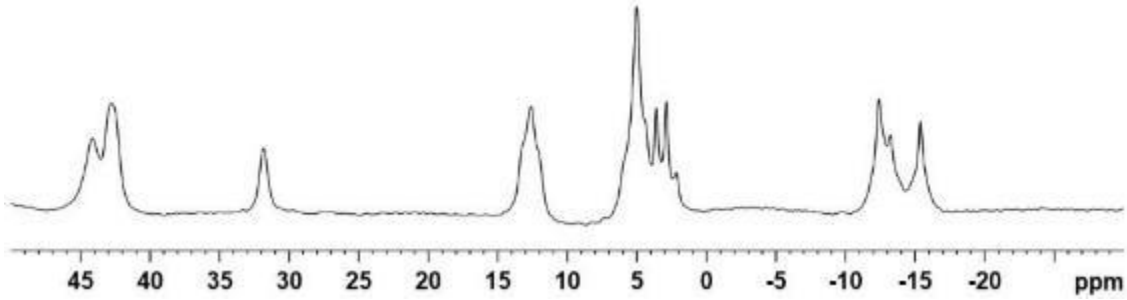

Fig. S82. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[3]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -30 ppm.

Table S7. ^{1}H NMR experimental chemical shifts for **[3]$^{3+}$** in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}i$	-228.91	-208.87	-190.94	-174.92	-160.43	-147.13	-135.01	-127.35	-161.94	21.54	8.35	-132.05	1
2: $CH_{ar}o$	-131.40	-121.49	-112.56	-104.57	-97.32	-90.78	-84.72	-80.96	-39.18	-61.03	7.98	-92.22	2
3: $CH_2\alpha i$	-105.73	-96.47	-88.11	-80.64	-73.86	-67.73	-62.00	-58.46	-74.22	-	4.64	-69.58	2
4: $CH_2\beta i$	-57.90	-53.02	-48.64	-44.70	-41.14	-37.90	-34.87	-33.02	-39.84	-	2.27	-37.57	2
5: $CH_2\gamma i$	-52.12	-47.63	-43.58	-39.96	-36.65	-33.69	-30.90	-29.22	-37.17	-	1.93	-35.24	2
6: $CH_2\alpha o$	-57.90	-51.64	-46.02	-41.00	-36.65	-32.45	-28.72	-26.47	-34.99	-	4.40	-30.59	2
7: CH_3i	-36.61	-33.71	-31.08	-28.71	-26.54	-24.58	-22.77	-21.60	-22.40	-	1.33	-21.07	3
8: $CH_2\beta o$	-27.84	-25.04	-22.49	-20.20	-18.12	-16.26	-14.54	-13.52	-12.94	-	2.10	-10.84	2
9: $CH_2\beta o$	-27.55	-24.74	-22.20	-19.93	-17.88	-16.01	-14.30	-13.29	-12.94	-	2.10	-10.84	2
10: $CH_2\alpha o$	-24.08	-21.41	-18.98	-16.82	-14.87	-13.10	-11.57	-10.75	-6.45	-	4.22	-2.23	2
11: $CH_2\gamma o$	-22.06	-19.81	-17.79	-15.98	-14.35	-12.91	-11.57	-10.75	-13.58	-	1.81	-11.77	2
12: $CH_2\gamma o$	-21.47	-19.26	-17.27	-15.50	-13.90	-12.48	-11.16	-10.39	-13.58	-	1.81	-11.77	2
13: CH_3o	-15.58	-14.02	-12.61	-11.34	-10.19	-9.18	-8.23	-7.68	-8.94	-	1.12	-7.82	6

[a]The δ_{orb} values of **[3]^0** were used. [a]The δ_{orb} values of **[3]$^{2+}$** were used.

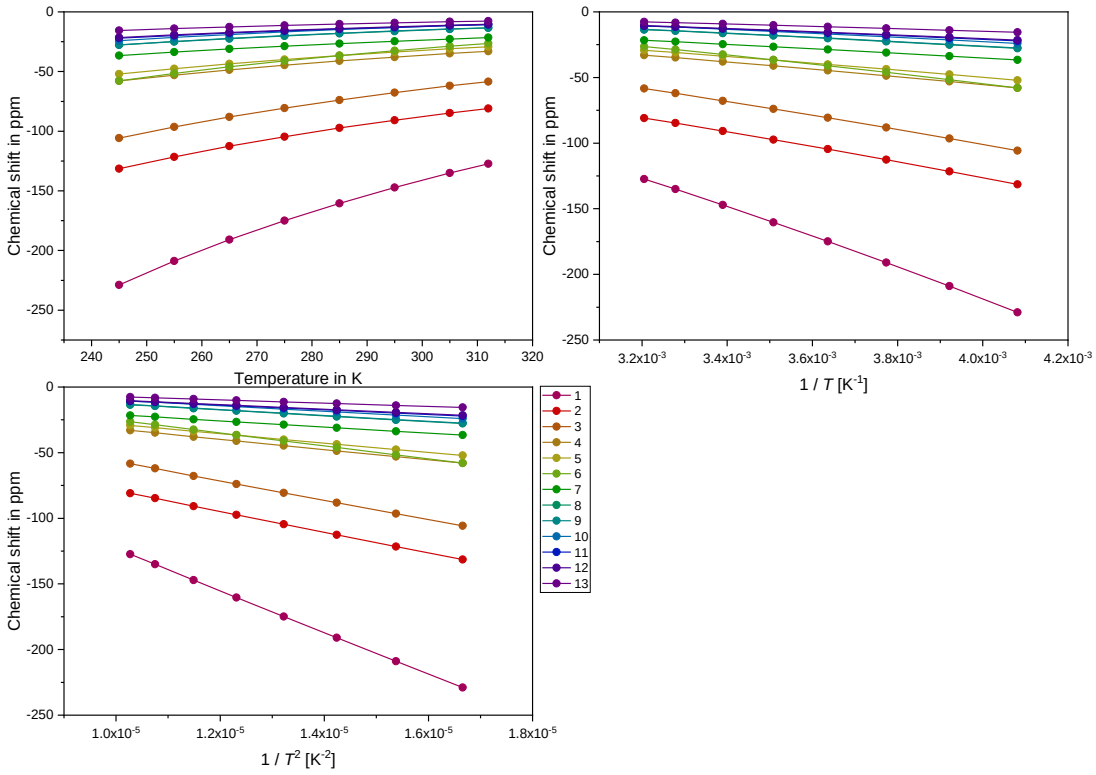

Fig. S83. Plot of the ^{1}H chemical shifts of **[3]$^{3+}$** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S8. ^{13}C NMR chemical shifts of **[3]$^{3+}$** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-170.5	s
2	-98.0	d
3	-15.4	t
4	-13.2	m
5	-12.5	q
6	3.3	q
7	4.9	q
8	5.2	t
9	12.6	t
10	31.7	s
11	42.8	t
12	44.1	d
13	131.6	s
14	207.6	s

3.6. Complex **[4]^{0}**

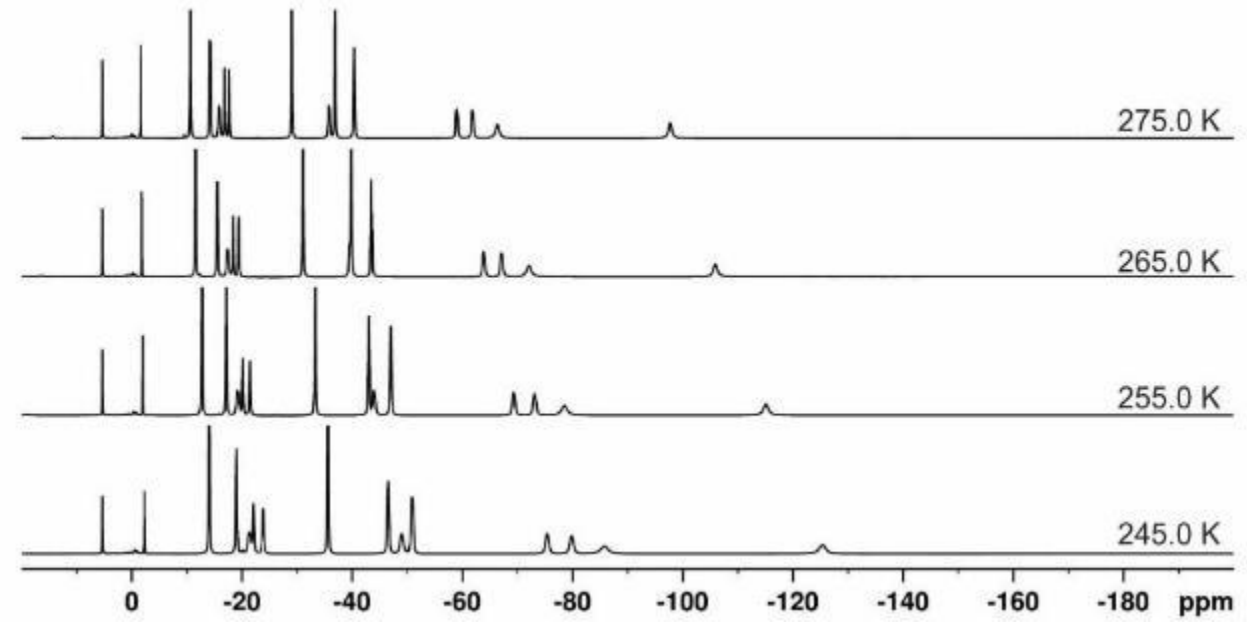

Fig. S84. Variable-temperature ^{1}H NMR spectra of complex **[4]^{0}** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

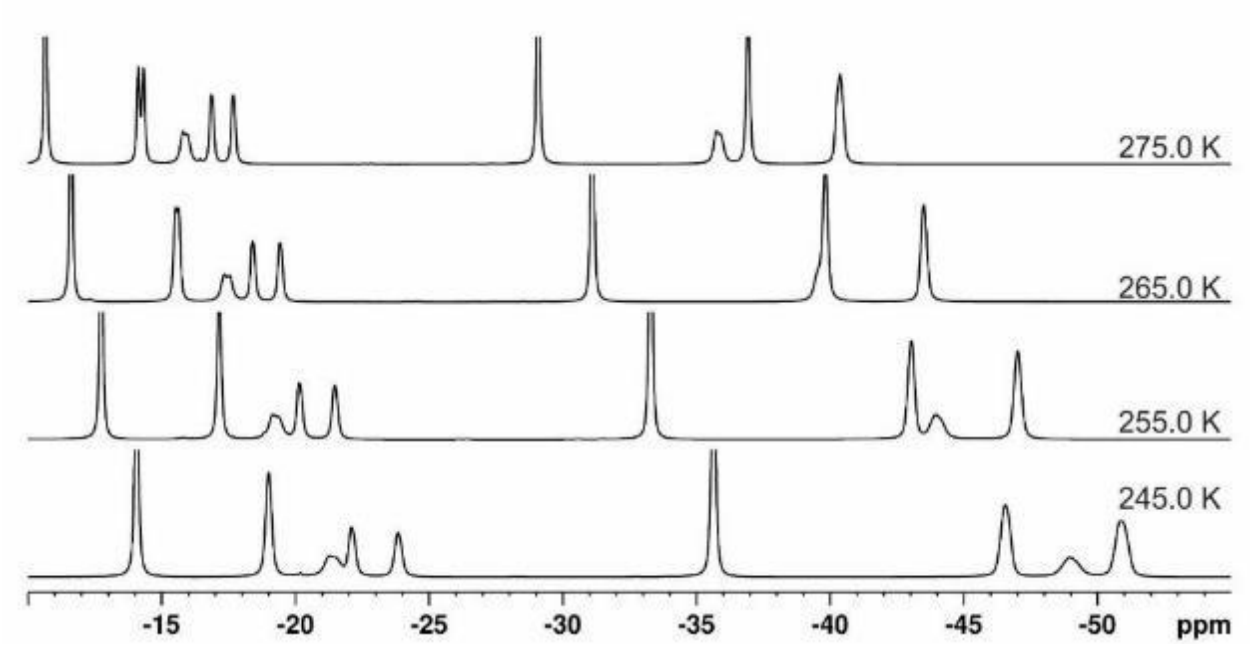

Fig. S85. Variable-temperature ^{1}H NMR spectra of complex **[4]^{0}** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -10 ppm to -55 ppm.

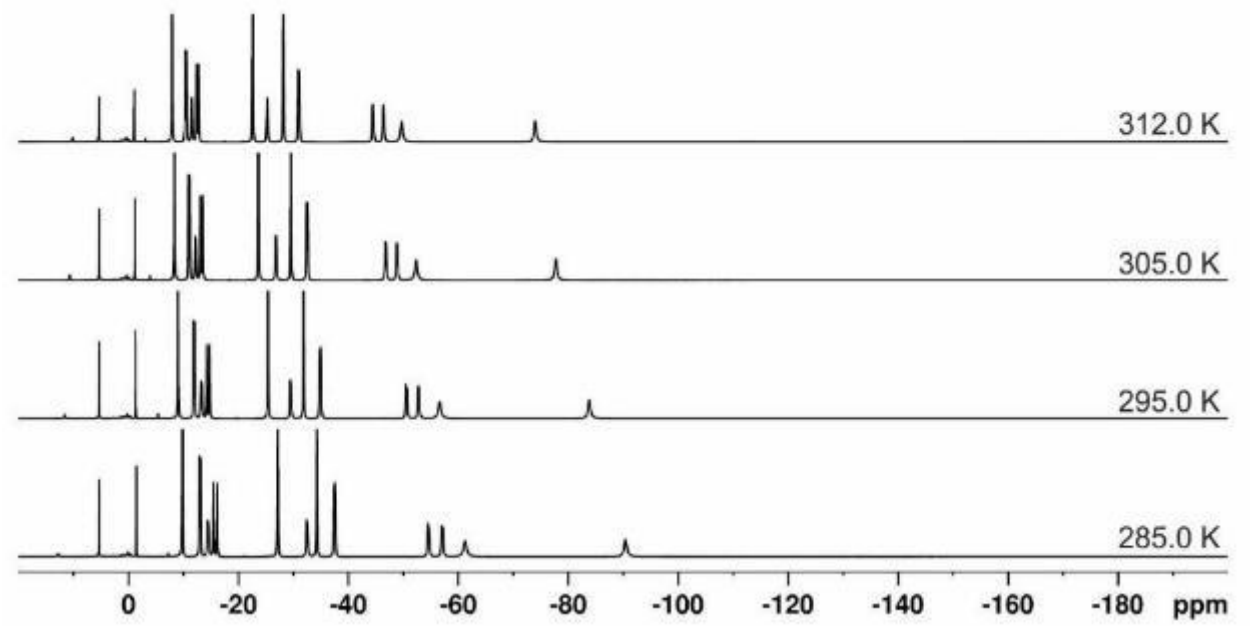

Fig. S86. Variable-temperature ^{1}H NMR spectra of complex **[4]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

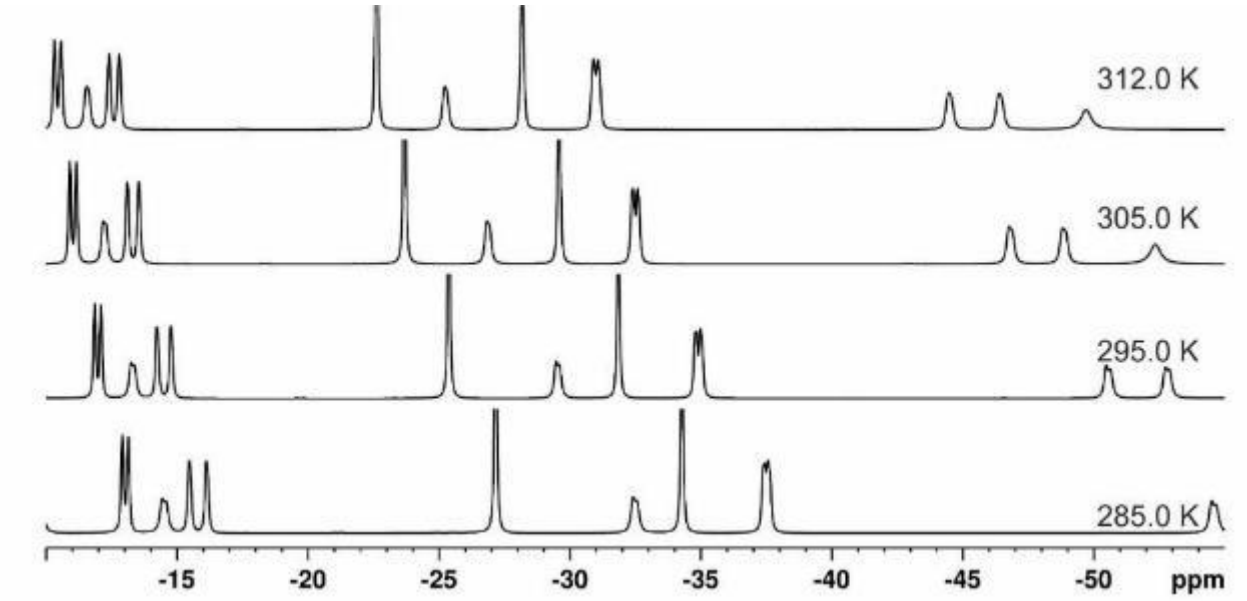

Fig. S87. Variable-temperature ^{1}H NMR spectra of complex **[4]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -20 ppm to -55 ppm.

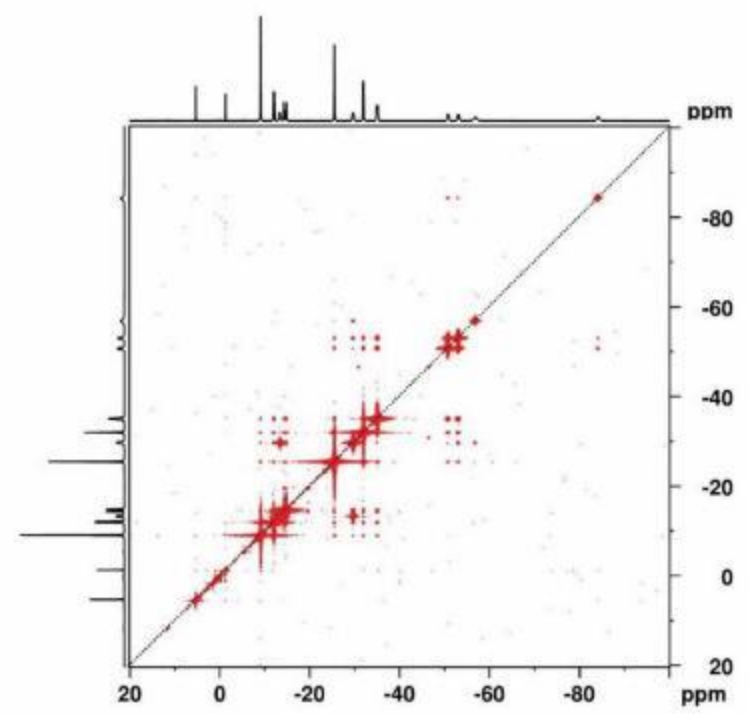

Fig. S88. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[4]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K.

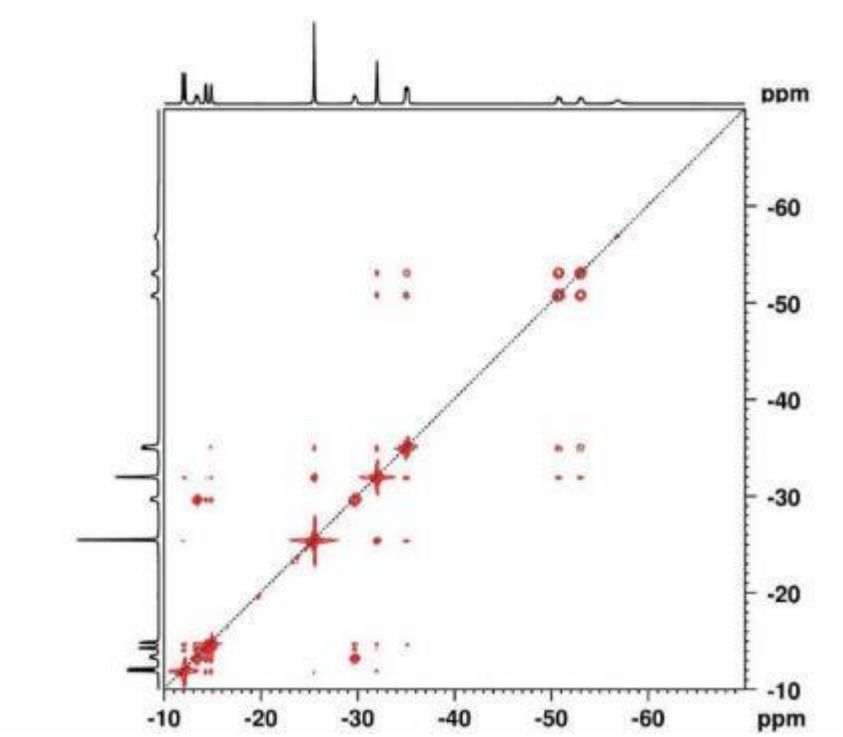

Fig. S89. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[4]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from -10 ppm to -70 ppm.

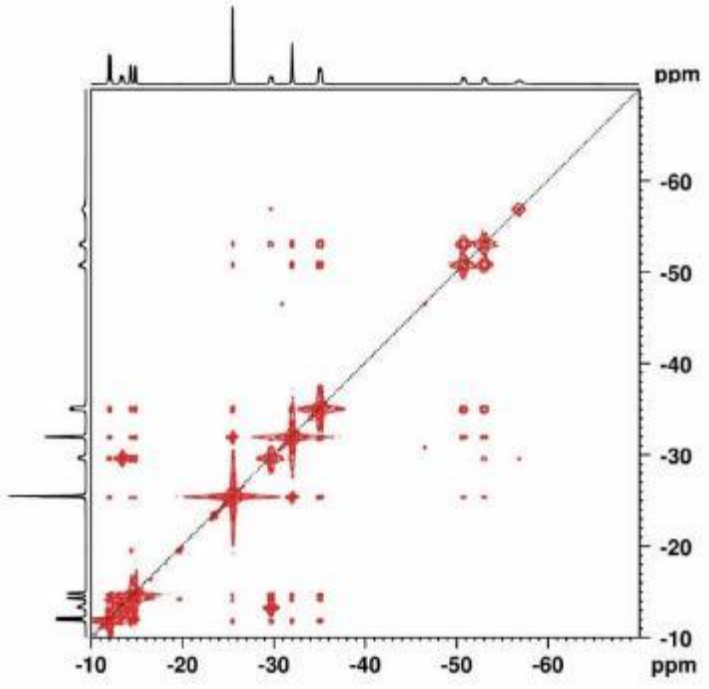

Fig. S90. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[4]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K.

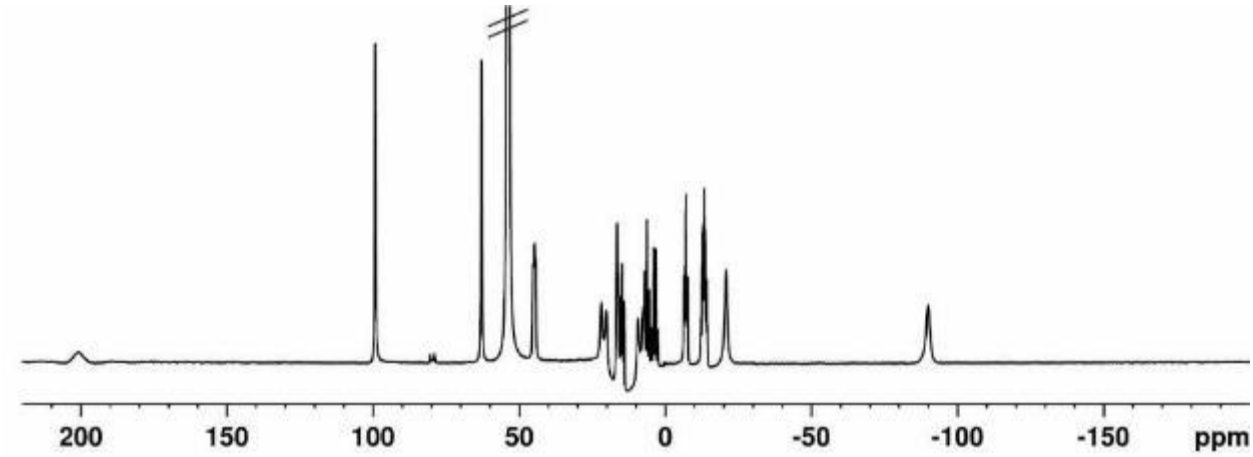

Fig. S91. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]^{0}** in CD_2Cl_2, recorded at 295.0 K.

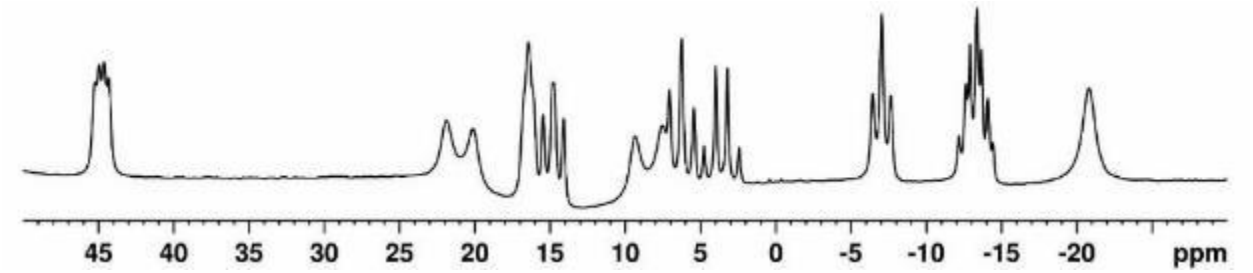

Fig. S92. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]^{0}** in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -30 ppm.

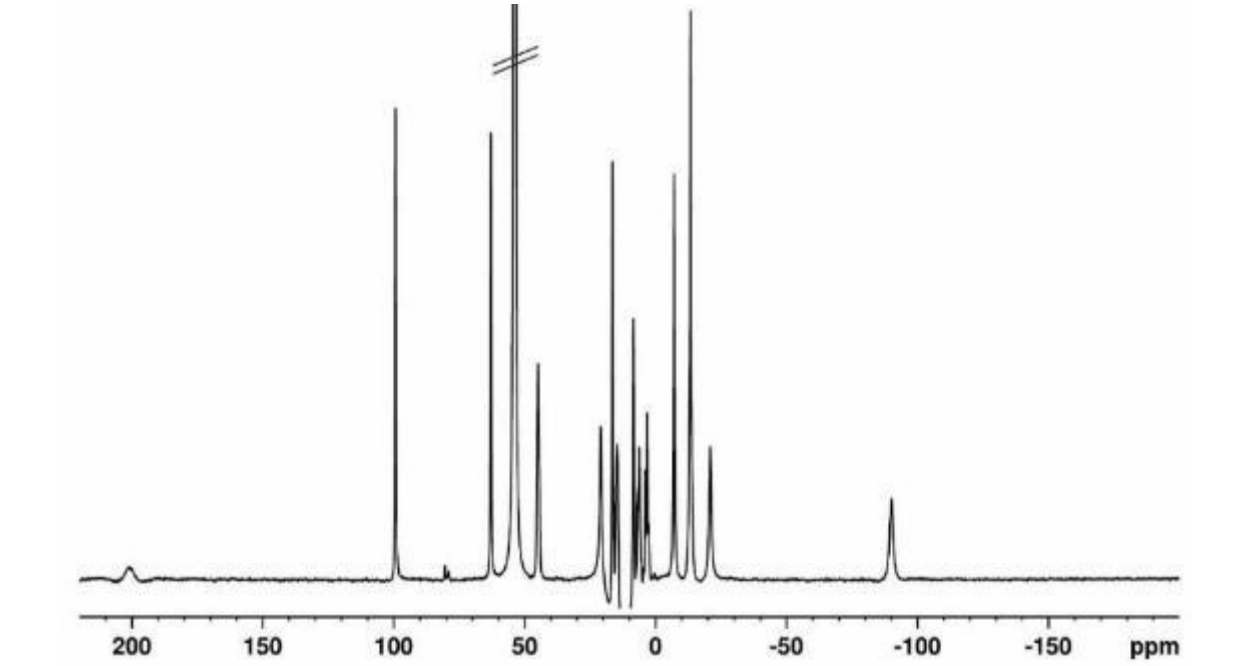

Fig. S93. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]^{0}** in CD_2Cl_2, recorded at 295.0 K.

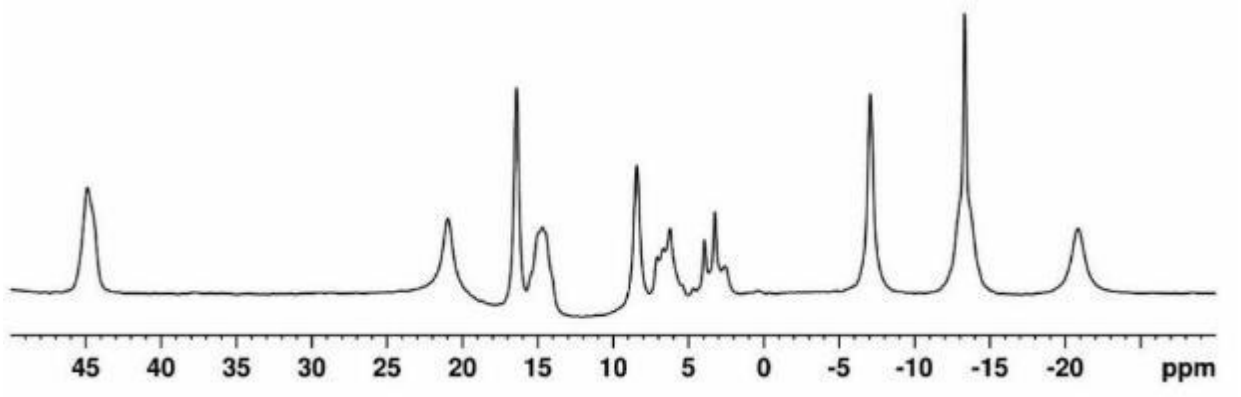

Fig. S94. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]^{0}** in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -30 ppm.

Table S9. ^{1}H NMR experimental chemical shifts for **[4]^0** in CD_2Cl_2. The naming convention for the ^{1}H nuclei is the same as for the triple-decker series (the presence of two inner ligands requires distinction between the diastereotopic ^{1}H of the CH_2 groups that point either towards the outer ligand or the other inner ligand). Signals which integrate to 0.5 are actually from the same ^{1}H resonance, but the additional splitting is caused by residual dipolar couplings (RDCs).

	T in K								Calculated@295 K			
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm											Integral
1: $CH_{ar}i$	-125.42	-115.14	-105.92	-97.75	-90.44	-83.85	-77.77	-74.00	-85.23	7.69	-77.54	1
2: $CH_{ar}o$	-85.76	-78.55	-72.10	-66.38	-61.25	-56.63	-52.35	-49.71	-66.09	7.69	-58.40	1
3: $CH_2\alpha i$	-79.83	-73.11	-67.12	-61.84	-57.10	-52.82	-48.66	-46.41	-56.10	4.65	-51.45	1
4: $CH_2\alpha i$	-75.39	-69.33	-63.86	-59.01	-54.59	-50.56	-46.82	-44.48	-52.32	4.76	-47.56	1
5: $CH_2\beta i$	-50.89	-47.02	-43.51	-40.37	-37.57	-34.99	-32.59	-31.09	-33.74	2.49	-31.25	1
6: $CH_2\beta i$	-50.89	-47.02	-43.51	-40.37	-37.45	-34.83	-32.40	-30.91	-33.74	2.49	-31.25	1
7: $CH_2\gamma i$	-46.56	-43.04	-39.83	-36.94	-34.29	-31.86	-29.59	-28.19	-32.03	2.18	-29.85	2
8: $CH_2\alpha o$	-48.98	-43.96	-39.57	-35.83	-32.49	-29.54	-26.87	-25.24	-42.67	4.42	-38.25	1
9: CH_3i	-35.65	-33.30	-31.11	-29.08	-27.17	-25.38	-23.69	-22.62	-21.02	1.54	-19.48	3
10: $CH_2\beta o$	-23.85	-21.47	-19.43	-17.67	-16.12	-14.76	-13.54	-12.79	-17.75	2.03	-15.72	1
11: $CH_2\beta o$	-22.11	-20.14	-18.40	-16.85	-15.47	-14.23	-13.10	-12.40	-17.75	2.03	-15.72	1
12: $CH_2\alpha o$	-21.39	-19.25	-17.45	-15.87	-14.50	-13.31	-12.23	-11.55	-20.24	4.13	-16.11	1
13: : $CH_2\gamma o$	-19.01	-17.16	-15.62	-14.32	-13.14	-12.10	-11.15	-10.58	-18.18	1.71	-16.47	1
14: : $CH_2\gamma o$	-19.01	-17.16	-15.53	-14.13	-12.92	-11.86	-10.91	-10.33	-18.18	1.71	-16.47	1
15: CH_3o	-14.06	-12.74	-11.62	-10.65	-9.80	-9.05	-8.37	-7.95	-11.85	1.14	-10.71	3

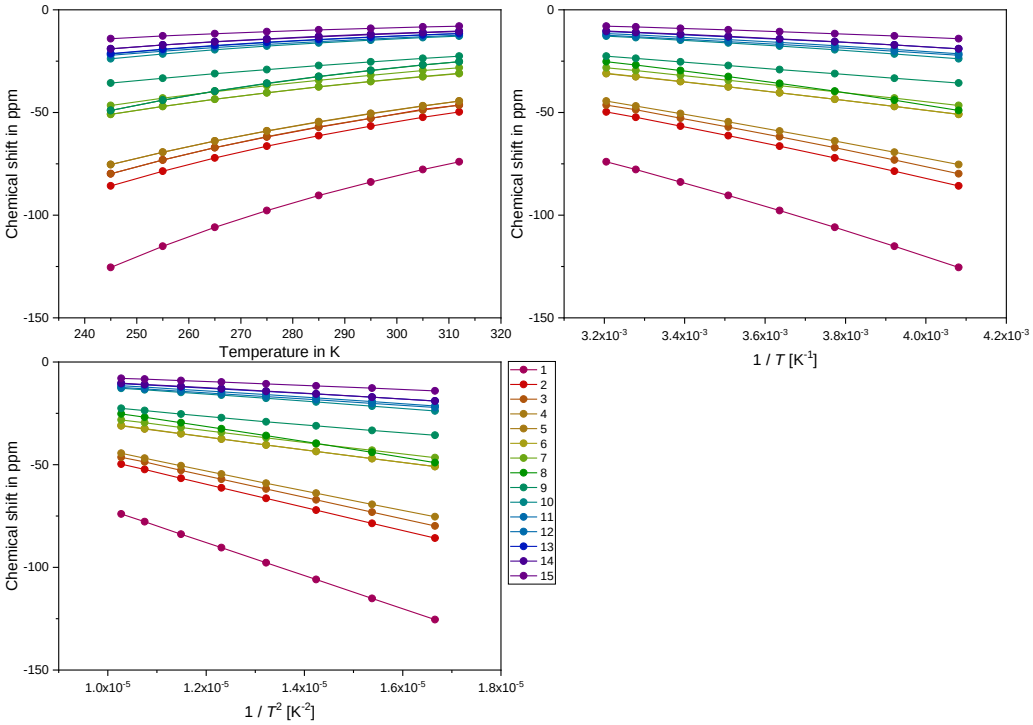

Fig. S95. Plot of the ^{1}H chemical shifts of **[4]^0** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S10. ^{13}C NMR chemical shifts of **[4]^{0}** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-90.0	s
2	-20.7	s
3	-13.3	t
4	-13.3	q
5	-7.0	t
6	3.7	q
7	6.3	t
8	8.5	d
9	14.8	t
10	14.8	t
11	16.5	t
12	20.9	d
13	44.9	t
14	62.9	s
15	99.3	s
16	201.1	s

3.7. Complex **[4]$^{+}$**

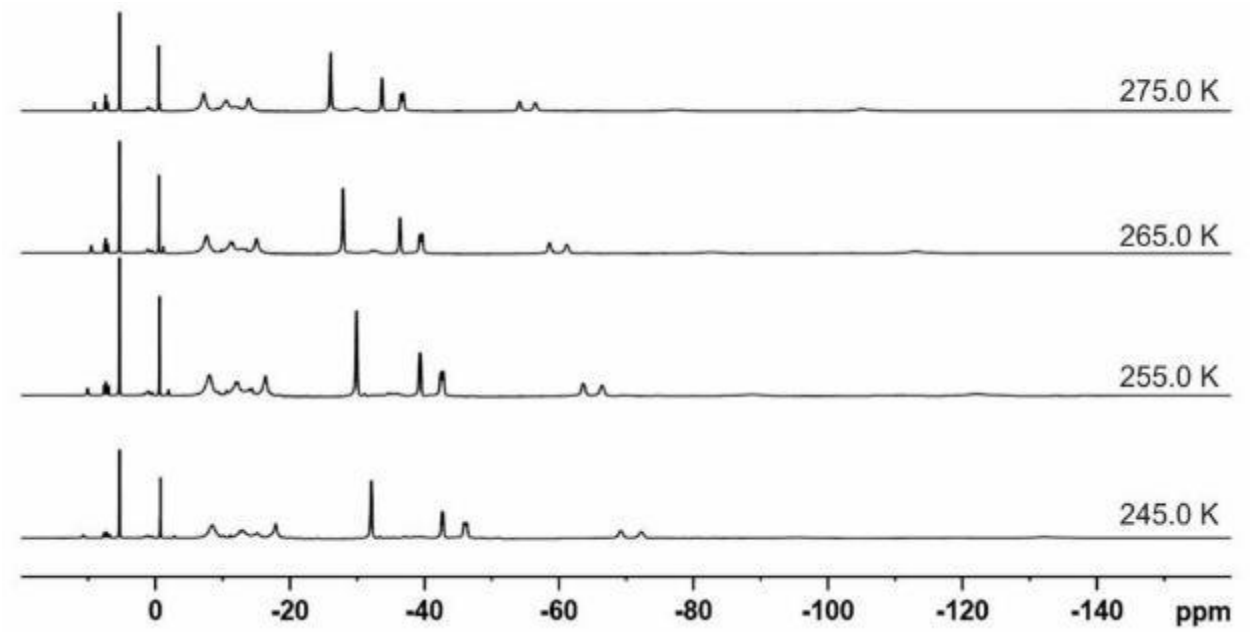

Fig. S96. Variable-temperature ^{1}H NMR spectra of complex **[4]$^{+}$** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

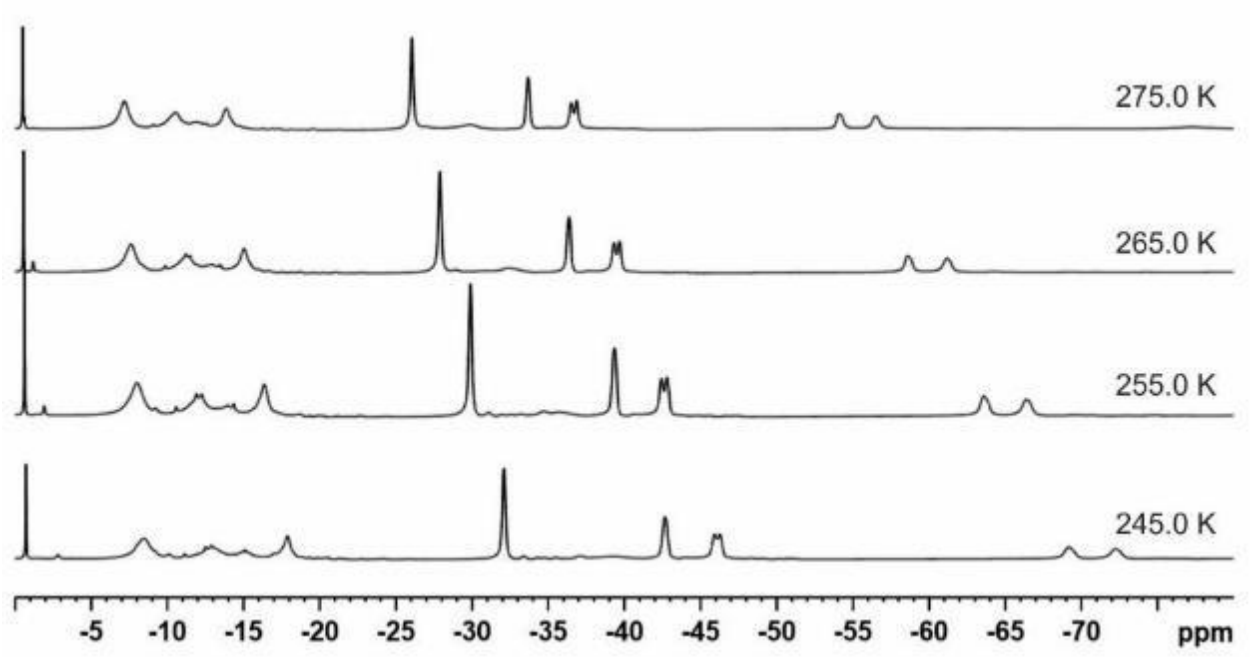

Fig. S97. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -80 ppm.

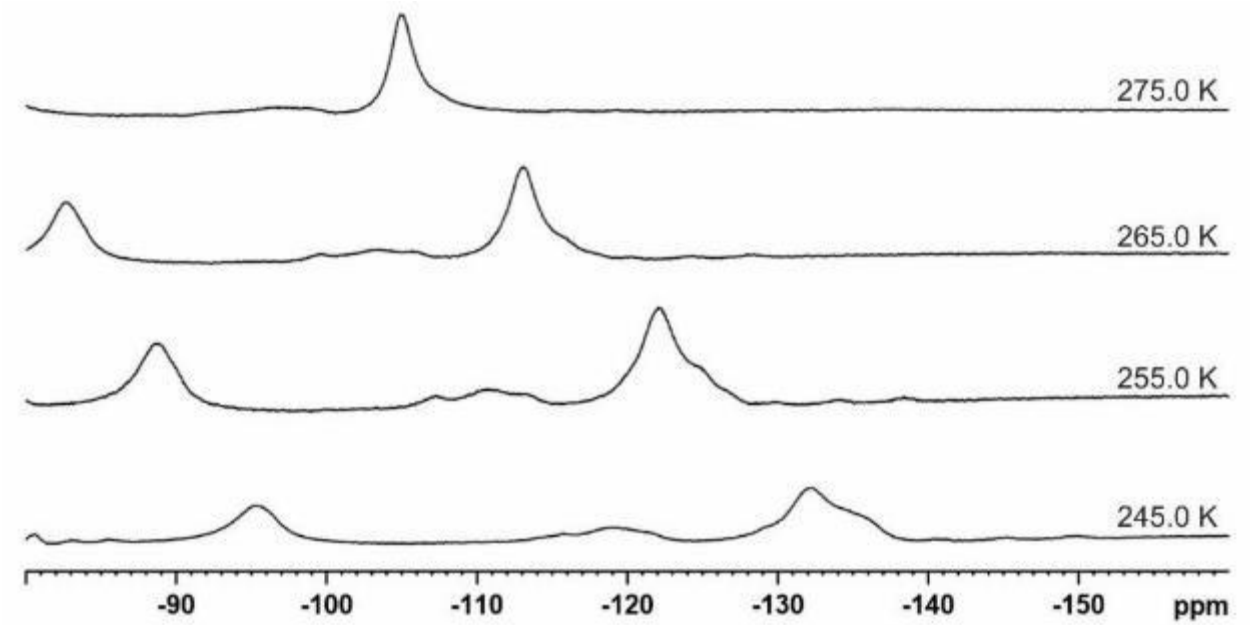

Fig. S98. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -80 ppm to -160 ppm.

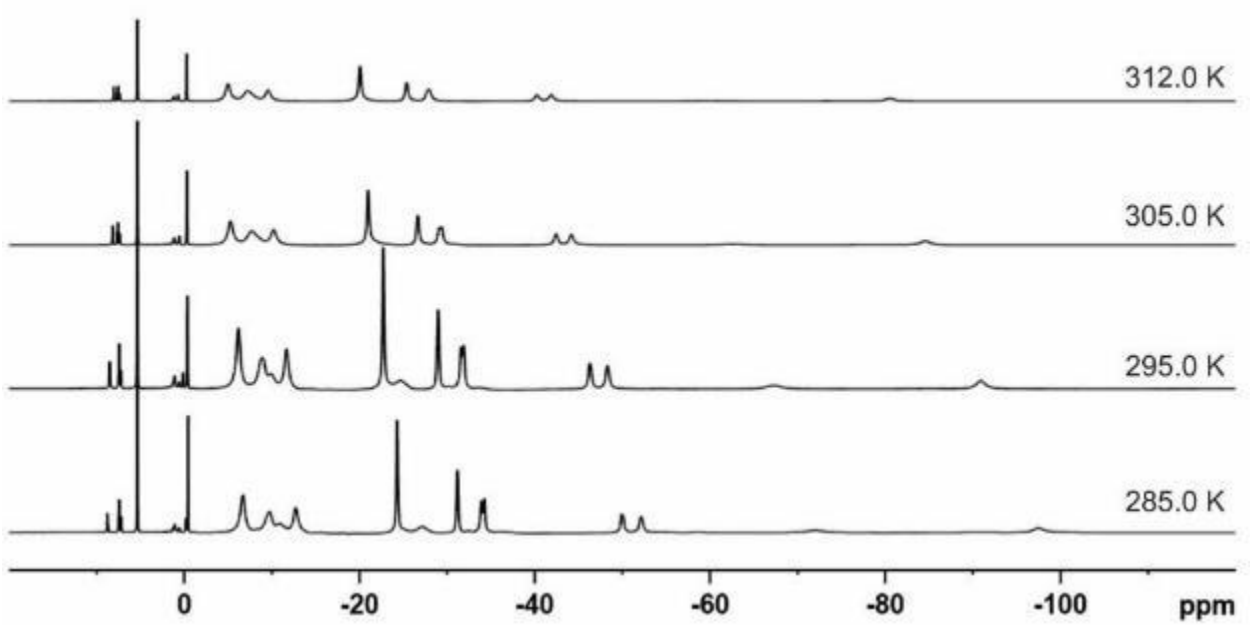

Fig. S99. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

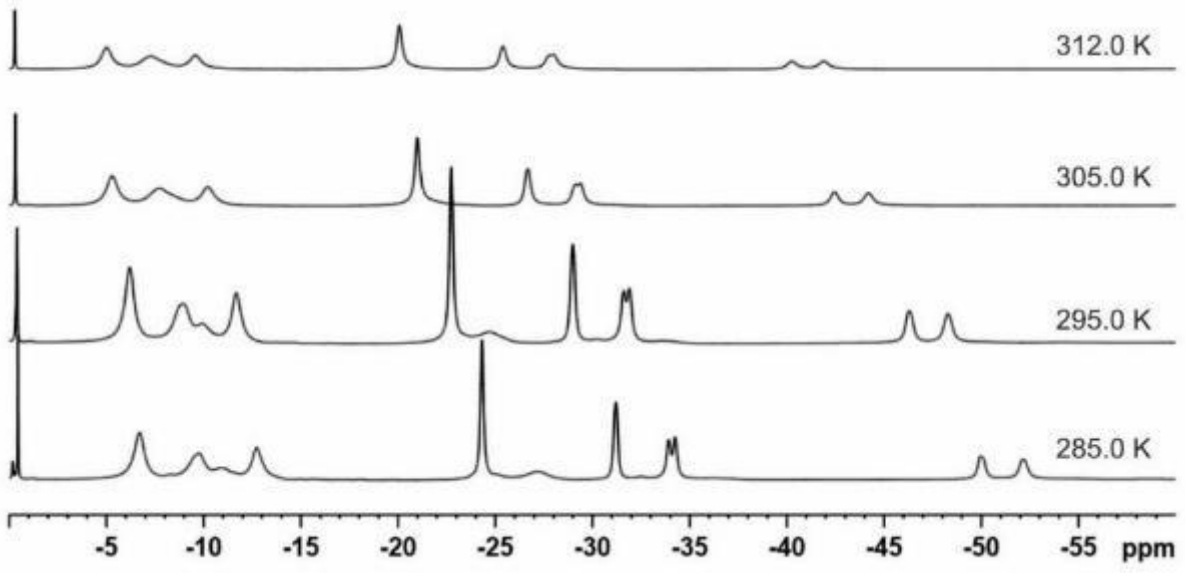

Fig. S100. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -60 ppm.

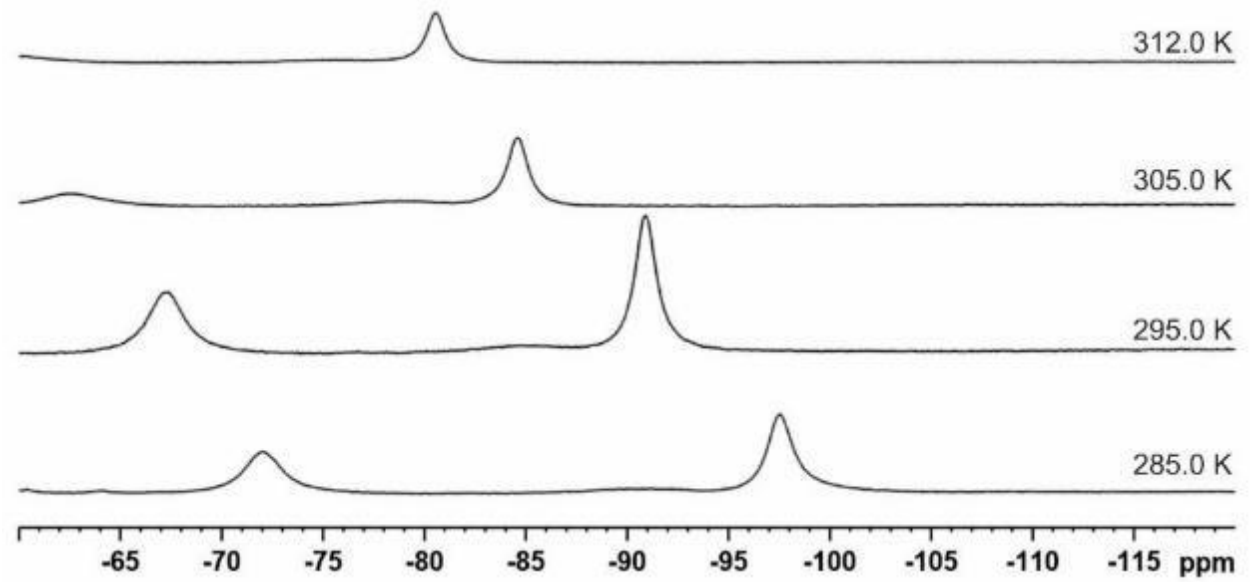

Fig. S101. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -60 ppm to -120 ppm.

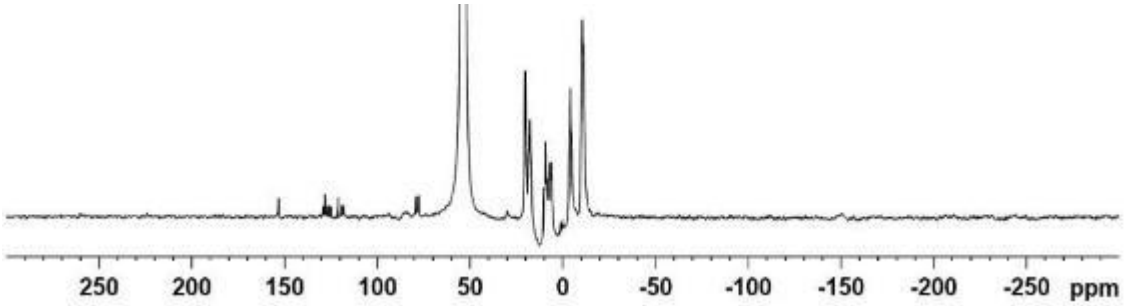

Fig. S102. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K.

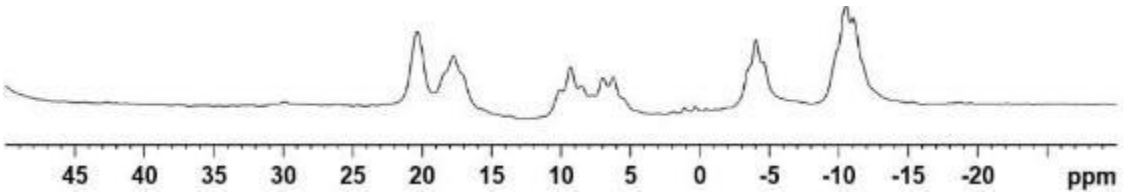

Fig. S103. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -30 ppm.

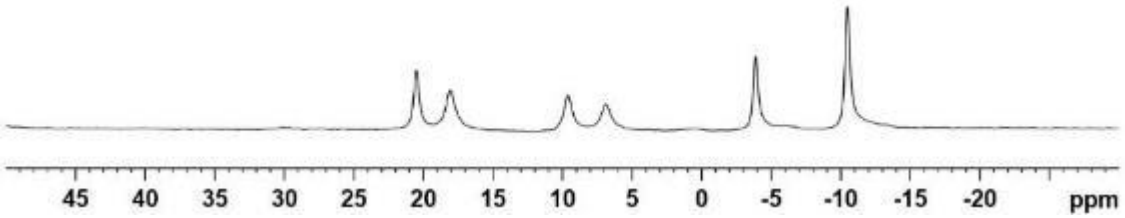

Fig. S104. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -30 ppm.

Table S11. ^{1}H NMR experimental chemical shifts for **[4]**$^{+}$ in CD_2Cl_2. The observed signals were quite broad. Some impurities (neutral quintuple-decker) were not avoidable even after repeating the sample preparation several times.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}i$	-132.31	-122.07	-113.01	-104.98	-97.53	-90.71	-84.65	-80.56	-80.92	-10.77	7.03[a]	-84.19	1
2: $CH_{ar}o$	-95.42	-88.67	-82.66	-77.26	-72.03	-67.06	-62.48	-59.76	-53.39	-24.53	7.03[a]	-70.42	1
3: $CH_2\alpha i$	-72.21	-66.41	-61.22	-56.48	-52.16	-48.19	-44.20	-41.92	-52.05	-	4.57[a]	-47.99	1
4: $CH_2\alpha i$	-69.10	-63.60	-58.65	-54.09	-49.96	-46.18	-42.45	-40.28	-49.07	-	4.57[a]	-45.01	1
5: $CH_2\beta i$	-46.21	-42.81	-39.67	-36.87	-34.26	-31.85	-29.39	-27.99	-31.82	-	2.43	-30.06	1
6: $CH_2\beta i$	-45.84	-42.45	-39.31	-36.52	-33.93	-31.55	-29.12	-27.83	-31.82	-	2.43	-30.06	1
7: $CH_2\gamma i$	-42.62	-39.36	-36.37	-33.69	-31.22	-28.94	-26.68	-25.41	-30.37	-	2.16	-28.92	2
8: $CH_2\alpha o$	-39.36	-35.70	-32.49	-29.87	-27.20	-24.57	-22.45	-20.75	-33.92	-	4.25[a]	-29.86	1
9: CH_3i	-32.00	-29.90	-27.88	-26.06	-24.33	-22.70	-21.00	-20.08	-20.02	-	1.5	-19.12	3
10: $CH_2\beta o$	-17.85	-16.37	-15.01	-13.86	-12.73	-11.66	-10.22	-9.58	-13.31	-	2.02	-11.55	2
11: $CH_2\alpha o$	-15.12	-13.96	-12.97	-11.87	-10.91	-9.87	-8.21	-7.78	-13.31	-	4.11[a]	-7.03	1
12: $CH_2\gamma o$	-12.95	-12.10	-11.31	-10.58	-9.70	-8.92	-7.72	-7.23	-13.07	-	1.73	-11.62	2
13: CH_3o	-8.36	-8.02	-7.61	-7.19	-6.71	-6.20	-5.30	-5.01	-8.79	-	1.10	-7.89	3

[a]The δ_{orb} values of **[4]**$^{4+}$ were used.

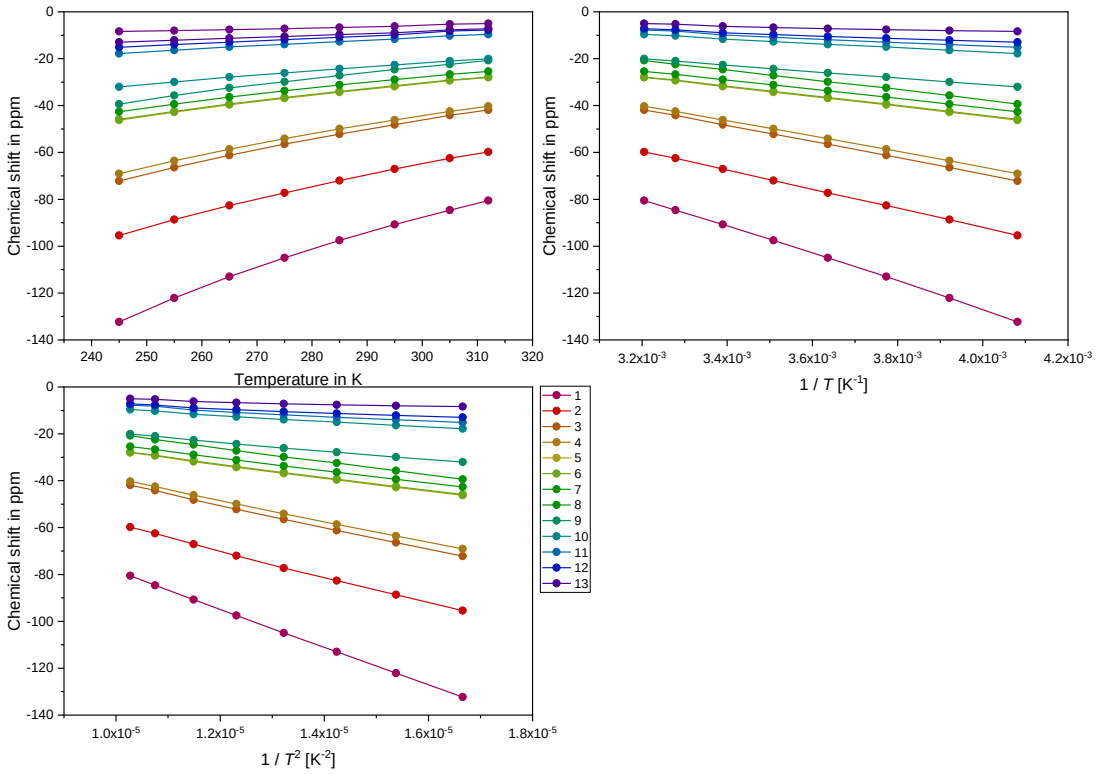

Fig. S105. Plot of the ^{1}H chemical shifts of **[4]**$^{+}$ in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S12. ^{13}C NMR chemical shifts of **[4]**$^{+}$ observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-10.5	t ?
2	-3.9	t
3	6.7	q
4	9.7	t
5	18.2	t
6	20.6	broad signal

3.8. Complex **[4]**$^{2+}$

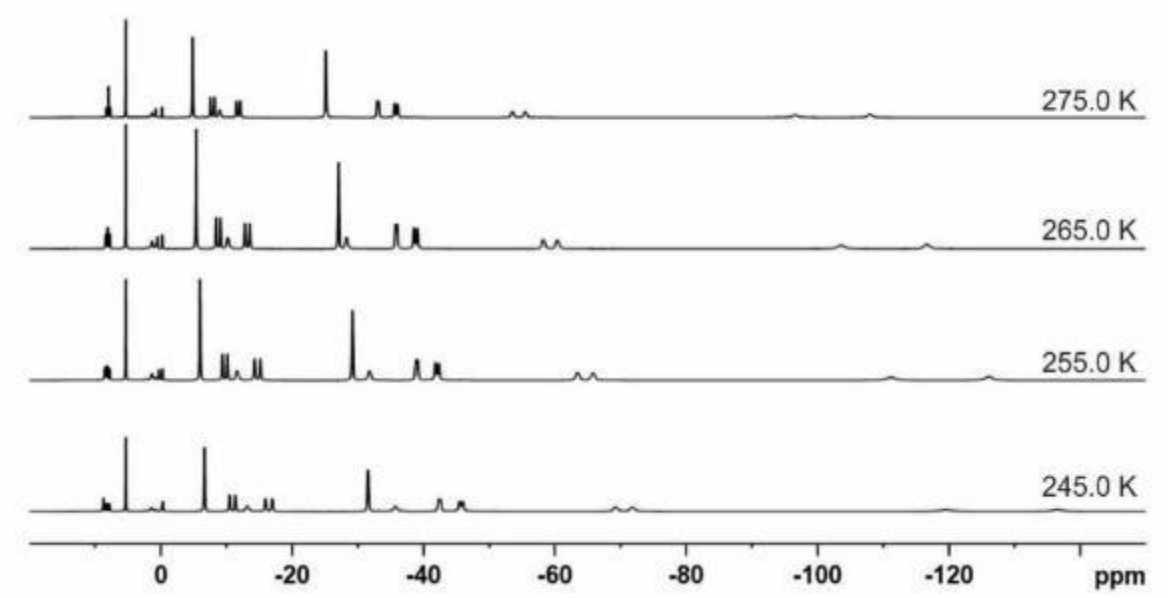

Fig. S106. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

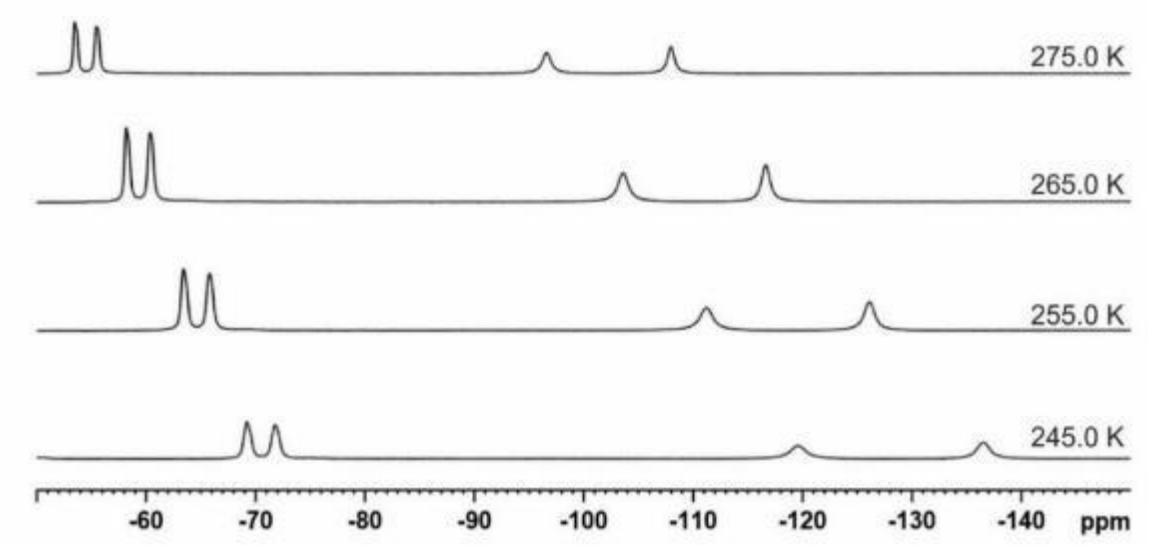

Fig. S107. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -50 ppm to -150 ppm.

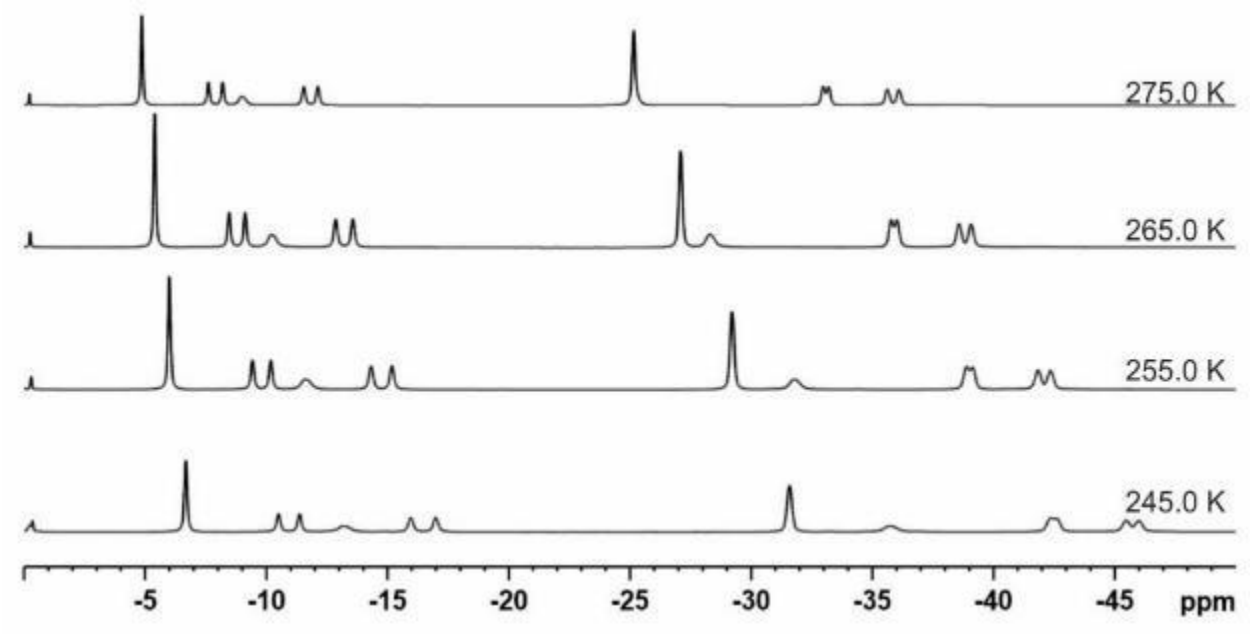

Fig. S108. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -50 ppm.

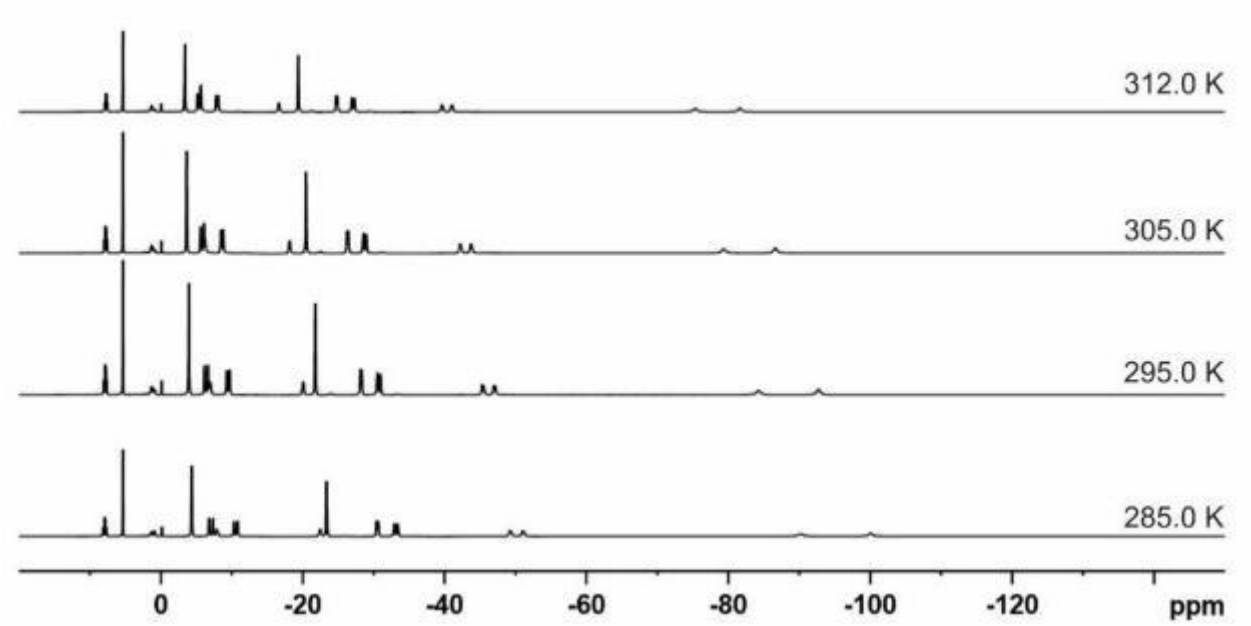

Fig. S109. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +20 ppm to -150 ppm.

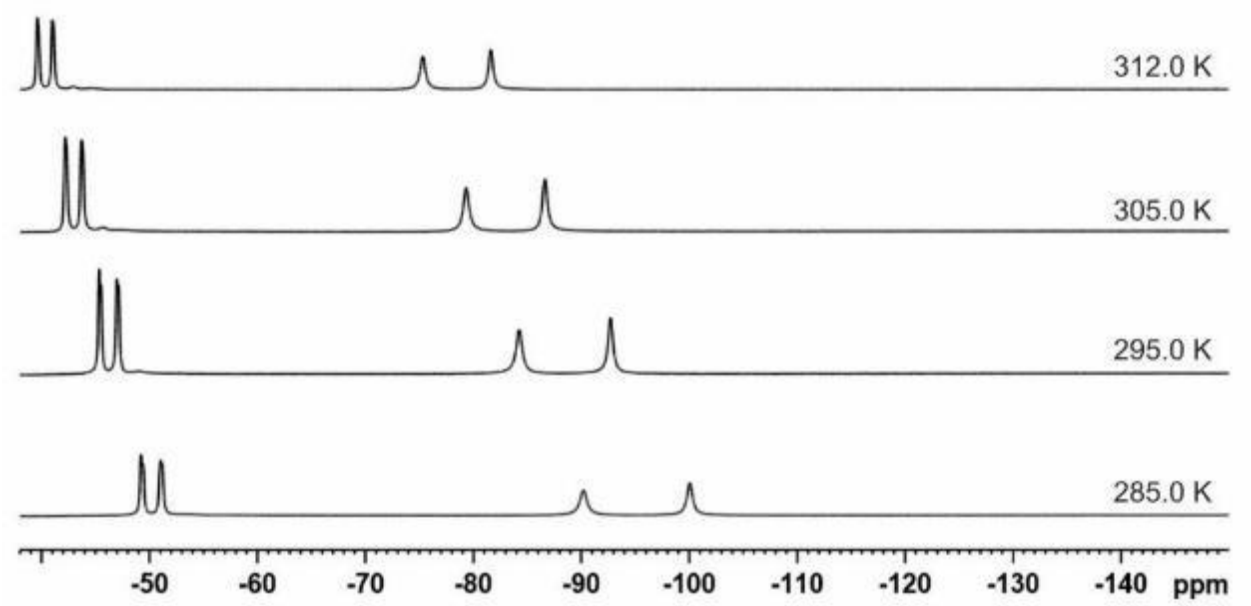

Fig. S110. Variable-temperature ^{1}H NMR spectra of complex $[4]^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -38 ppm to -150 ppm.

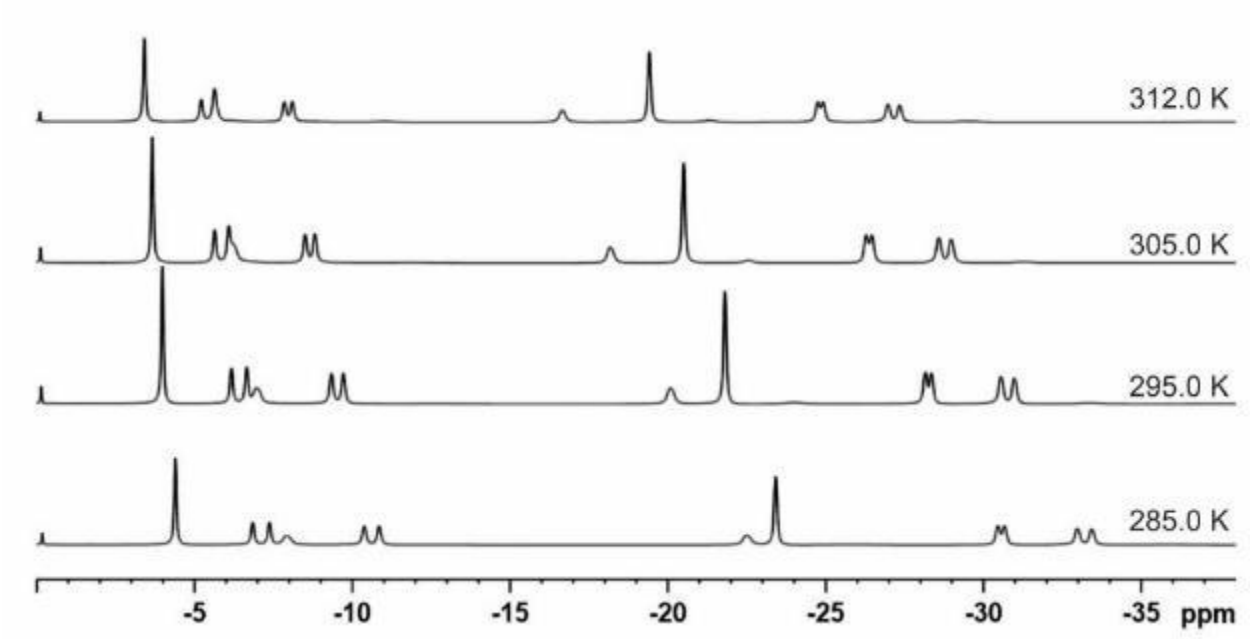

Fig. S111. Variable-temperature ^{1}H NMR spectra of complex $[4]^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -40 ppm.

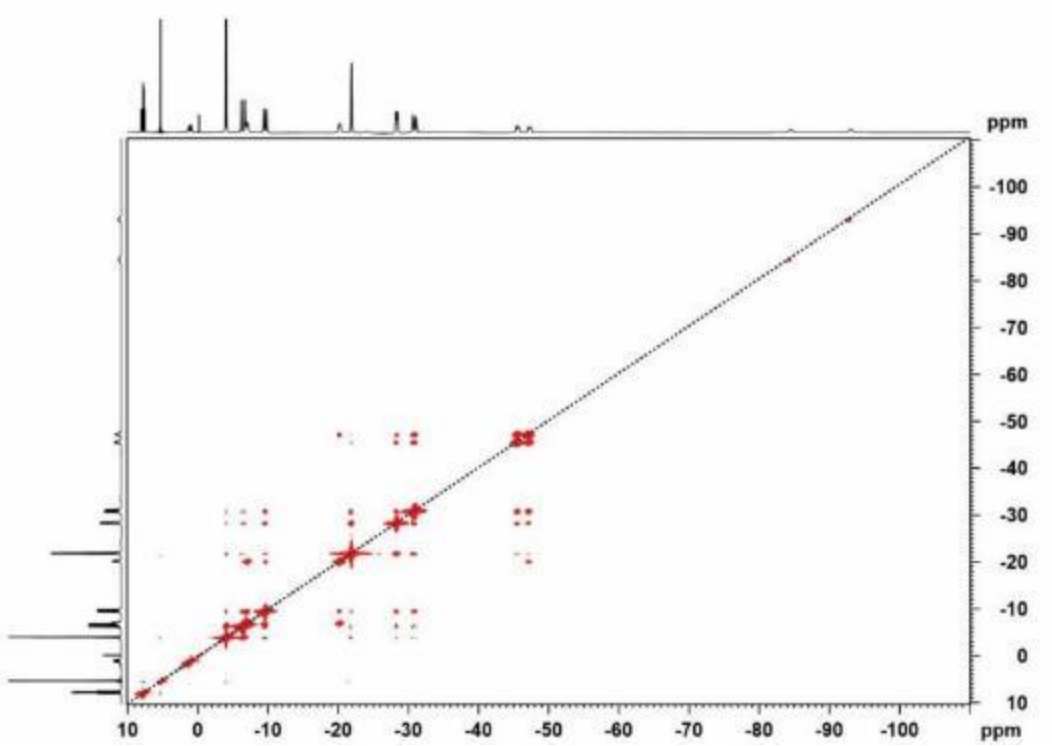

Fig. S112. H, ^{1}H NMR correlation (COSY) spectrum of complex **[4]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from +10 ppm to -110 ppm.

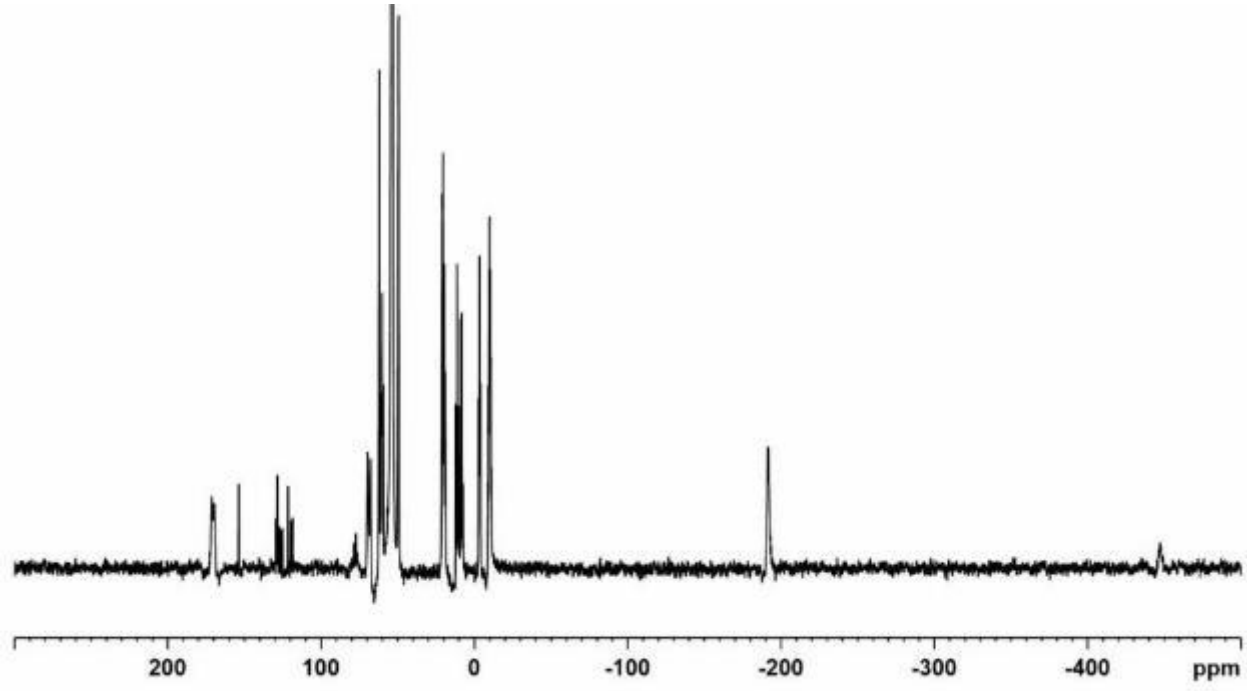

Fig. S113. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K.

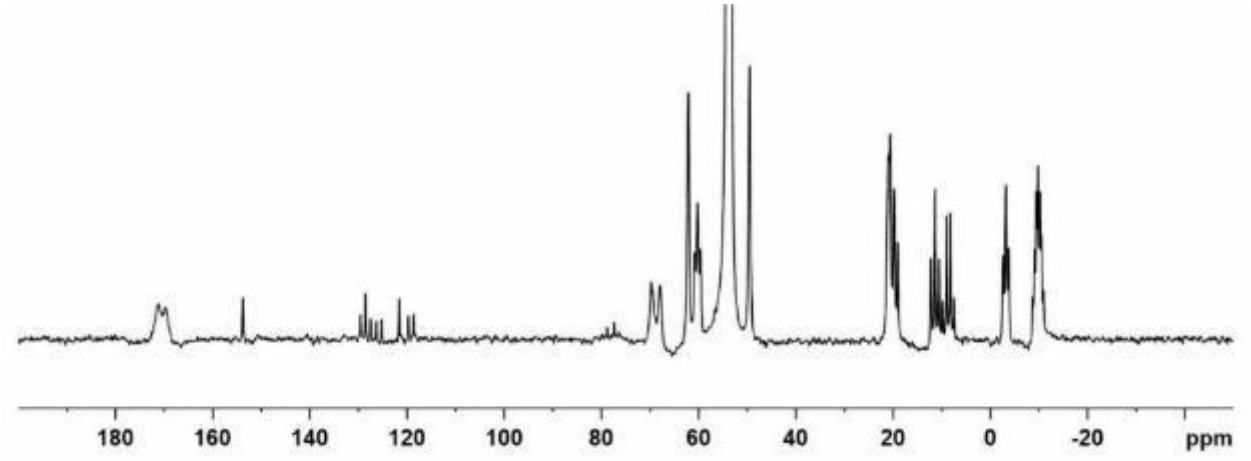

Fig. S114. ^{13}C NMR spectrum (^{1}H coupled) of complex $\mathbf{[4]^{2+}}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +200 ppm to -50 ppm.

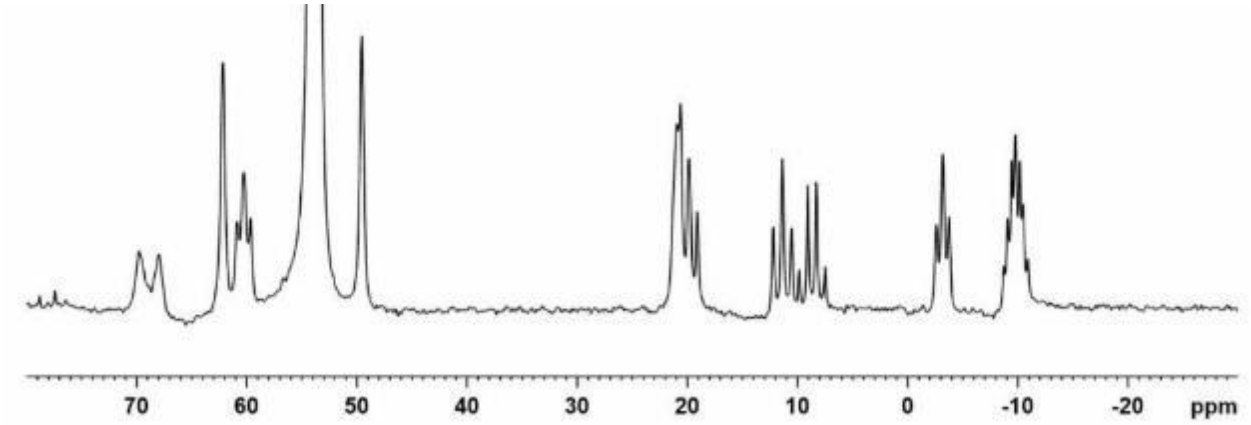

Fig. S115. ^{13}C NMR spectrum (^{1}H coupled) of complex $\mathbf{[4]^{2+}}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +80 ppm to -30 ppm.

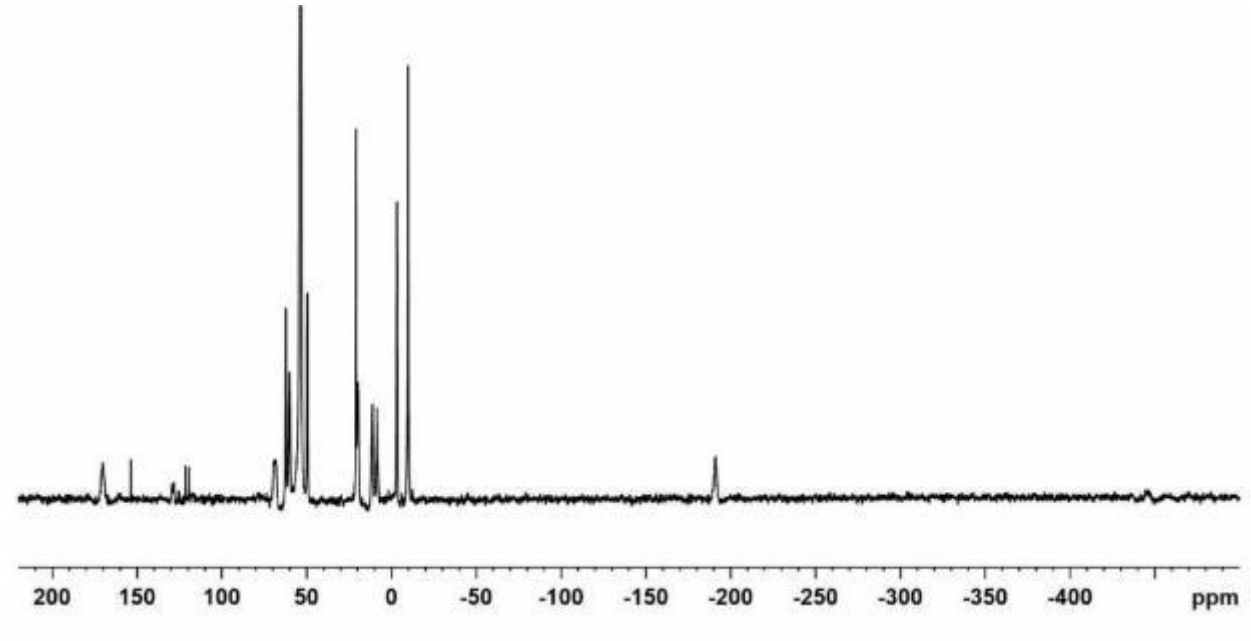

Fig. S116. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K.

Table S13. ^{1}H NMR experimental chemical shifts for **[4]**$^{2+}$ in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}o$	-136.54	-126.12	-116.64	-107.98	-100.08	-92.74	-86.64	-81.64	-51.81	-59.23	7.03[a]	-104.01	1
2: $CH_{ar}i$	-119.67	-111.23	-103.63	-96.64	-90.22	-84.26	-79.35	-75.35	-82.82	-21.54	7.03[a]	-97.33	1
3: $CH_2\alpha i$	-71.81	-65.81	-60.39	-55.52	-51.11	-47.07	-43.74	-41.07	-53.11	-	4.57[a]	-48.54	1
4: $CH_2\alpha i$	-69.24	-63.45	-58.27	-53.56	-49.32	-45.44	-42.22	-39.68	-49.82	-	4.57[a]	-45.25	1
5: $CH_2\beta i$	-45.99	-42.36	-39.07	-36.10	-33.42	-30.97	-28.98	-27.35	-31.92	-	2.38	-29.54	1
6: $CH_2\beta i$	-45.48	-41.85	-38.57	-35.62	-32.96	-30.55	-28.58	-26.80	-31.92	-	2.38	-29.54	1
7: $CH_2\gamma i$	-42.61	-39.14	-36.02	-33.20	-30.66	-28.35	-26.46	-24.92	-30.34	-	2.11	-28.23	1
8: $CH_2\gamma i$	-42.37	-38.90	-35.78	-32.98	-30.46	-28.16	-26.28	-24.76	-30.34	-	2.11	-28.23	1
9: CH_3i	-31.59	-29.22	-27.06	-25.16	-23.41	-21.81	-20.49	-19.42	-19.84	-	1.46	-18.38	3
10: $CH_2\alpha o$	-35.74	-31.79	-28.30	-25.16	-22.45	-20.07	-18.17	-16.66	-33.48	-	4.25[a]	-29.23	1
11: $CH_2\beta o$	-16.99	-15.18	-13.57	-12.13	-10.85	-9.72	-8.82	-8.10	-13.01	-	2.02	-10.99	1
12: $CH_2\beta o$	-15.96	-14.33	-12.86	-11.55	-10.38	-9.34	-8.52	-7.85	-13.01	-	2.02	-10.99	1
13: $CH_2\alpha o$	-13.17	-11.60	-10.20	-8.98	-7.91	-6.96	-6.23	-5.64	-10.24	-	4.11[a]	-6.13	1
14: $CH_2\gamma o$	-11.38	-10.19	-9.13	-8.20	-7.38	-6.66	-6.09	-5.64	-12.66	-	1.73	-10.93	1
15: $CH_2\gamma o$	-10.51	-9.44	-8.47	-7.61	-6.84	-6.18	-5.64	-5.22	-12.66	-	1.73	-10.93	1
16: CH_3o	-6.68	-6.00	-5.40	-4.87	-4.40	-3.99	-3.67	-3.41	-8.56	-	1.05	-7.51	3

[a]The δ_{orb} values of **[4]**$^{4+}$ were used.

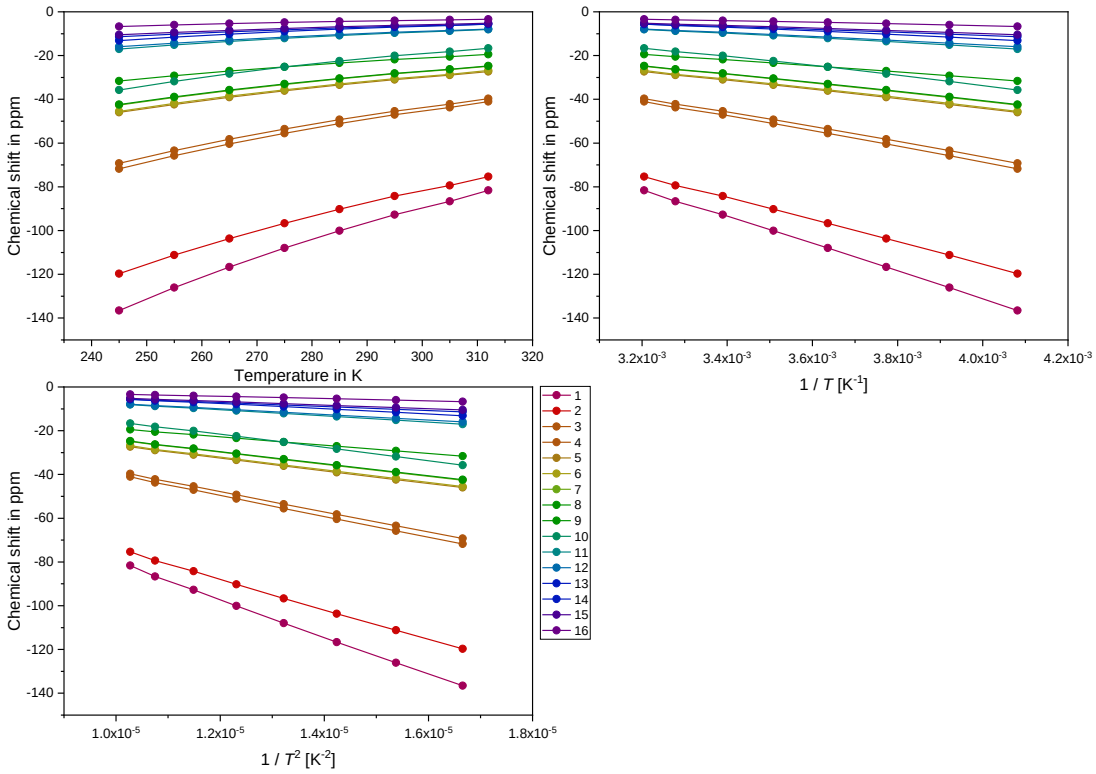

Fig. S117. Plot of the ^{1}H chemical shifts of **[4]$^{2+}$** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S14. ^{13}C NMR chemical shifts of **[4]$^{2+}$** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-447.4	s
2	-191.5	s
3	-9.8	q
4	-9.8	t
5	-3.2	t
6	8.7	q
7	11.4	t
8	19.9	t
9	20.9	m
10	49.6	s
11	60.3	t
12	62.2	s
13	69.0	d
14	170.5	d

3.9. Complex **[4]**$^{3+}$

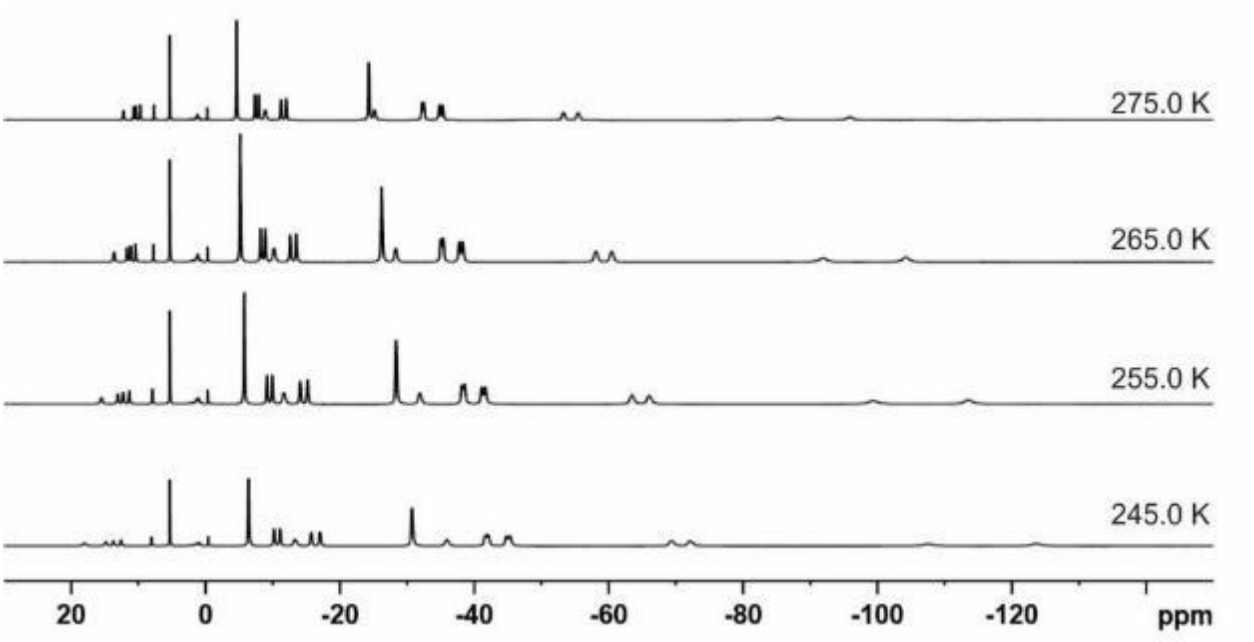

Fig. S118. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

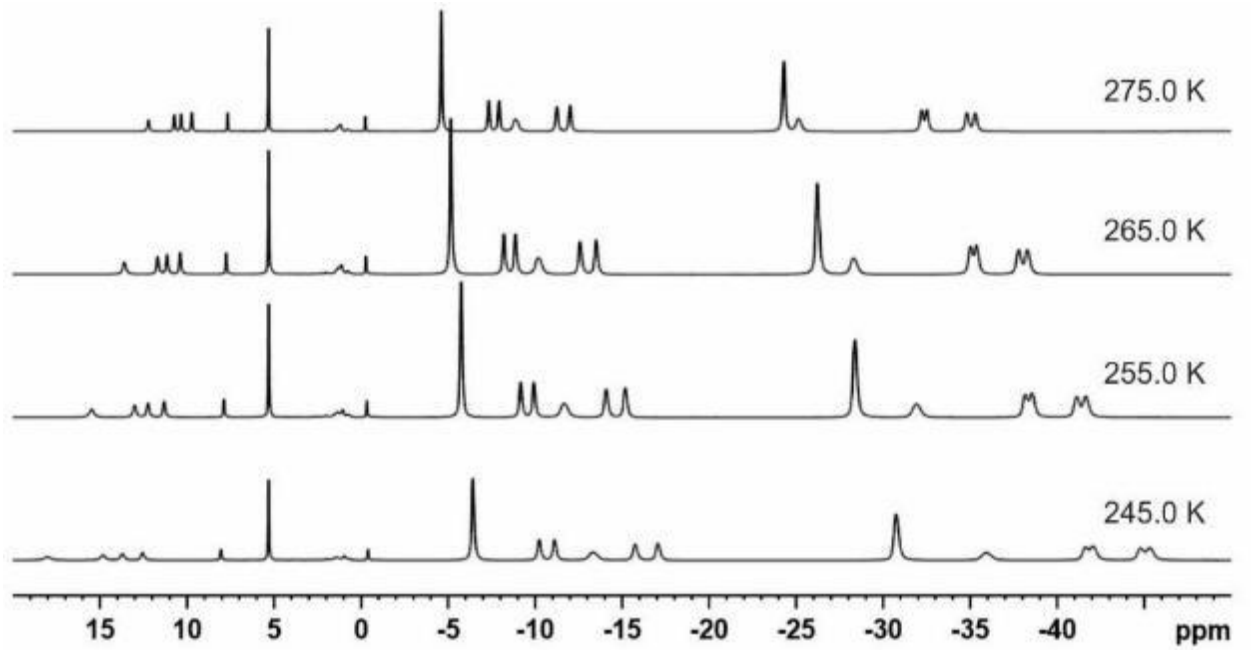

Fig. S119. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +20 ppm to -50 ppm.

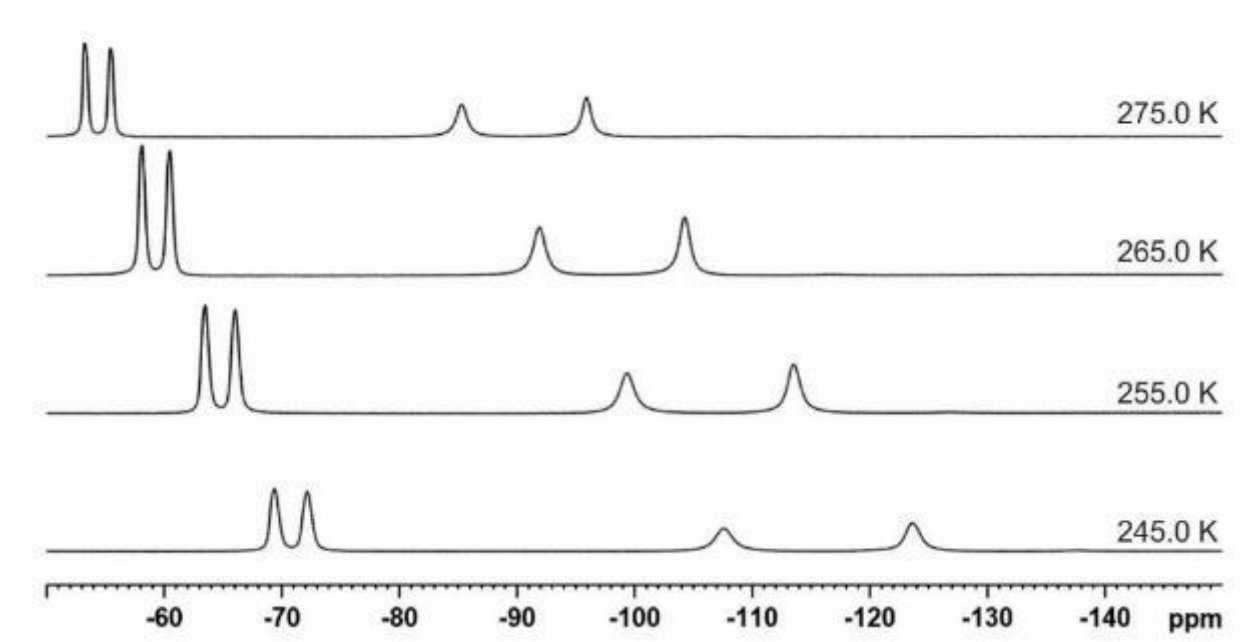

Fig. S120. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -50 ppm to -150 ppm.

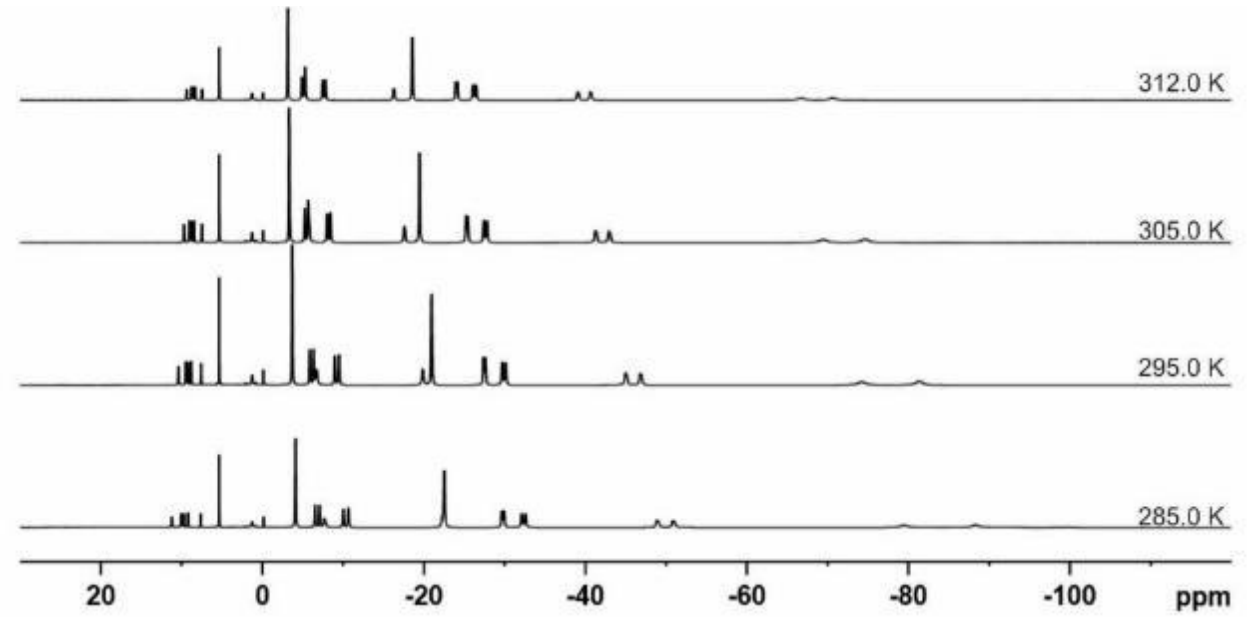

Fig. S121. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

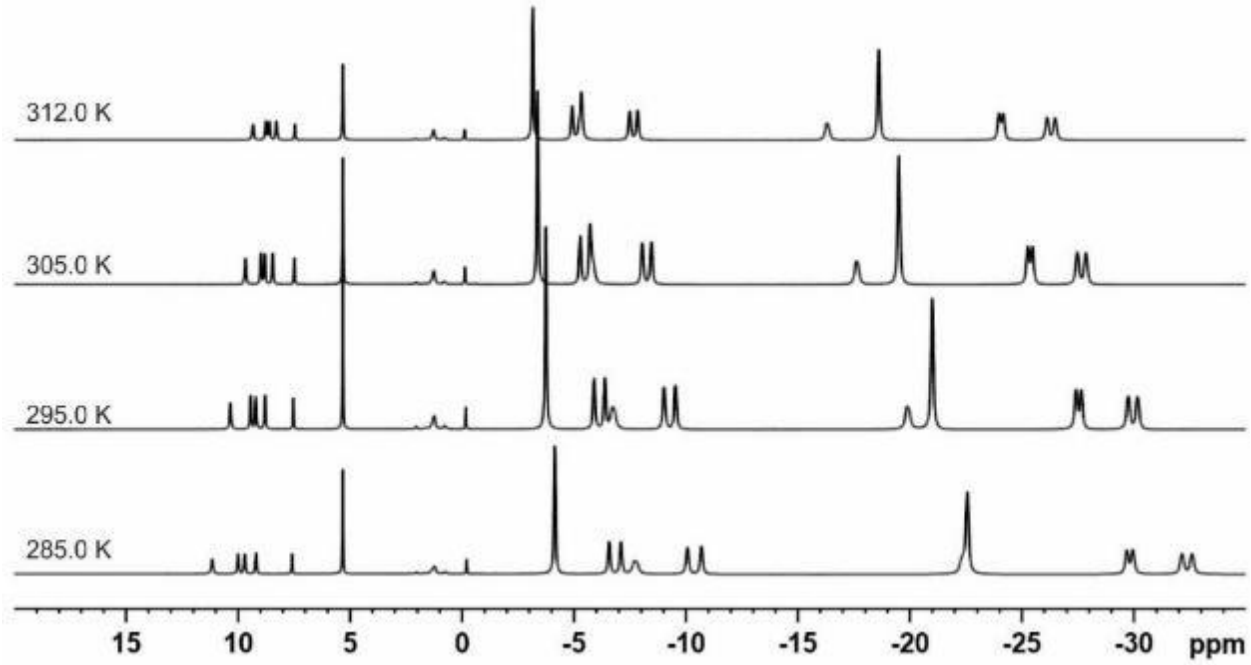

Fig. S122. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +20 to -35 ppm.

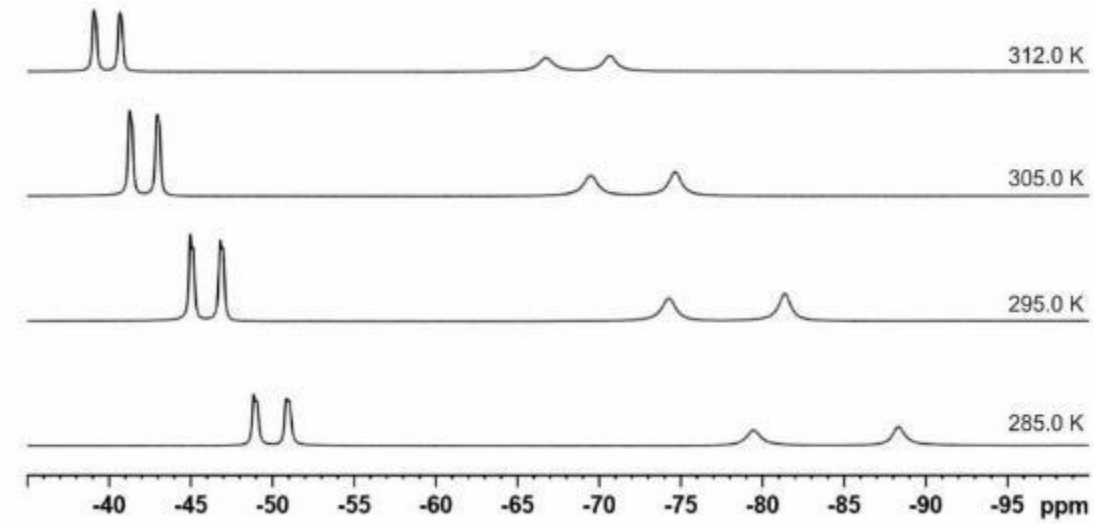

Fig. S123. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -35 ppm to -100 ppm.

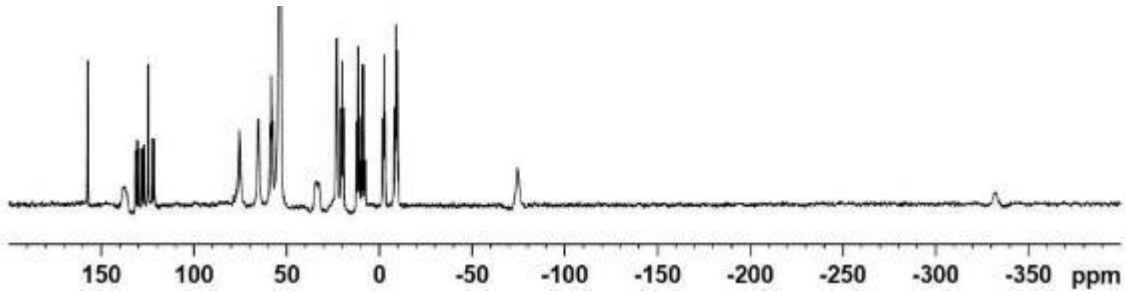

Fig. S124. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K.

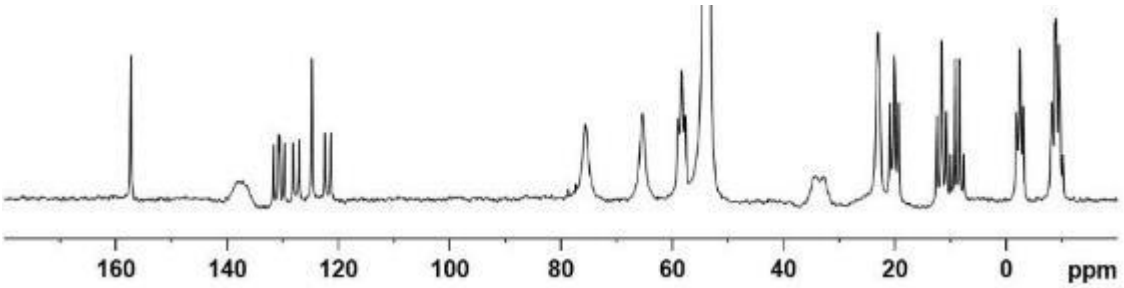

Fig. S125. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +180 ppm to -20 ppm.

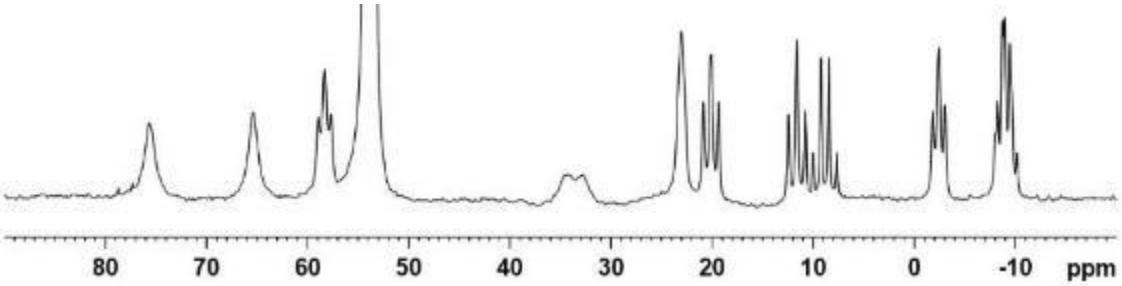

Fig. S126. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +90 ppm to -20 ppm.

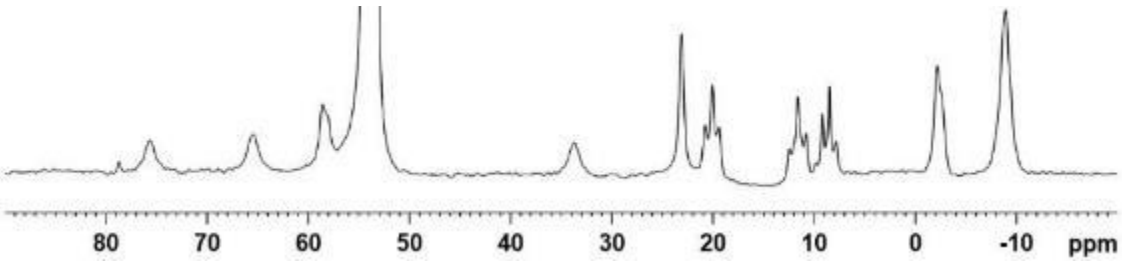

Fig. S127. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +90 ppm to -20 ppm.

Table S15. ^{1}H NMR experimental chemical shifts for **[4]**$^{3+}$ in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}i$	-123.64	-113.53	-104.28	-95.94	-88.35	-81.38	-74.66	-70.69	-81.64	-5.38	7.03[a]	-79.99	1
2: $CH_{ar}o$	-107.61	-99.42	-91.92	-85.33	-79.44	-74.29	-69.5	-66.77	-43.69	-35.90	7.03[a]	-72.55	1
3: $CH_2\alpha i$	-72.19	-66.06	-59.3	-55.47	-50.95	-46.89	-43.01	-40.67	-51.86	-	4.57[a]	-47.29	1
4: $CH_2\alpha i$	-69.42	-63.49	-58.12	-53.3	-48.97	-45.06	-41.33	-39.11	-48.41	-	4.57[a]	-43.84	1
5: $CH_2\beta i$	-45.32	-41.64	-38.29	-35.3	-32.59	-30.17	-27.86	-26.49	-31.26	-	2.32	-28.94	1
6: $CH_2\beta i$	-44.79	-41.12	-37.8	-34.83	-32.15	-29.75	-27.48	-26.13	-31.26	-	2.32	-28.94	1
7: $CH_2\gamma i$	-42.06	-38.54	-35.36	-32.52	-29.95	-27.66	-25.47	-24.17	-29.65	-	2.03	-27.62	1
8: $CH_2\gamma i$	-41.63	-38.17	-35.03	-32.22	-29.69	-27.43	-25.27	-23.99	-29.65	-	2.03	-27.62	1
9: CH_3i	-30.75	-28.37	-26.23	-24.3	-22.56	-21	-19.51	-18.61	-19.39	-	1.41	-17.98	1
10: $CH_2\alpha o$	-35.93	-31.91	-28.32	-25.15	-22.56	-19.88	-17.62	-16.31	-28.84	-	4.25[a]	-24.59	3
11: $CH_2\beta o$	-17.06	-15.19	-13.51	-12.02	-10.7	-9.54	-8.46	-7.84	-9.87	-	2.03	-7.84	1
12: $CH_2\beta o$	-15.74	-14.09	-12.59	-11.26	-10.07	-9.03	-8.06	-7.49	-9.87	-	2.03	-7.84	1
13: $CH_2\alpha o$	-13.31	-11.67	-10.19	-8.87	-7.72	-6.72	-5.73	-5.33	-5.31	-	4.11[a]	-1.20	1
14: $CH_2\gamma o$	-11.12	-9.94	-8.88	-7.94	-7.11	-6.38	-5.73	-5.33	-10.27	-	1.68	-8.59	1
15: $CH_2\gamma o$	-10.24	-9.18	-8.21	-7.34	-6.58	-5.9	-5.28	-4.93	-10.27	-	1.68	-8.59	1
16: CH_3o	-6.42	-5.56	-5.16	-4.62	-4.15	-3.75	-3.38	-3.17	-6.83	-	1.04	-5.79	3

[a]The δ_{orb} values of **[4]**$^{4+}$ were used.

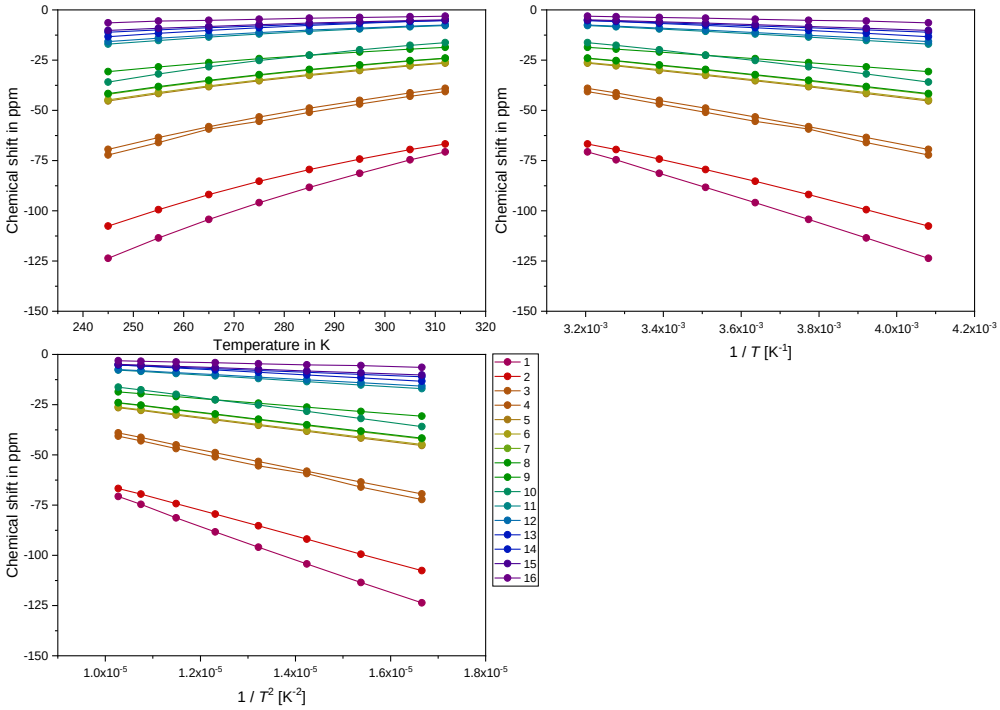

Fig. S128. Plot of the ^{1}H chemical shifts of **[4]**$^{3+}$ in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S16. ^{13}C NMR chemical shifts of **[4]$^{3+}$** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-332.0	s
2	-74.6	s
3	-9.3	q
4	-9.1	q
5	-2.4	t
6	8.9	q
7	11.7	t
8	20.1	t
9	23.1	t
10	33.7	d
11	58.3	t
12	65.5	s
13	75.8	s
14	137.5	s

Complex **[4]$^{4+}$**

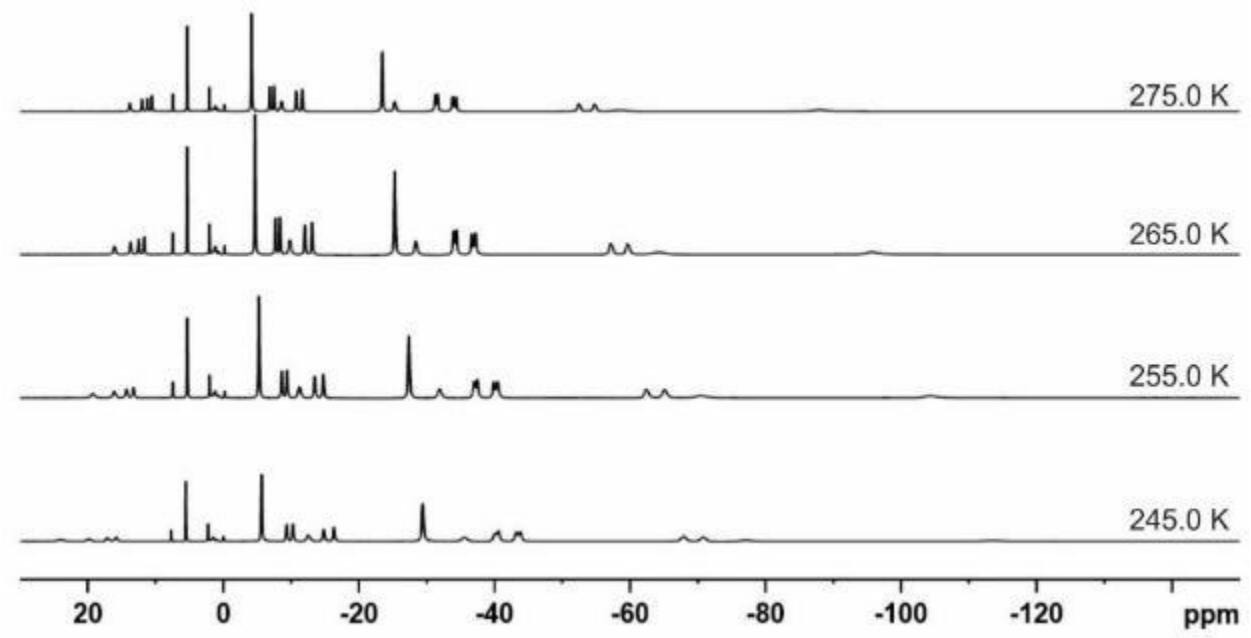

Fig. S129. Variable-temperature ^1H NMR spectra of complex **[4]$^{4+}$** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

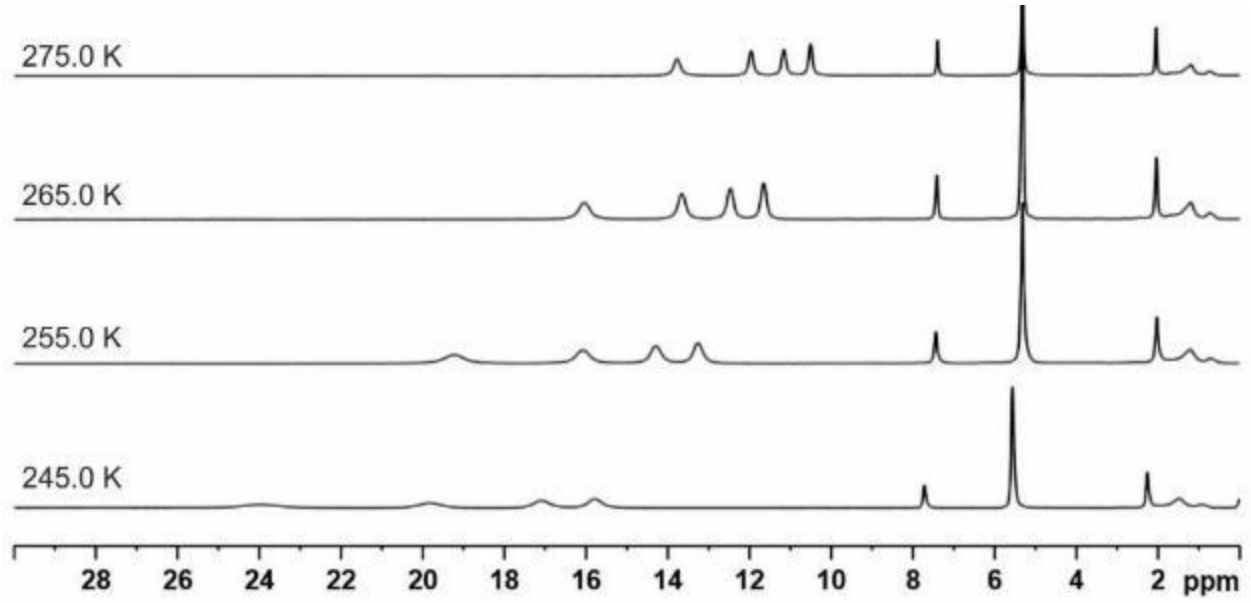

Fig. S130. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +30 ppm to 0 ppm.

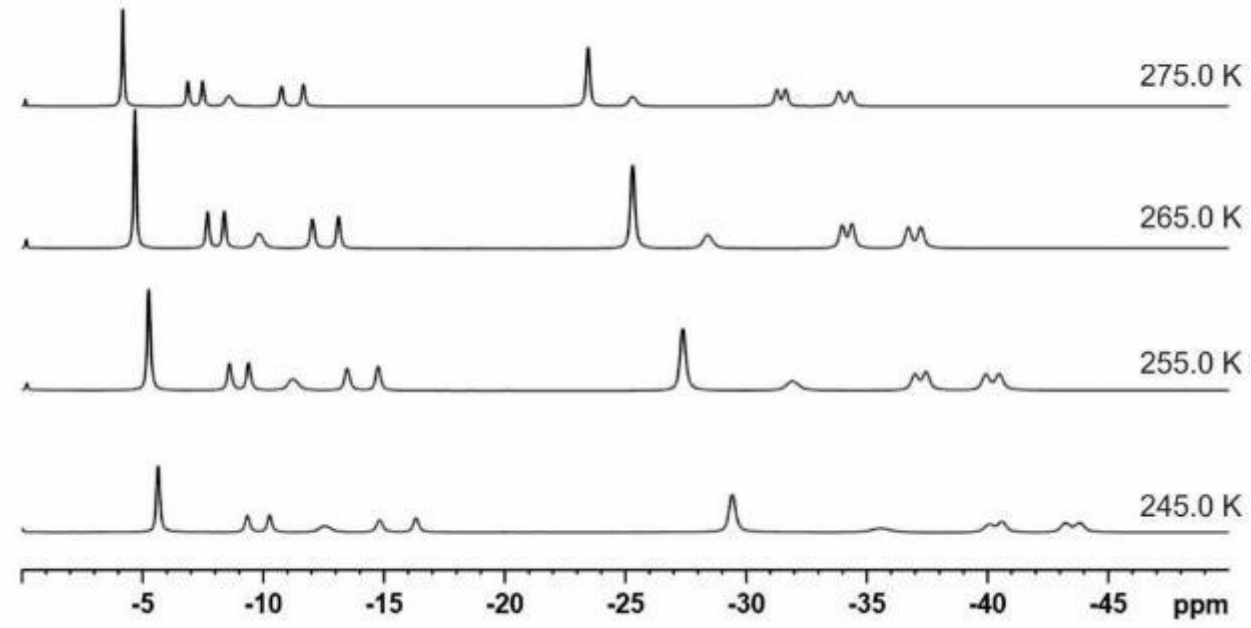

Fig. S131. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -50 ppm.

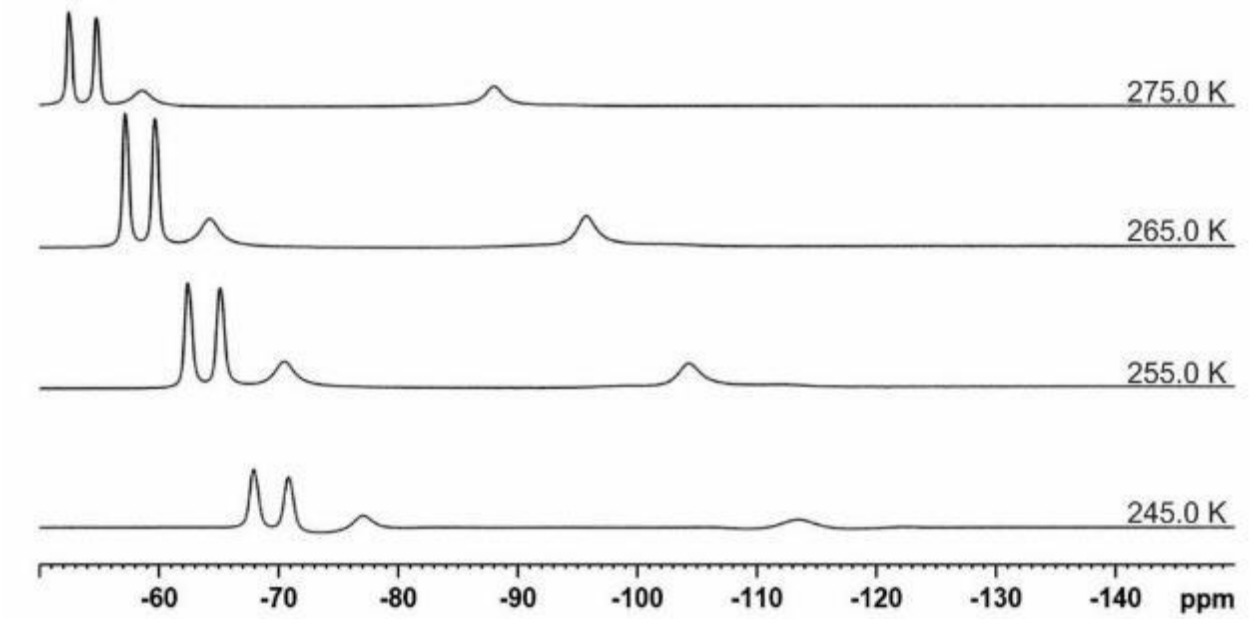

Fig. S132. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -50 ppm to -150 ppm.

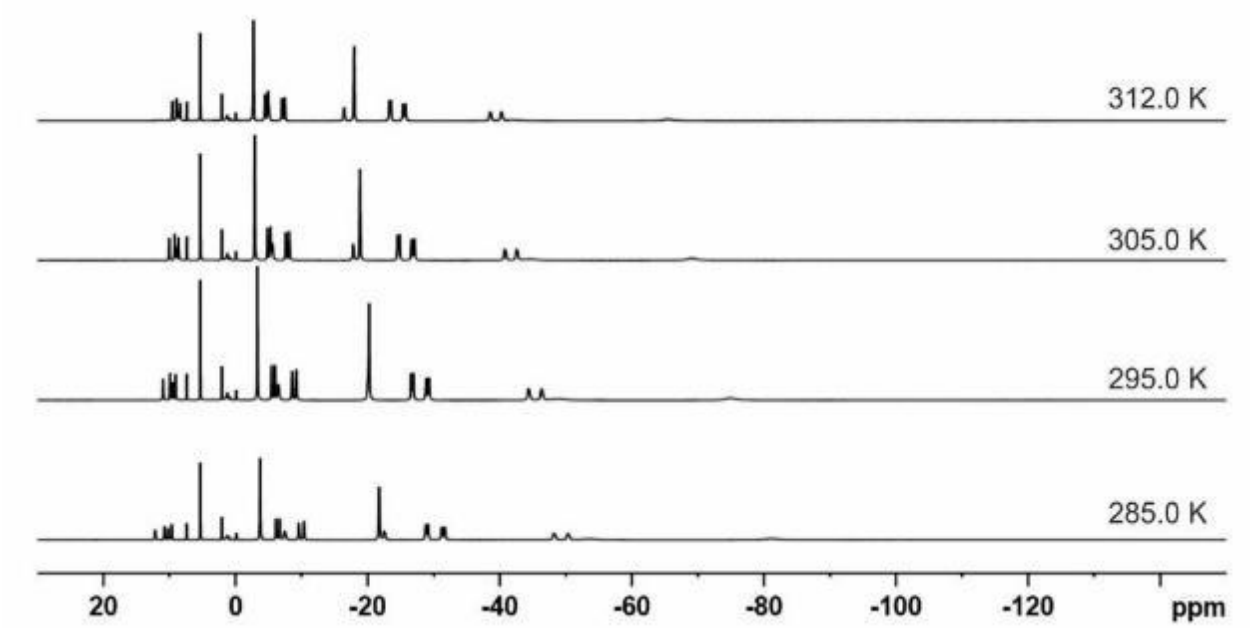

Fig. S133. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

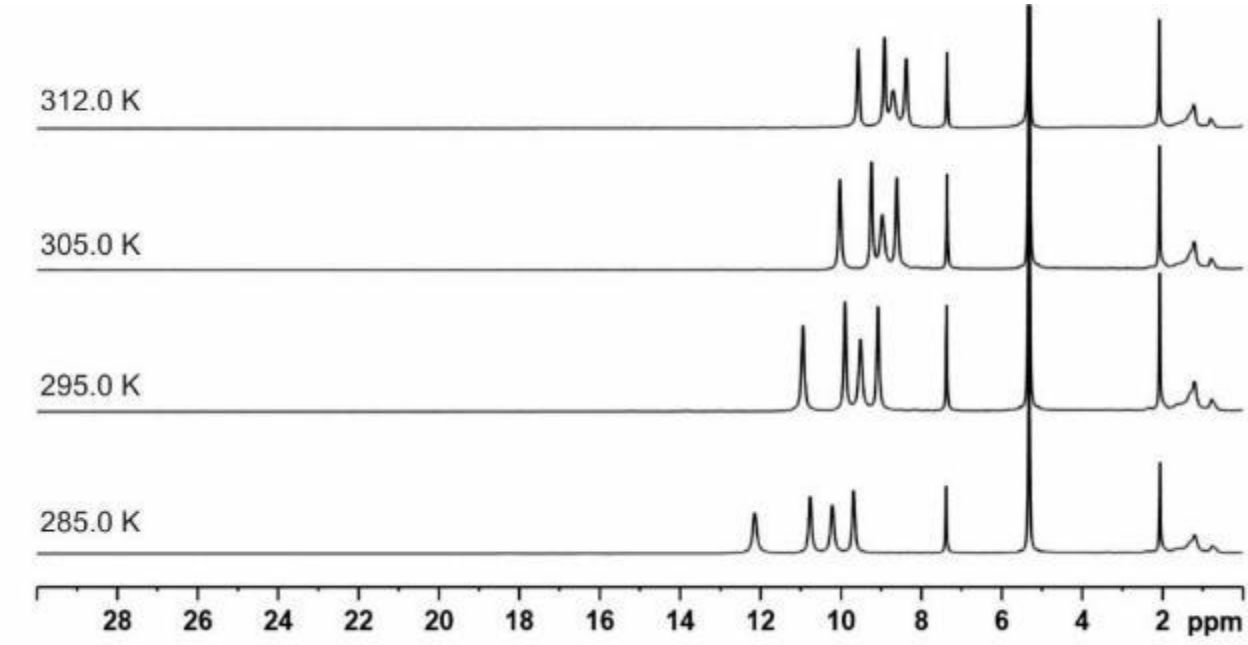

Fig. S134. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +30 ppm to 0 ppm.

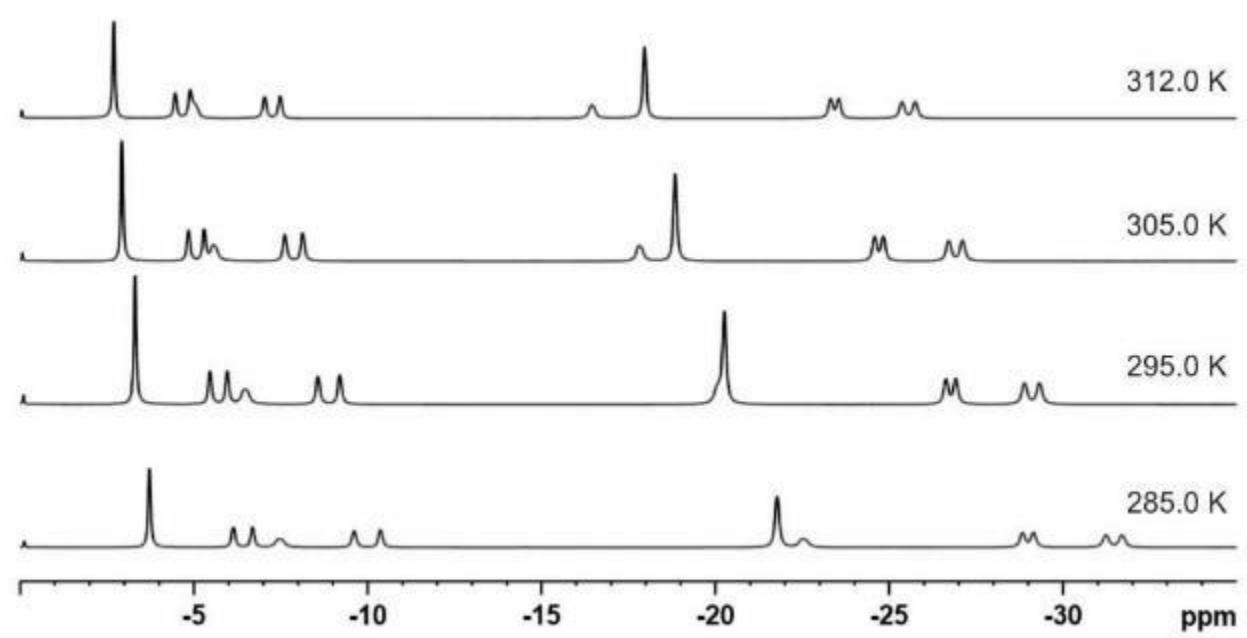

Fig. S135. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -35 ppm.

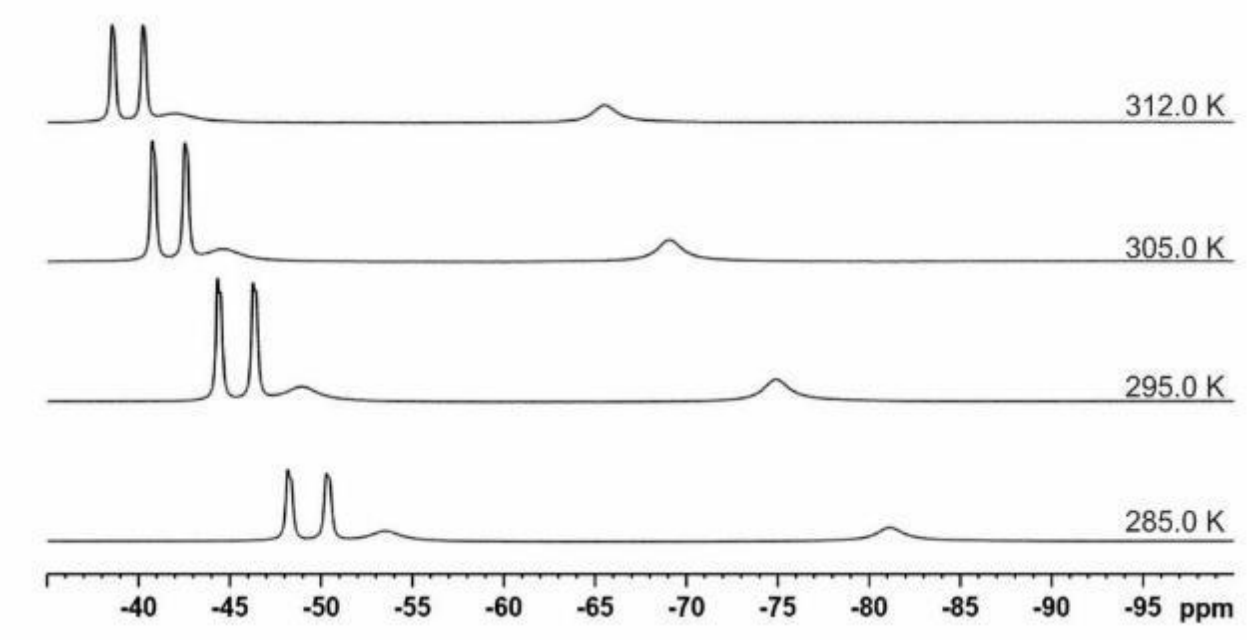

Fig. S136. Variable-temperature ^{1}H NMR spectra of complex **[4]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -35 ppm to -100 ppm.

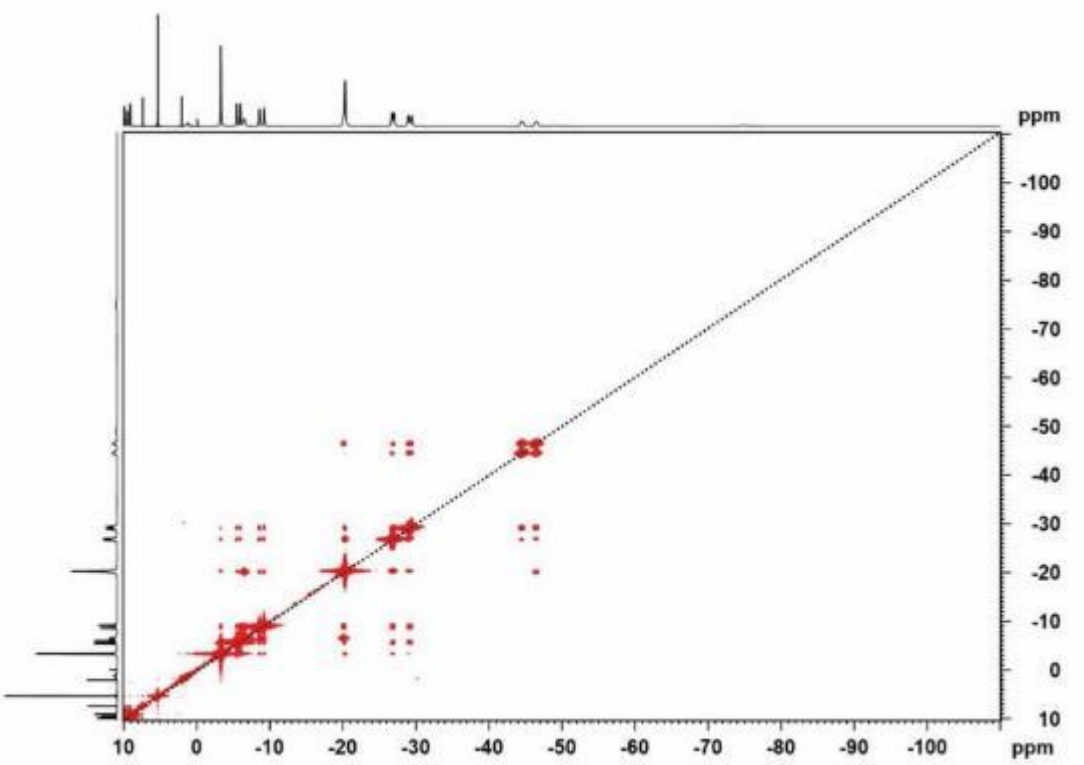

Fig. S137. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[4]**$^{4+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K.

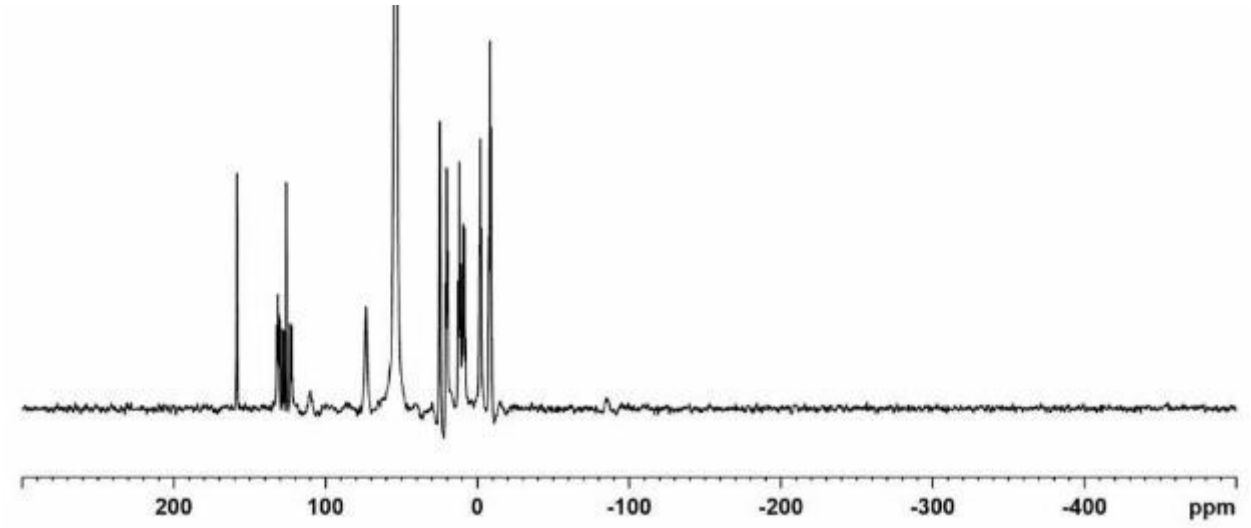

Fig. S138. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K.

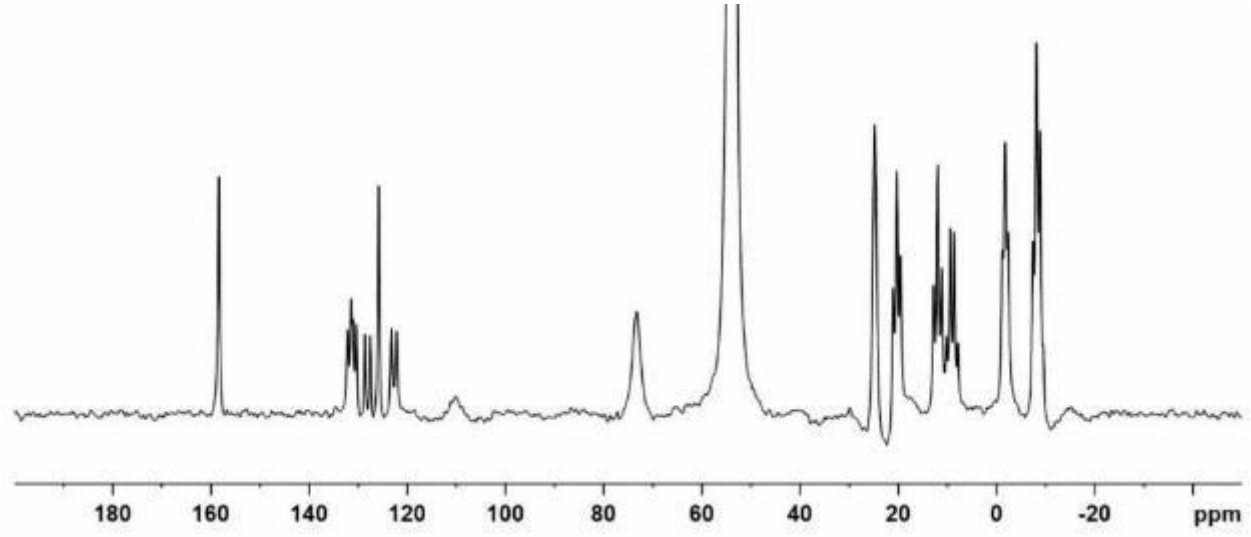

Fig. S139. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +200 ppm to -50 ppm.

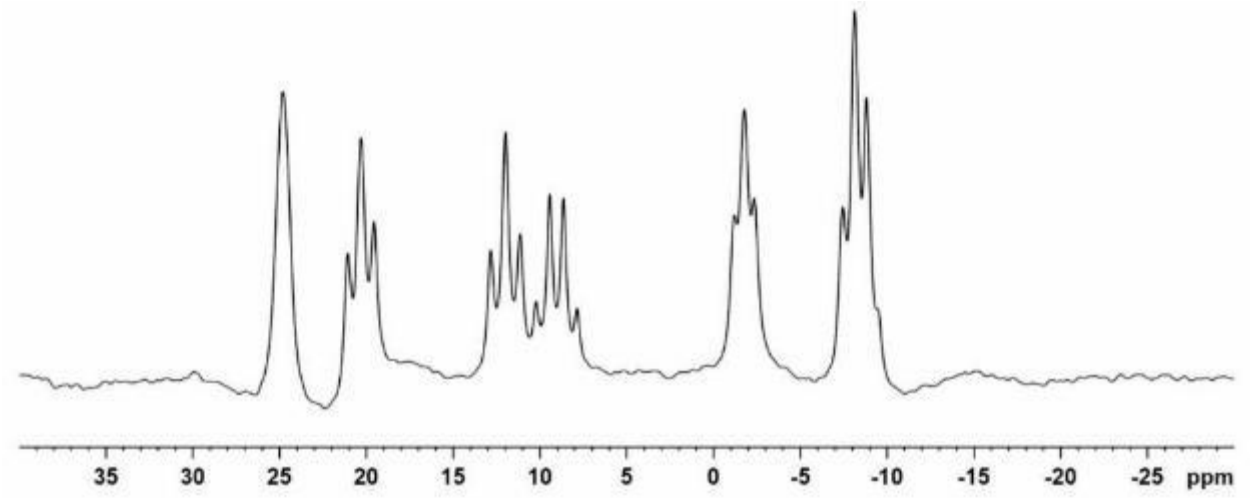

Fig. S140. ^{13}C NMR spectrum (^{1}H coupled) of complex **[4]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +40 ppm to -30 ppm.

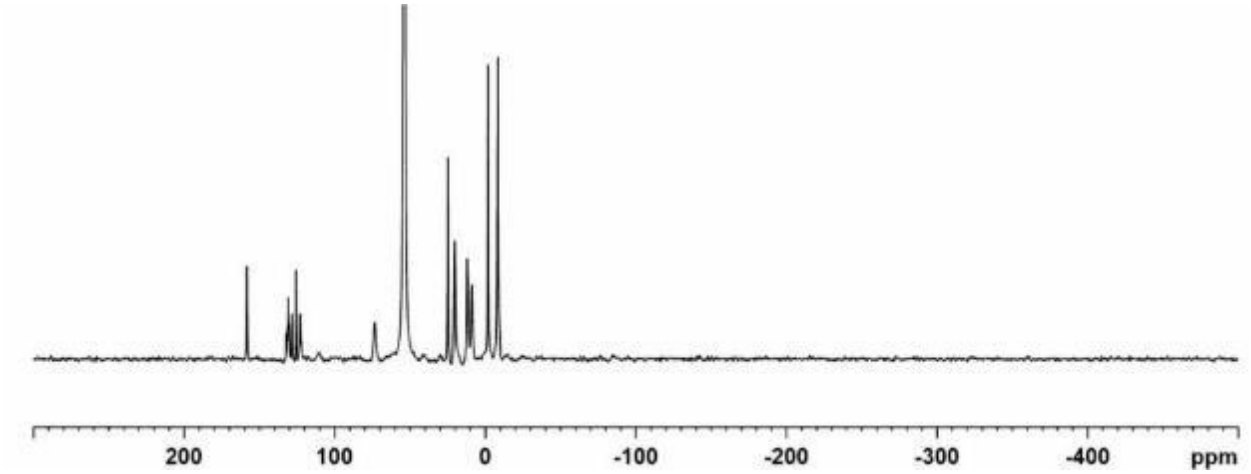

Fig. S141. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K.

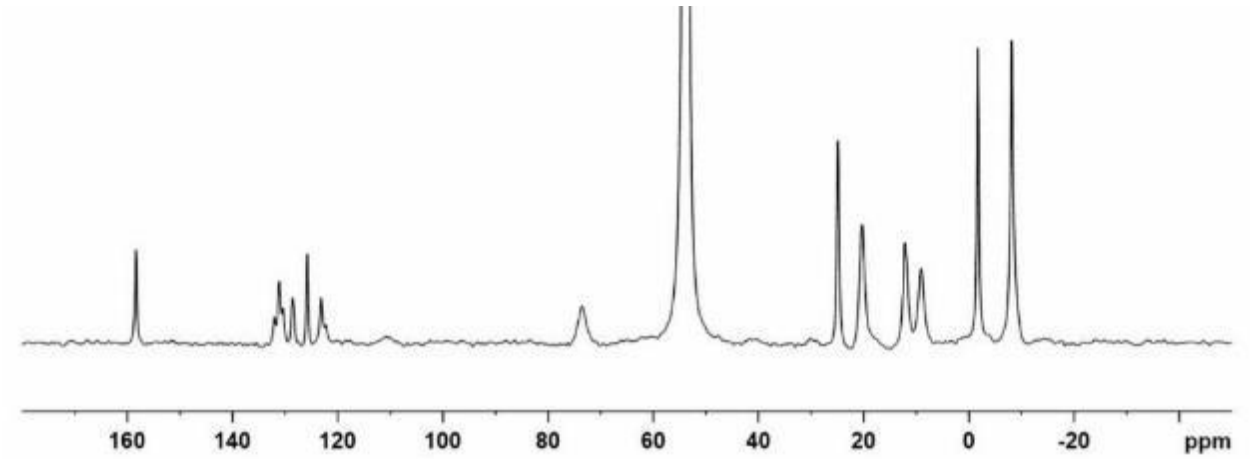

Fig. S142. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[4]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +200 ppm to -50 ppm.

Table S17. ^{1}H NMR experimental chemical shifts for **[4]**$^{4+}$ in CD_2Cl_2.

	T in K								Theoretical@295 K			
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm											Integral
1: $CH_{ar}i$	-113.42	-104.34	-95.75	-88.01	-81.16	-74.91	-69.02	-65.52	-81.23	7.03	-74.20	1
2: $CH_{ar}o$	-77.06	-70.45	-64.20	-58.54	-53.56	-48.94	-44.52	-41.95	-41.12	7.03	-34.09	1
3: $CH_2\alpha i$	-70.84	-65.12	-59.67	-54.80	-50.38	-46.37	-42.60	-40.30	-51.61	4.57	-47.04	1
4: $CH_2\alpha i$	-67.93	-62.41	-57.18	-52.51	-48.27	-44.42	-40.82	-38.61	-48.01	4.57	-43.44	1
5: $CH_2\beta i$	-43.82	-40.49	-37.24	-34.33	-31.70	-29.32	-27.11	-25.75	-30.97	2.27	-28.70	1
6: $CH_2\beta i$	-43.25	-39.94	-37.24	-33.84	-31.24	-28.89	-26.71	-25.37	-30.97	2.27	-28.70	1
7: $CH_2\gamma i$	-40.61	-37.46	-34.39	-31.63	-29.15	-26.91	-24.83	-23.55	-29.22	1.92	-27.30	1
8: $CH_2\gamma i$	-40.10	-37.01	-33.99	-31.28	-28.84	-26.64	-24.58	-23.32	-29.22	1.92	-27.30	1
9: CH_3i	-29.43	-27.39	-25.31	-23.45	-21.78	-20.26	-18.84	-17.97	-19.09	1.36	-17.73	3
10: $CH_2\alpha o$	-35.59	-31.93	-28.40	-25.29	-22.52	-20.26	-17.81	-16.45	-27.24	4.25	-22.99	1
11: $CH_2\beta o$	-16.33	-14.76	-13.12	-11.67	-10.36	-9.20	-8.13	-7.48	-8.84	1.92	-6.92	1
12: $CH_2\beta o$	-14.82	-13.48	-12.04	-10.76	-9.61	-8.57	-7.62	-7.04	-8.84	1.92	-6.92	1
13: $CH_2\alpha o$	-12.53	-11.22	-9.80	-8.56	-7.45	-6.46	-5.56	-5.02	-3.76	4.11	0.35	1
14: $CH_2\gamma o$	-10.27	-9.40	-8.39	-7.49	-6.69	-5.96	-5.30	-4.90	-9.31	1.57	-7.74	1
15: $CH_2\gamma o$	-9.35	-8.61	-7.70	-6.88	-6.14	-5.47	-4.85	-4.47	-9.31	1.57	-7.74	1
16: CH_3o	-5.65	-5.26	-4.69	-4.19	-3.73	-3.31	-2.93	-2.70	-6.14	1.03	-5.11	3

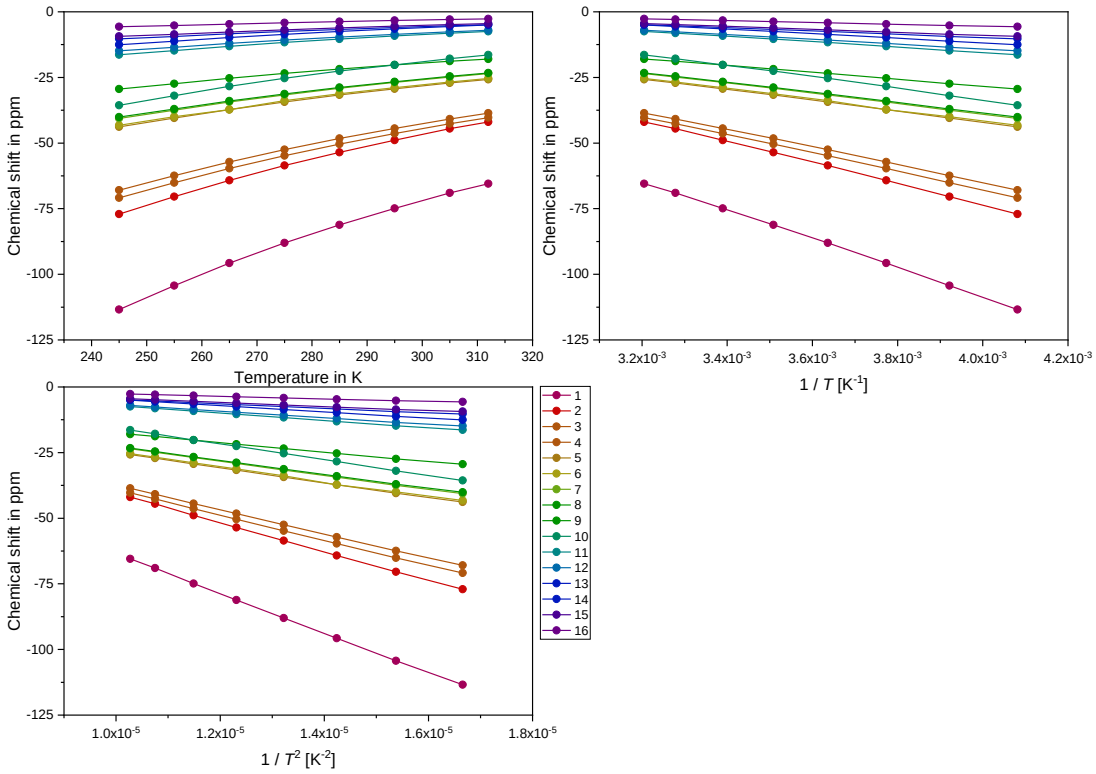

Fig. S143. Plot of the ^{1}H chemical shifts of **[4]**$^{4+}$ in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S18. ^{13}C NMR chemical shifts of **[4]**$^{4+}$ observed at 295.0 K in CD_2Cl_2. * Possible that there are seeral peaks under the solvent signal, please see predicted values.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-85.4	s
2	-14.3	s
3	-8.5	q
4	-8.1	t
5	-1.8	t
6	9.1	q
7	12.0	t
8	20.3	t
9	24.8	t
10	40.9	s
11	73.4	s
12	110.3	s
13*	53.4	t (overlap)

3.10. Complex **[5]^0**

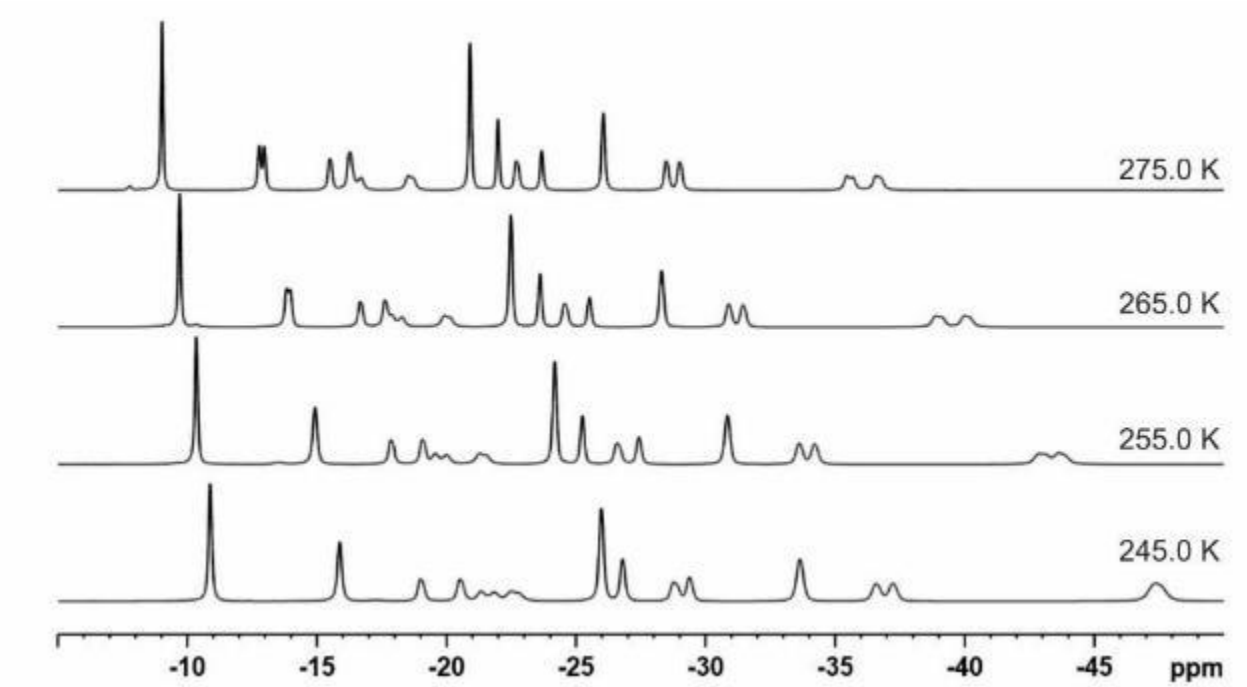

Fig. S144. Variable-temperature ^{1}H NMR spectra of complex **[5]^0** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -5 ppm to -50 ppm.

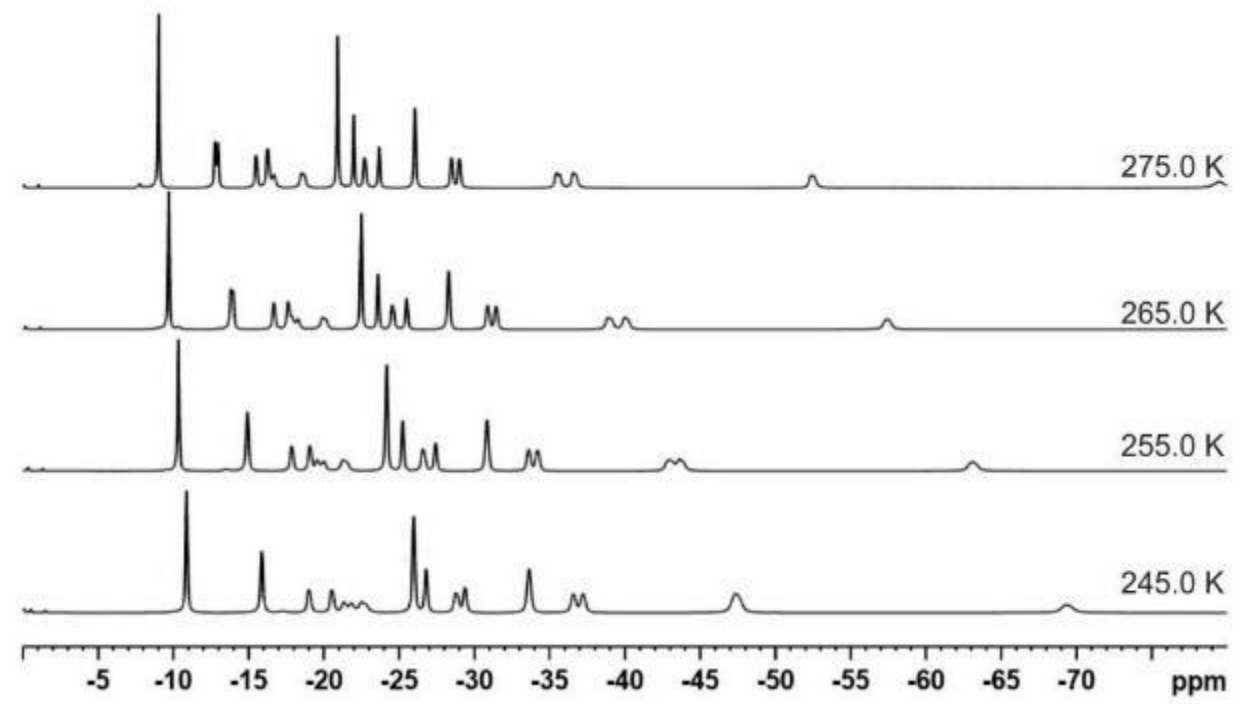

Fig. S145. Variable-temperature ^{1}H NMR spectra of complex **[5]^0** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -80 ppm.

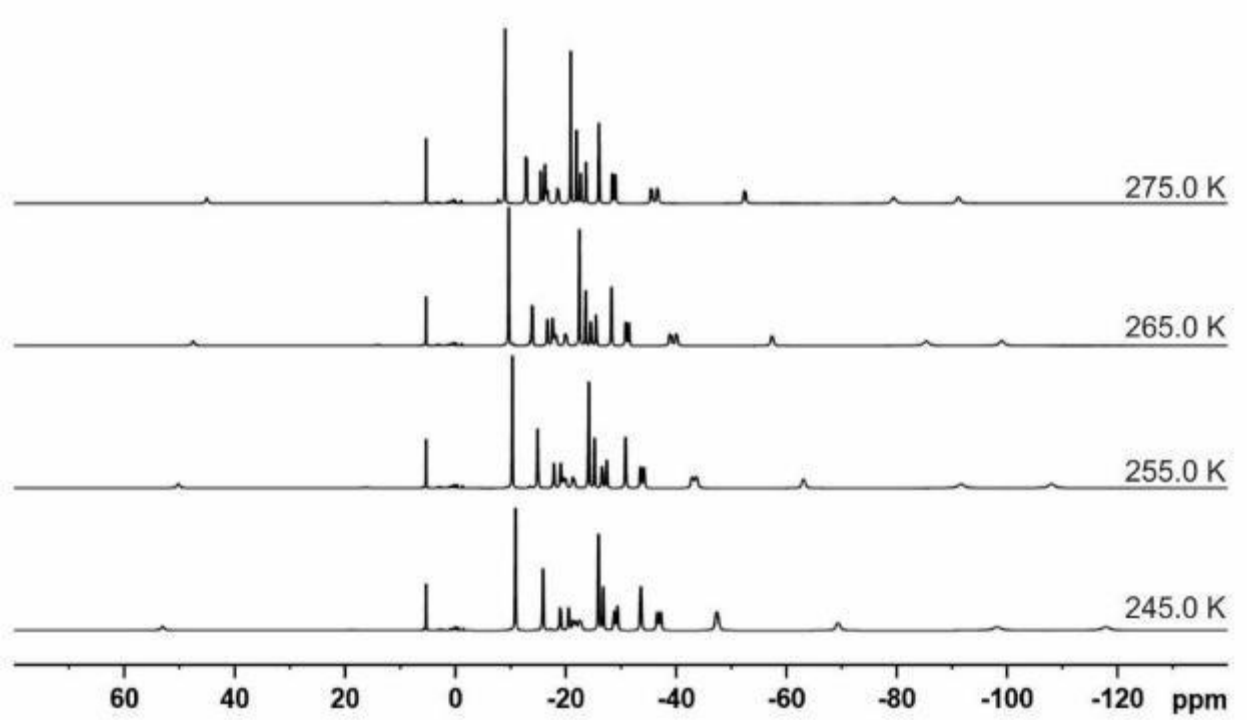

Fig. S146. Variable-temperature ^{1}H NMR spectra of complex **[5]^{0}** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

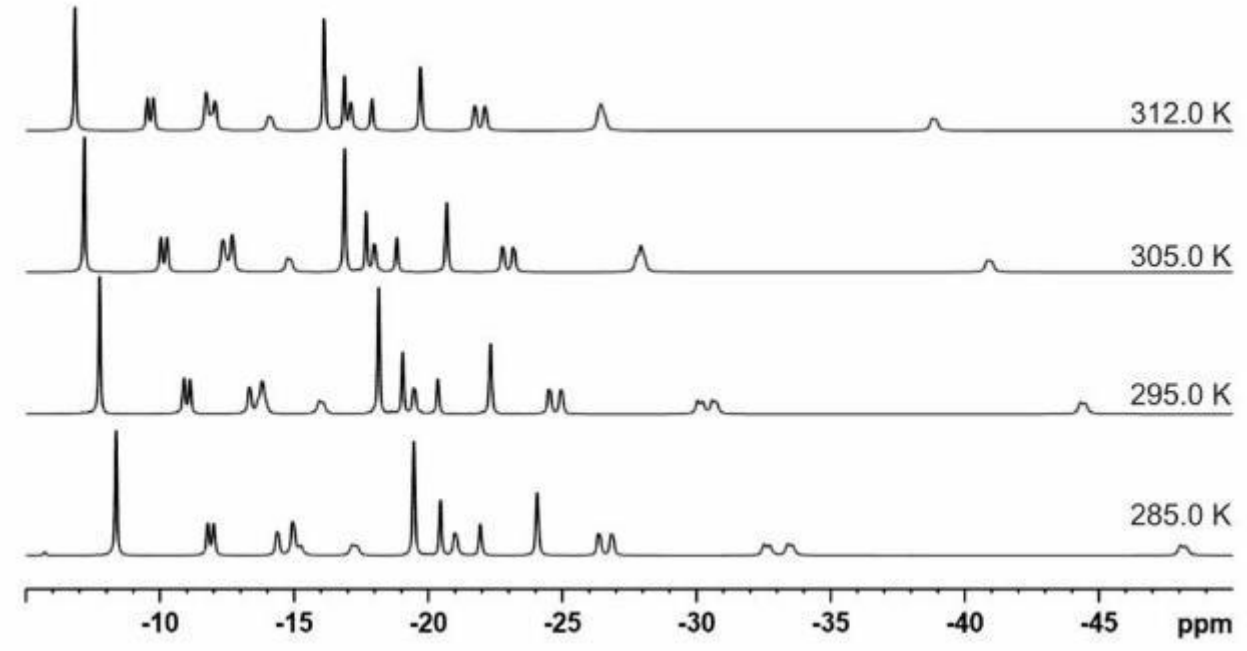

Fig. S147. Variable-temperature ^{1}H NMR spectra of complex **[5]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -5 ppm to -50 ppm.

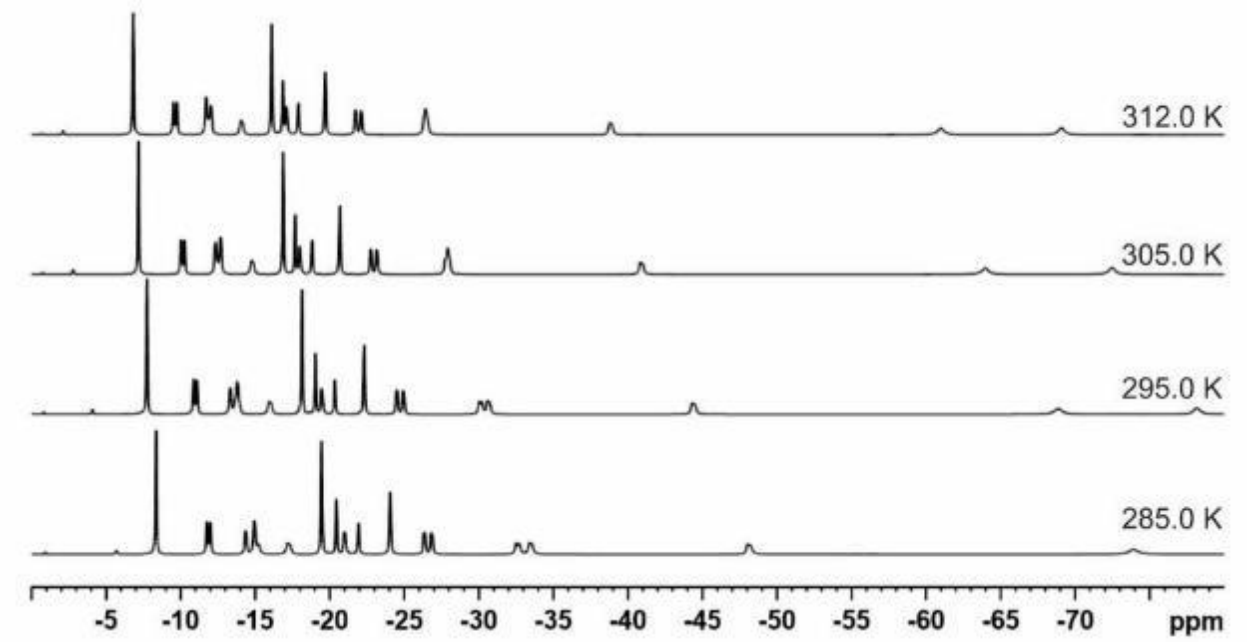

Fig. S148. Variable-temperature ^{1}H NMR spectra of complex **[5]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -80 ppm.

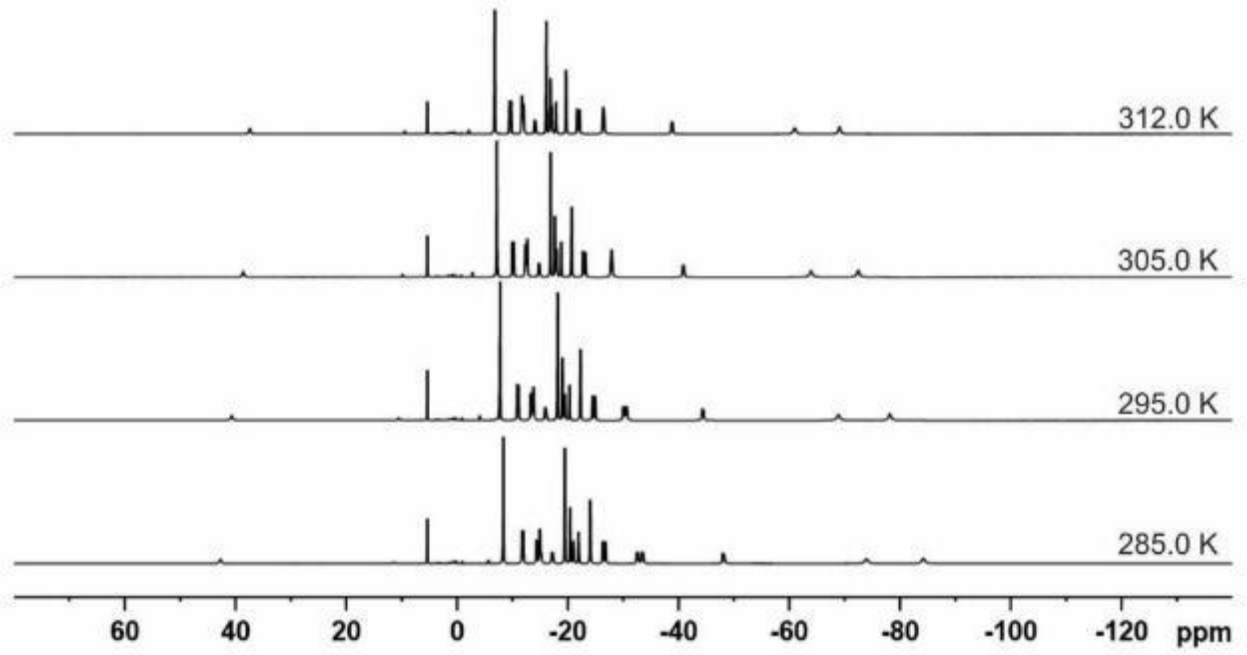

Fig. S149. Variable-temperature ^{1}H NMR spectra of complex **[5]^{0}** recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

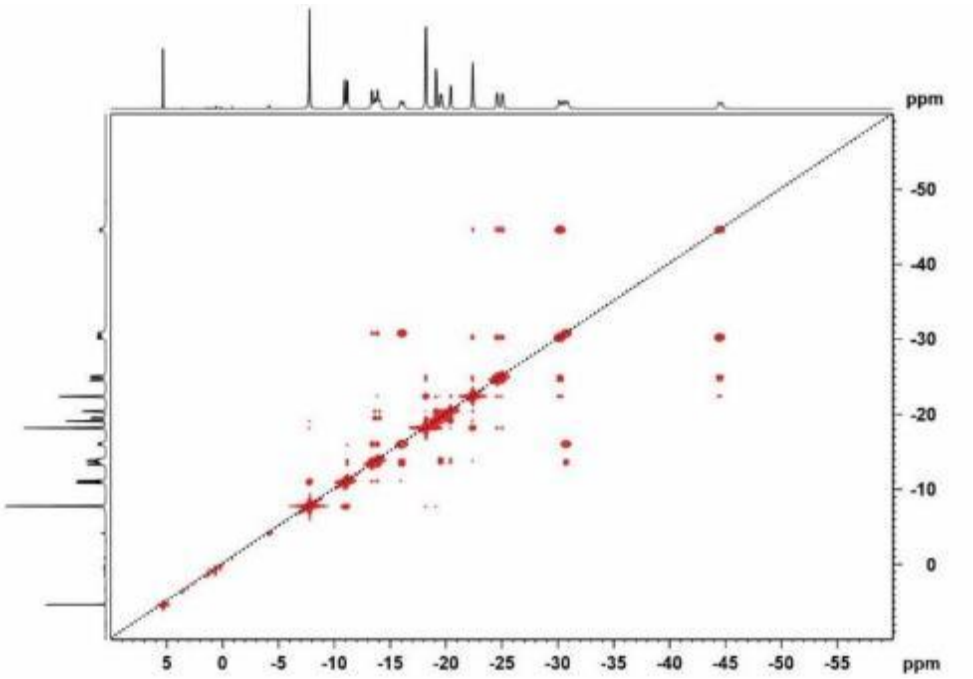

Fig. S150. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[5]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from +10 ppm to -60 ppm.

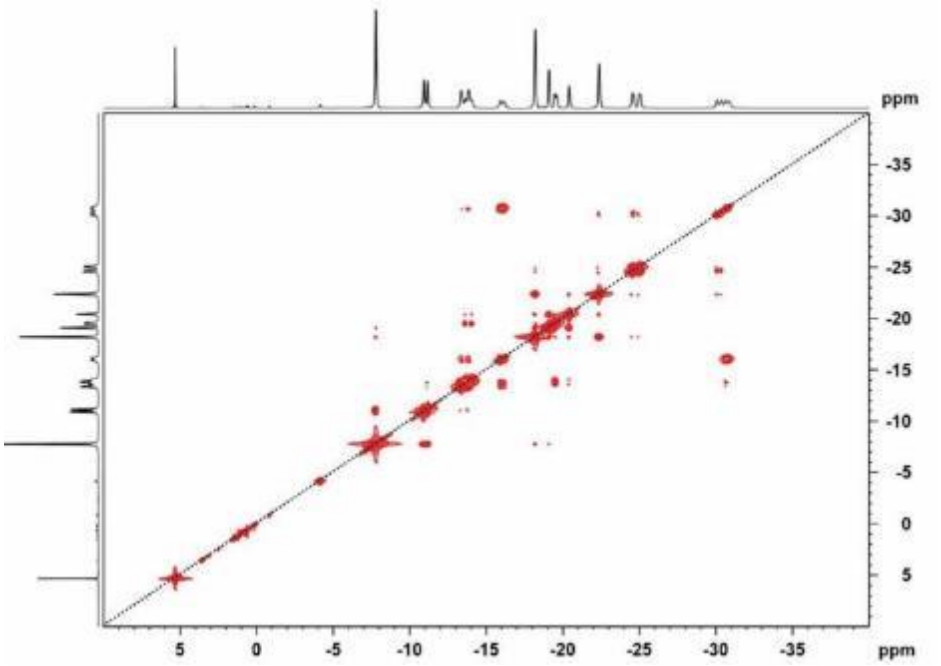

Fig. S151. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[5]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from +10 ppm to -40 ppm.

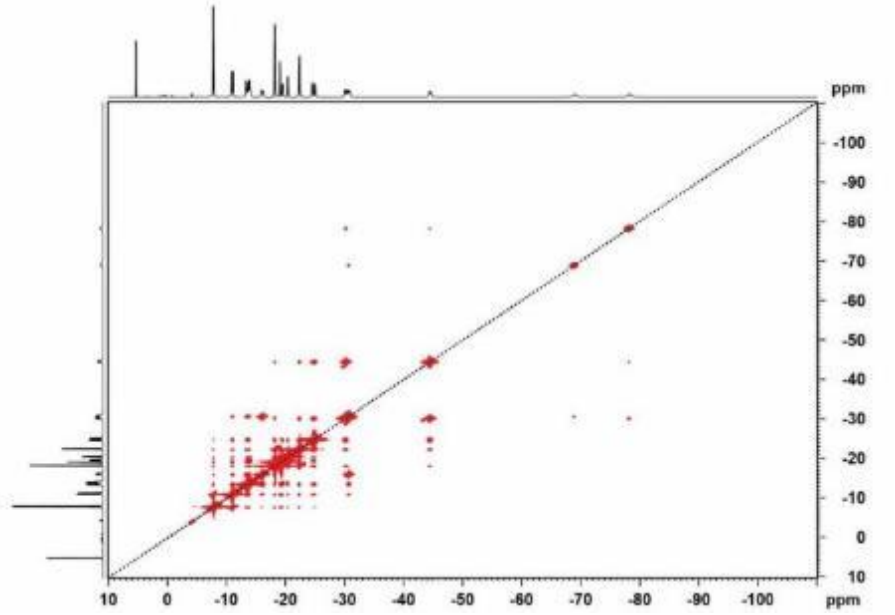

Fig. S152. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[5]^{0}** in CD_2Cl_2 (COSY), recorded at 295.0 K.

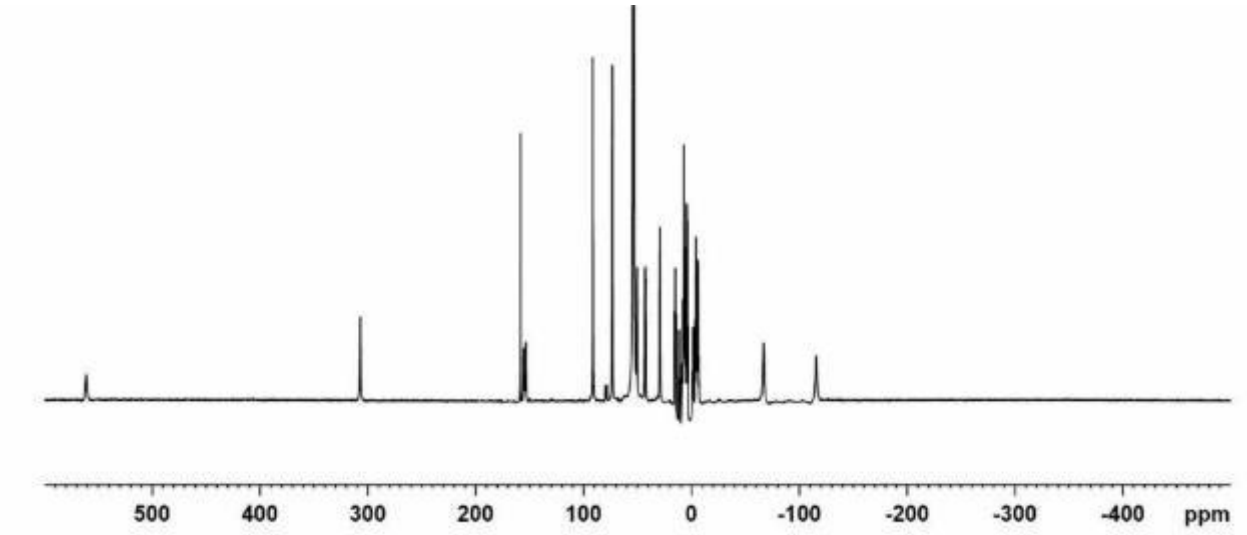

Fig. S153. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]^{0}** in CD_2Cl_2, recorded at 295.0 K.

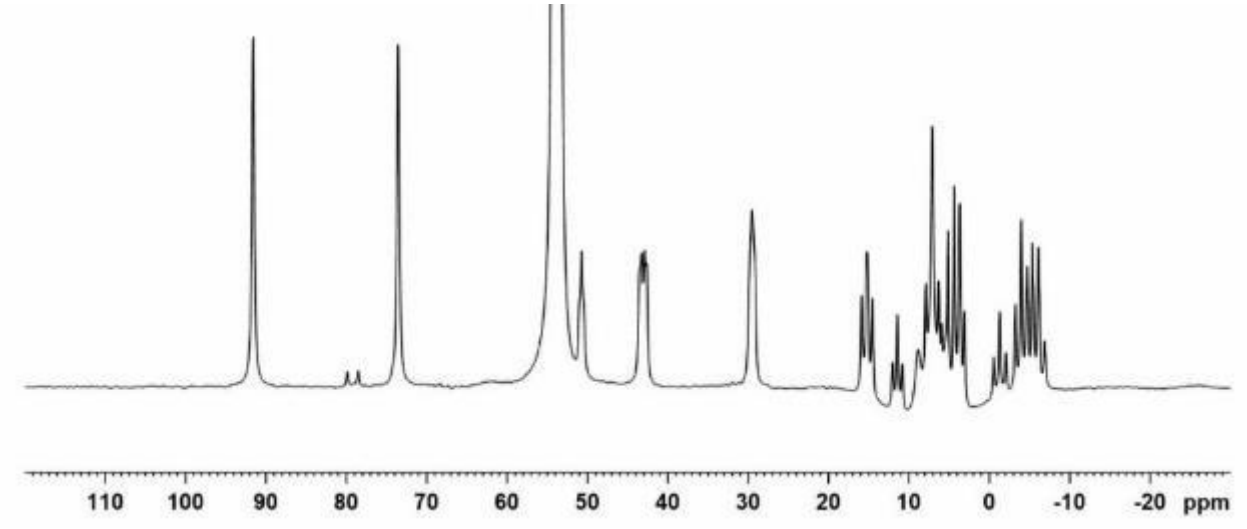

Fig. S154. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]^{0}** in CD_2Cl_2, recorded at 295.0 K. Expansion from +120 ppm to -30 ppm.

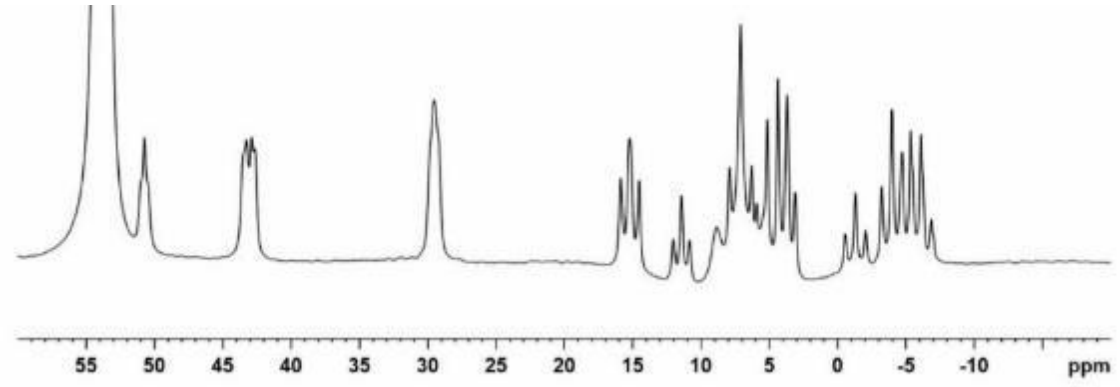

Fig. S155. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]^{0}** in CD_2Cl_2, recorded at 295.0 K. Expansion from +60 ppm to -20 ppm.

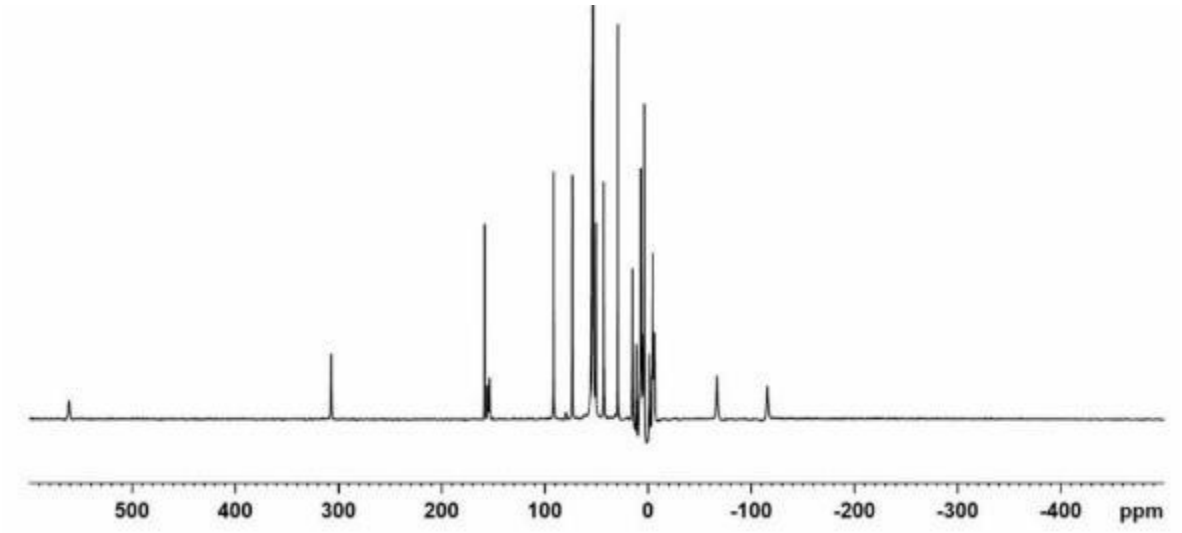

Fig. S156. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]^{0}** in CD_2Cl_2, recorded at 295.0 K.

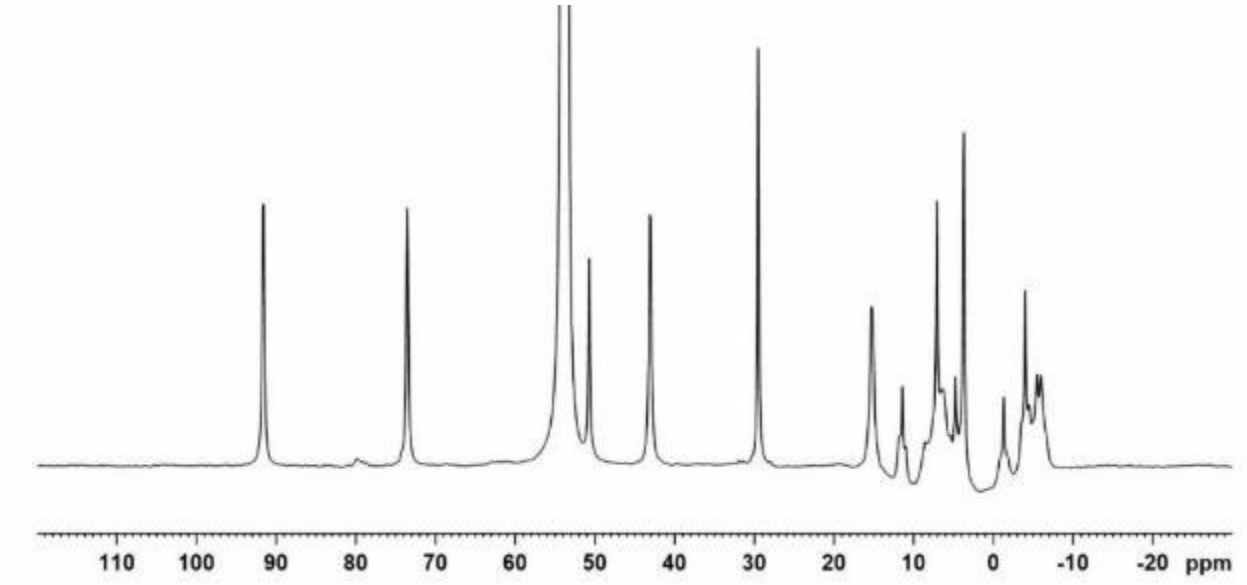

Fig. S157. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]^{0}** in CD_2Cl_2, recorded at 295.0 K. Expansion from +120 ppm to -30 ppm.

Table S19. ^{1}H NMR experimental chemical shifts for **[5]^0** in CD_2Cl_2. The signal assignment convention for the quintuple-decker series is the same as for the triple-decker and quadruple-decker series; the ^{1}H belonging to the outer ligand are marked with an "o", those of the two following inner ligands with an "i", and those of the middle ligand with an "ii".

	T in K								Calculated@295 K			
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm											Integral
1: CH_{ar}i	-117.96	-108.06	-99.07	-91.19	-84.23	-78.17	-72.48	-69.10	-80.11	7.52	-72.59	2
2: CH_{ar}o	-98.22	-91.70	-85.41	-79.48	-73.93	-68.87	-63.97	-61.00	-77.91	7.38	-70.53	2
3: CH_2αi	-69.35	-63.09	-57.39	-52.39	-48.15	-44.41	-40.92	-38.86	-50.63	4.54	-46.09	2
4: CH_2αo	-47.37	-43.64	-40.07	-36.66	-33.49	-30.67	-27.93	-25.44	-42.50	4.30	-38.20	2
5: CH_2αi	-47.37	-42.90	-38.99	-35.57	-32.63	-30.14	-27.86	-26.44	-32.20	4.54	-27.66	2
6: CH_2βi	-37.23	-34.21	-31.45	-29.00	-26.82	-24.94	-23.17	-22.12	-24.17	2.39	-21.78	2
7: CH_2βi	-36.59	-33.62	-30.89	-28.48	-26.35	-24.50	-22.77	-21.74	-24.17	2.39	-21.78	2
8: CH_2γi	-33.64	-30.85	-28.31	-26.06	-24.07	-22.33	-20.69	-19.72	-24.01	2.10	-21.91	4
9: CH_2γii	-29.82	-27.43	-25.52	-23.68	-21.95	-20.36	-18.83	-17.91	-18.47	2.16	-16.31	2
10: CH_2βii	-28.77	-26.59	-24.56	-22.69	-20.99	-19.46	-17.99	-17.11	-18.63	2.44	-16.19	2
11: CH_3ii	-26.80	-25.25	-23.61	-21.99	-20.46	-19.05	-17.70	-16.88	-15.28	1.56	-13.72	3
12: CH_3i	-25.98	-24.19	-22.49	-20.93	-19.47	-18.15	-17.37	-16.13	-15.67	1.49	-14.18	6
13: CH_2αo	-22.63	-21.39	-20.02	-18.61	-17.26	-16.02	-14.83	-14.10	-22.89	4.03	-18.86	2
14: CH_2αii	-21.60	-19.79	-18.09	-16.50	-15.10	-13.71	-12.69	-12.05	-14.14	4.53	-9.61	2
15: CH_2βo	-20.53	-19.08	-17.63	-16.29	-14.95	-13.79	-12.36	-11.73	-16.31	1.95	-14.36	2
16: CH_2βo	-19.00	-17.86	-16.68	-15.49	-14.39	-13.32	-12.36	-11.73	-16.31	1.95	-14.36	2
17: CH_2γo	-15.88	-14.93	-13.97	-12.97	-12.00	-11.12	-10.27	-7.76	-16.36	1.65	-14.71	2
18: CH_2γo	-15.88	-14.93	-13.84	-12.78	-11.79	-10.89	-10.04	-9.54	-16.36	1.65	-14.71	2
19: CH_3o	-10.89	-10.35	-9.71	-9.03	-8.36	-7.76	-7.18	-6.84	-9.88	1.09	-8.79	6
20: CH_{ar}ii	53.07	50.20	47.52	45.03	42.71	40.63	38.65	37.37	36.95	6.98	43.93	1

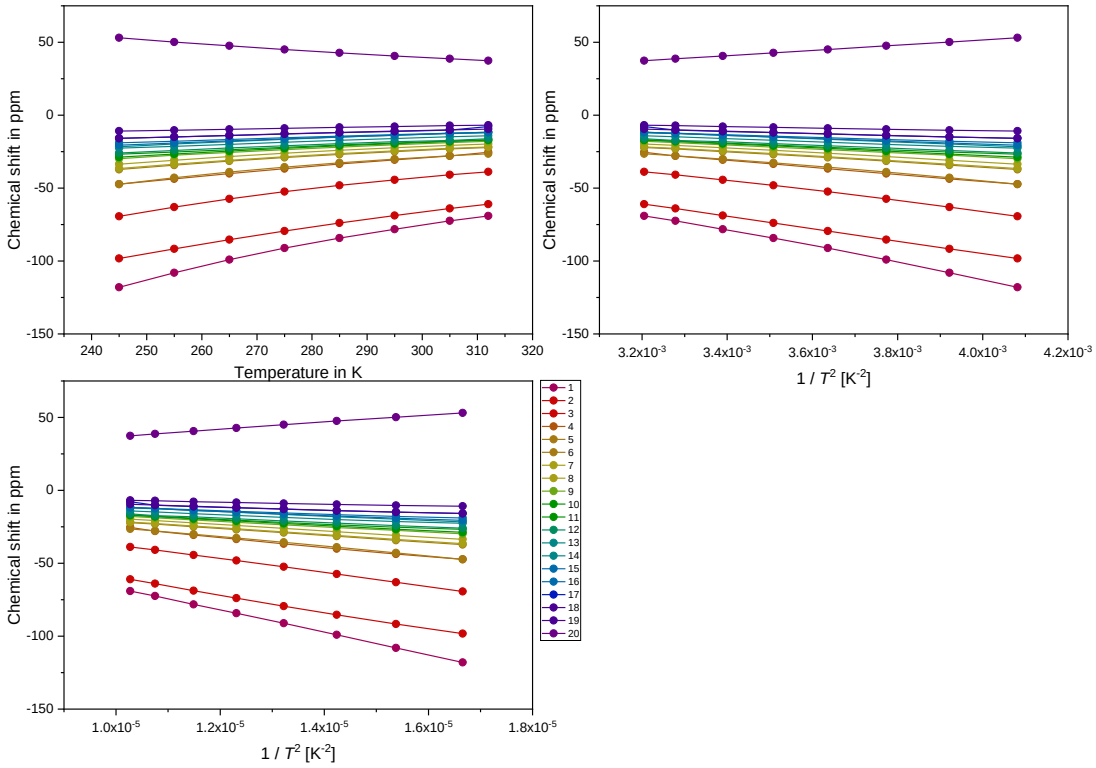

Fig. S158. Plot of the ^{1}H chemical shifts of **[5]^{0}** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S20. ^{13}C NMR chemical shifts of **[5]^{0}** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-115.5	s
2	-66.7	s
3	-5.8	q
4	-5.7	q
5	-4.0	t
6	-1.3	t
7	3.7	t
8	4.8	q
9	6.4	s ?
10	7.1	t
11	8.9	s or d
12	11.5	t
13	15.3	t
14	29.6	t
15	43.1	t
16	50.8	t
17	73.6	s
18	79.3	d / impurity
19	91.6	s
20	154.8	d
21	158.5	s
22	307.14	s
23	561.3	s
24	53.0	overlaped

3.11. Complex **[5]$^{+}$**

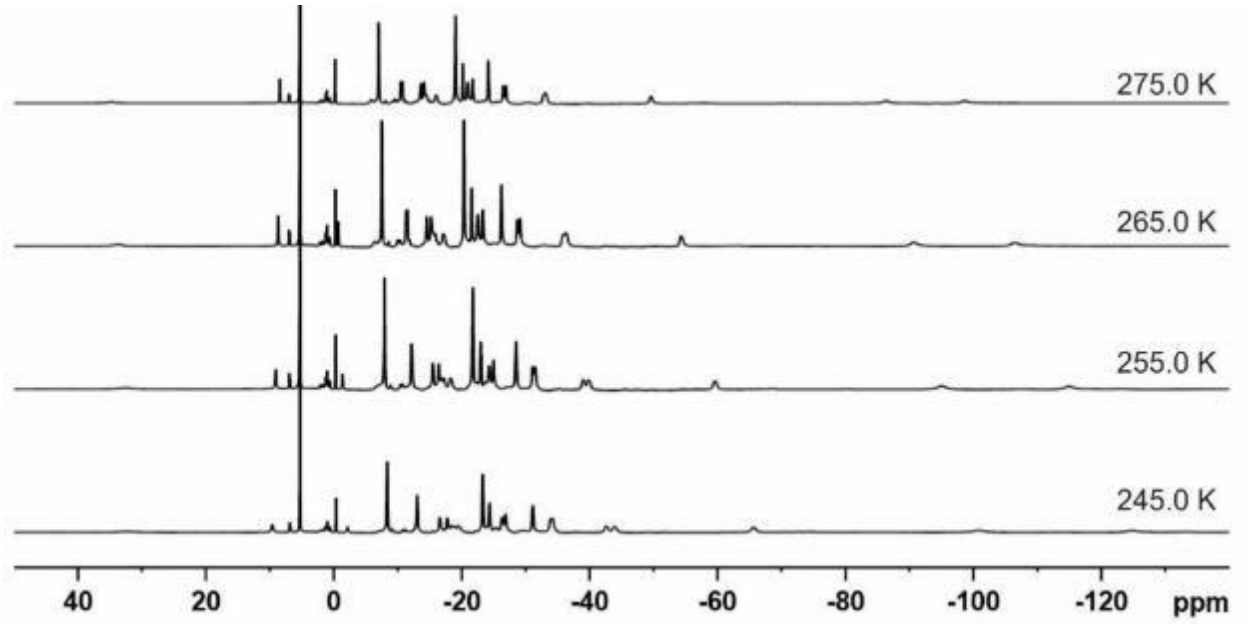

Fig. S159. Variable-temperature ^{1}H NMR spectra of complex **[5]$^{+}$** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

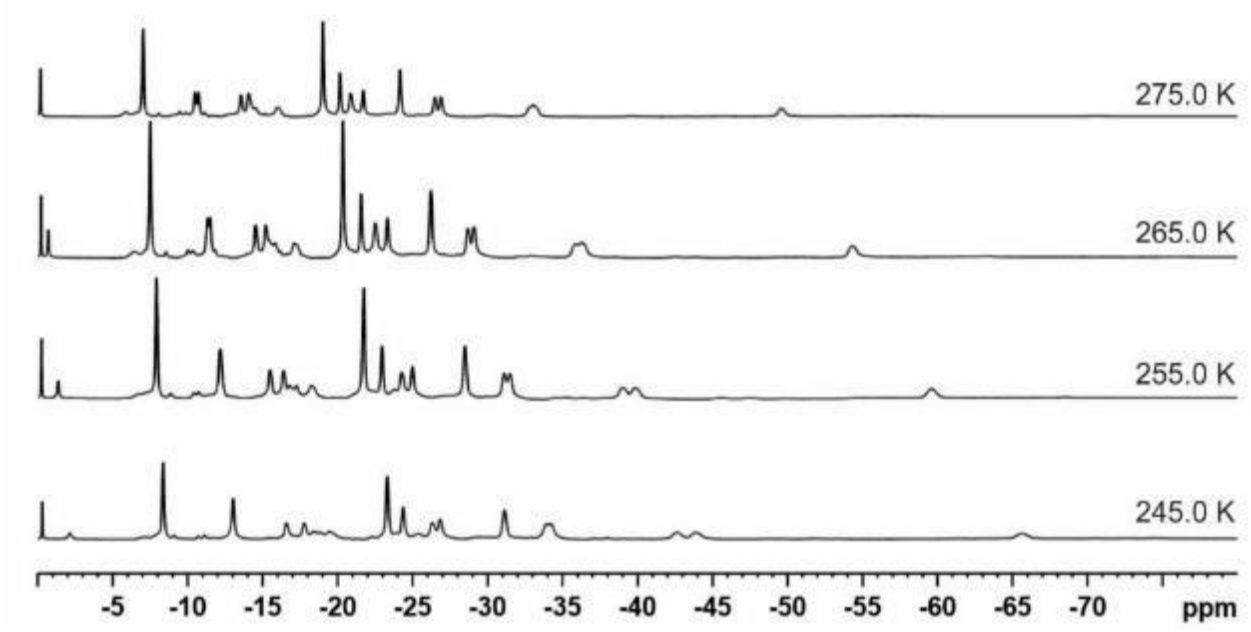

Fig. S160. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -80 ppm.

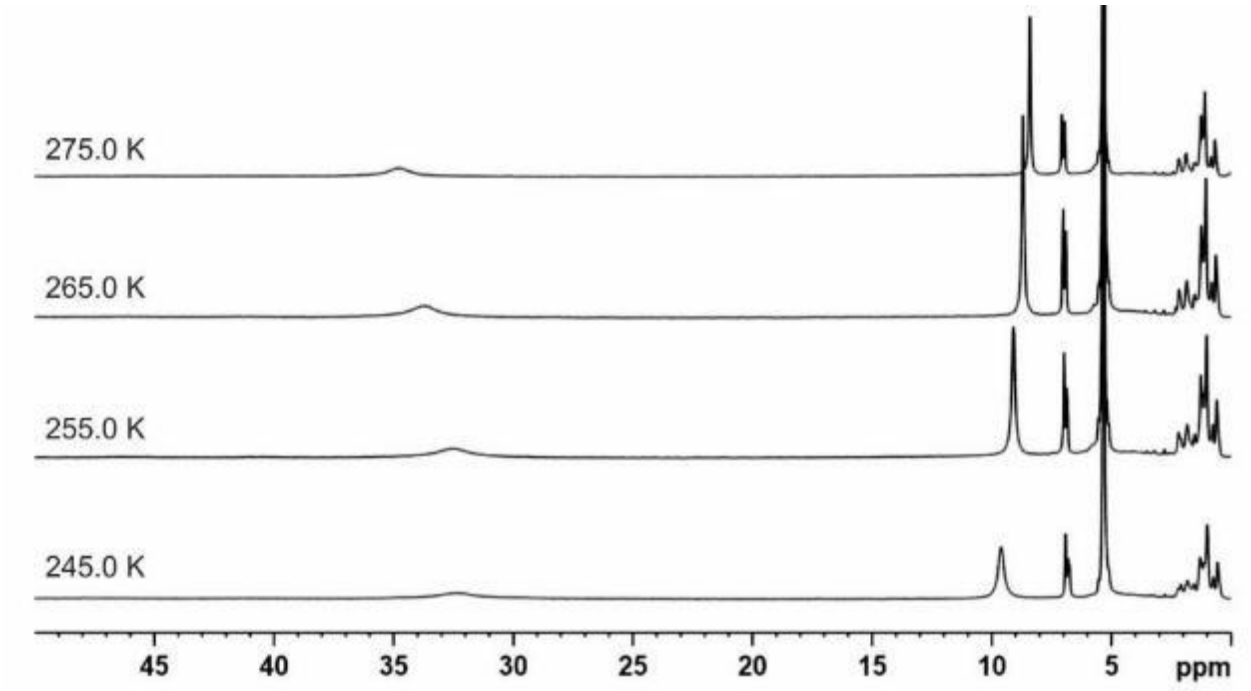

Fig. S161. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +50 ppm to 0 ppm.

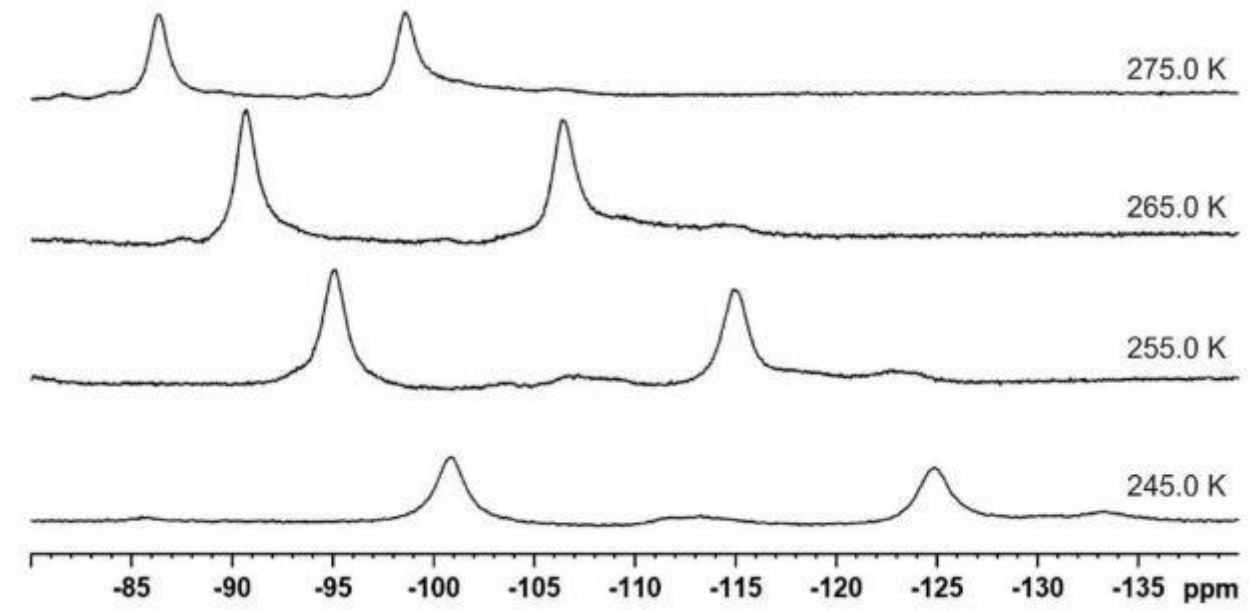

Fig. S162. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -80 ppm to -140 ppm.

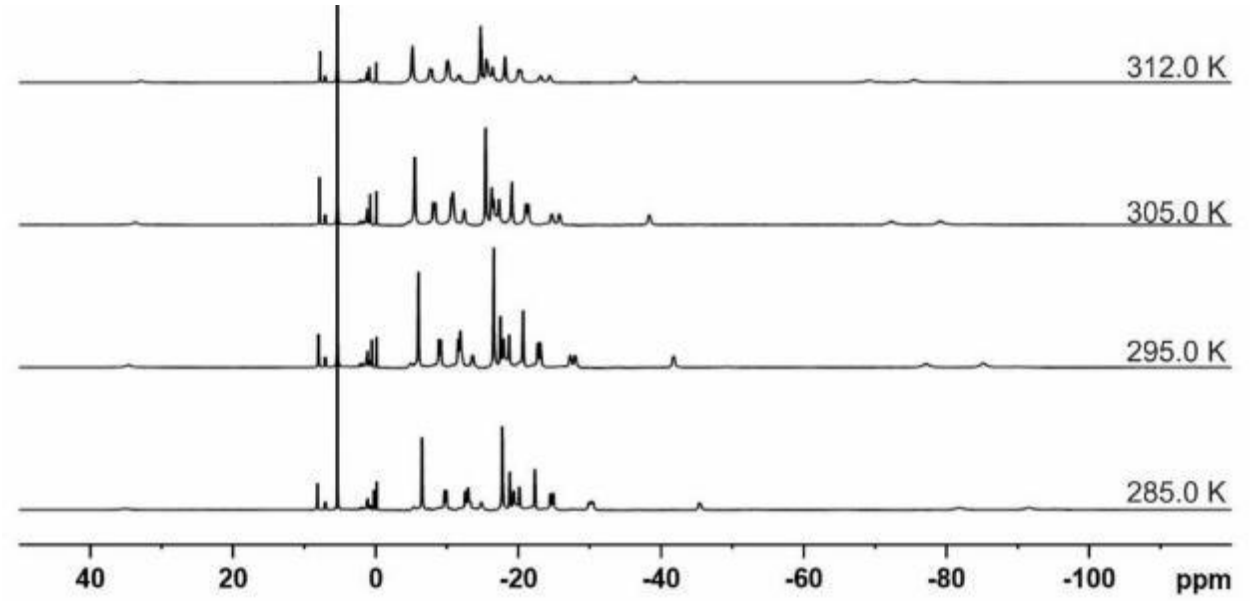

Fig. S163. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

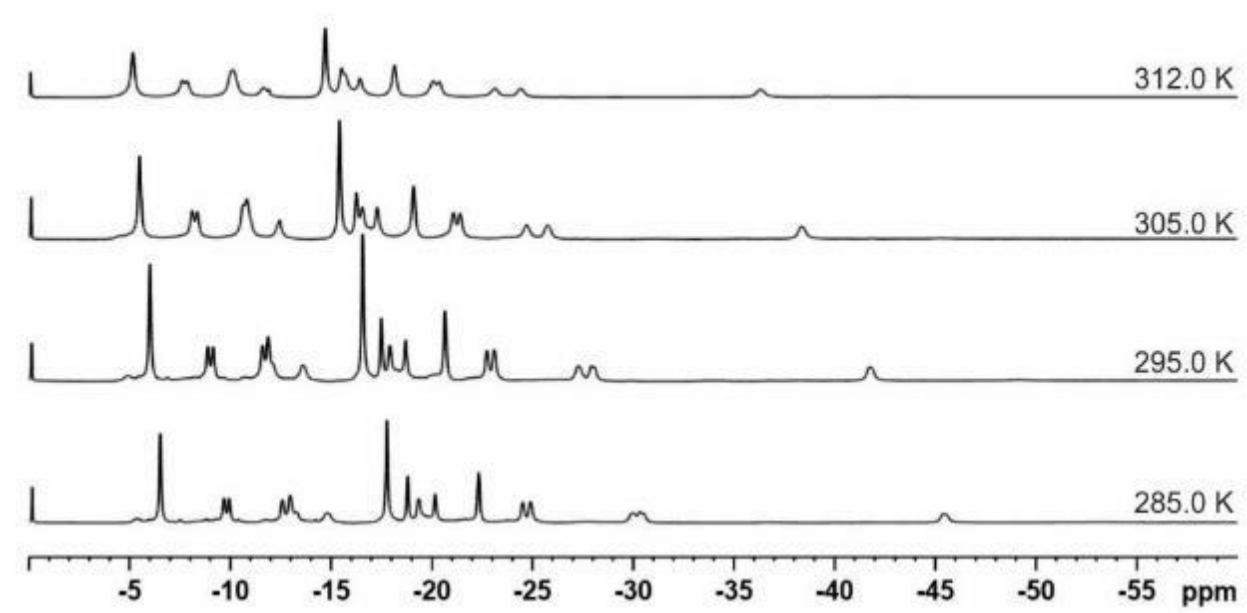

Fig. S164. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -60 ppm.

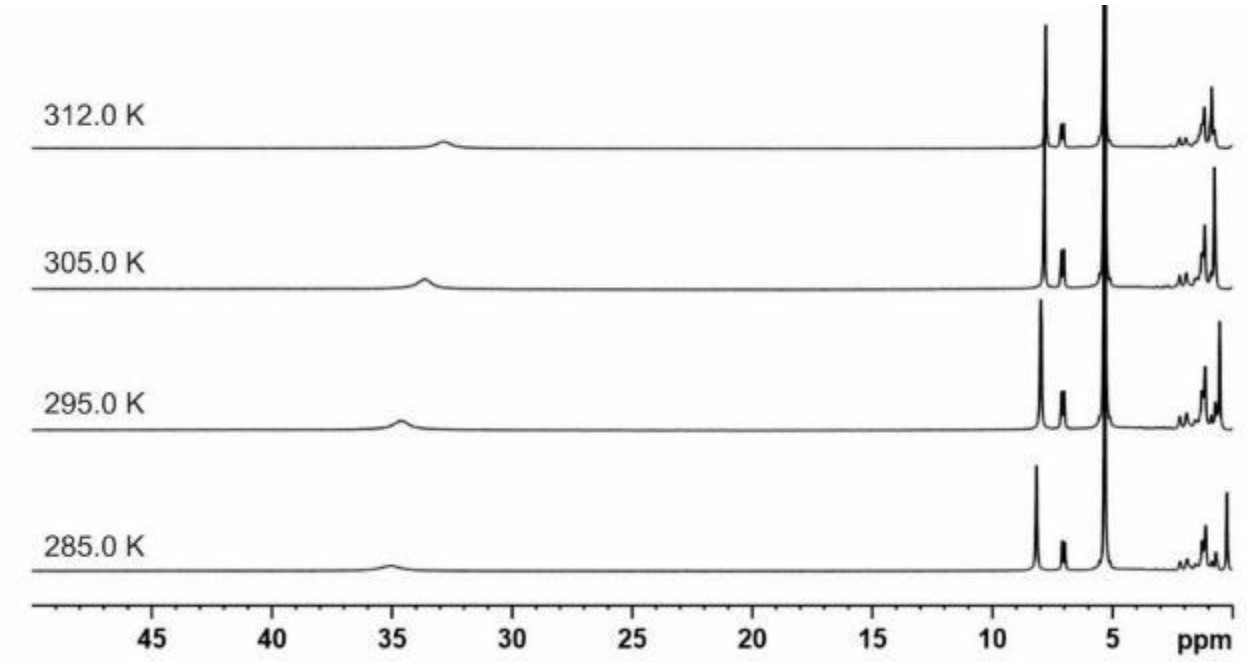

Fig. S165. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +50 ppm to 0 ppm.

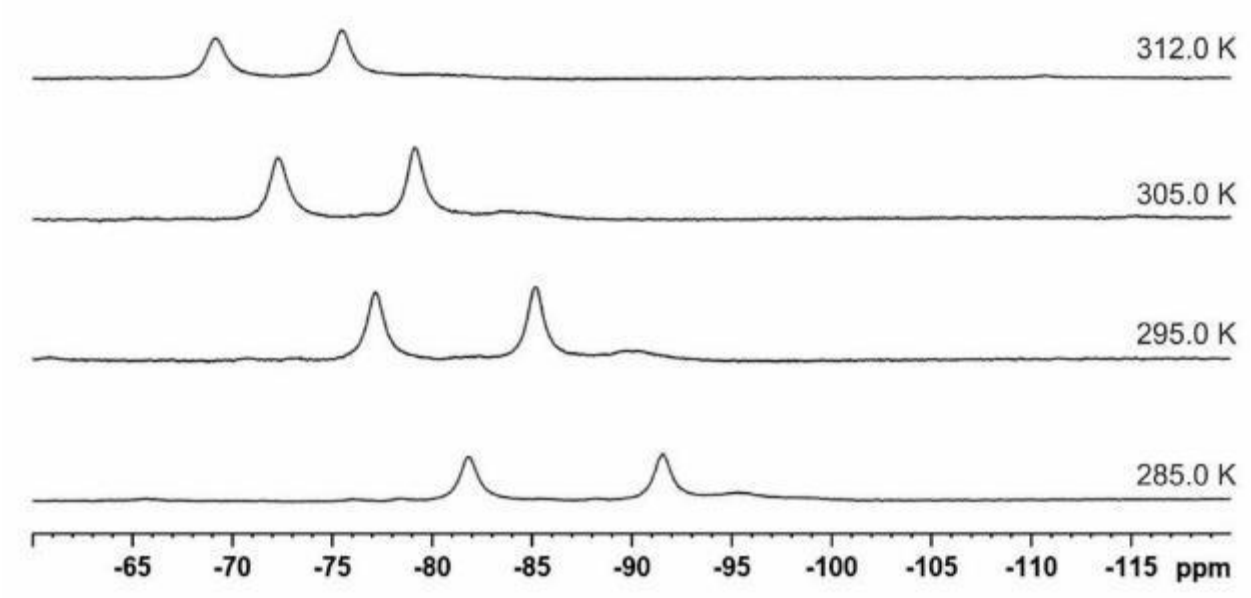

Fig. S166. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -60 ppm to -120 ppm.

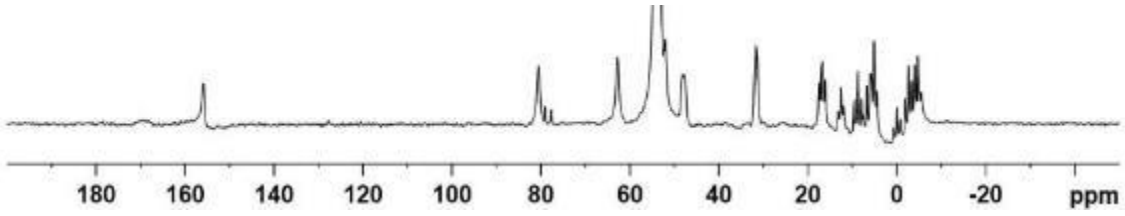

Fig. S167. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K.

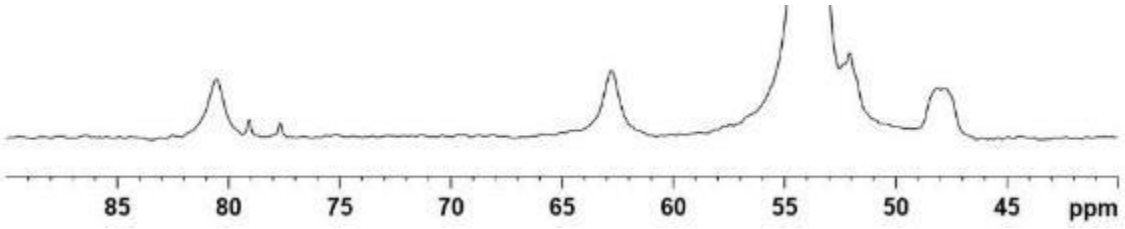

Fig. S168. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +90 ppm to +40 ppm.

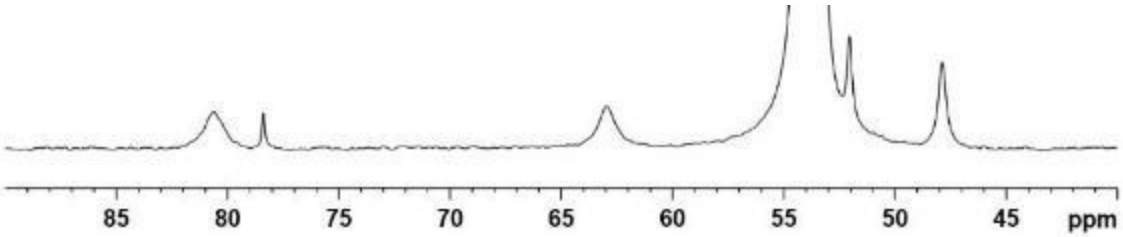

Fig. S169. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +90 ppm to +40 ppm.

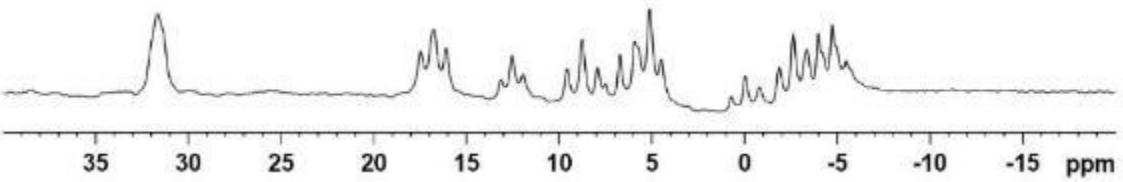

Fig. S170. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +40 ppm to -20 ppm.

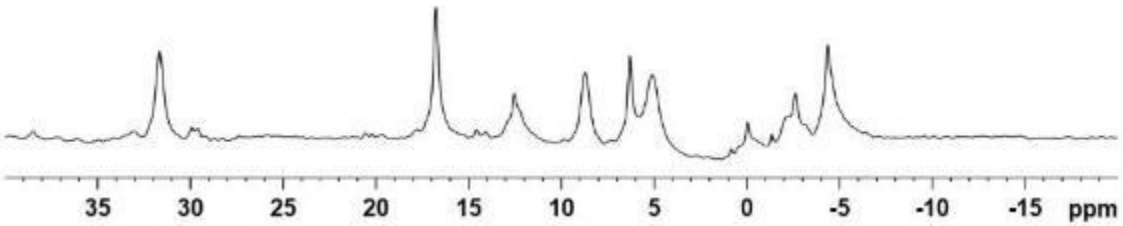

Fig. S171. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +40 ppm to -20 ppm.

Table S21. ^{1}H NMR experimental and calculated chemical shifts for **[5]**$^{+}$ in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
*Impurity	-133.43	-122.72	-114.66	-106.07	-95.42	-89.82	-83.94	-80.02	-	-	-	-	-
1: CH_{ar}i	-125.03	-114.87	-106.40	-98.61	-91.55	-85.17	-79.16	-75.45	-80.06	-9.57	7.52[a]	-82.12	2
2: CH_{ar}o	-100.87	-95.13	-90.70	-86.31	-81.80	-77.17	-72.28	-69.14	-70.35	-25.13	7.38[a]	-88.10	2
3: CH_2αi	-65.63	-59.61	-54.31	-49.57	-45.39	-41.74	-38.38	-36.33	-48.30	-	4.54[a]	-43.76	2
4: CH_2αo	-43.86	-39.82	-36.31	-33.17	-30.34	-27.98	-25.75	-24.42	-37.32	-	4.05[b]	-33.27	2
5: CH_2αi	-42.60	-38.99	-35.84	-32.86	-29.94	-27.28	-24.71	-23.14	-30.01	-	4.54[a]	-25.47	2
6: CH_2βi	-34.23	-31.50	-29.10	-26.89	-24.90	-23.11	-21.42	-20.38	-24.04	-	2.35	-21.69	2
7: CH_2βi	-33.87	-31.12	-28.70	-26.49	-24.52	-22.75	-21.09	-20.07	-24.04	-	2.35	-21.69	4
8: CH_2γi	-31.13	-28.51	-26.23	-24.17	-22.33	-20.68	-19.11	-18.16	-22.80	-	2.09	-20.71	2
9: CH_2γii	-26.84	-25.00	-23.34	-21.72	-20.17	-18.71	-17.30	-16.45	-18.70	-	2.09	-16.61	2
10: CH_2βii	-26.31	-24.28	-22.52	-20.88	-19.35	-17.93	-16.56	-15.69	-18.84	-	2.39	-16.45	3
11: CH_3ii	-25.42	-22.97	-21.59	-20.18	-18.80	-17.51	-16.27	-15.53	-15.36	-	1.52	-13.84	6
12: CH_3i	-24.36	-21.75	-20.36	-19.02	-17.78	-16.58	-15.43	-14.73	-15.49	-	1.46	-14.03	2
13: CH_2αo	-19.32	-18.26	-17.19	-15.98	-14.77	-13.59	-12.46	-11.67	-15.42	-	3.91[b]	-11.51	2
14: CH_2αii	-18.64	-17.05	-15.67	-14.55	-13.32	-12.02	-10.98	-10.15	-14.80	-	4.53[a]	-10.27	2
15: CH_2βo	-17.77	-16.41	-15.23	-14.08	-12.97	-11.89	-10.83	-10.15	-13.81	-	1.96	-11.85	2
16: CH_2βo	-16.58	-15.51	-14.54	-13.57	-12.59	-11.61	-10.66	-10.04	-13.81	-	1.96	-11.85	2
17: CH_2γo	-13.04	-12.19	-11.50	-10.74	-9.95	-9.16	-8.37	-7.86	-12.84	-	1.67	-11.17	2
18: CH_2γo	-13.04	-10.75	-11.33	-10.51	-9.69	-8.89	-8.11	-7.63	-12.84	-	1.67	-11.17	6
19: CH_3o	-8.37	-7.94	-7.51	-7.04	-6.53	-6.02	-5.50	-5.17	-8.02	-	1.05	-6.97	1
20: CH_{ar}ii	32.51	32.54	33.81	34.77	35.05	34.62	33.61	32.85	35.54	1.20	6.98[a]	43.72	

[a]The δ_{orb} values of **[5]**^{0} were used. [b]The δ_{orb} values of **[5]**$^{4+}$ were used.

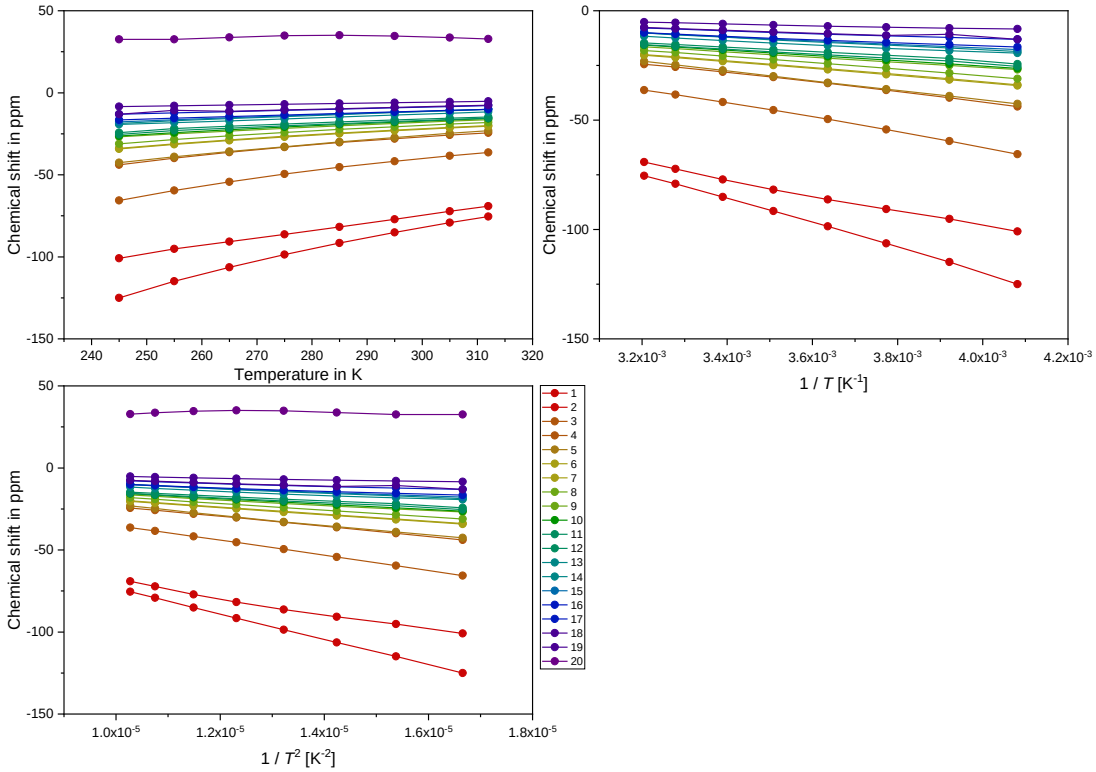

Fig. S172. Plot of the ^{1}H chemical shifts of **[5]**$^{+}$ in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S22. ^{13}C NMR chemical shifts of **[5]**$^{+}$ observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-4.5	q
2	-4.2	q
3	-2.6	t
4	0.0	t
5	5.1	t
6	6.4	q
7	8.8	t
8	12.6	t
9	16.9	t
10	31.7	t
11	48.0	d ?
12	52.1	s?
13	62.8	s
14	77.7	s
15	79.1	s
16	80.7	s
17	156.1	s
18	169.7	s / impurity

3.12. Complex **[5]**$^{2+}$

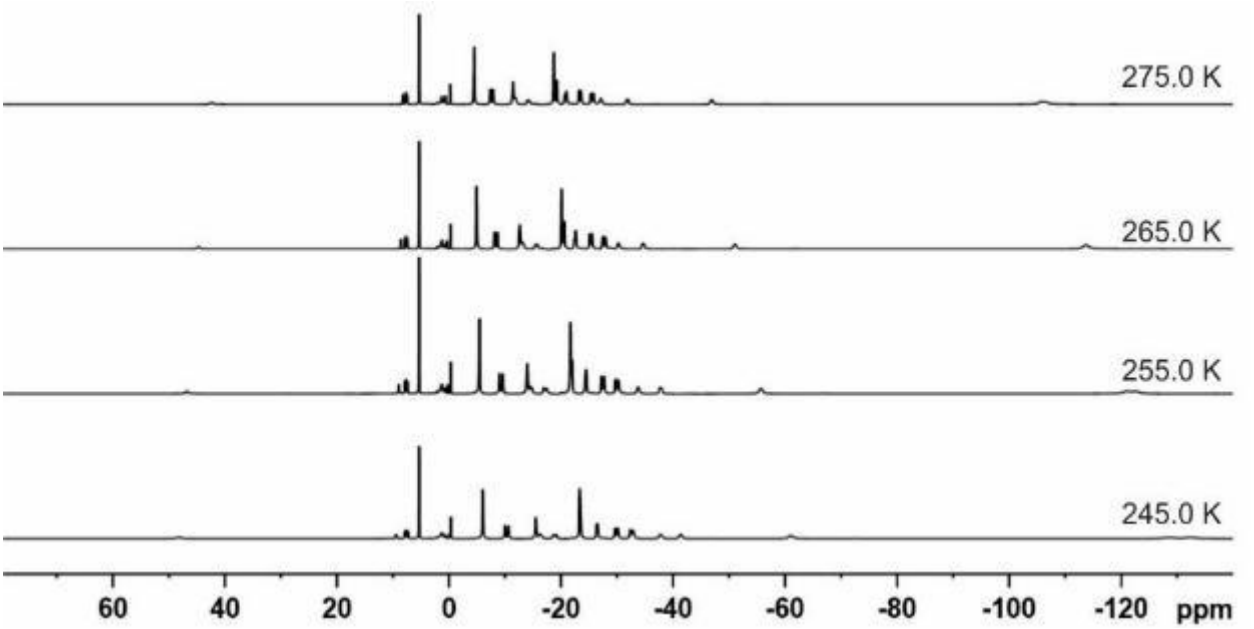

Fig. S173. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

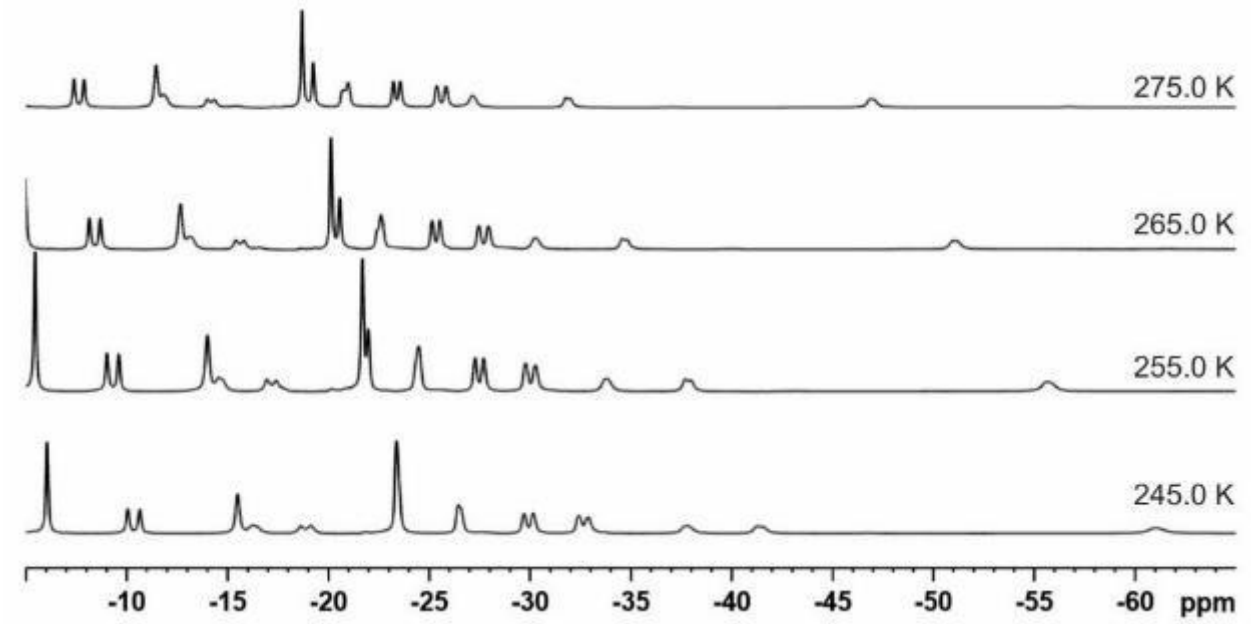

Fig. S174. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -5 ppm to -65 ppm.

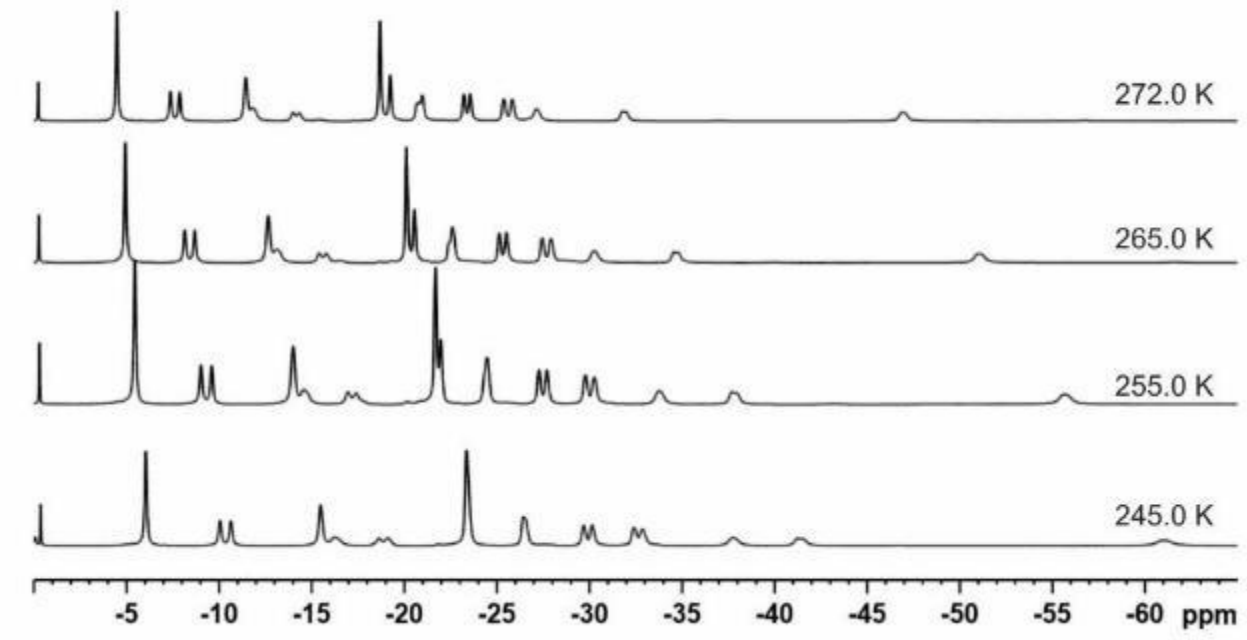

Fig. S175. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -65 ppm.

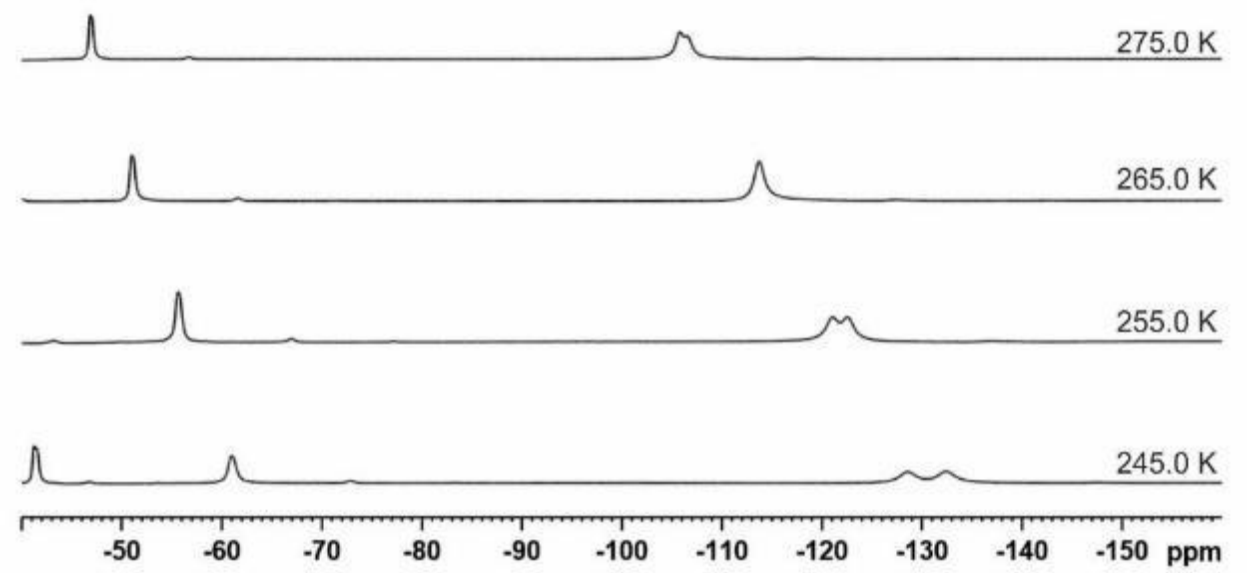

Fig. S176. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -45 ppm to -155 ppm.

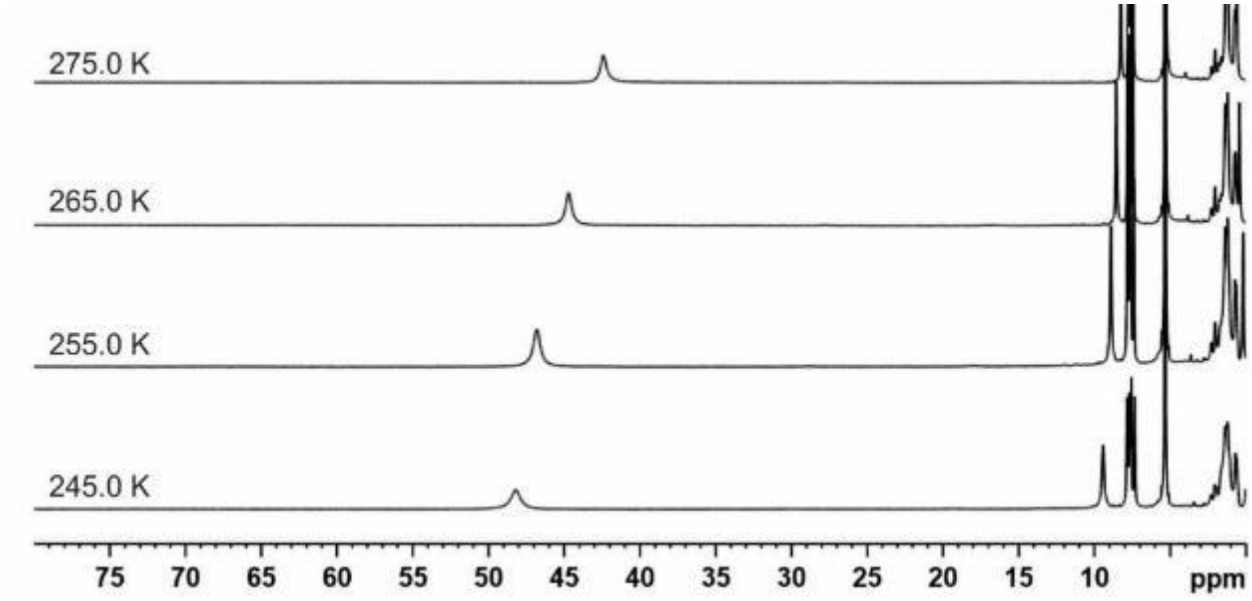

Fig. S177. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +80 ppm to -5 ppm.

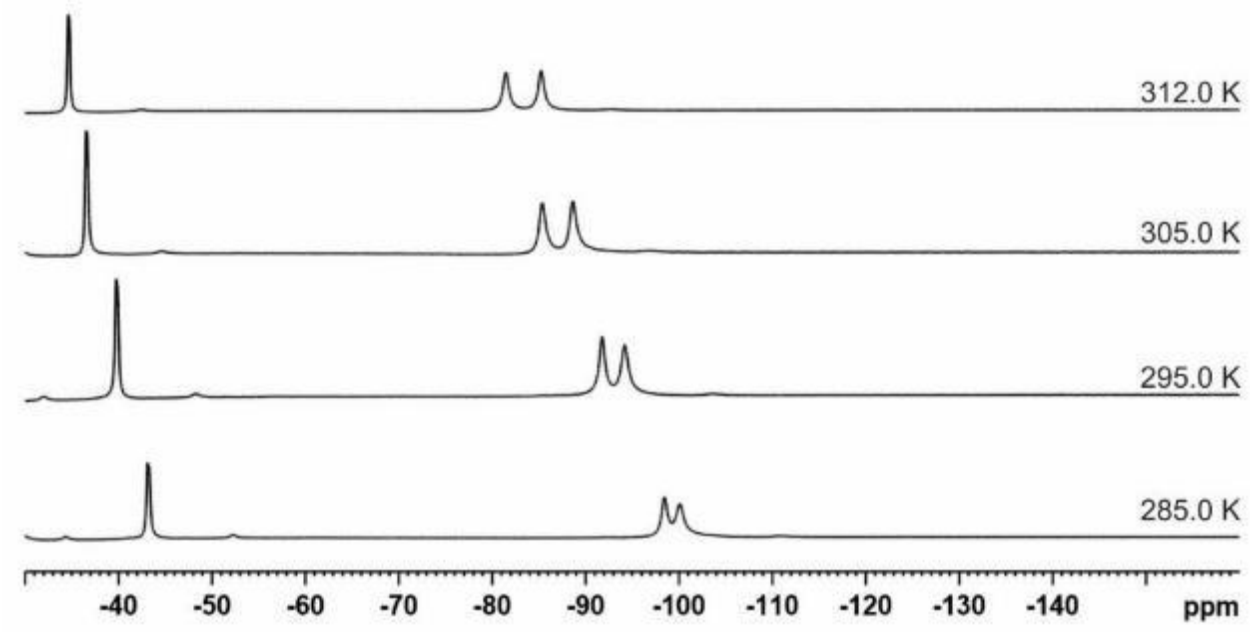

Fig. S178. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -30 ppm to -160 ppm.

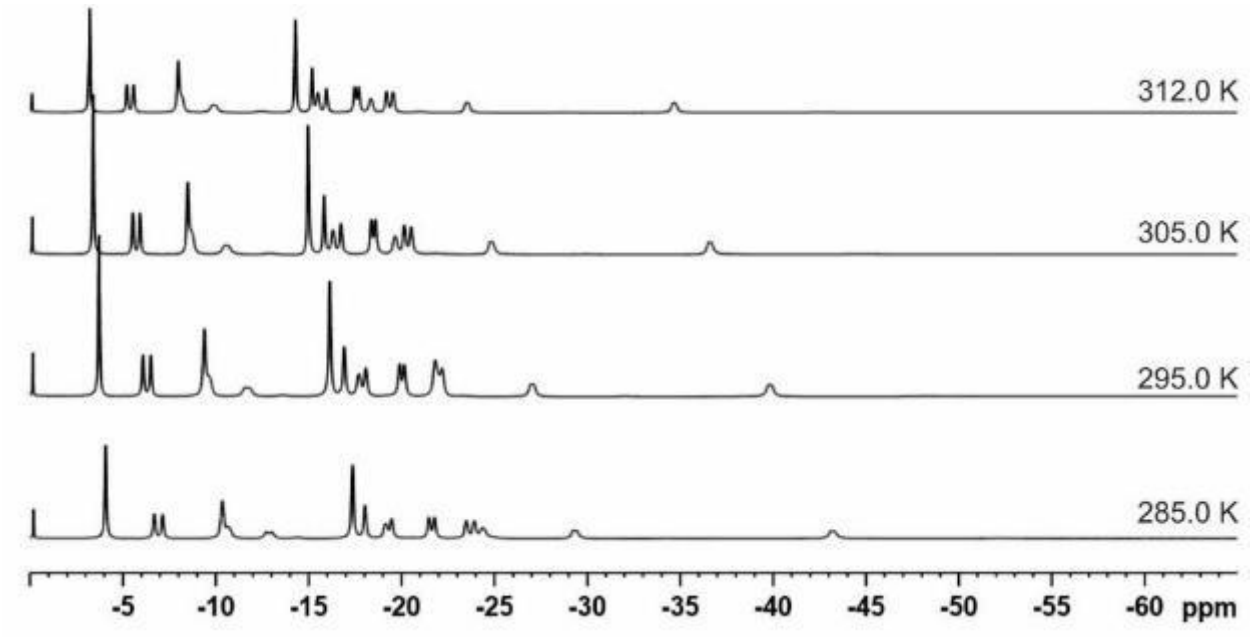

Fig. S179. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -65 ppm.

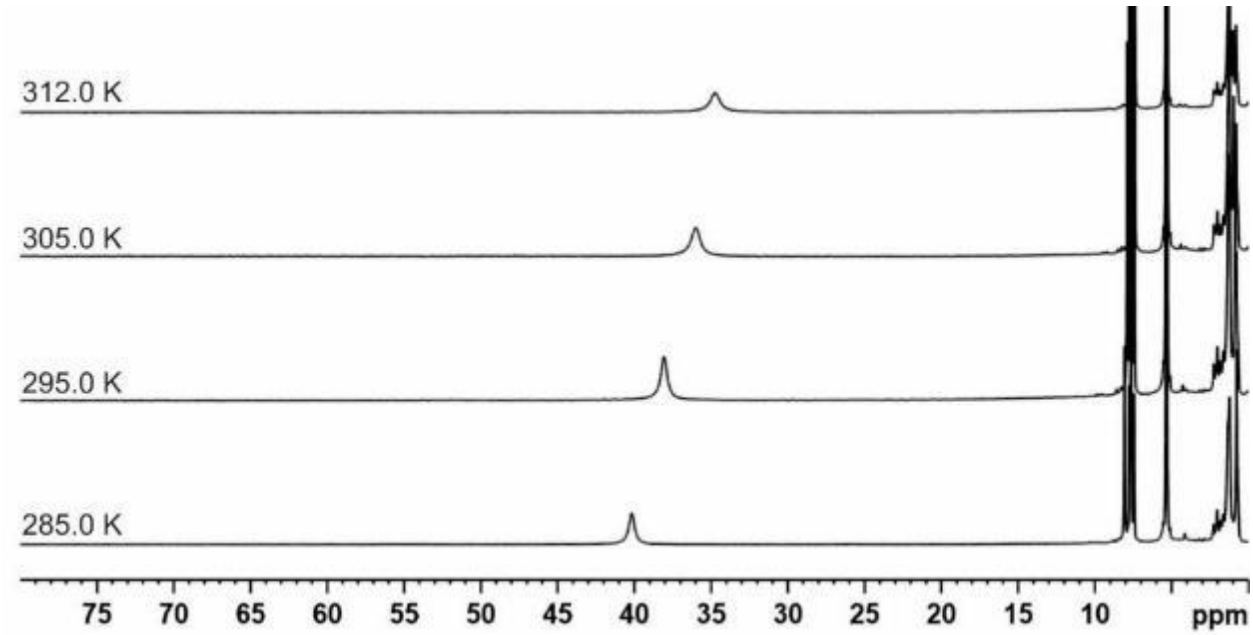

Fig. S180. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{2+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +80 ppm to 0 ppm.

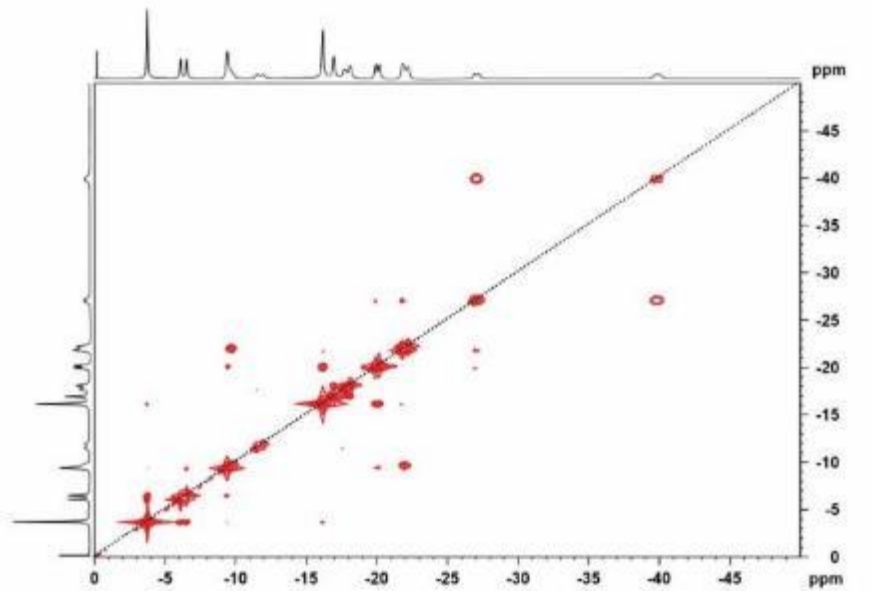

Fig. S181. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[5]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from 0 ppm to -50 ppm.

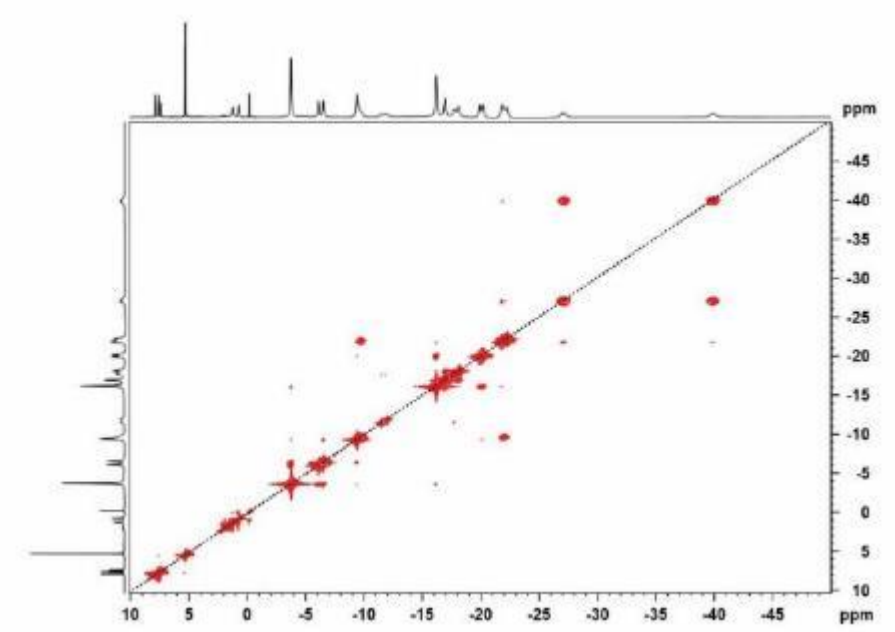

Fig. S182. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[5]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from +10 ppm to -50 ppm.

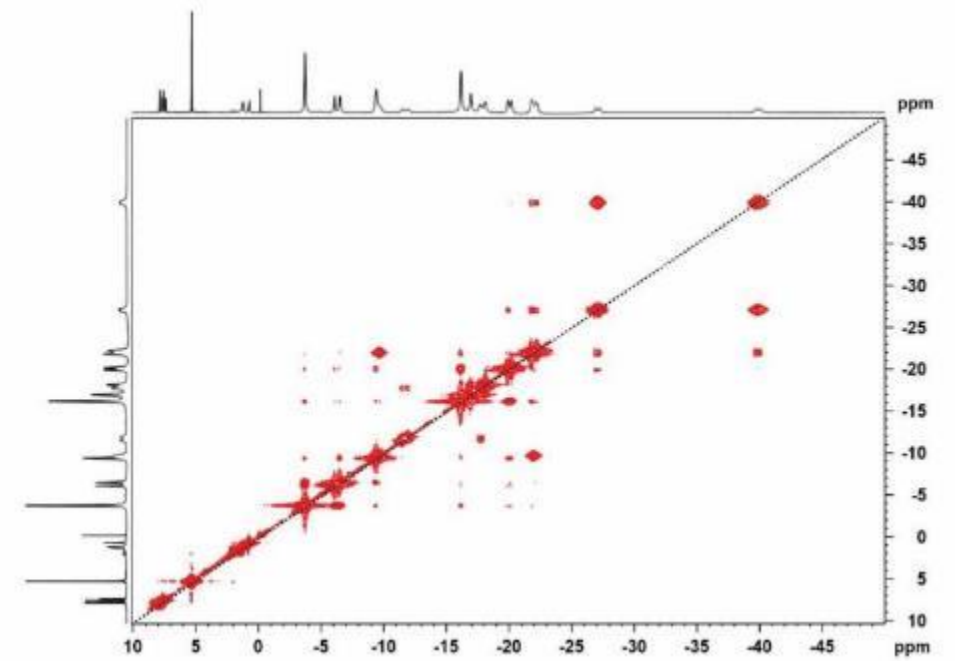

Fig. S183. ^{1}H, ^{1}H NMR correlation (COSY) spectrum of complex **[5]**$^{2+}$ in CD_2Cl_2 (COSY), recorded at 295.0 K. Expansion from +10 ppm to -45 ppm.

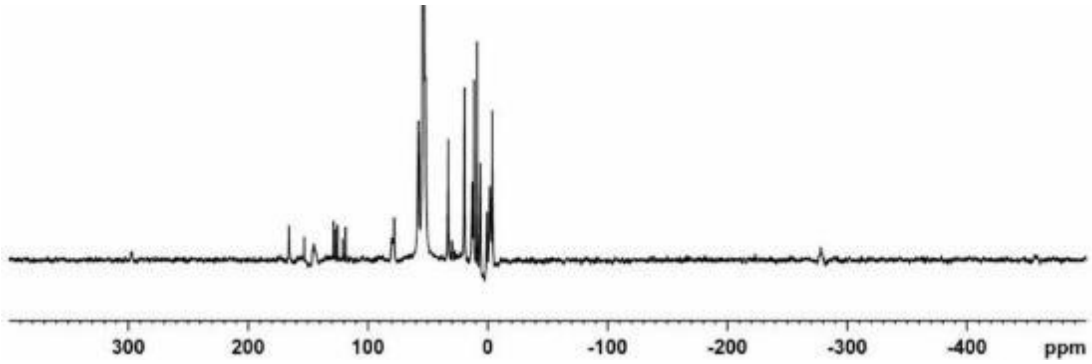

Fig. S184. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K.

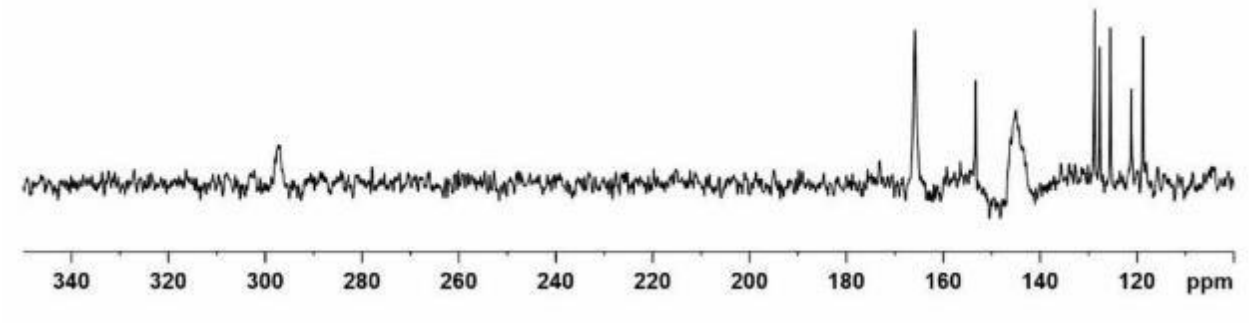

Fig. S185. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +350 ppm to +100 ppm.

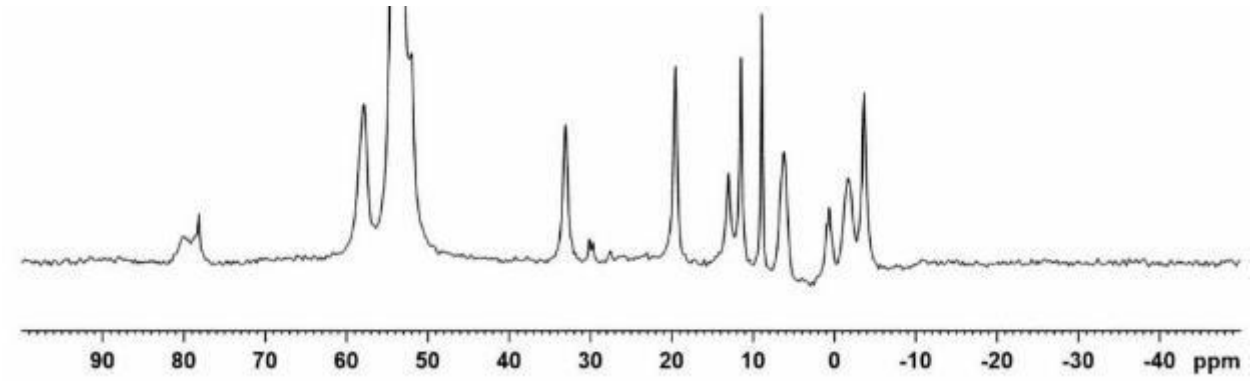

Fig. S186. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +100 ppm to -50 ppm.

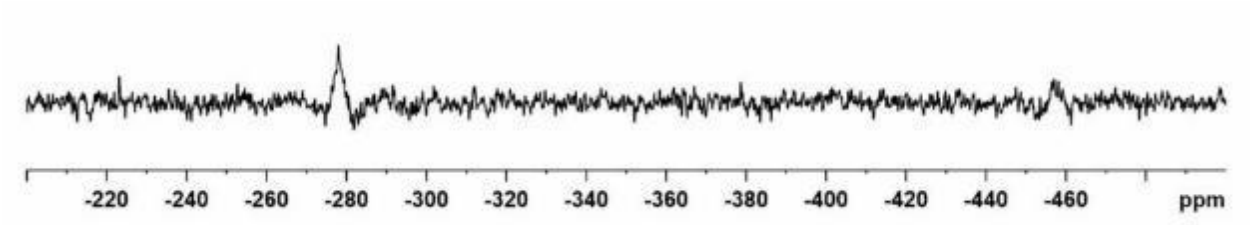

Fig. S187. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from -200 ppm to -500 ppm.

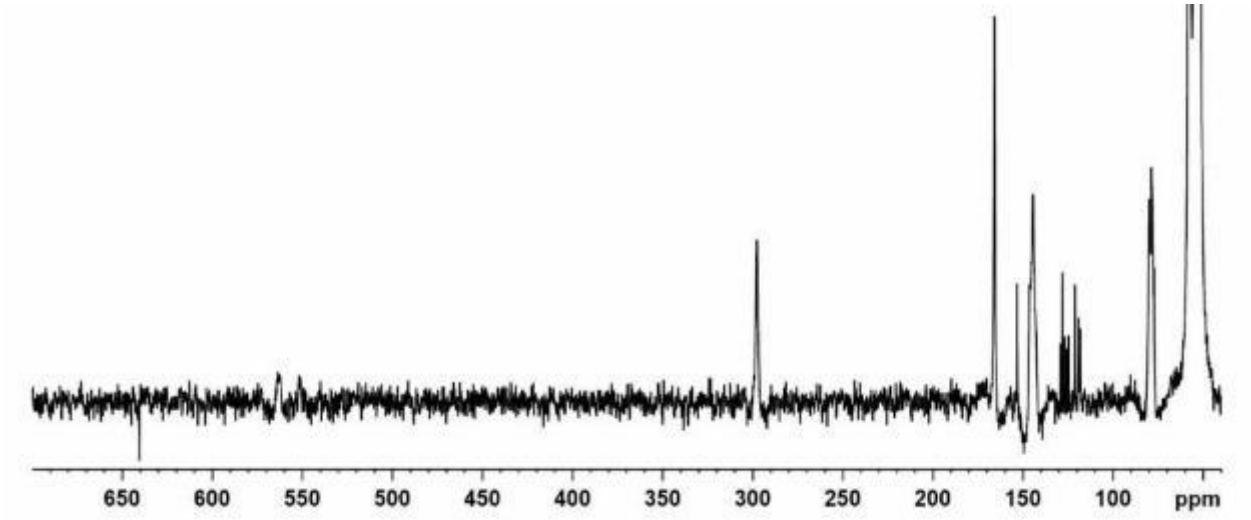

Fig. S188. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +700 ppm to +40 ppm.

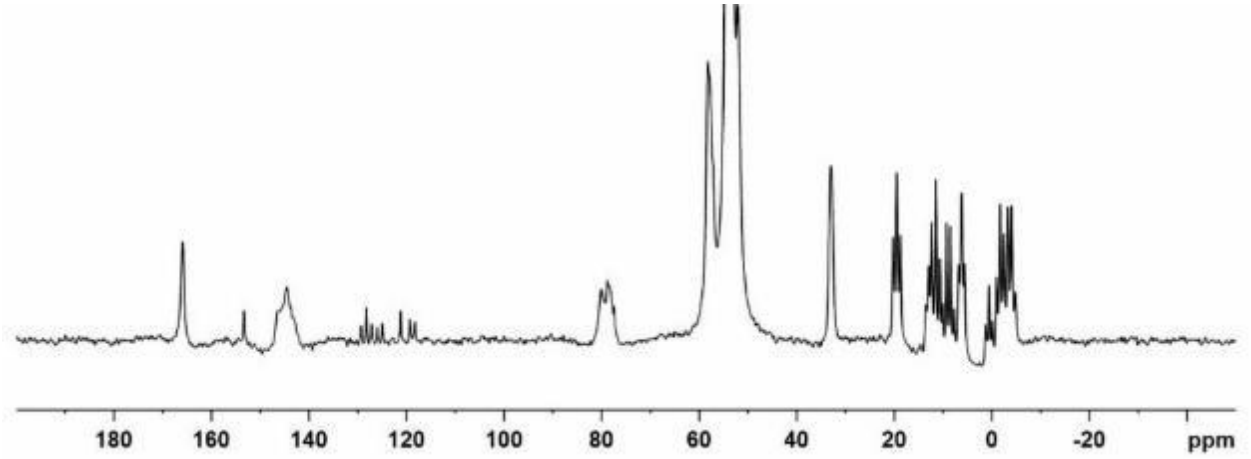

Fig. S189. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +200 ppm to -50 ppm.

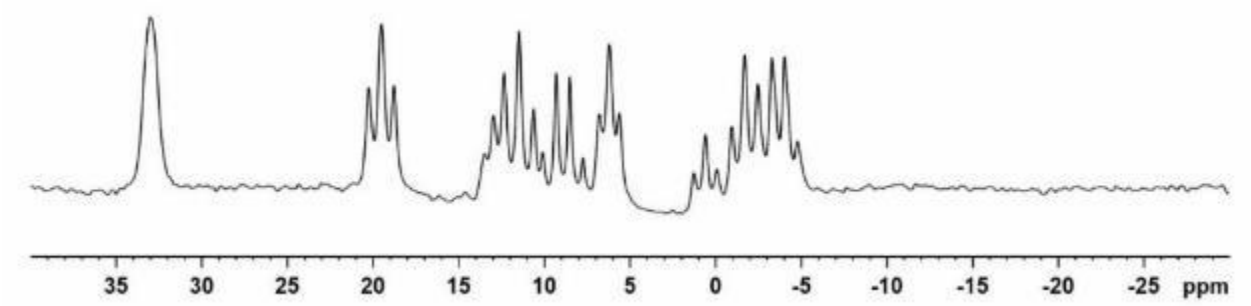

Fig. S190. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +40 ppm to -30 ppm.

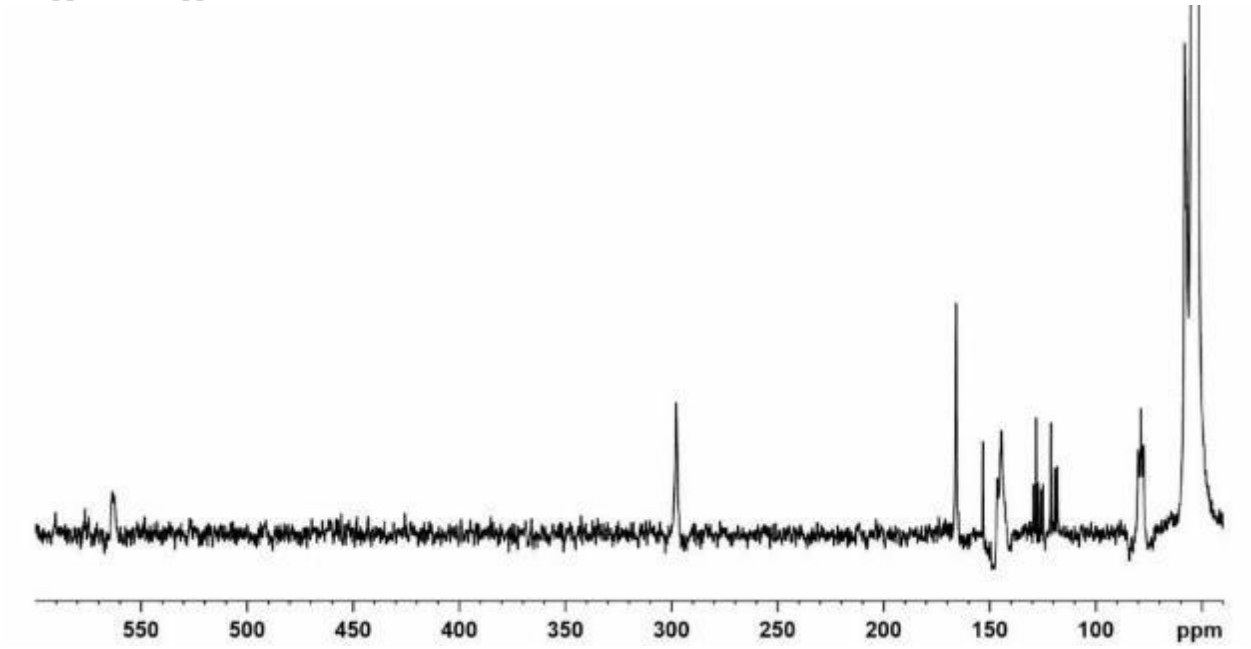

Fig. S191. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +600 ppm to +40 ppm.

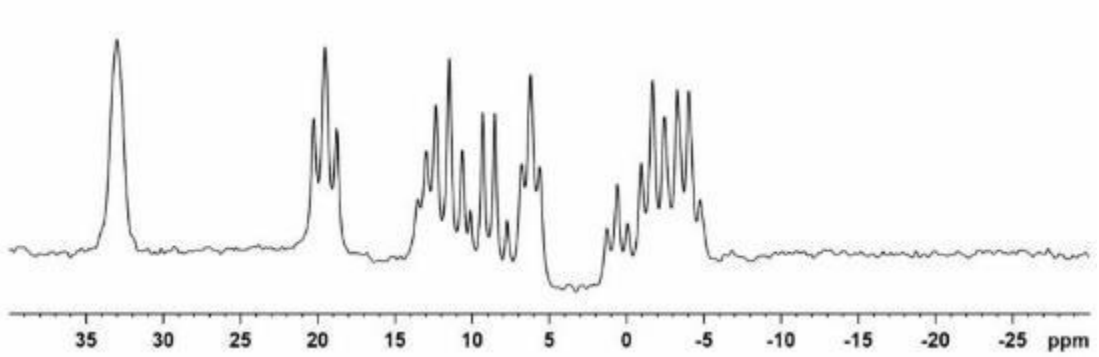

Fig. S192. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +40 ppm to -30 ppm.

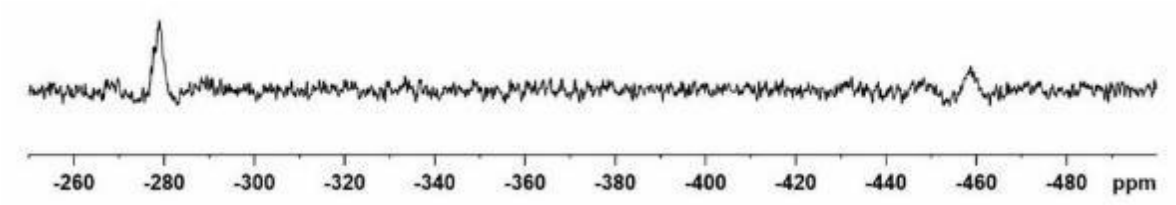

Fig. S193. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from -270 ppm to -500 ppm.

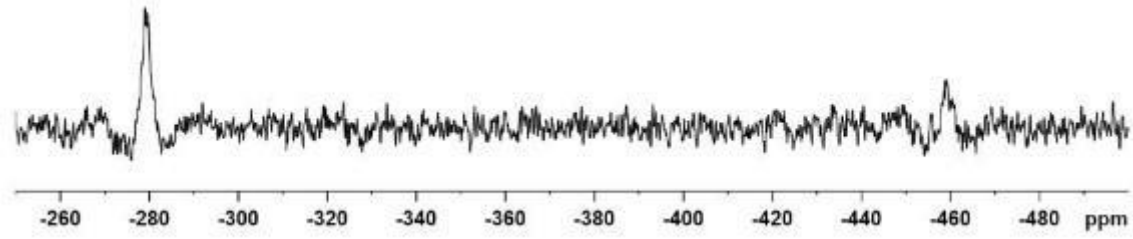

Fig. S194. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{2+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from -250 ppm to -500 ppm.

Table S23. ^{1}H NMR experimental chemical shifts for **[5]$^{2+}$** in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}o$	-134.41	-122.56	-113.70	-106.52	-100.14	-94.20	-88.67	-85.27	-61.84	-52.65	7.38[a]	-107.11	2
2: $CH_{ar}i$	-128.52	-121.05	-113.70	-105.79	-98.48	-91.81	-85.38	-81.49	-76.29	-19.15	7.52[a]	-87.91	2
3: $CH_2\alpha i$	-61.04	-55.66	-50.99	-46.95	-43.22	-39.84	-36.58	-34.66	-45.13	-	4.54[a]	-40.59	2
4: $CH_2\alpha i$	-41.39	-37.83	-34.68	-31.89	-29.35	-27.05	-24.85	-23.54	-28.19	-	4.54[a]	-23.65	2
5: $CH_2\alpha o$	-37.77	-33.78	-30.25	-27.14	-24.38	-22.00	-19.66	-18.36	-33.89	-	4.05[b]	-29.84	2
6: $CH_2\beta i$	-32.89	-30.27	-27.93	-25.83	-23.92	-21.82	-20.17	-19.56	-23.31	-	2.34	-20.97	2
7: $CH_2\beta i$	-32.44	-29.79	-27.45	-25.38	-23.49	-21.82	-20.53	-19.21	-23.31	-	2.34	-20.97	2
8: $CH_2\gamma i$	-30.17	-27.71	-25.52	-23.57	-21.78	-20.16	-18.61	-17.71	-22.24	-	2.09	-20.15	2
9: $CH_2\gamma i$	-29.71	-27.28	-25.14	-23.23	-21.49	-19.90	-18.39	-17.50	-22.24	-	2.09	-20.15	2
10: $CH_2\gamma ii$	-26.45	-24.48	-22.61	-20.99	-19.47	-18.08	-16.76	-15.98	-17.99	-	2.09	-15.90	2
11: $CH_2\beta ii$	-26.45	-24.48	-22.43	-20.75	-19.16	-17.71	-16.32	-15.51	-18.22	-	2.39	-15.83	2
12: CH_3ii	-23.38	-21.98	-20.56	-19.26	-18.04	-16.93	-15.84	-15.21	-14.75	-	1.51	-13.24	3
13: CH_3i	-23.38	-21.69	-20.13	-18.70	-17.38	-16.16	-14.99	-14.30	-14.86	-	1.46	-13.40	6
14: $CH_2\alpha ii$	-18.89	-17.19	-15.61	-14.18	-12.89	-11.72	-10.59	-9.92	-14.51	-	4.53[a]	-9.98	2
15: $CH_2\alpha o$	-16.32	-14.65	-13.16	-11.87	-10.66	-9.63	-8.69	-8.14	-33.89	-	4.05[b]	-29.84	2
16: $CH_2\beta o$	-15.50	-14.01	-12.66	-11.46	-10.37	-9.40	-8.51	-7.99	-11.89	-	1.96	-9.93	4
17: $CH_2\gamma o$	-10.65	-9.61	-8.69	-7.89	-7.16	-6.52	-5.93	-5.59	-11.42	-	1.67	-9.75	2
18: $CH_2\gamma o$	-10.06	-9.02	-8.15	-7.39	-6.70	-6.10	-5.55	-5.23	-11.42	-	1.67	-9.75	2
19: CH_3o	-6.06	-5.46	-4.95	-4.49	-4.09	-3.73	-3.41	-3.23	-7.07	-	1.03	-6.04	6
20: $CH_{ar}ii$	48.20	46.79	44.71	42.39	40.15	38.05	35.99	34.75	32.02	-1.20	6.98[a]	39.00	1

[a]The δ_{orb} values of **[5]^0** were used. [b]The δ_{orb} values of **[5]$^{4+}$** were used.

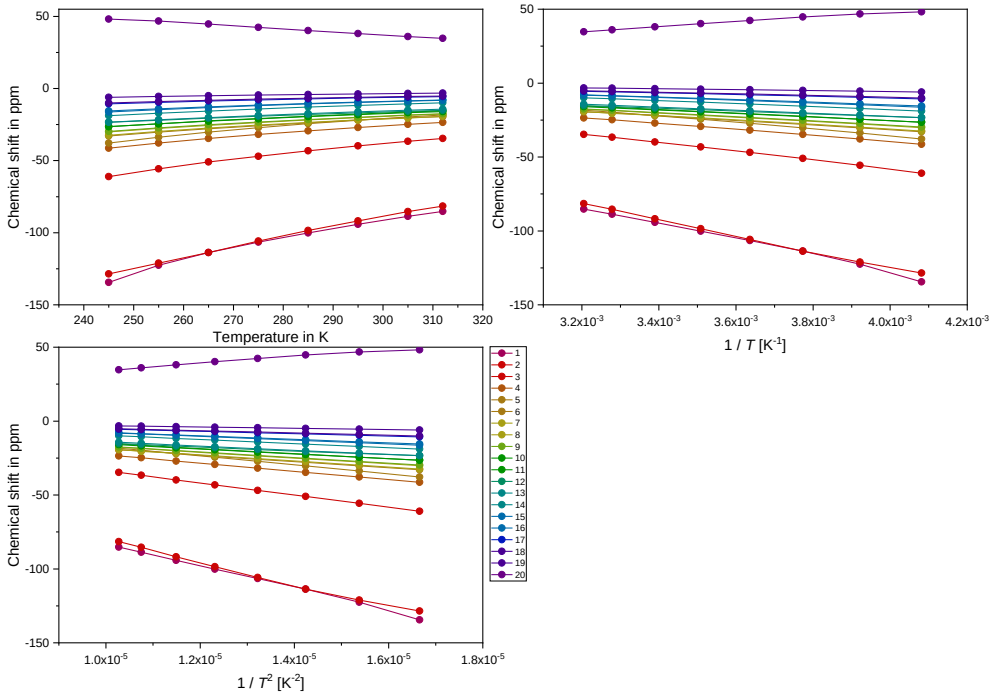

Fig. S195. Plot of the ^{1}H chemical shifts of **[5]$^{2+}$** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S24. ^{13}C NMR chemical shifts of **[5]$^{2+}$** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-459.7	s
2	-279.6	s
3	-3.7	q
4	-1.7	t
5	0.6	t
6	6.2	t
7	8.9	q
8	11.6	t
9	11.8	q
10	12.4	t ?
11	13.1	d ?
12	19.6	t
13	33	t
14	52.4	?
15	58.1	?
16	78.3	d or t
17	79.4	d
18	144.8	d ?
19	145.7	d
20	166	s
21	297.9	s
22	563.1	s

3.13. Complex **[5]$^{3+}$**

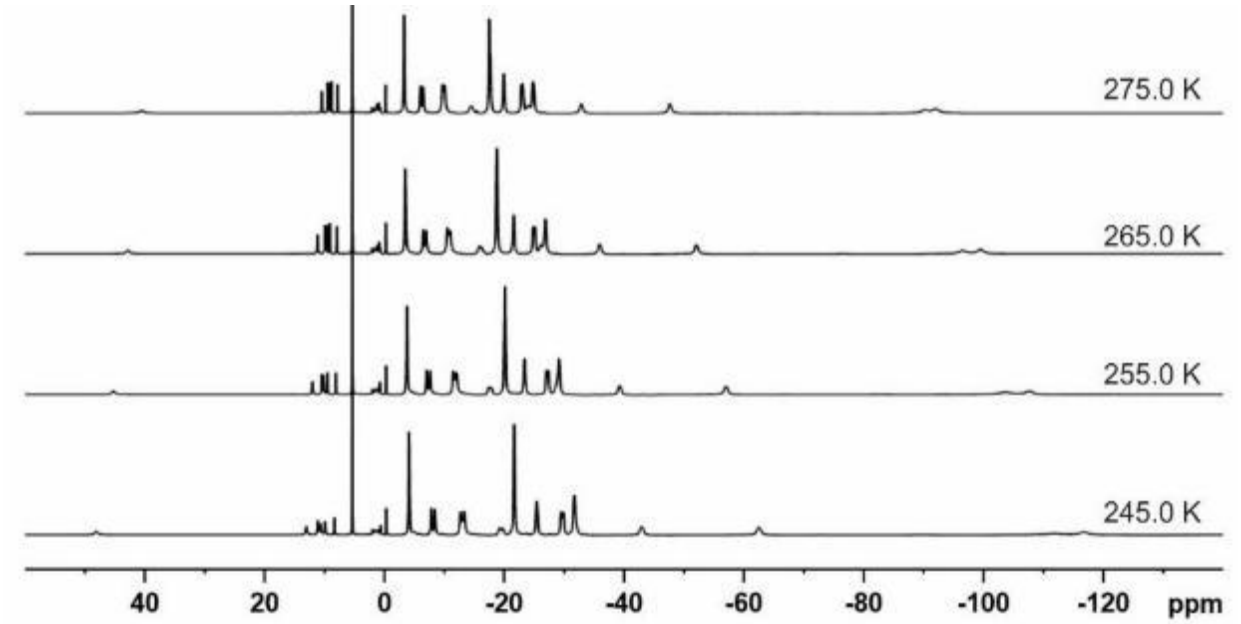

Fig. S196. Variable-temperature ^1H NMR spectra of complex **[5]$^{3+}$** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

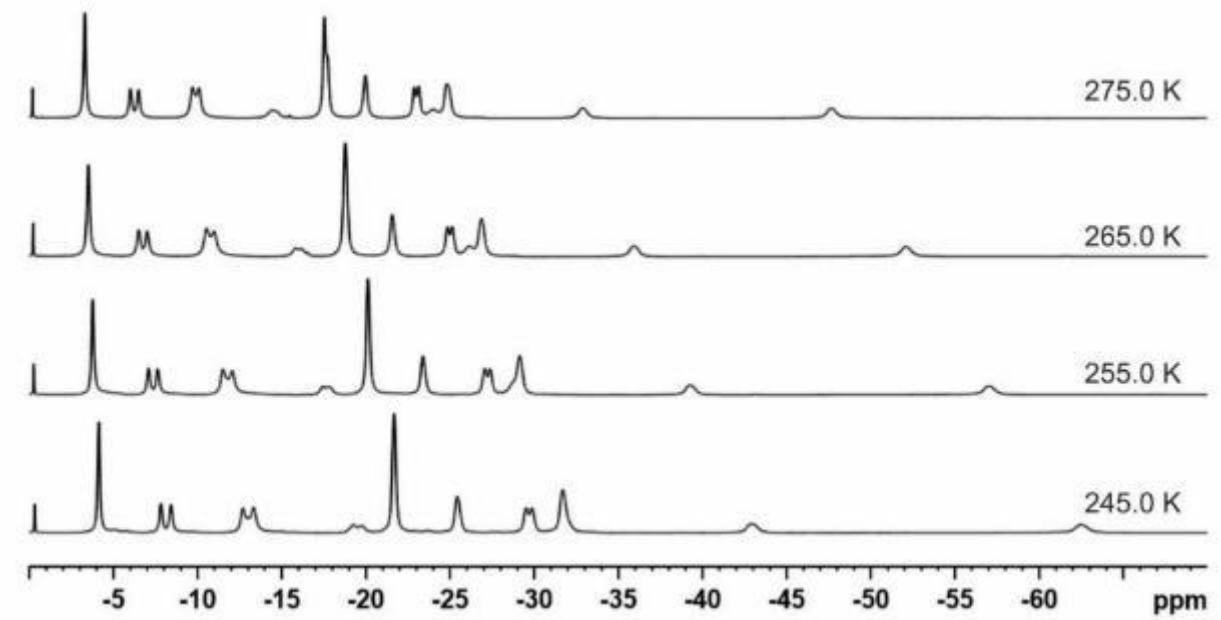

Fig. S197. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -70 ppm.

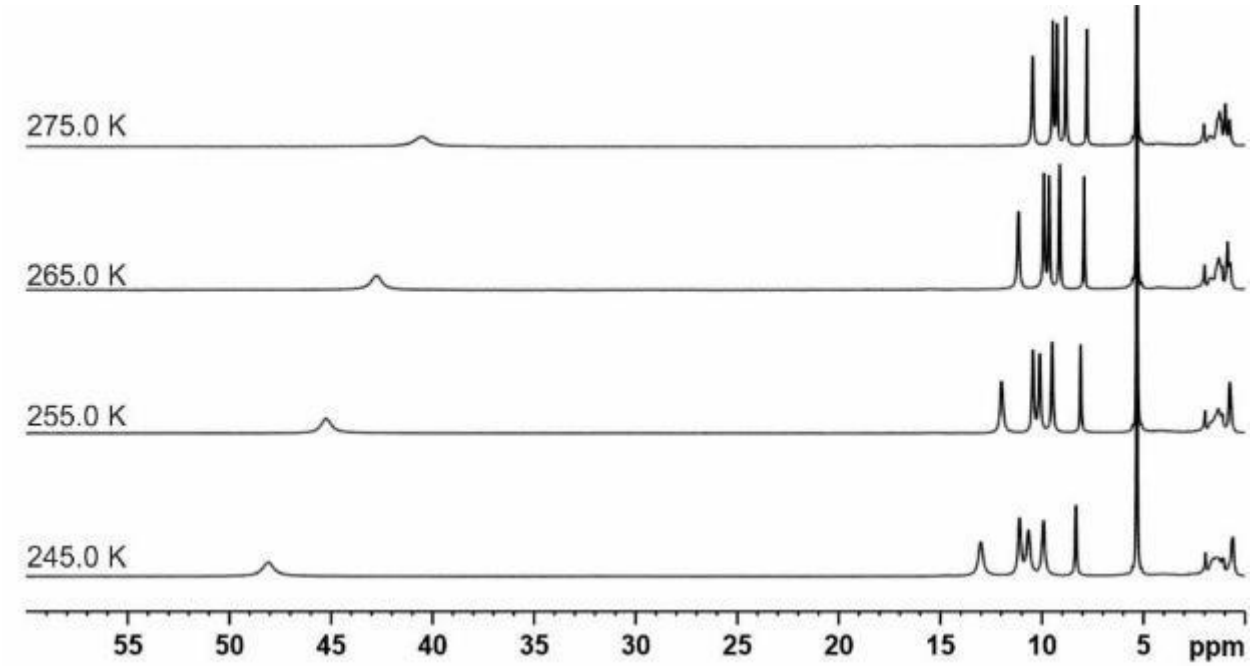

Fig. S198. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +60 ppm to 0 ppm.

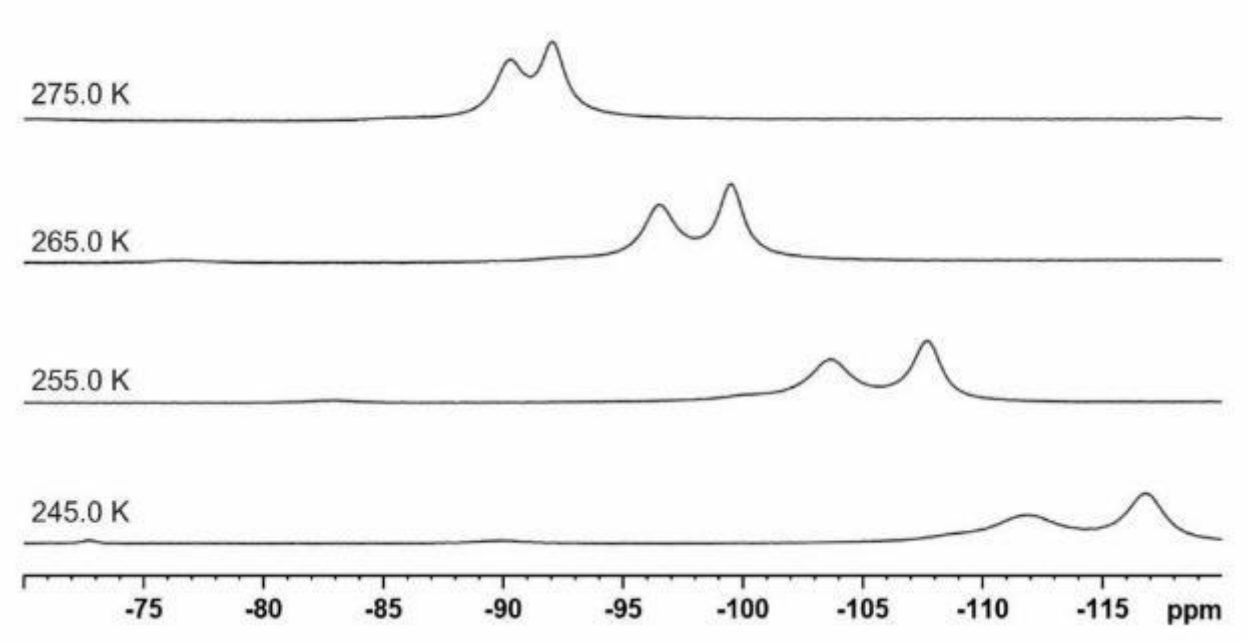

Fig. S199. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -70 ppm to -120 ppm.

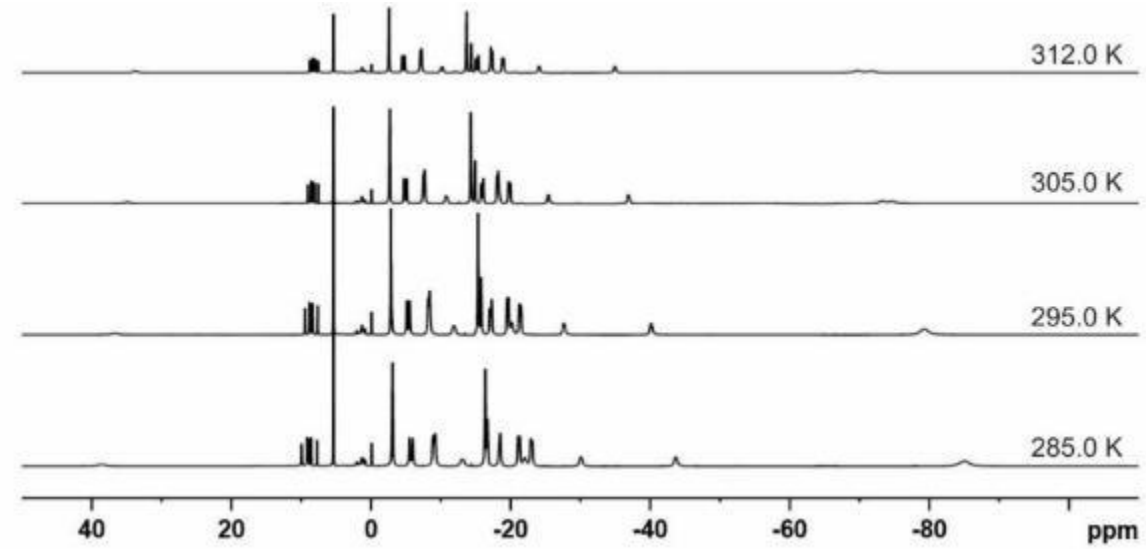

Fig. S200. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

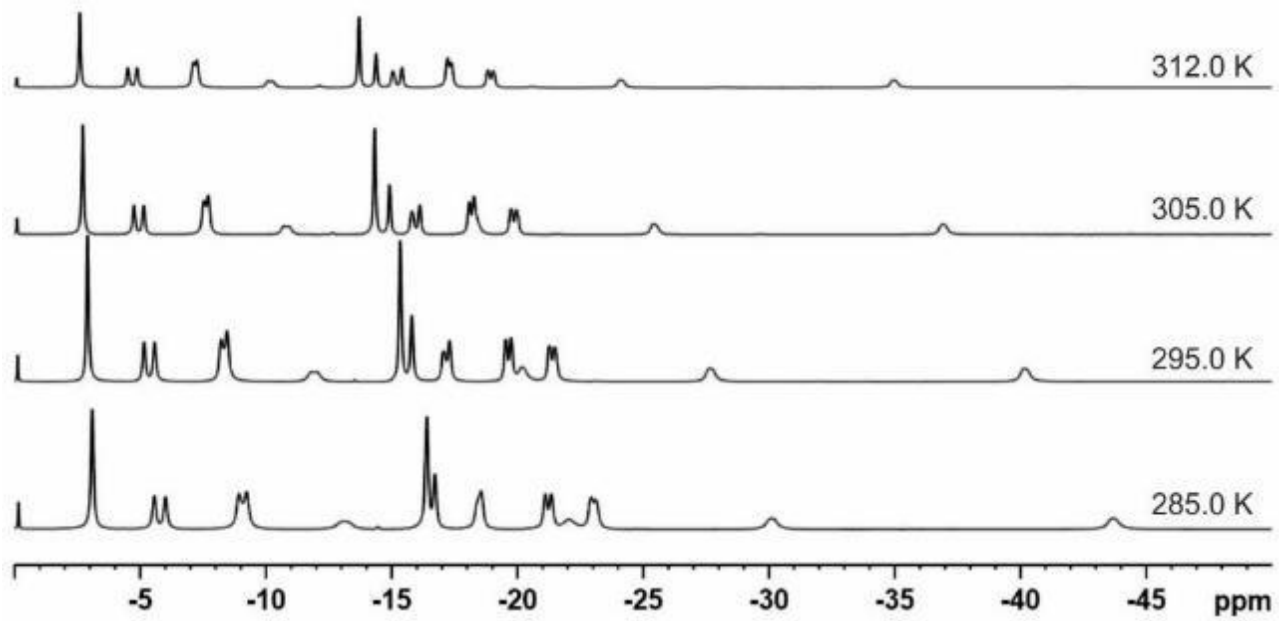

Fig. S201. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -50 ppm.

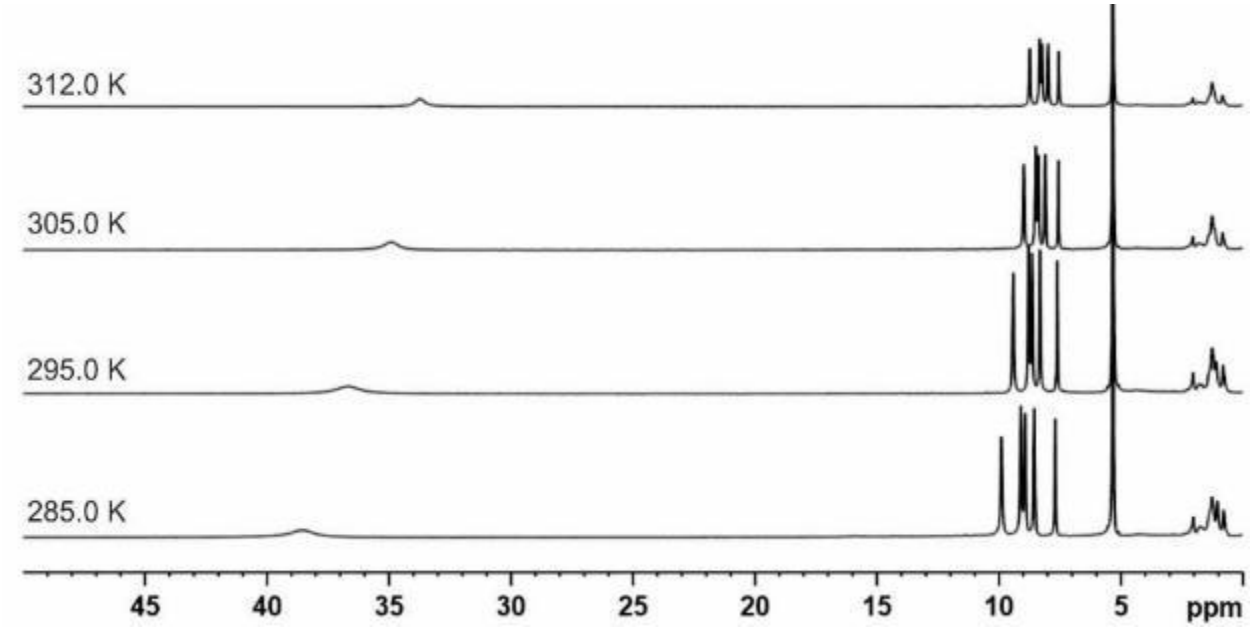

Fig. S202. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +50 ppm top 0 ppm.

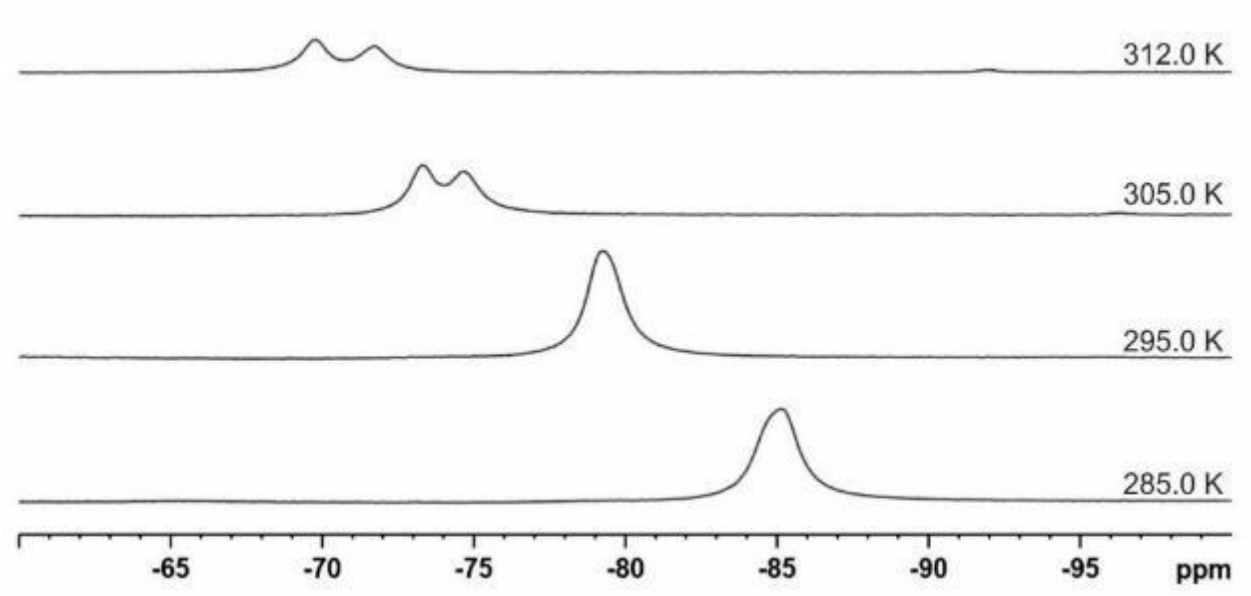

Fig. S203. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{3+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -60 ppm to -100 ppm.

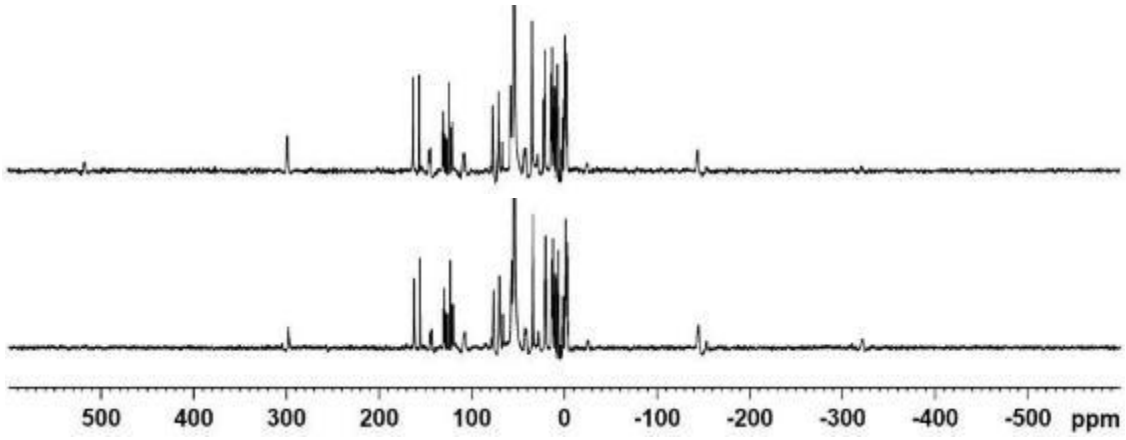

Fig. S204. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Different o1p values were needed in order to see all the signals.

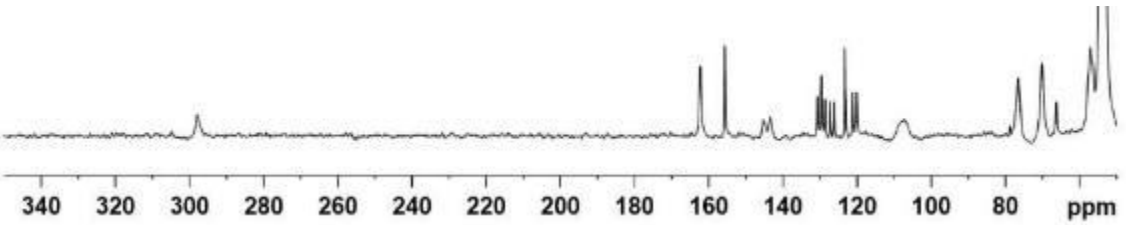

Fig. S205. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +350 ppm to +50 ppm.

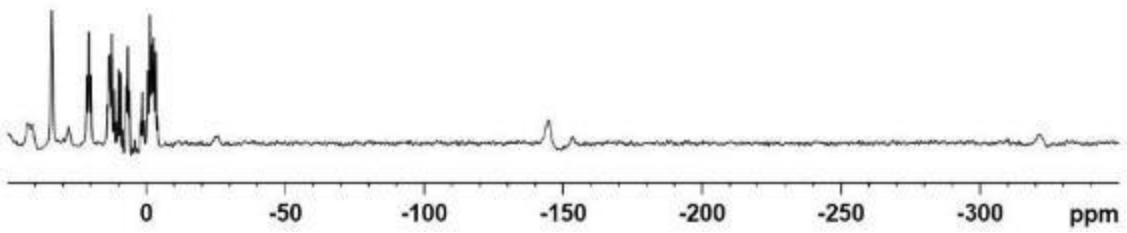

Fig. S206. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -350 ppm.

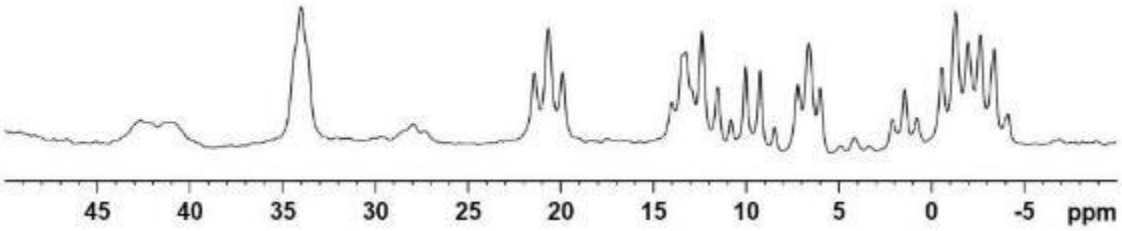

Fig. S207. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -10 ppm.

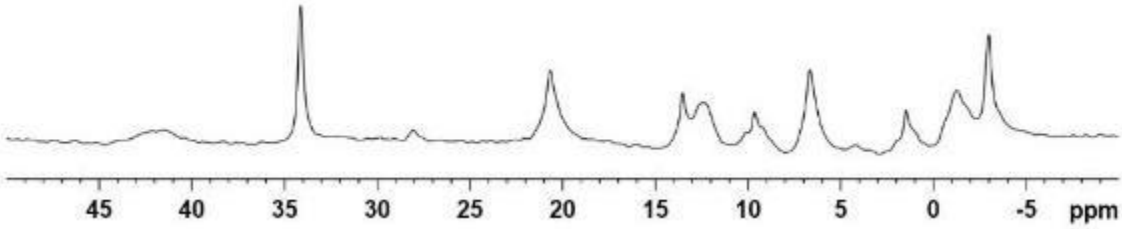

Fig. S208. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{3+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -10 ppm.

Table S25. ^{1}H NMR experimental chemical shifts for **[5]$^{3+}$** in CD_2Cl_2.

	T in K								Calculated@295 K				
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{LFC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm												Integral
1: $CH_{ar}o$	-116.77	-107.77	-99.53	-92.03	-85.15	-79.23	-74.68	-71.73	-56.25	-35.90	7.38[a]	-84.77	2
2: $CH_{ar}i$	-111.73	-103.63	-96.84	-90.28	-85.15	-79.23	-73.32	-69.77	-75.33	-2.99	7.52[a]	-70.80	2
3: $CH_2\alpha i$	-62.50	-57.03	-52.09	-47.65	-43.68	-40.13	-36.89	-34.95	-46.60	-	4.54[a]	-42.06	2
4: $CH_2\alpha o$	-42.89	-39.24	-35.91	-32.88	-30.08	-27.62	-25.39	-24.08	-31.03	-	4.05[a]	-26.98	2
5: $CH_2\beta i$	-31.70	-29.15	-26.88	-24.81	-23.12	-21.49	-19.96	-19.04	-23.05	-	2.26	-20.79	2
6: $CH_2\beta i$	-31.70	-29.15	-26.88	-24.81	-22.94	-21.29	-19.75	-18.83	-23.05	-	2.26	-20.79	2
7: $CH_2\alpha i$	-31.70	-28.82	-26.16	-24.00	-22.06	-20.20	-18.28	-17.38	-28.41	-	4.54[a]	-23.87	2
8: $CH_2\gamma i$	-29.87	-27.38	-25.14	-23.13	-21.35	-19.75	-18.28	-17.38	-21.87	-	2.00	-19.87	2
9: $CH_2\gamma i$	-29.53	-27.07	-24.86	-22.88	-21.12	-19.55	-18.09	-17.23	-21.87	-	2.00	-19.87	2
10: $CH_2\gamma ii$	-25.44	-23.39	-21.58	-19.97	-18.56	-17.31	-16.12	-15.41	-17.81	-	2.00	-15.81	2
11: $CH_2\beta ii$	-25.44	-23.39	-21.58	-19.79	-18.56	-17.08	-15.81	-10.06	-18.05	-	2.35	-15.70	2
12: CH_3ii	-21.68	-20.13	-18.78	-17.54	-16.72	-15.81	-14.93	-14.39	-14.56	-	1.44	-13.12	3
13: CH_3i	-21.68	-20.13	-18.78	-17.53	-16.40	-15.35	-14.33	-13.71	-14.61	-	1.39	-13.22	6
14: $CH_2\alpha ii$	-19.51	-17.60	-16.00	-14.52	-13.14	-11.93	-10.83	-10.19	4.86	-	-14.75	-9.89	2
15: $CH_2\alpha o$	-13.34	-12.06	-10.99	-10.08	-9.23	-8.46	-7.71	-7.26	-8.87	-	3.91[b]	-4.96	2
16: $CH_2\beta o$	-13.34	-12.06	-10.99	-10.08	-9.23	-8.46	-7.71	-7.26	-10.10	-	1.89	-8.21	2
17: $CH_2\beta o$	-12.70	-11.51	-10.54	-9.71	-8.94	-8.23	-7.54	-7.13	-10.10	-	1.89	-8.21	2
18: $CH_2\gamma o$	-8.42	-7.64	-7.01	-6.49	-6.02	-5.58	-5.15	-4.89	-10.04	-	1.57	-8.47	2
19: $CH_2\gamma o$	-7.82	-7.09	-6.50	-6.02	-5.57	-5.16	-4.76	-4.52	-10.04	-	1.57	-8.47	2
20: CH_3o	-4.13	-3.77	-3.51	-3.30	-3.10	-2.92	-2.73	-2.61	-6.12	-	0.99	-5.13	6
21: $CH_{ar}ii$	48.08	45.23	42.75	40.50	38.56	36.67	34.91	33.73	32.42	-1.20	6.98[a]	38.20	1

[a]The δ_{orb} values of **[5]^0** were used. [b]The δ_{orb} values of **[5]$^{4+}$** were used.

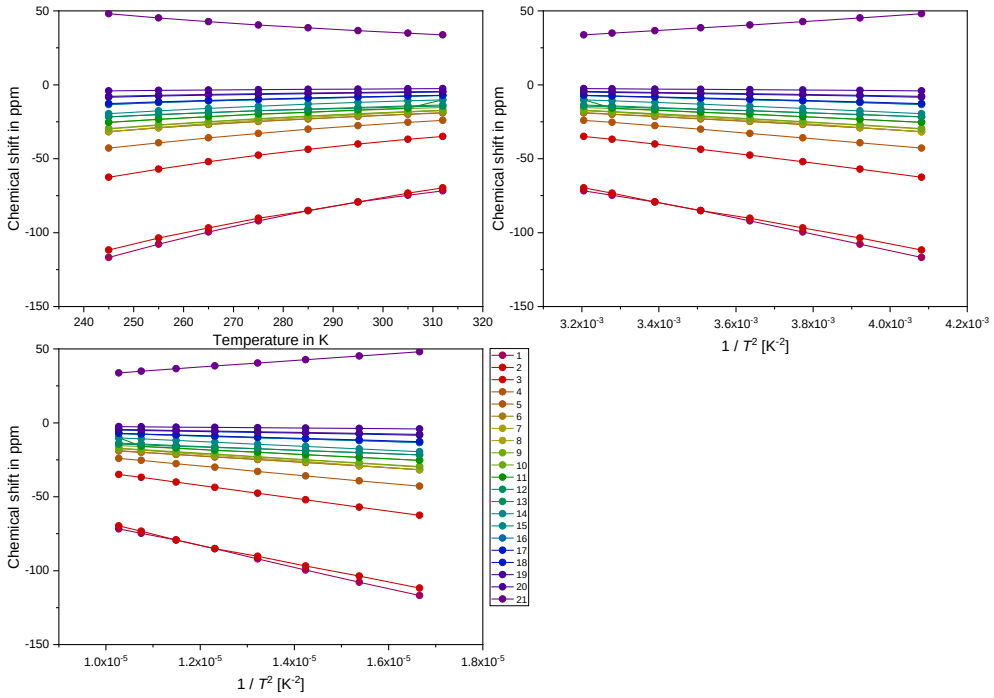

Fig. S209. Plot of the ^{1}H chemical shifts of **[5]$^{3+}$** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S26. ^{13}C NMR chemical shifts of **[5]$^{3+}$** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-321.4	s
2	-153.1	s / impurity
3	-144.3	s
4	-2.9	q
5	-1.2	t
6	1.5	t
7	6.7	q
8	9.7	q
9	12.4	t
10	13.4	t
11	20.8	t
12	34.1	t
13	41.9	d
14	57.1	t?
15	66.2	s
16	70.2	s
17	76.6	s
18	107.6	s
19	144.3	d
20	155.8	s
21	162.4	s
22	298	s
23	516.1	s

3.14. Complex **[5]$^{4+}$**

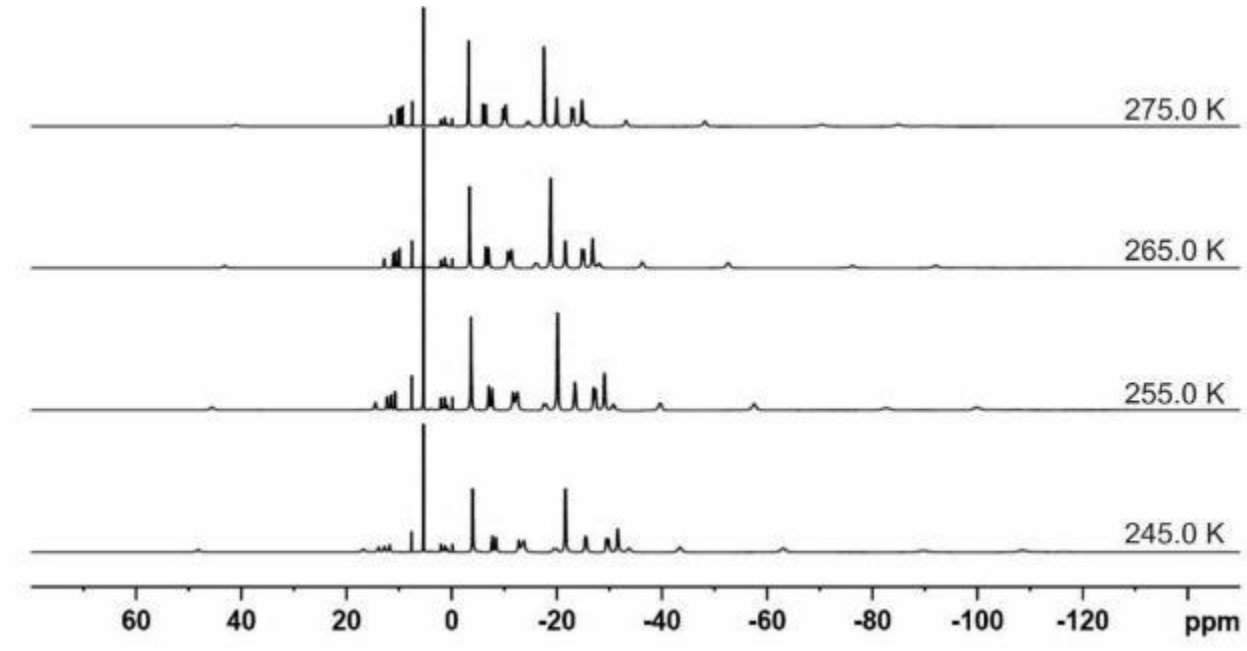

Fig. S210. Variable-temperature ^1H NMR spectra of complex **[5]$^{4+}$** recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K.

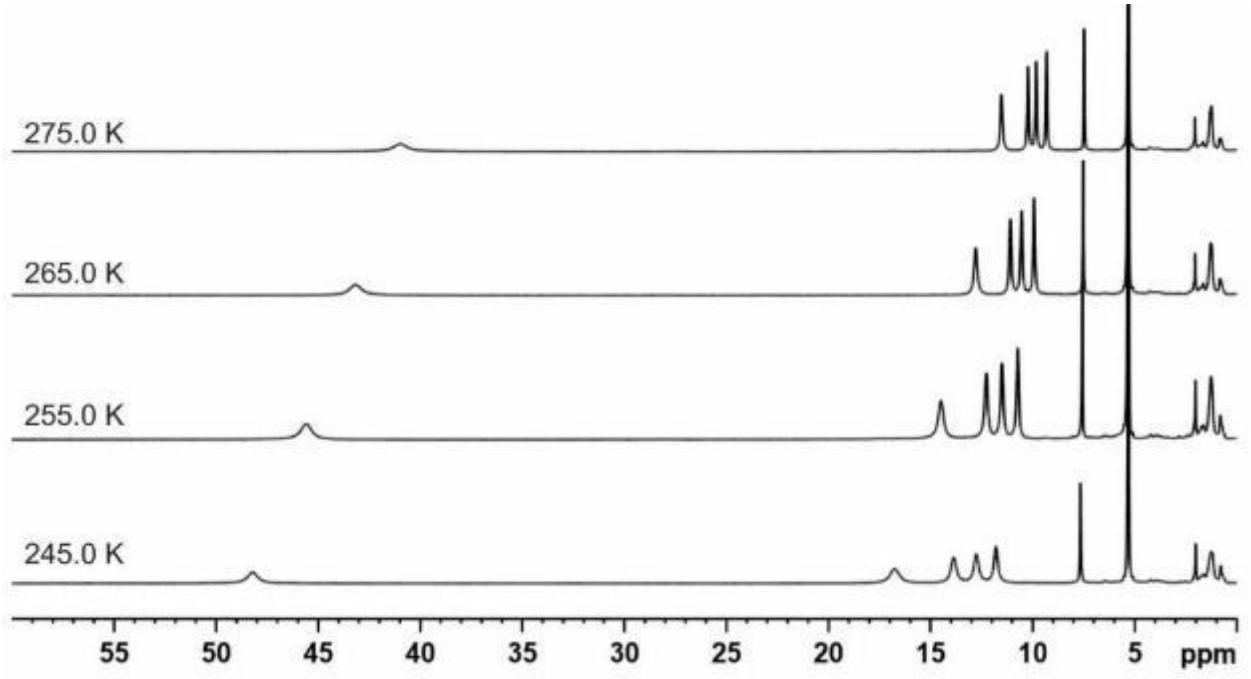

Fig. S211. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from +60 ppm to 0 ppm.

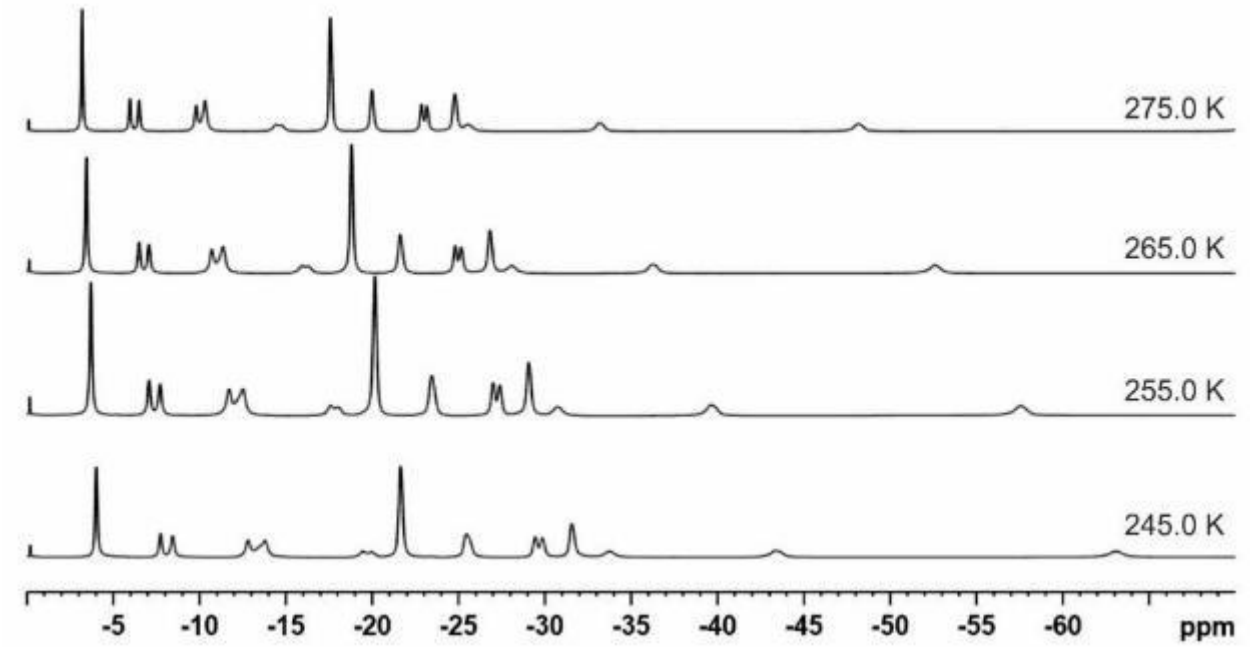

Fig. S212. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from 0 ppm to -70 ppm.

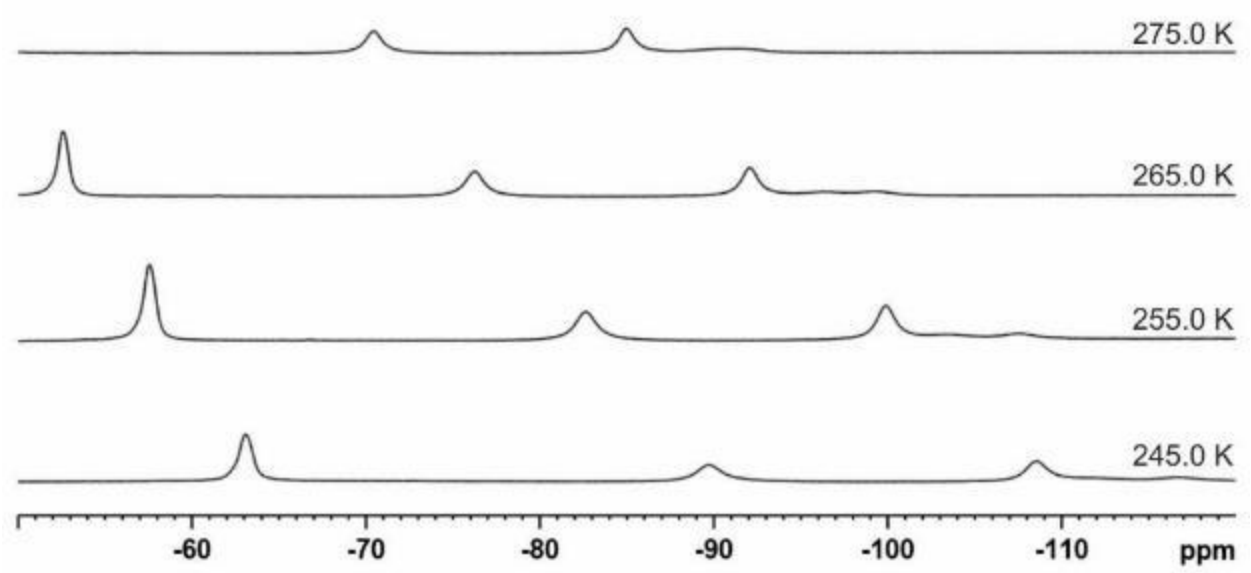

Fig. S213. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 245.0 K to 275.0 K. Expansion from -50 ppm to -120 ppm.

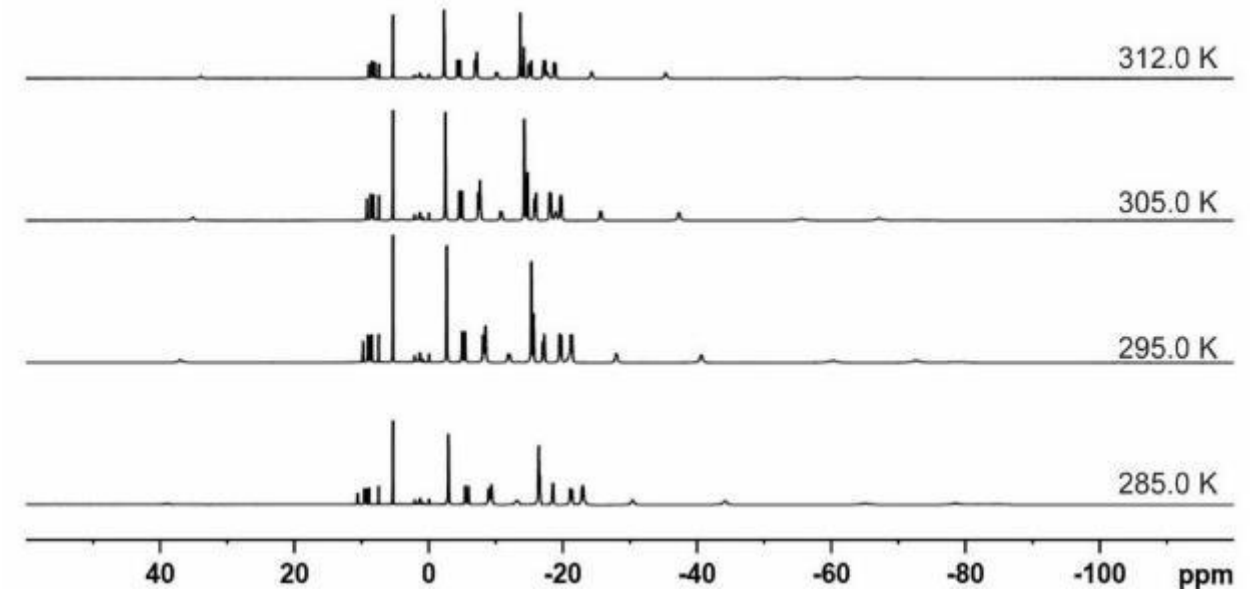

Fig. S214. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K.

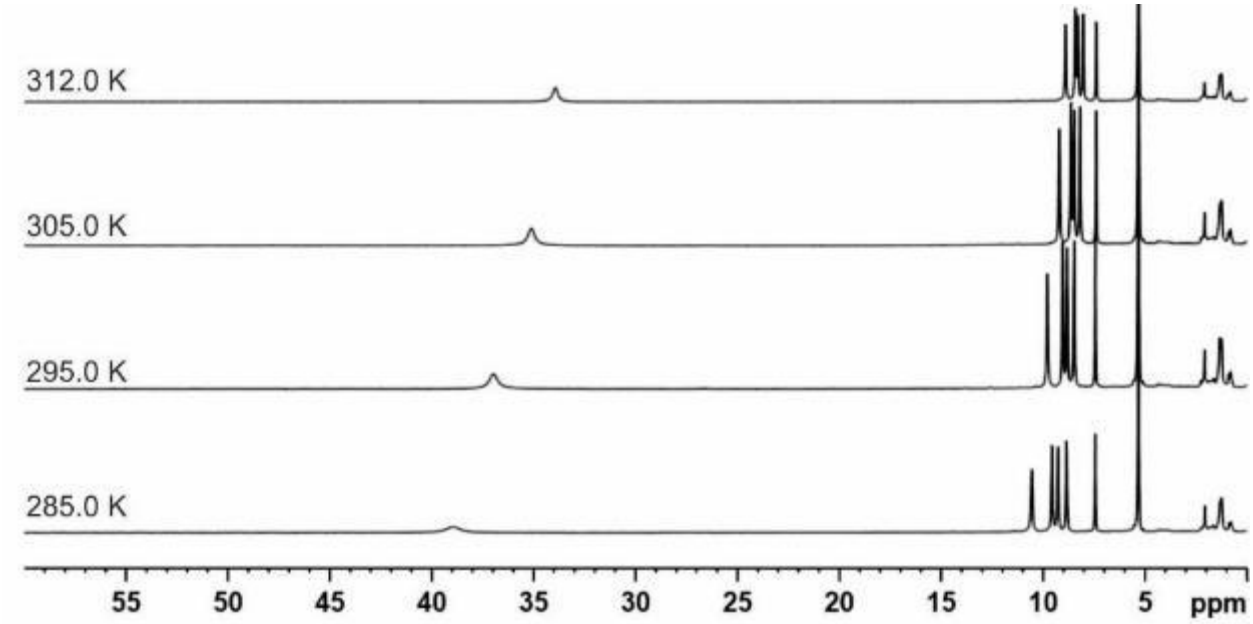

Fig. S215. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from +60 ppm to 0 ppm.

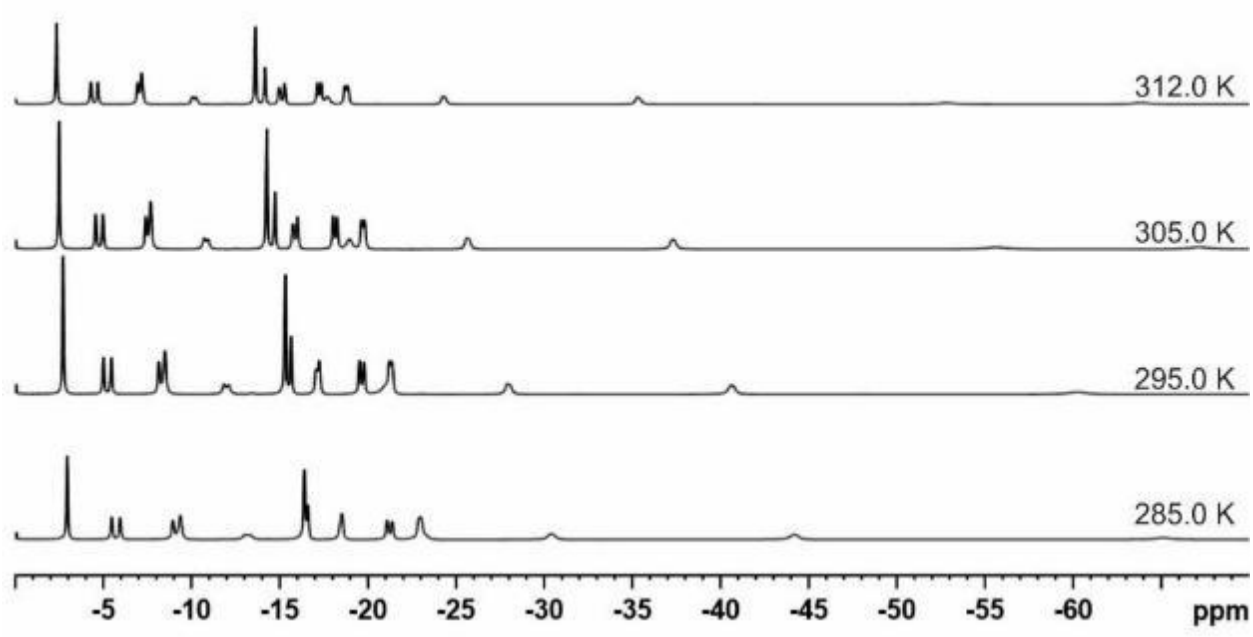

Fig. S216. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from 0 ppm to -70 ppm.

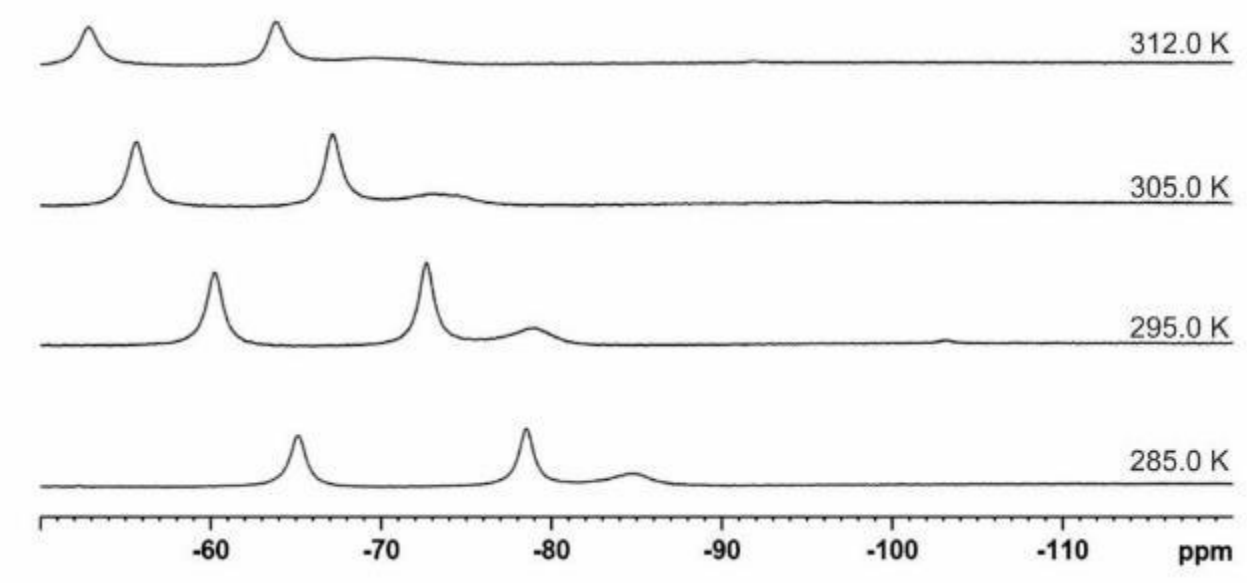

Fig. S217. Variable-temperature ^{1}H NMR spectra of complex **[5]**$^{4+}$ recorded in CD_2Cl_2, in the temperature range from 285.0 K to 312.0 K. Expansion from -50 ppm to -120 ppm.

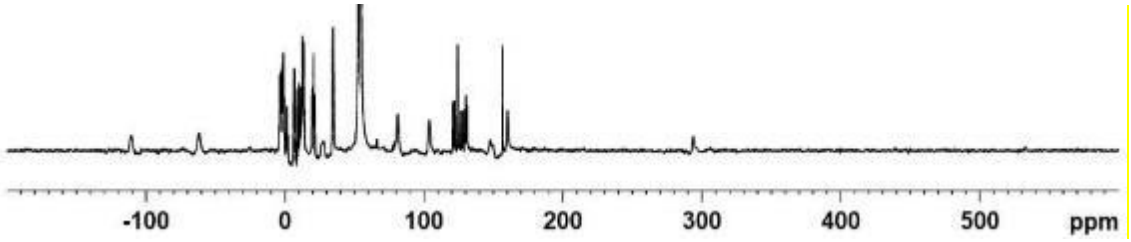

Fig. S218. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K.

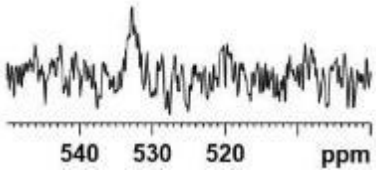

Fig. S219. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +550 ppm to +500 ppm.

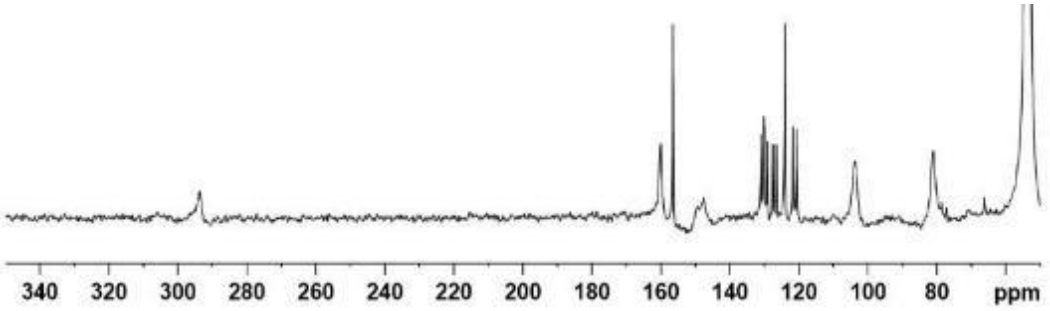

Fig. S220. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +350 ppm to +50 ppm.

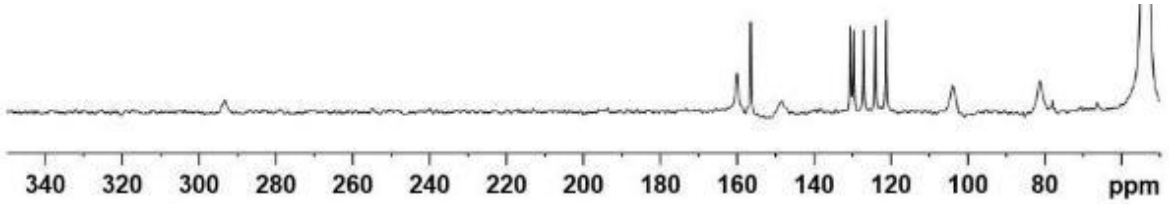

Fig. S221. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +350 ppm to +50 ppm.

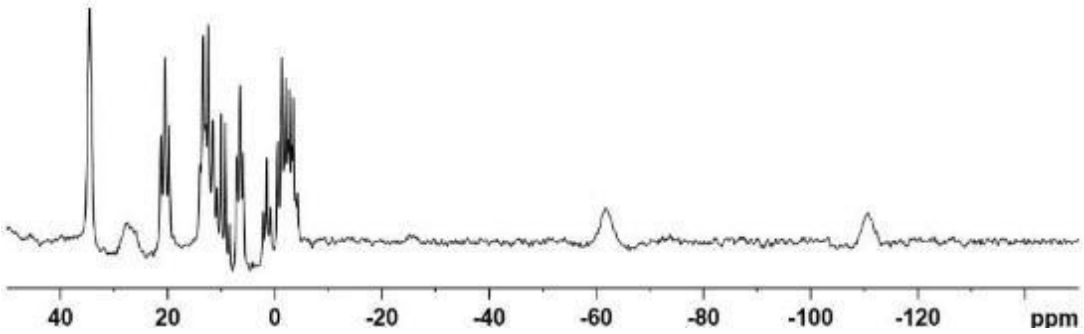

Fig. S222. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -200 ppm.

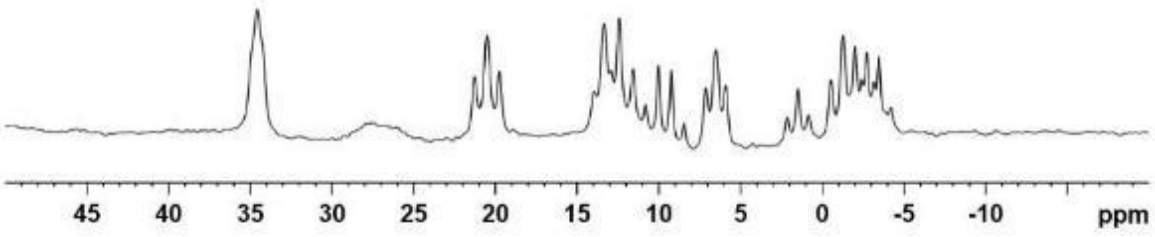

Fig. S223. ^{13}C NMR spectrum (^{1}H coupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -20 ppm.

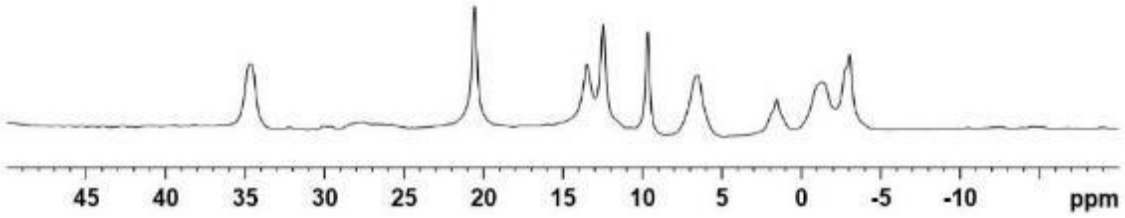

Fig. S224. ^{13}C NMR spectrum (^{1}H decoupled) of complex **[5]**$^{4+}$ in CD_2Cl_2, recorded at 295.0 K. Expansion from +50 ppm to -20 ppm.

Table S27. ^{1}H NMR experimental chemical shifts for **[5]$^{4+}$** in CD_2Cl_2.

	T in K								Calculated@295 K			
	245	255	265	275	285	295	305	312	δ_{MPC}	δ_{orb}	δ_{calcd}	
Assignment	Chemical shift in ppm											Integral
Impurity*	-114.29	-105.64	-97.77	-90.94	-84.65	-79.22	-73.19	-69.91	-	-	-	-
1: CH_{ar}i	-108.55	-99.92	-92.03	-84.99	-78.55	-72.80	-67.17	-63.88	-76.00	7.52[a]	-68.48	2
2: CH_{ar}o	-89.68	-82.66	-76.27	-70.45	-65.16	-60.37	-55.63	-52.87	-54.81	7.38[a]	-47.43	2
3: CH_2αi	-63.09	-57.57	-52.59	-48.17	-44.18	-40.72	-37.32	-35.31	-46.80	4.54[a]	-42.26	2
4: CH_2αo	-43.38	-39.63	-36.23	-33.16	-30.38	-27.97	-25.66	-24.26	-30.13	4.05	-26.08	2
5: CH_2βi	-33.76	-30.77	-28.07	-25.58	-23.00	-21.39	-19.81	-18.87	-23.11	2.22	-20.89	2
6: CH_2βi	-31.58	-29.08	-26.83	-24.81	-22.92	-21.27	-19.67	-18.72	-23.11	2.22	-20.89	2
7: CH_2αi	-31.58	-29.08	-26.83	-24.72	-23.21	-20.99	-18.97	-17.72	-28.65	4.54[a]	-24.11	2
8: CH_2γi	-29.87	-27.40	-25.17	-23.18	-21.39	-19.81	-18.27	-17.36	-21.90	1.90	-20.00	2
9: CH_2γi	-29.45	-27.02	-24.82	-22.87	-21.11	-19.56	-18.05	-17.16	-21.90	1.90	-20.00	2
10: CH_2γii	-25.56	-23.46	-21.64	-20.00	-18.54	-17.27	-16.03	-15.29	-17.84	1.99	-15.85	2
11: CH_2βii	-25.47	-23.46	-21.64	-20.00	-18.43	-17.12	-15.76	-14.98	-18.08	2.32	-15.76	2
12: CH_3ii	-21.66	-20.16	-18.82	-17.67	-16.61	-15.67	-14.74	-14.18	-14.57	1.41	-13.16	3
13: CH_3i	-21.66	-20.16	-18.82	-17.59	-16.41	-15.35	-14.28	-13.64	-14.57	1.35	-13.22	6
14: CH_2αo	-17.81	-16.12	-14.59	-13.20	-11.99	-10.84	-10.17	-17.81	-7.86	3.91	-3.95	2
15: CH_2βo	-13.80	-12.52	-11.37	-10.33	-9.38	-8.53	-7.69	-7.19	-9.50	1.80	-7.70	2
16: CH_2αii	-13.46	-12.25	-11.23	-10.24	-9.38	-8.53	-7.69	-7.19	-14.52	4.53[a]	-9.99	2
17: CH_2βo	-12.82	-11.72	-10.73	-9.81	-8.96	-8.19	-7.42	-6.96	-9.50	1.80	-7.70	2
18: CH_2γo	-8.45	-7.72	-7.09	-6.51	-5.97	-5.48	-4.99	-4.69	-9.50	1.49	-8.01	2
19: CH_2γo	-7.75	-7.09	-6.51	-5.98	-5.48	-5.03	-4.58	-4.31	-9.50	1.49	-8.01	2
20: CH_3o	-4.03	-3.72	-3.45	-3.21	-2.96	-2.74	-2.50	-2.36	-5.73	0.97	-4.76	6
21: CH_{ar}ii	48.20	45.57	43.18	40.97	38.93	37.07	35.11	33.92	32.28	6.98[a]	39.26	1

[a]The δ_{orb} values of **[5]^0** were used.

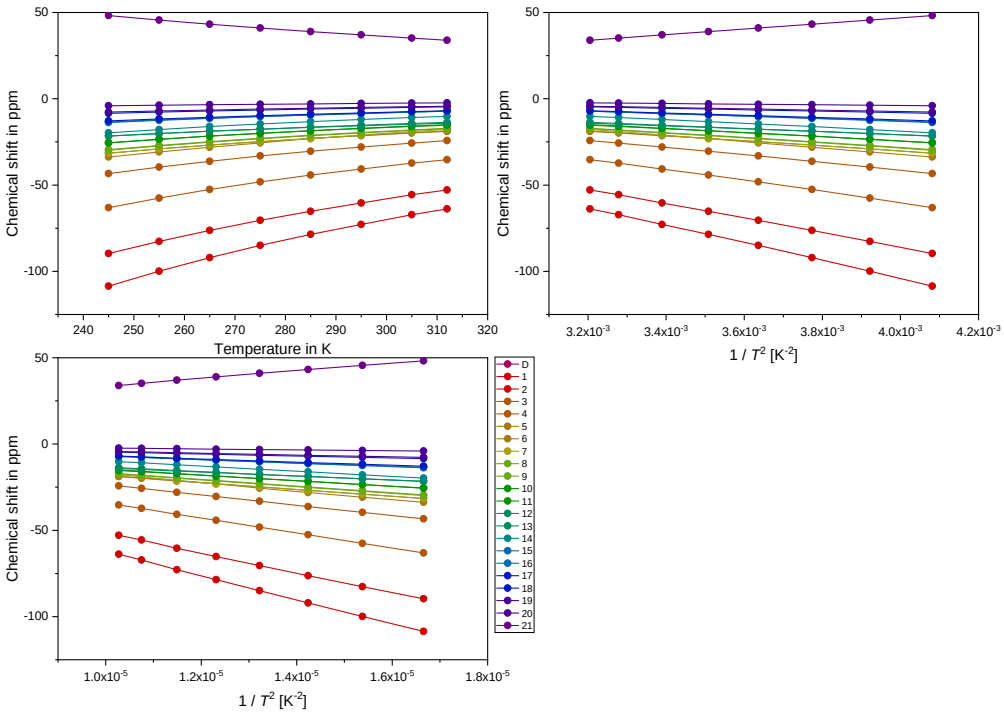

Fig. S225. Plot of the ^{1}H chemical shifts of **[5]$^{4+}$** in CD_2Cl_2 at various temperatures. Assignments are given in the previous table.

Table S28. ^{13}C NMR chemical shifts of **[5]$^{4+}$** observed at 295.0 K in CD_2Cl_2.

Signal Nr.:	Chemical Shift [ppm]:	Shape:
1	-110.5	s
2	-61.6	s
3	-3.1	q
4	-2.7	q
5	-1.8	t
6	1.6	t
8	6.5	t
9	9.7	q
10	12.5	t
11	13.4	t
12	20.6	t
13	27.1	d ?
14	34.7	t
18	81.2	s
19	103.8	s
20	148.7	d
21	156.6	s
22	160.1	s
23	293.9	s
24	532.8	s

3.15. Diamagnetic contributions to the ^{1}H chemical shifts

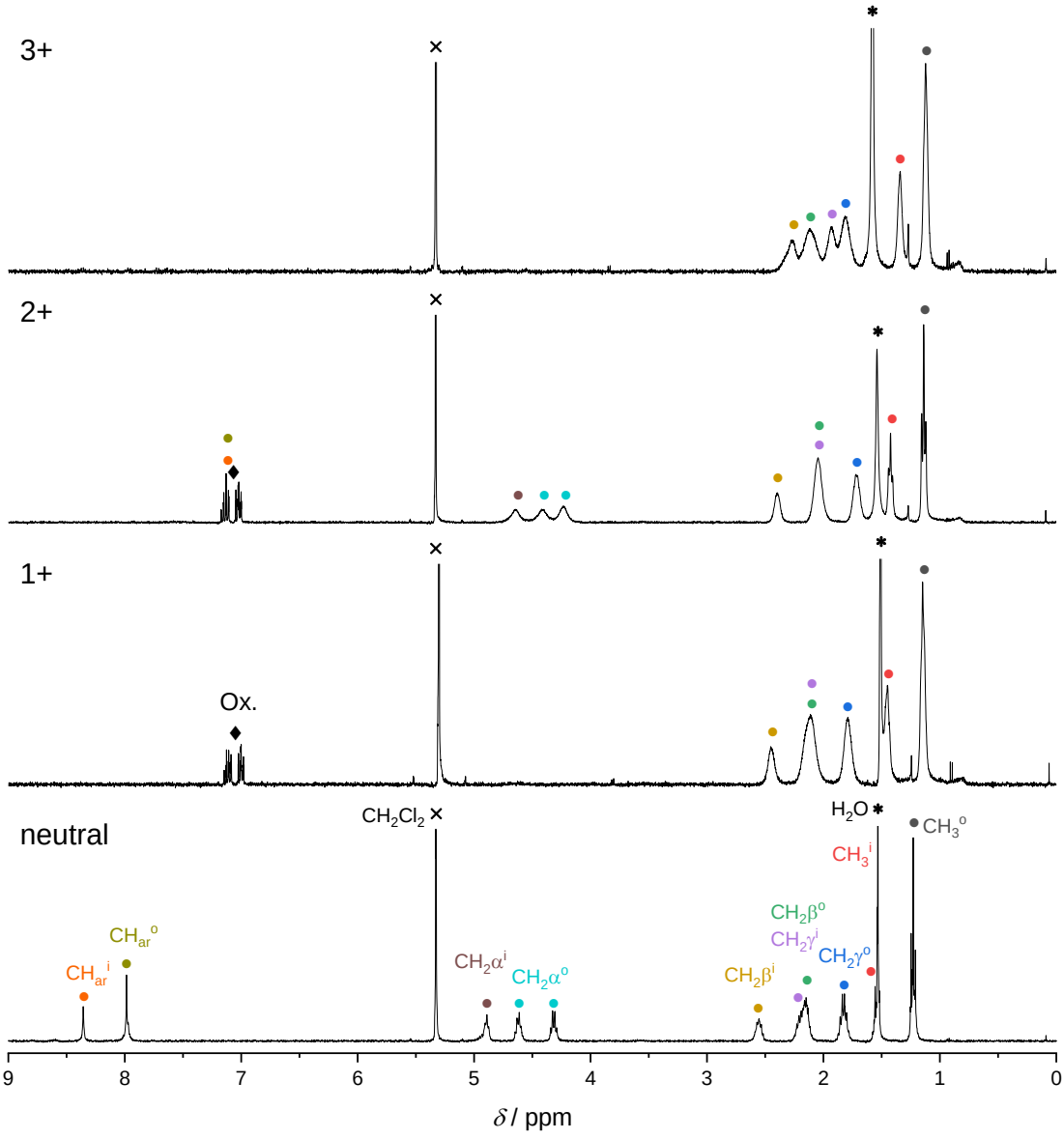

Fig. S226. ^{1}H NMR for Y(III) analogues of **[3]** series in CD_2Cl_2 and at room temperature (ca. 24 °C). Multiplet singnals around 7 ppm are attributed to the neutral form of phenoxathiin (Ox.).

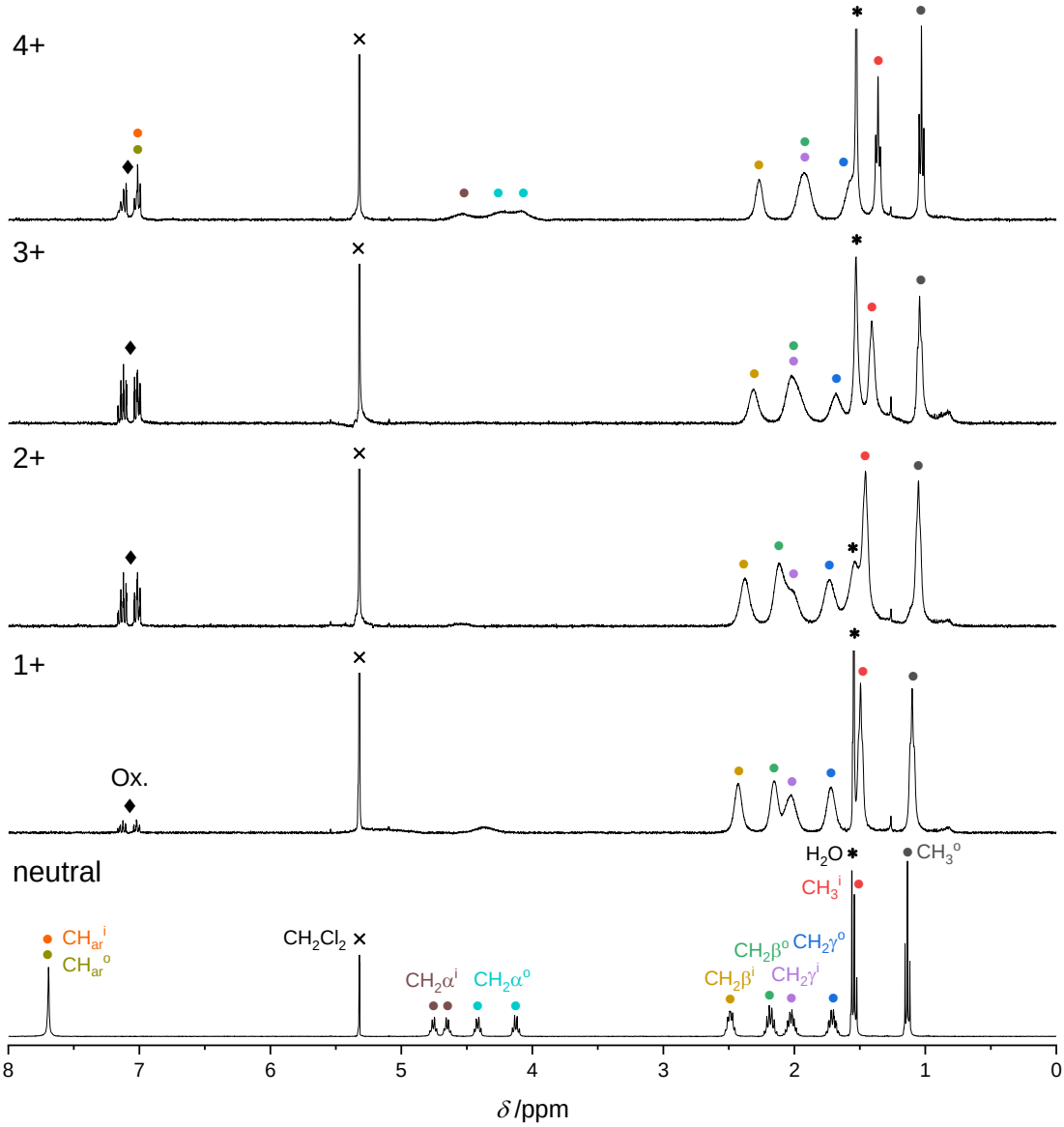

Fig. S227. ^{1}H NMR for Y(III) analogues of **[4]** series in CD_2Cl_2 and at room temperature (ca. 24 °C). Multiplet signals around 7 ppm are attributed to neutral form of phenoxathiin (Ox.).

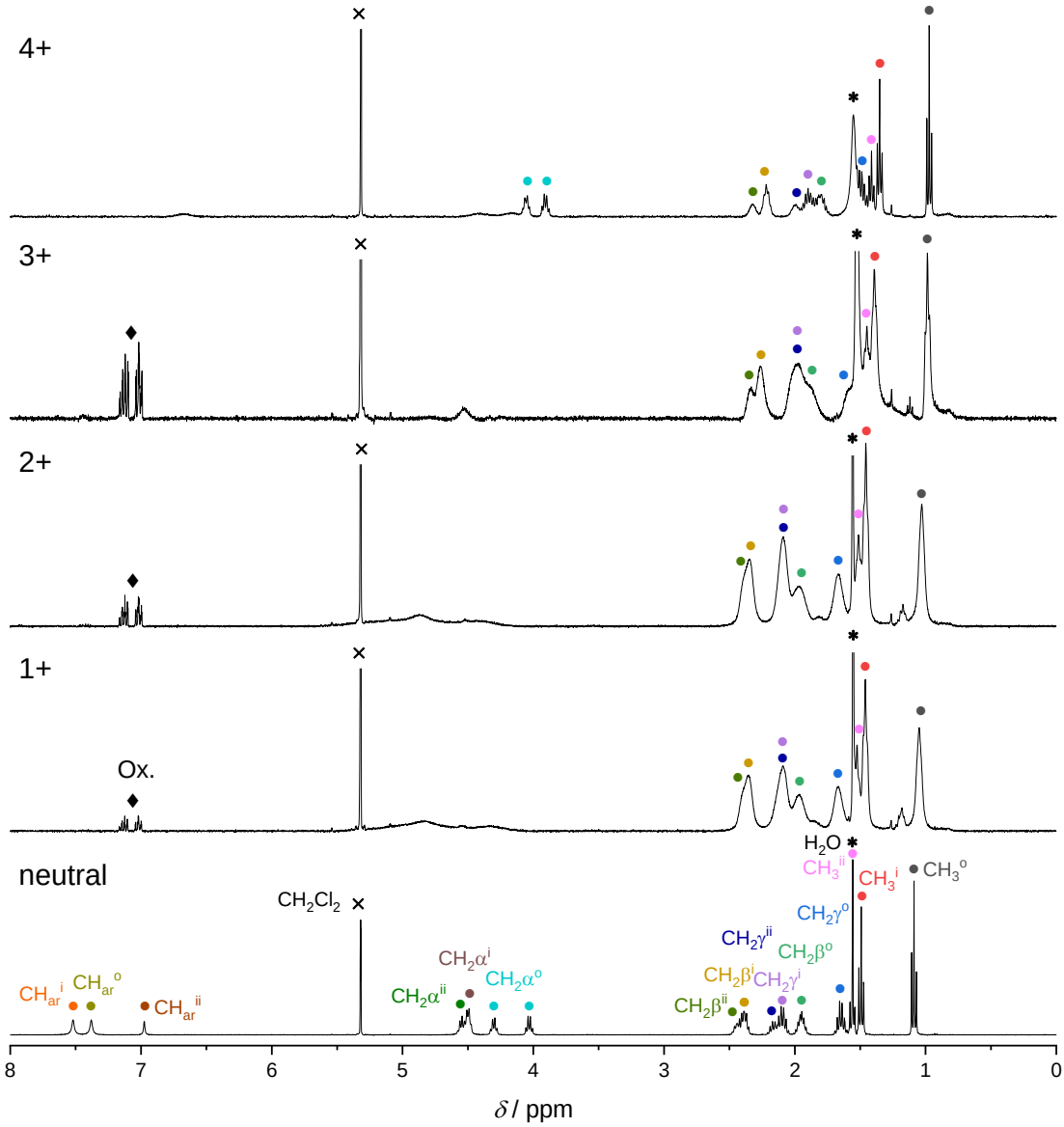

Fig. S228. ^{1}H NMR for Y(III) analogues of **[5]** series in CD_2Cl_2 and at room temperature (ca. 24 °C). Multiplet signals around 7 ppm are attributed to neutral form of phenoxathiin (Ox.).

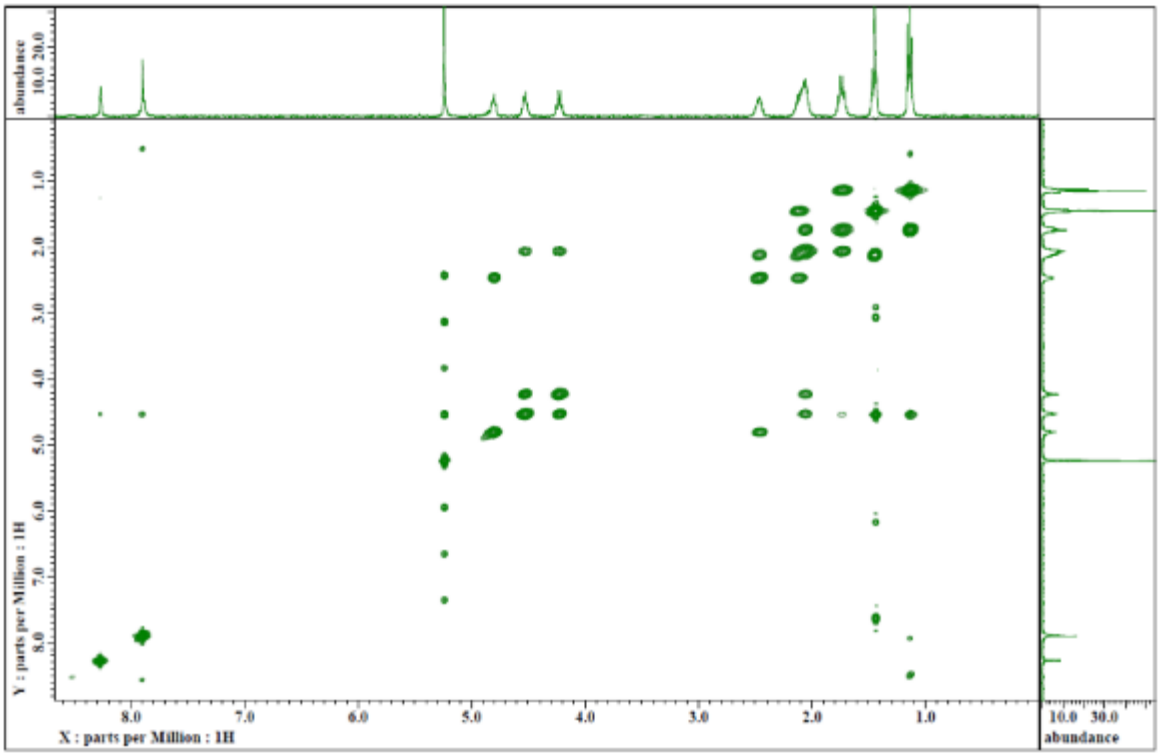

Fig. S229. ^{1}H-^{1}H COSY spectrum of complex **[3]^{0}** in CD_2Cl_2 and at room temperature (ca. 24 °C).

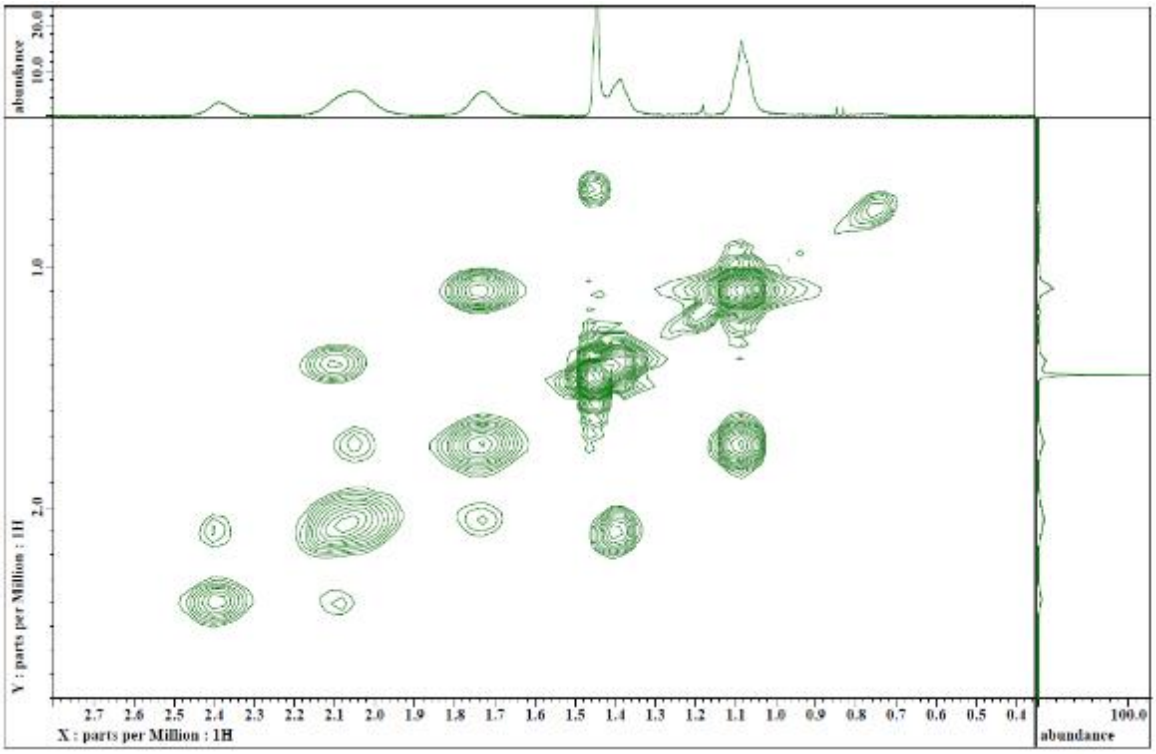

Fig. S230. ^{1}H-^{1}H COSY spectrum of complex **[3]$^{+}$** in CD_2Cl_2 and at room temperature (ca. 24 °C).

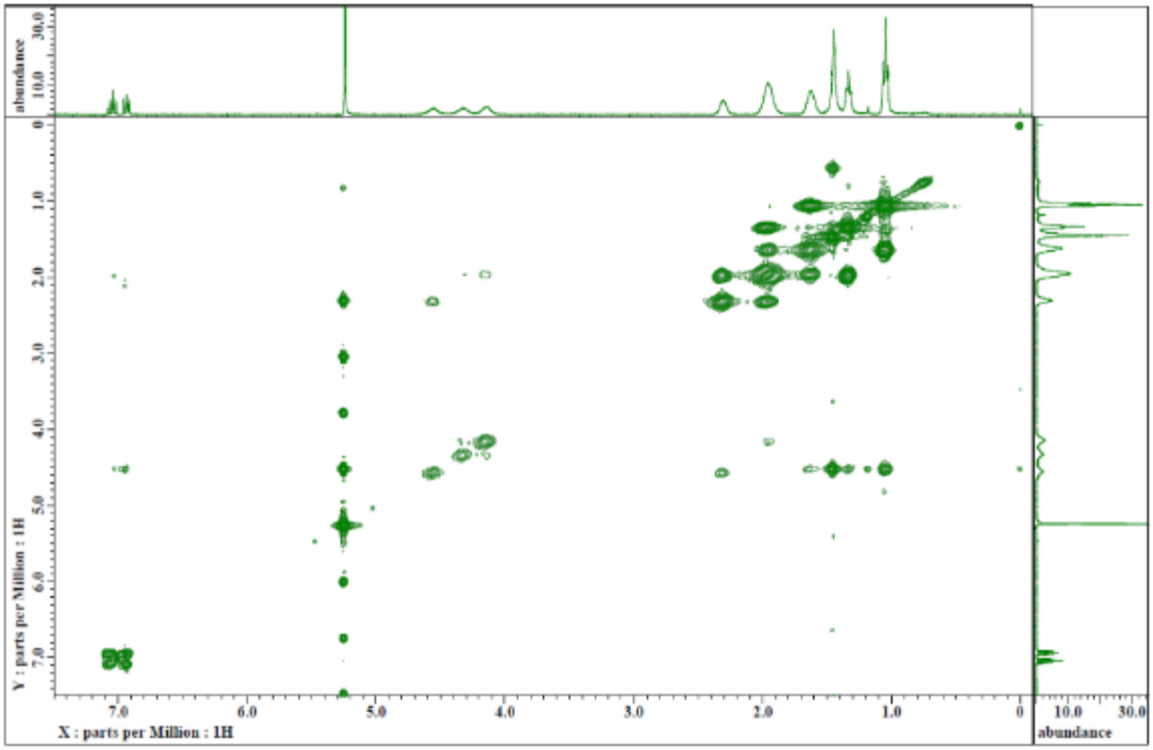

Fig. S231. ^{1}H-^{1}H COSY spectrum of complex **[3]**$^{2+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

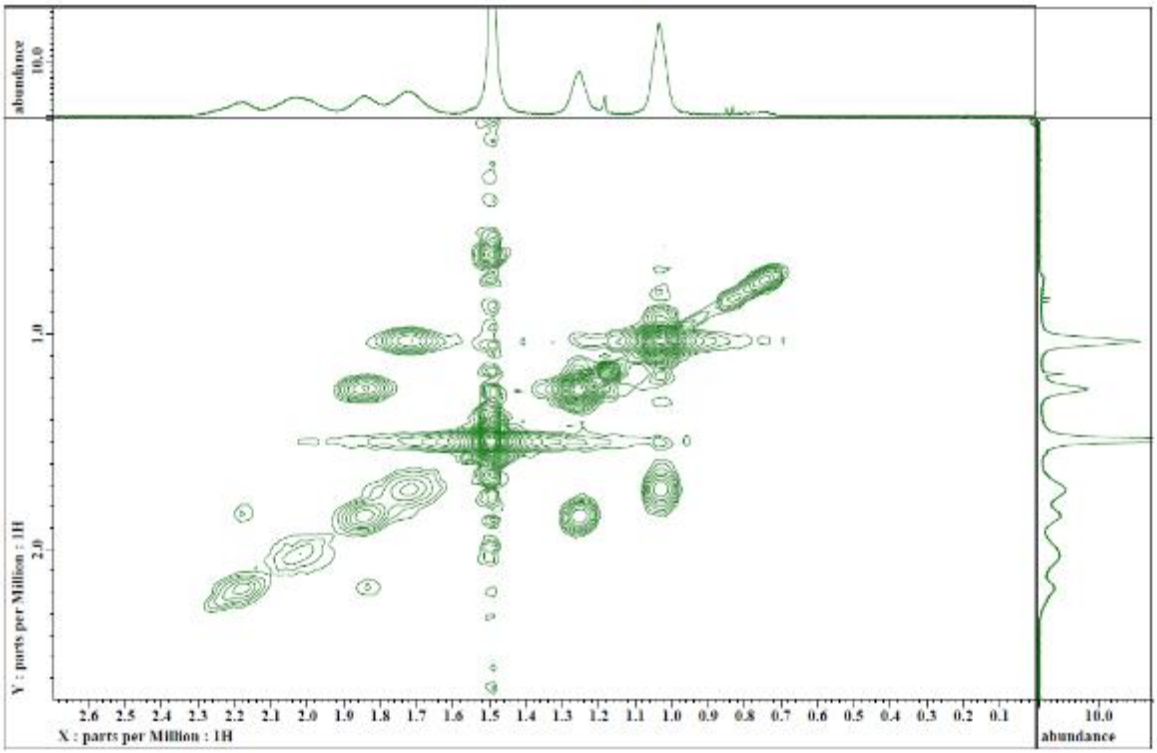

Fig. S232. ^{1}H-^{1}H COSY spectrum of complex **[3]**$^{3+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

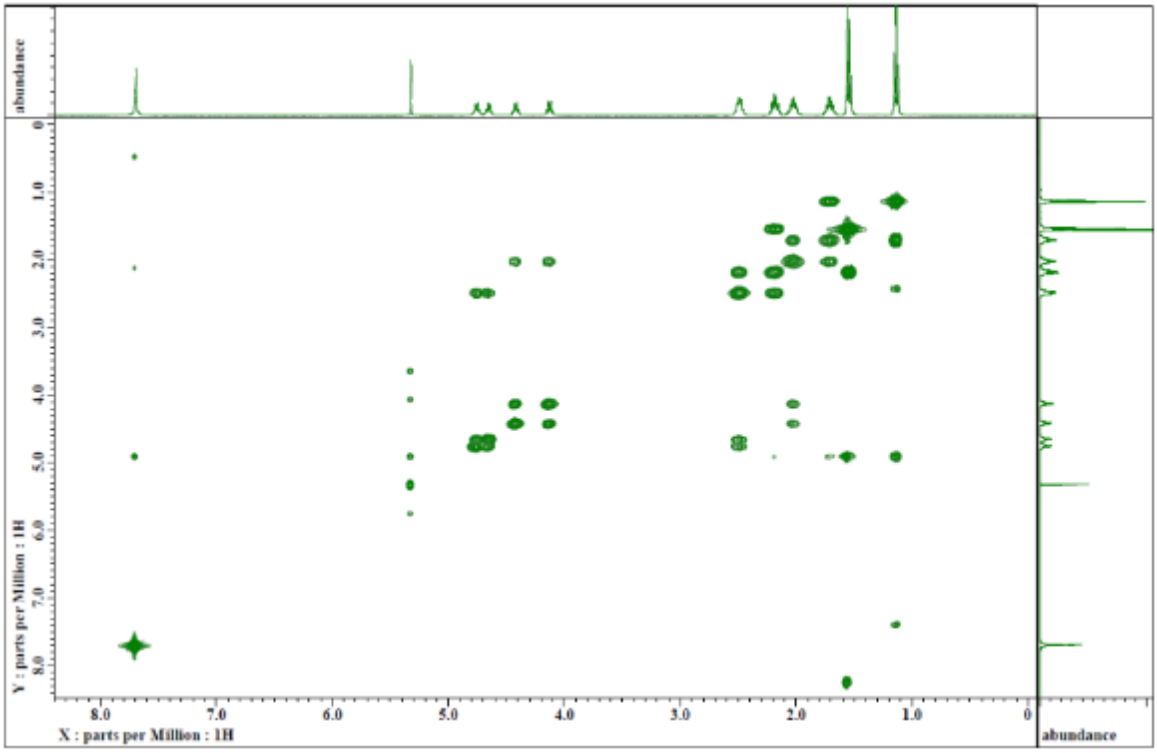

Fig. S233. ^{1}H-^{1}H COSY spectrum of complex **[4]^{0}** in CD_2Cl_2 and at room temperature (ca. 24 °C).

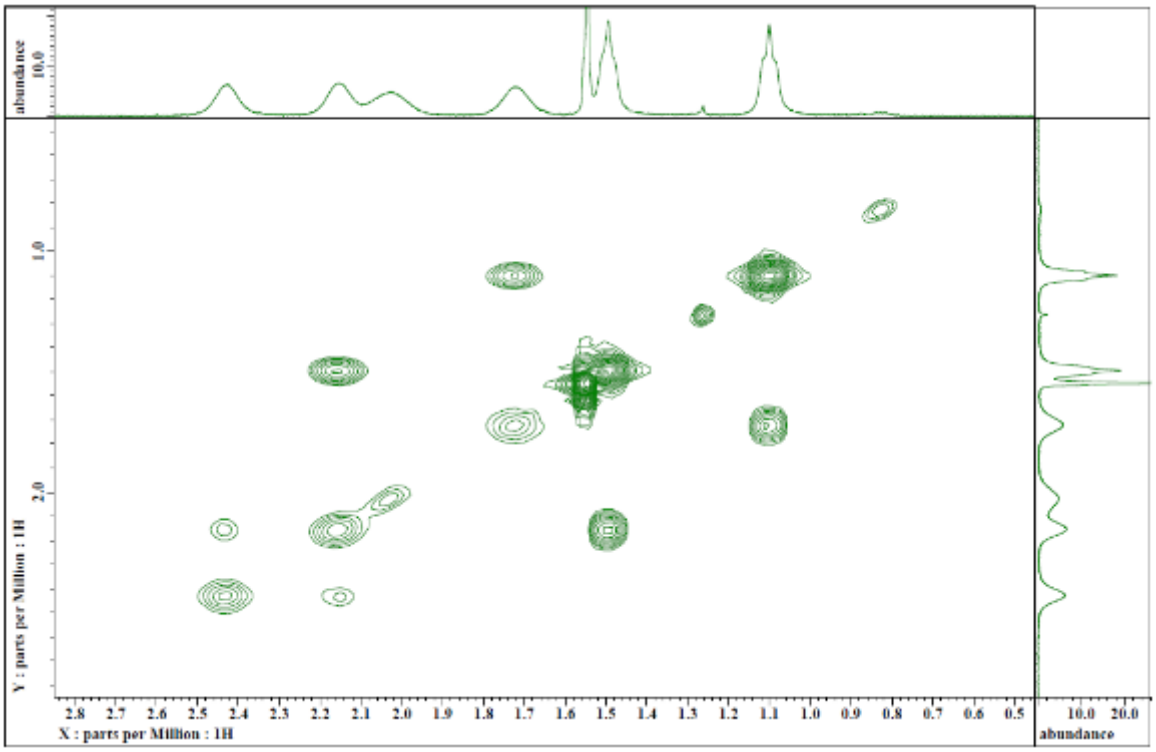

Fig. S234. ^{1}H-^{1}H COSY spectrum of complex **[4]$^{+}$** in CD_2Cl_2 and at room temperature (ca. 24 °C).

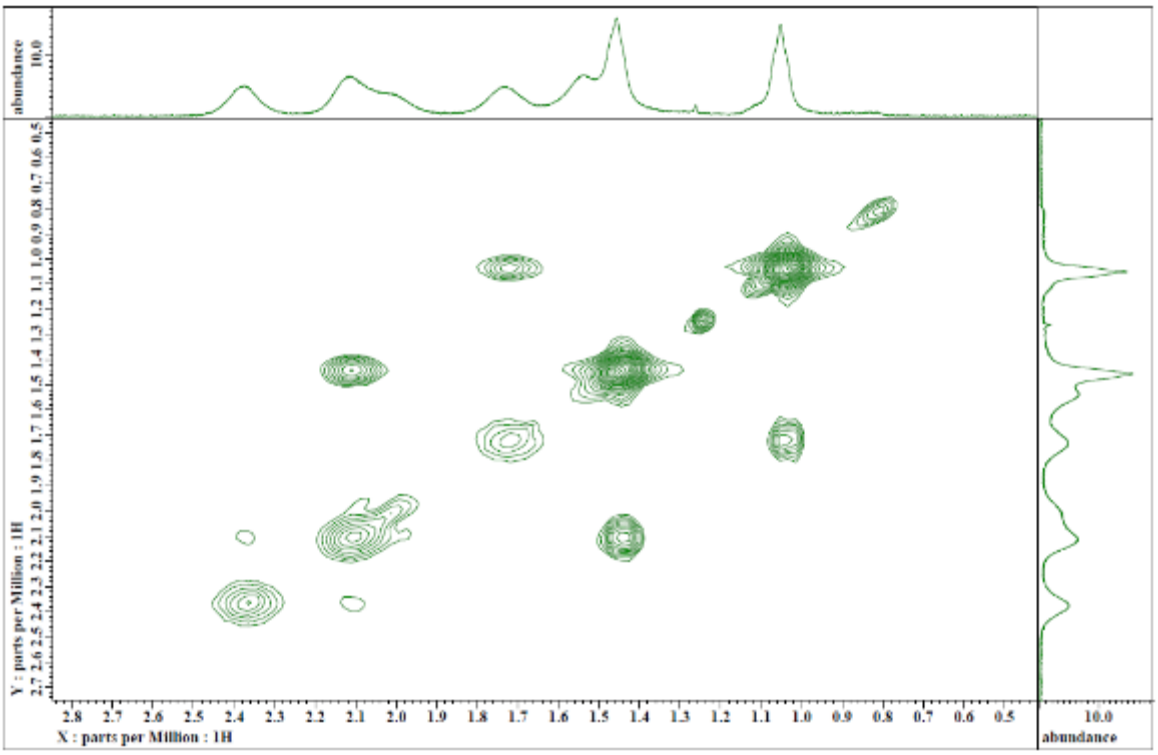

Fig. S235. ^{1}H-^{1}H COSY spectrum of complex **[4]**$^{2+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

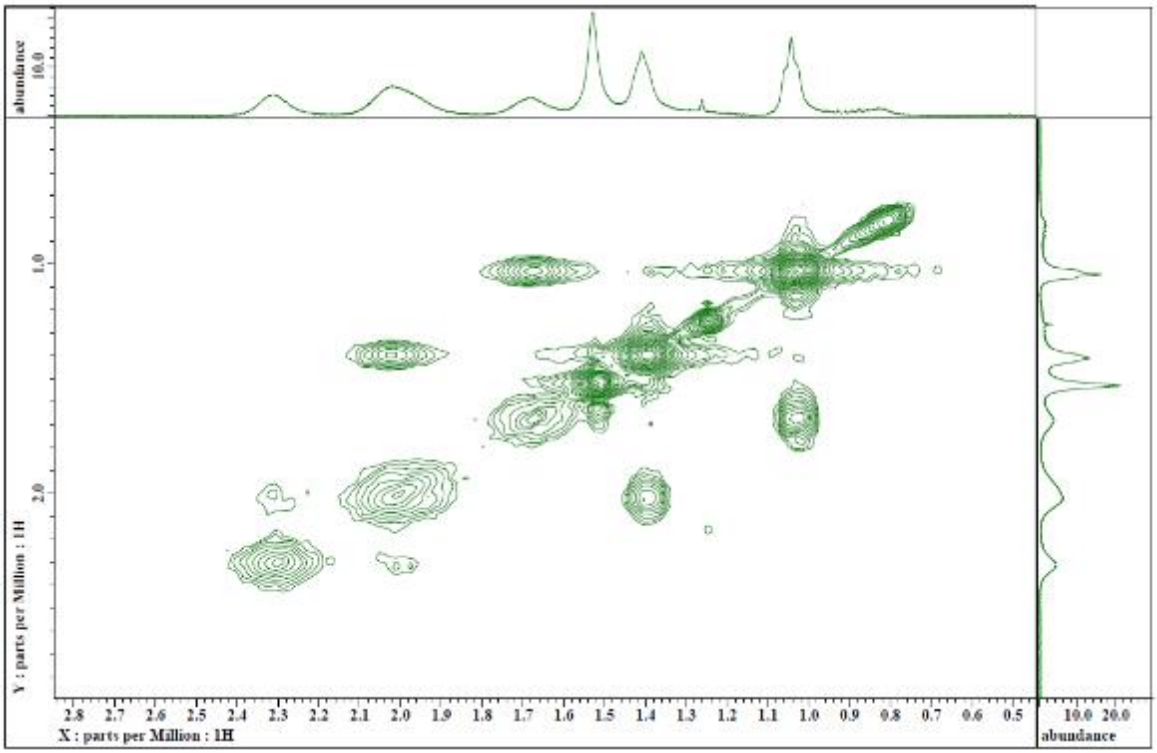

Fig. S236. ^{1}H-^{1}H COSY spectrum of complex **[4]**$^{3+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

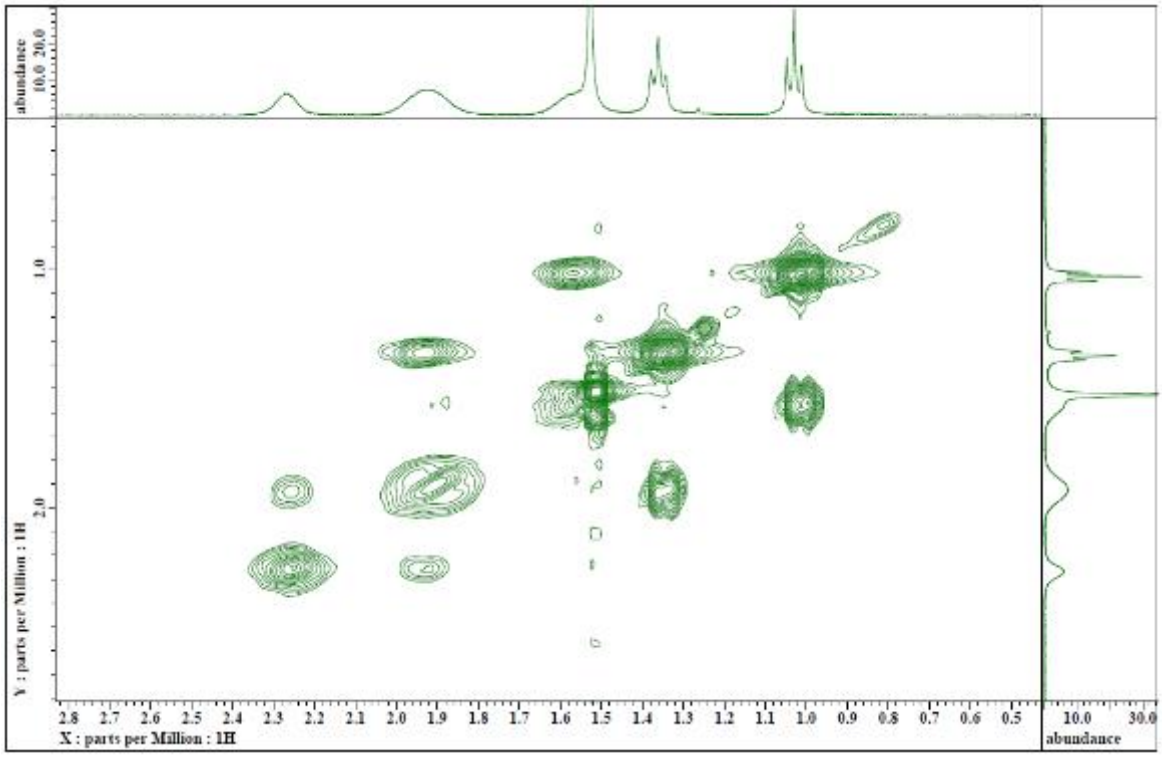

Fig. S237. ^{1}H-^{1}H COSY spectrum of complex **[4]**$^{4+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

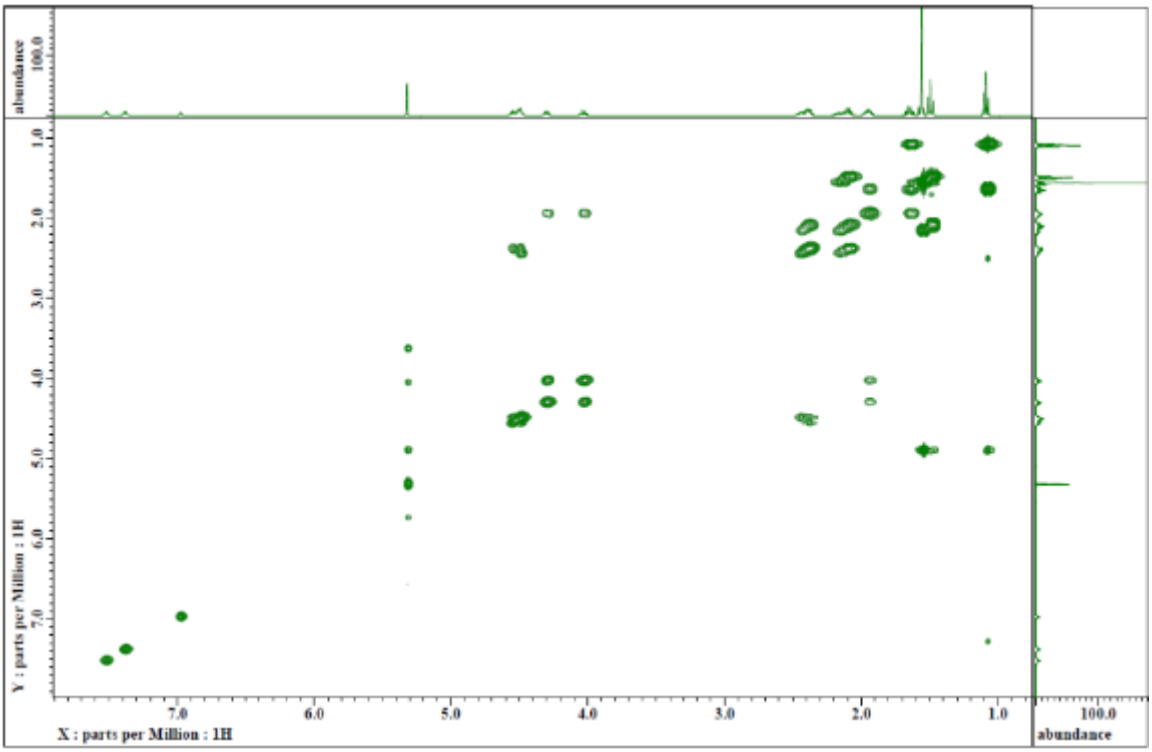

Fig. S238. ^{1}H-^{1}H COSY spectrum of complex **[5]**^{0} in CD_2Cl_2 and at room temperature (ca. 24 °C).

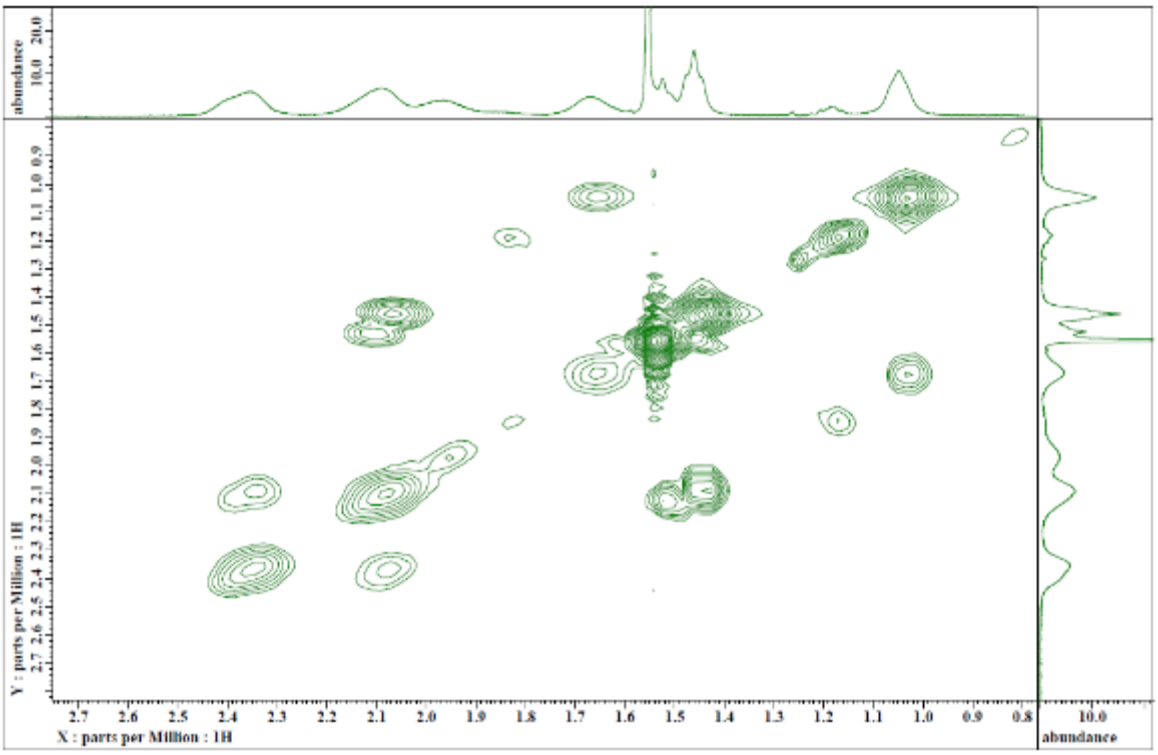

Fig. S239. ^{1}H-^{1}H COSY spectrum of complex **[5]**$^{+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

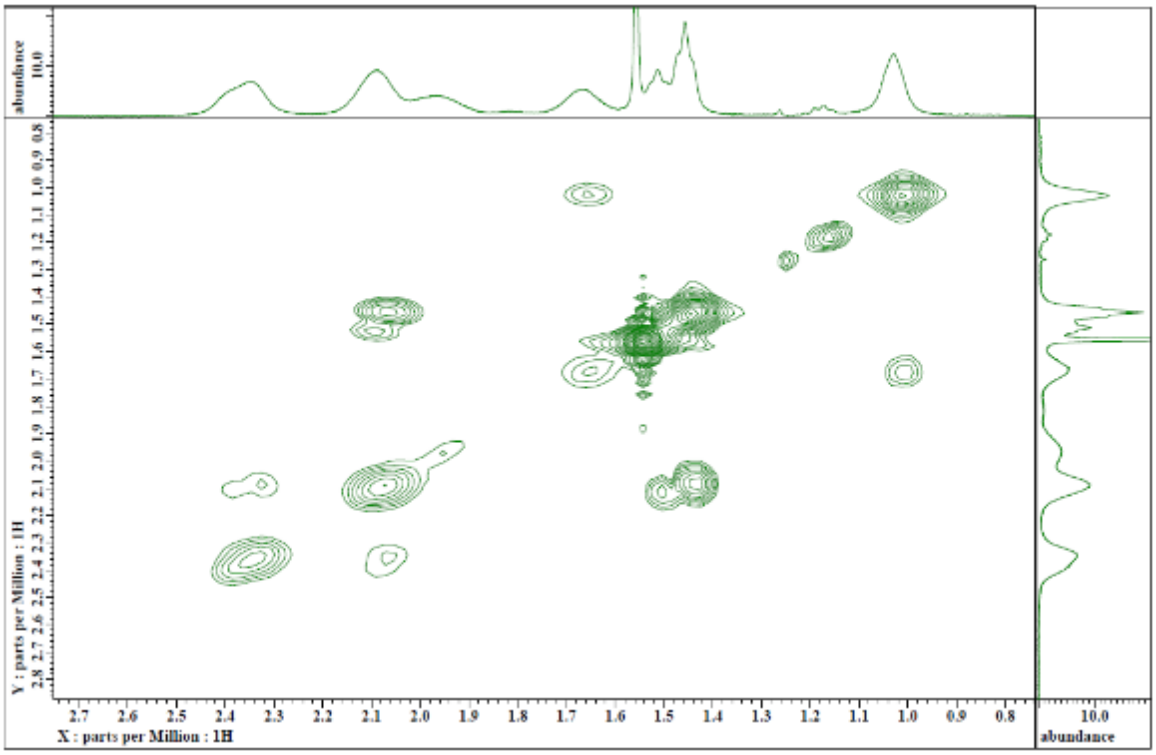

Fig. S240. ^{1}H-^{1}H COSY spectrum of complex **[5]**$^{2+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

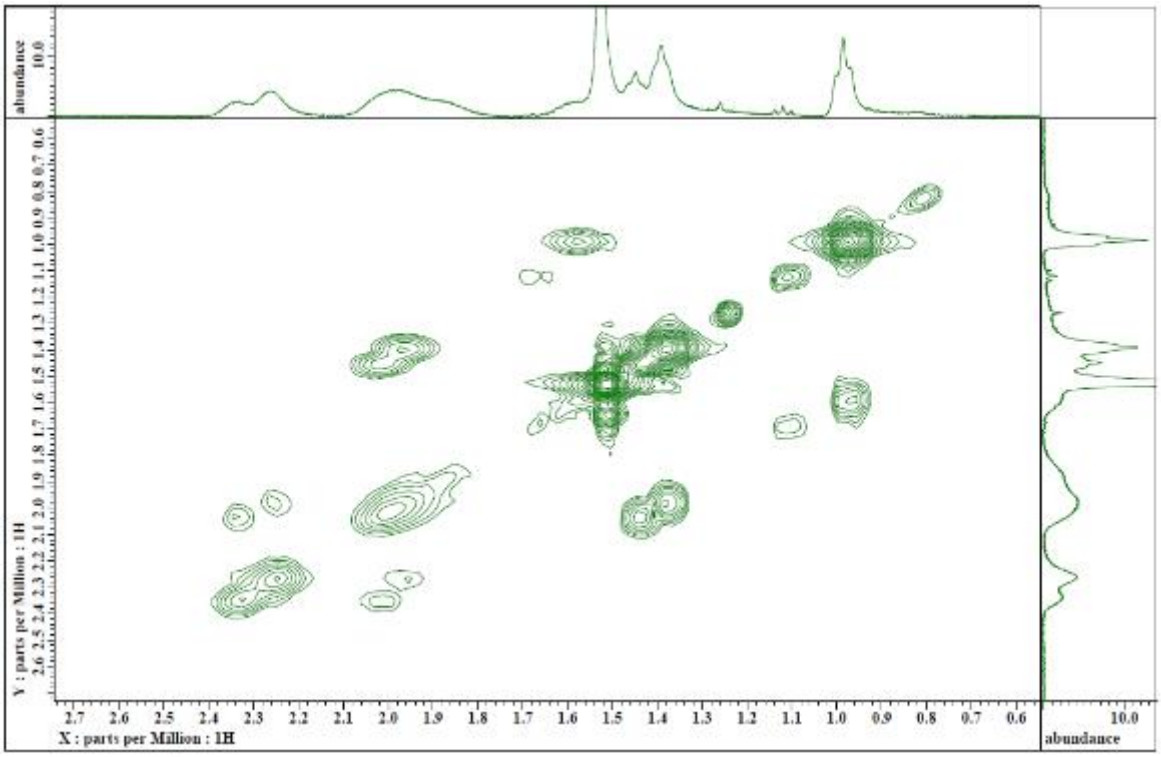

Fig. S241. ^{1}H-^{1}H COSY spectrum of complex **[5]**$^{3+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

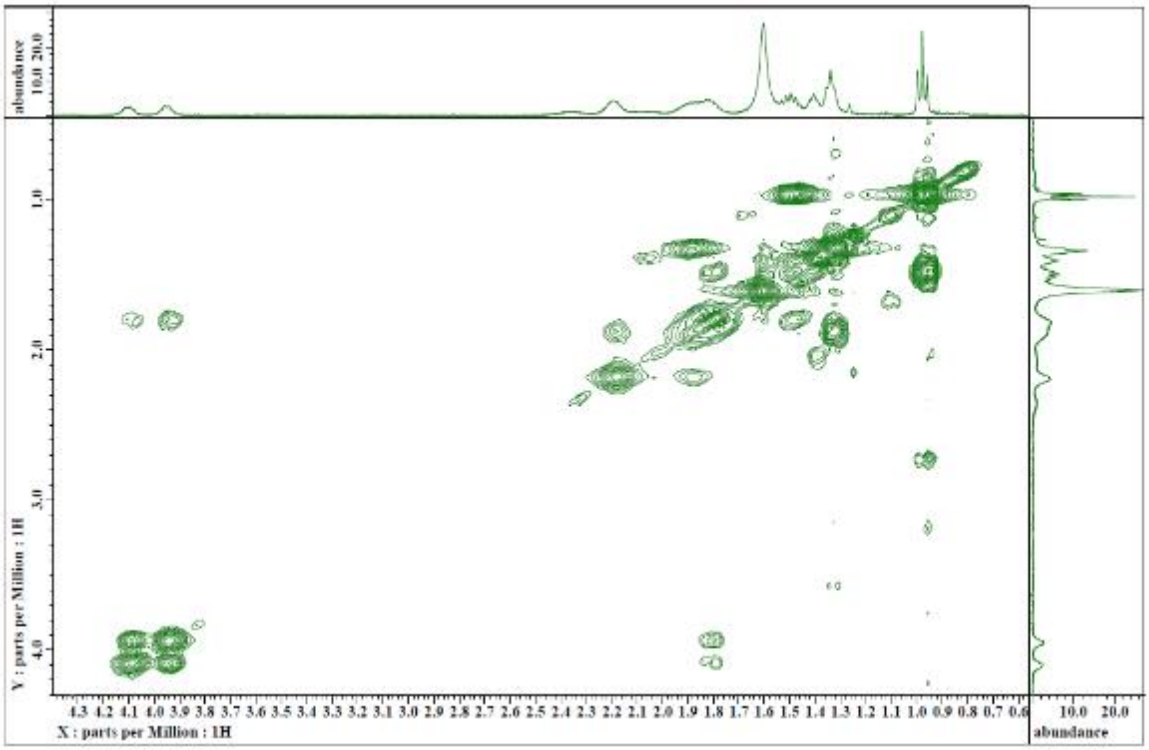

Fig. S242. ^{1}H-^{1}H COSY spectrum of complex **[5]**$^{4+}$ in CD_2Cl_2 and at room temperature (ca. 24 °C).

3.16. Analysis of ^{13}C NMR data

The observed ^{13}C NMR shifts of the studied triple-, quadruple- and quintuple-decker series were compared to predicted values, where the latter were obtained as the sum of the diamagnetic contribution[11], the pseudocontact shift as obtained from DFT refined models with the axial susceptibility anisotropy obtained from fitting ^{1}H data (see above) and, where applicable, the Fermi contact shift due to the organic radical (spin density values obtained from single-point DFT calculations of optimised structures). In general, the agreement is quite good for all aliphatic groups. Outliers are marked, and possible reasons for discrepancies are: neglect of the Fermi contact contribution for the nuclei close to the Tb(III) ion (C_q, C_N were not considered in the analysis for this reason), not accurate spin density values of organic radicals as obtained from DFT (CH_{ar}), presence of impurities or not possible reliable assigment of signals. In some cases, considerably fewer signals were observed than the maximum possible number. Possible reasons for this are that some of the signals are too broad (due to fast relaxation of some nuclei or fast electron exchange due to the difficulty in preparing samples with the perfect amount of oxidant) and disappear after data processing or the already very broad (ca. 2000 ppm) window of frequencies in which the measurements were performed.

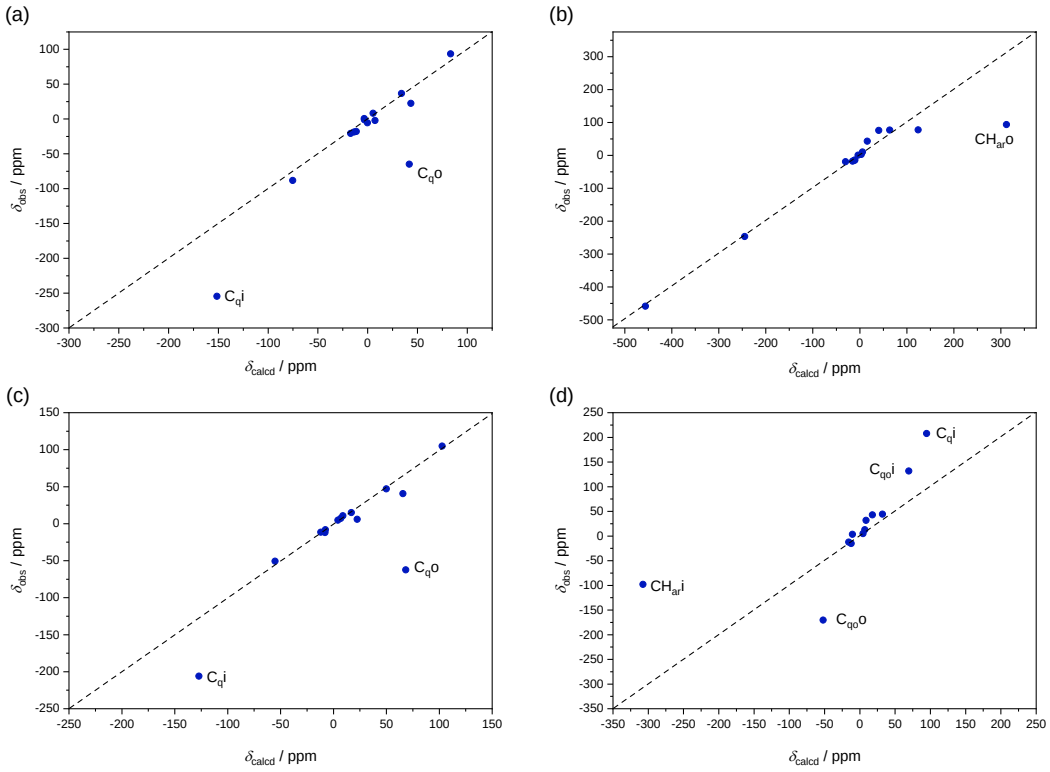

Fig. S243. Comparison of calculated and observed experimental ^{13}C NMR shifts for (a) **[3]^{0}**, (b) **[3]$^{+}$**, (c) **[3]$^{2+}$** and (d) **[3]$^{3+}$**.

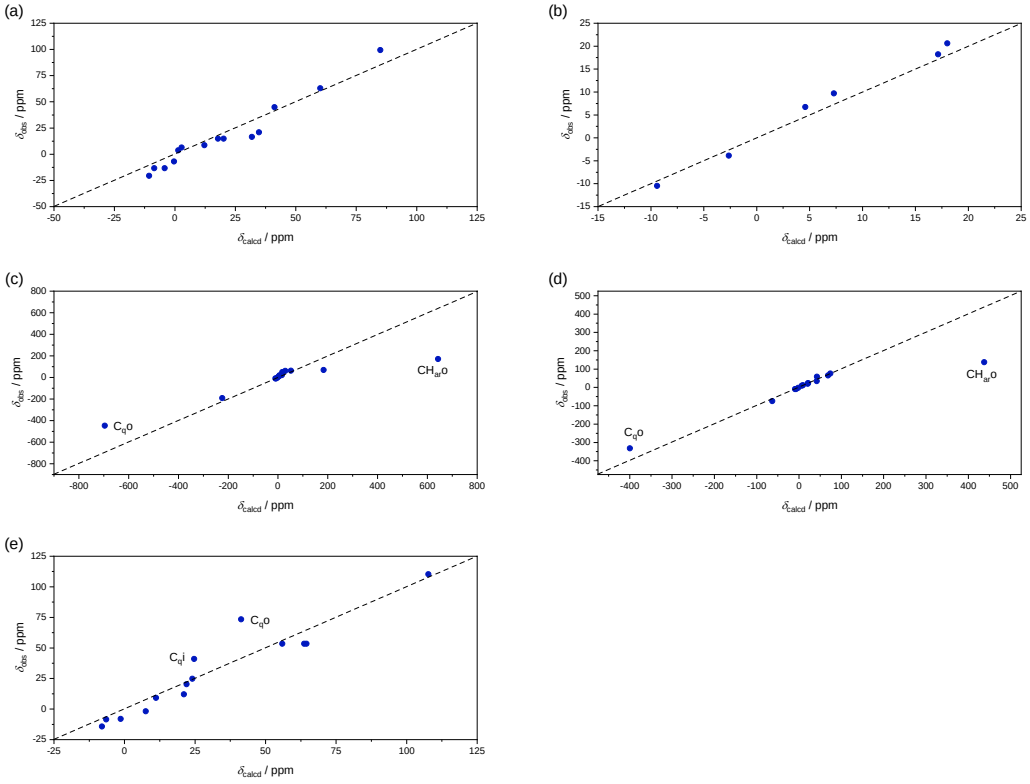

Fig. S244. Comparison of calculated and observed experimental ^{13}C NMR shifts for (a) **[4]^{0}**, (b) **[4]$^{+}$**, (c) **[4]$^{2+}$**, (d) **[4]$^{3+}$** and (e) **[4]$^{4+}$**.

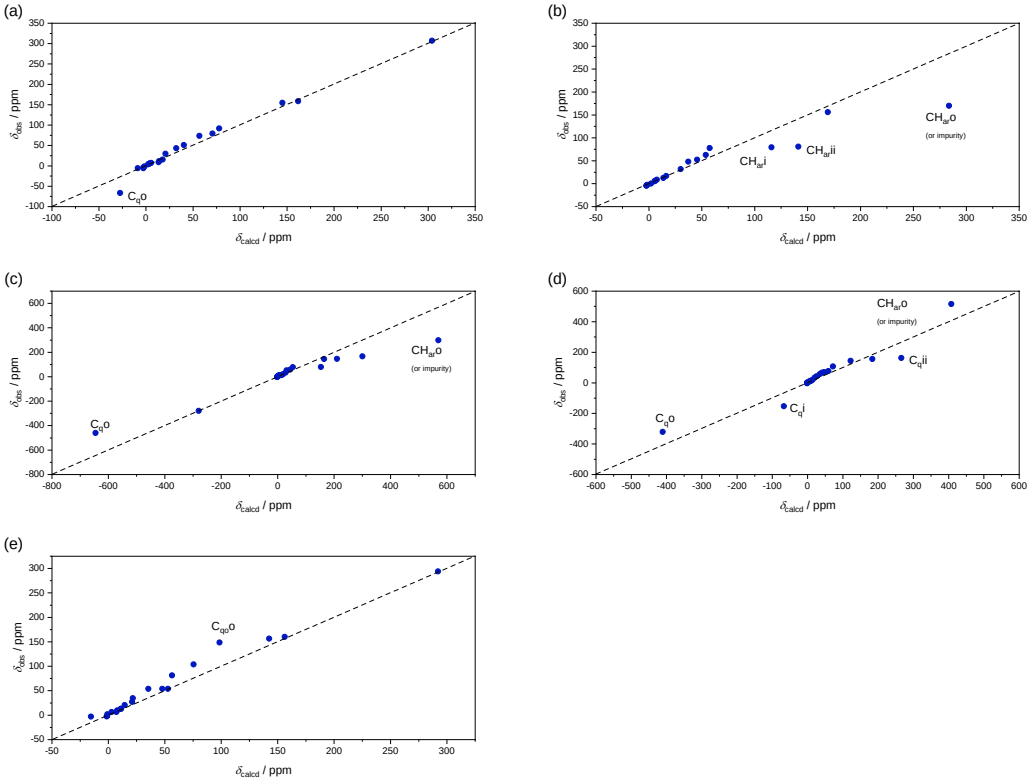

Fig. S245. Comparison of calculated and observed experimental ^{13}C NMR shifts for (a) **[5]^{0}**, (b) **[5]$^{+}$**, (c) **[5]$^{2+}$**, (d) **[5]$^{3+}$** and (e) **[5]$^{4+}$**.

4. DFT Calculations

4.1. General Information

In order to reduce the computational time, the input structures made from the XRD data were symmetrized in order to belong to the C_4 point group. In some instances, the optimized structure deviates from this symmetry due to a rotation of one of the ligands away from the ideal square antiprismatic coordination environment for the metal ion. Also, all butoxy groups were turned into methoxy groups, for the purpose of saving computational time. All calculations were done with Gaussian 09 (revision D.01)[12], with the (U)TPSSH functional[13] and with the def2svp[14-15] basis functions on all atoms. A "superfine" grid was also used in the optimization procedure. True minima were proven by the absence of negative frequencies for the triple-decker series. Since optimizations of the triple-deckers did not lead to negative frequencies (if these at all appeared, they were related to the waggling of the ligand by a few degrees around the Tb-Tb axis and not to any other structural distortion that would influence the interligand, intermetal or metal-ligand distances). The frequency calculations of the quintuple- and quadruple-deckers were beyond our resources. For the reasons above, we assumed that minima were reached and, if not, that the converged structures were good enough for analysis.

TD-DFT calculations were done with B3LYP/6-31G*[16-18],[19-22] with SDD[23] for Y(III) and Cd(II). Such calculations for the quintuple-deckers were unfortunately beyond our current resources for computations.

4.2. Triple-Deckers **[3]**

Fig. S246. Comparison of DFT optimized structures of the triple-decker (Y^{III} analogue) in various oxidation states.

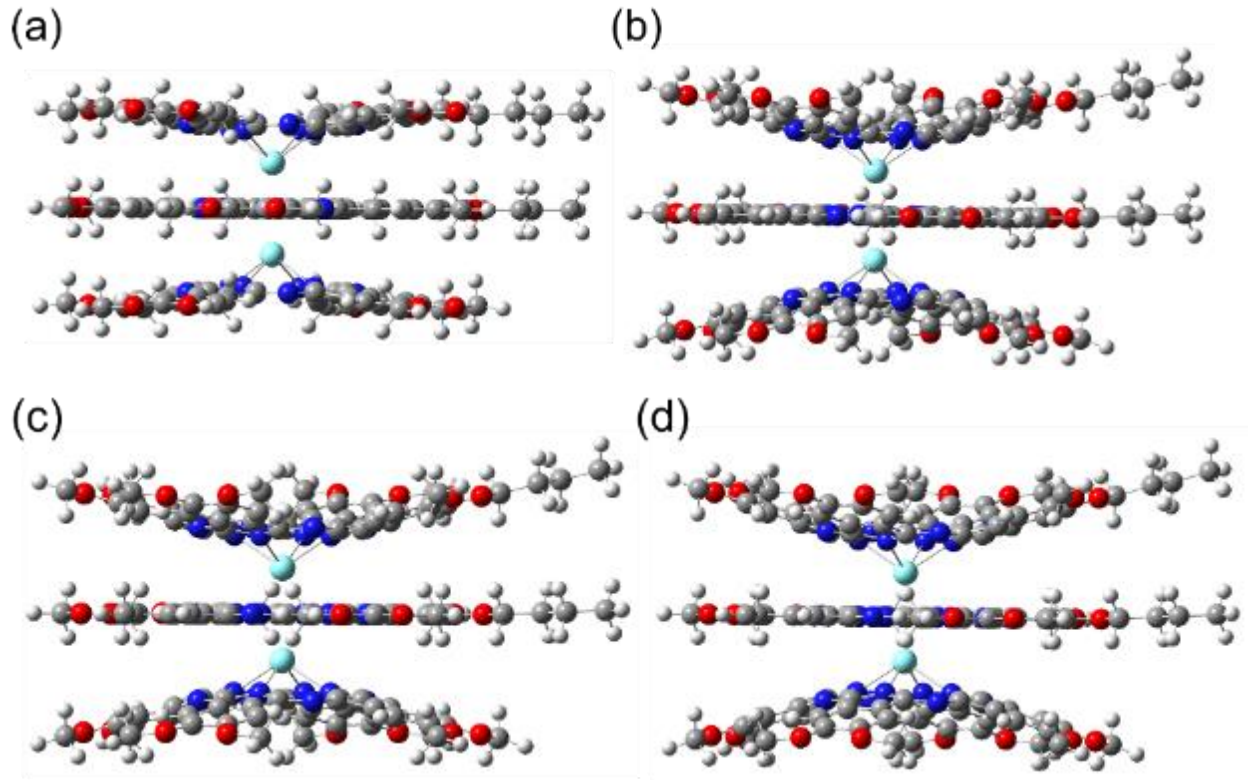

Fig. S247. Optimized structures of (a) **[3]**^{0}, (b) **[3]**$^{+}$, (c) **[3]**$^{2+}$ and (d) **[3]**$^{3+}$. The parts of the methoxy groups of the optimized structures shown in Fig. S237 were replaced to butoxy ones, followed by the optimization of butoxy chains.

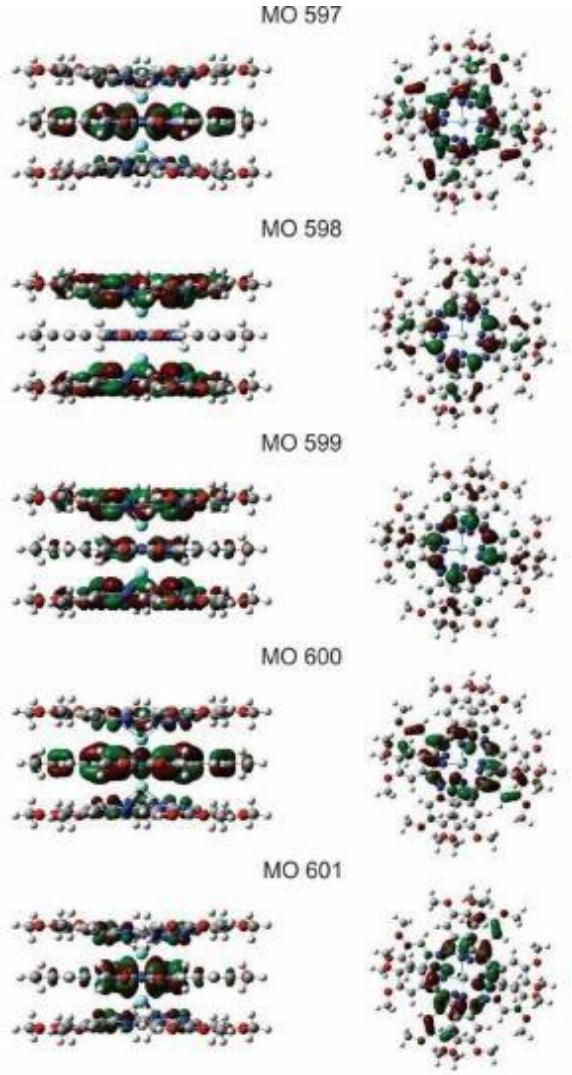

Fig. S248. Molecular orbitals of the triple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the neutral state. MO 599 is HOMO.

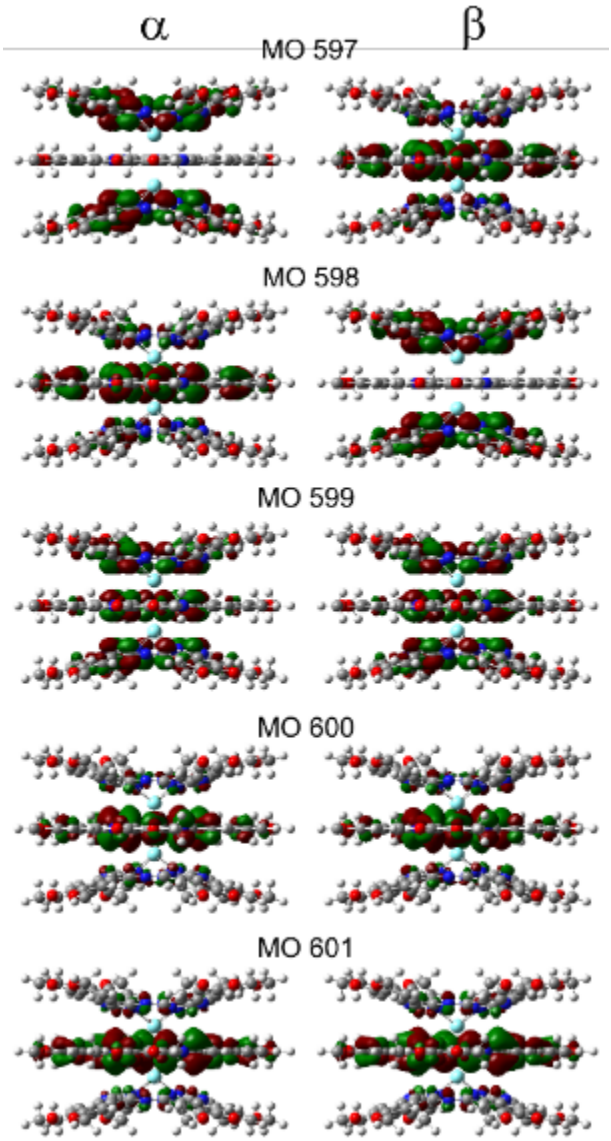

Fig. S249. Molecular orbitals of the triple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +1 state. MO 599α is SOMO.

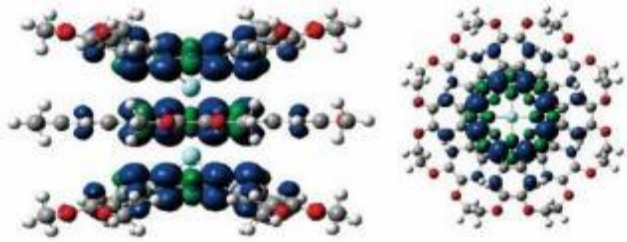

Fig. S250. Spin density (isosurface value 0.0004) of the organic radical of the triple-decker, from the DFT optimized Y^{III} analogue in the +1 state.

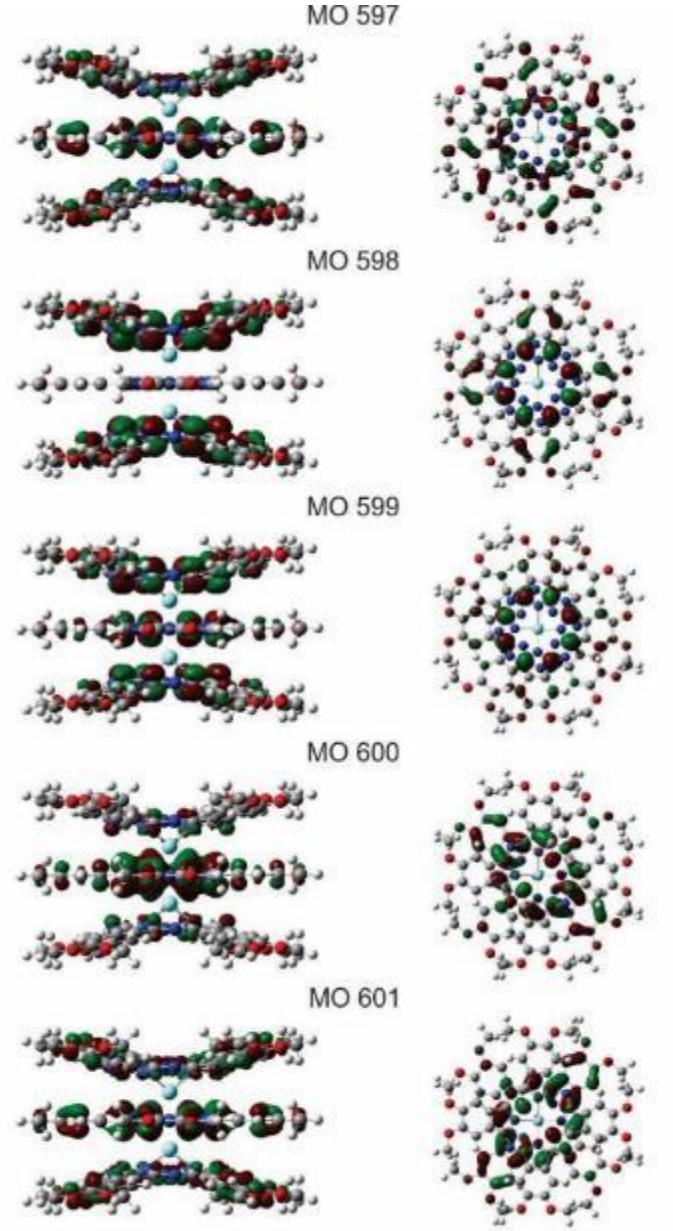

Fig. S251. Molecular orbitals of the triple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +2 state. MO 598 is HOMO.

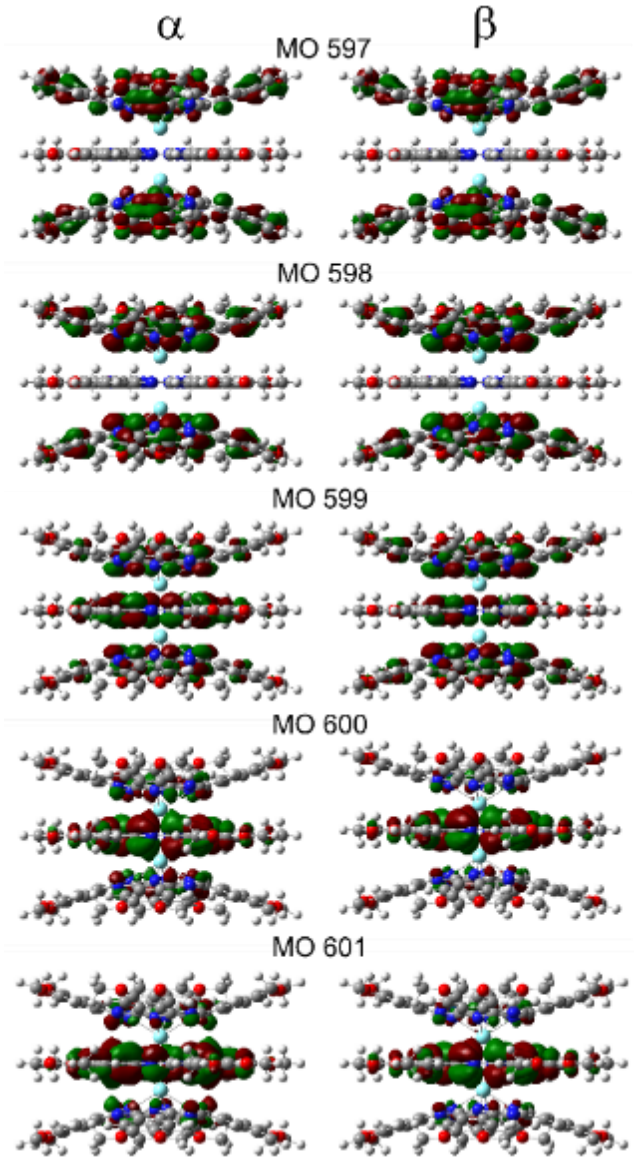

Fig. S252. Molecular orbitals of the triple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +3 state. MO 598α is SOMO.

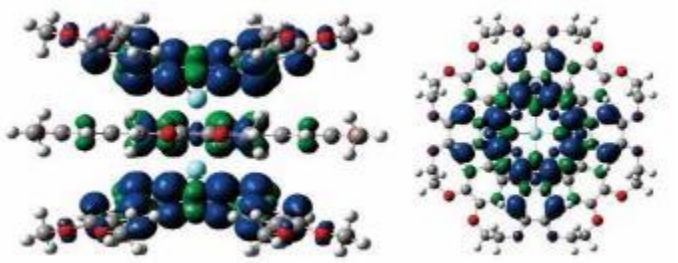

Fig. S253. Spin density (isosurface value 0.0004) of the organic radical of the triple-decker, from the DFT optimized Y^{III} analogue in the +3 state.

4.3. Quadruple-Deckers **[4]**

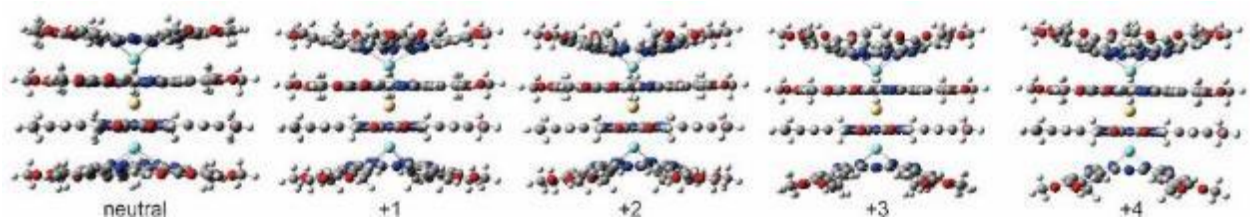

Fig. S254. Comparison of DFT optimized structures of the quadruple-decker (Y^{III} analogue) in various oxidation states.

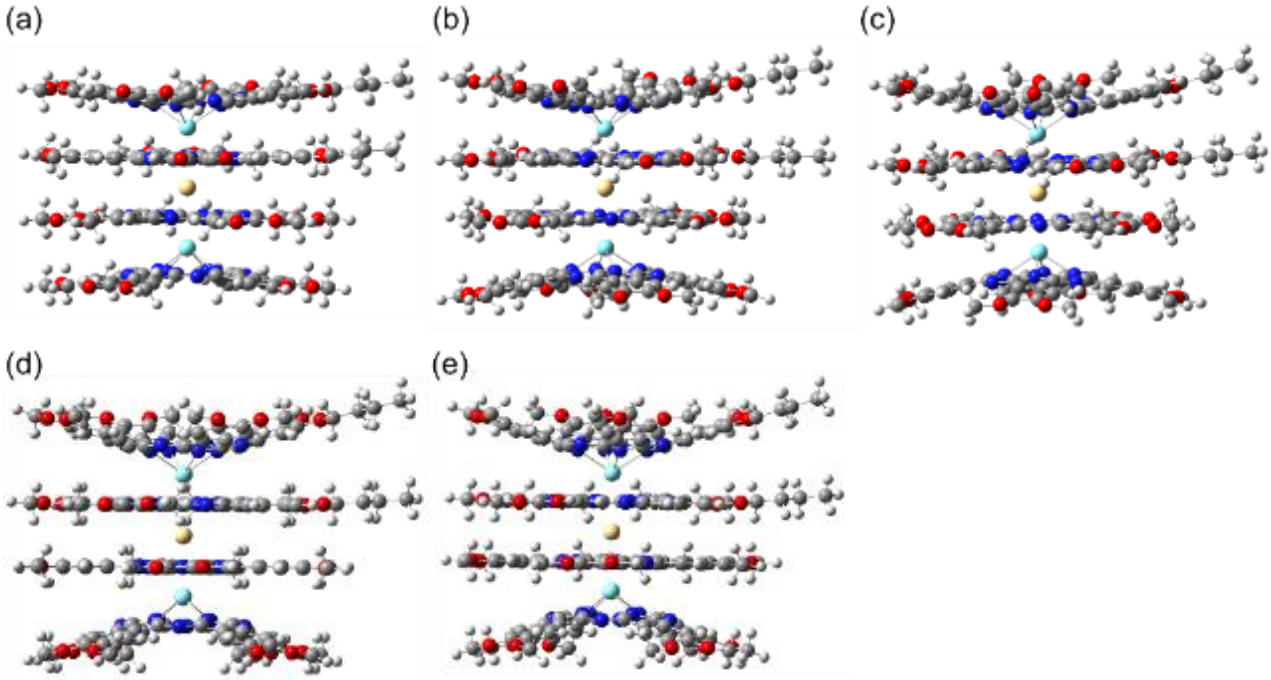

Fig. S255. Optimized structures of (a) $\mathbf{[4]^0}$, (b) $\mathbf{[4]^+}$, (c) $\mathbf{[4]^{2+}}$, (d) $\mathbf{[4]^{3+}}$ and (e) $\mathbf{[4]^{4+}}$.The parts of the methoxy groups of the optimized structures shown in Fig. S244 were replaced to butoxy ones, followed by the optimization of butoxy chains.

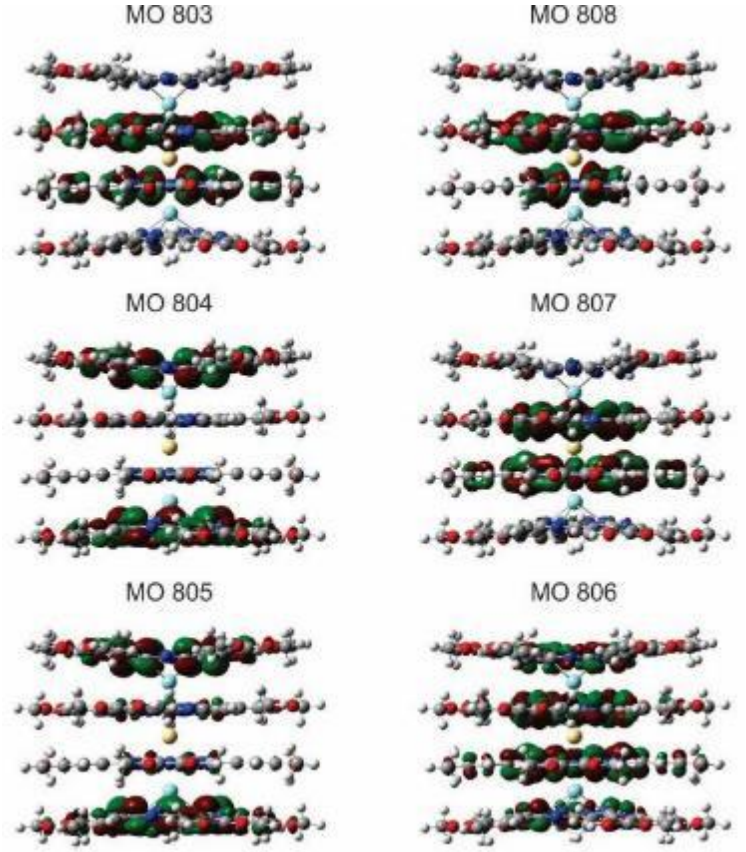

Fig. S256. Molecular orbitals of the quadruple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the neutral state. MO 805 is HOMO.

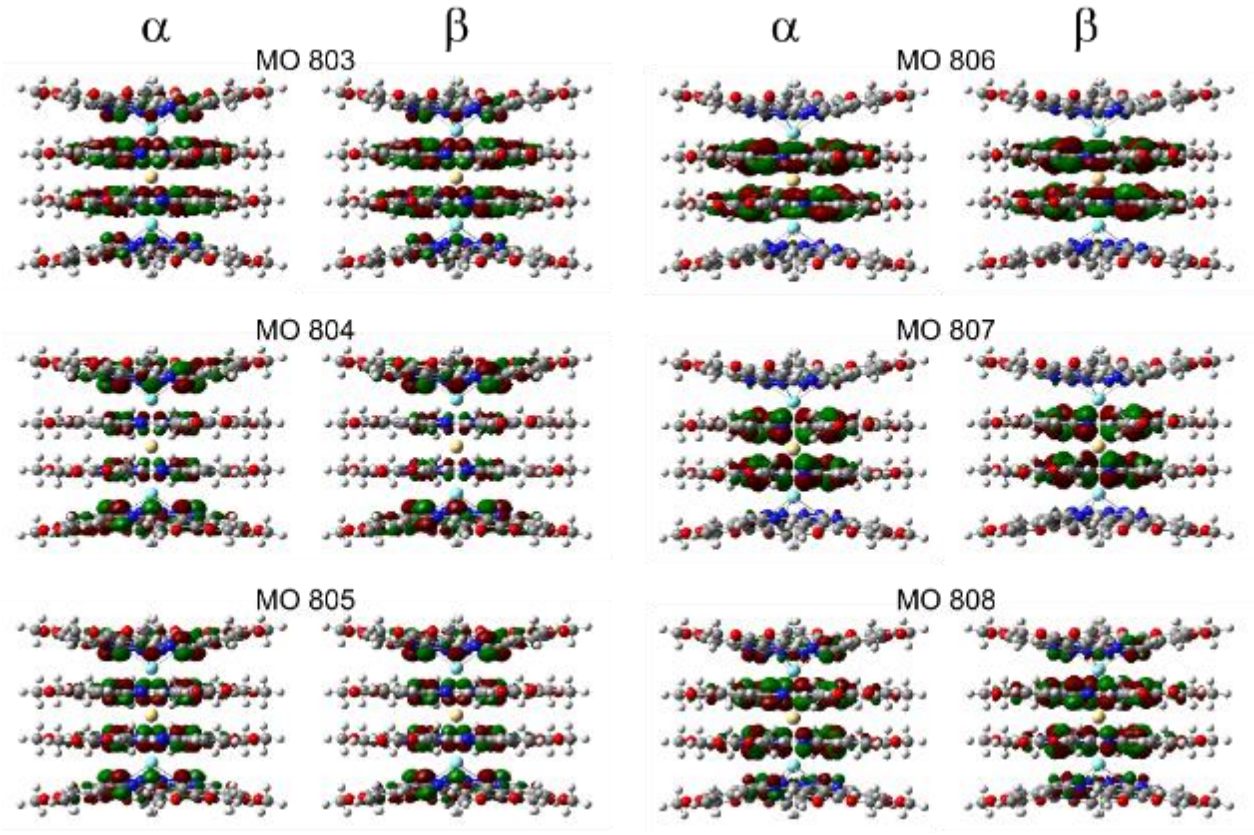

Fig. S257. Molecular orbitals of the quadruple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +1 state. MO 805α is SOMO.

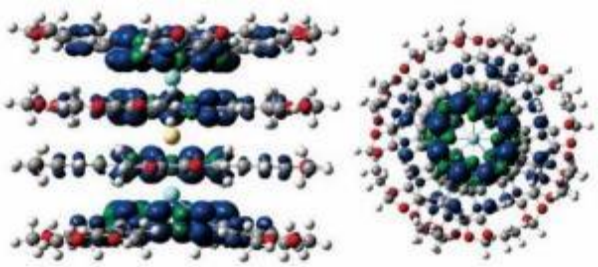

Fig. S258. Spin density (isosurface value 0.0004) of the organic radical of the quadruple-decker, from the DFT optimized Y^{III} analogue in the +1 state.

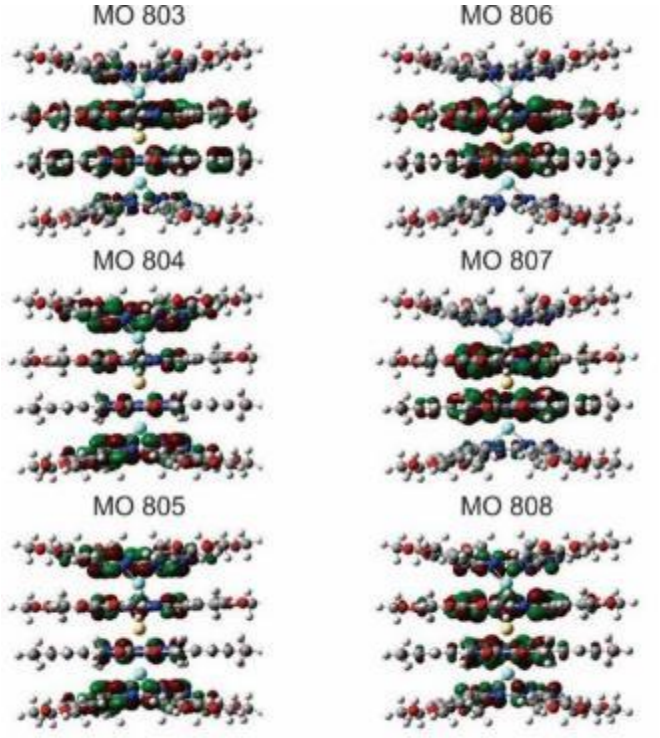

Fig. S259. Molecular orbitals of the quadruple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +2 state. MO 804 is HOMO.

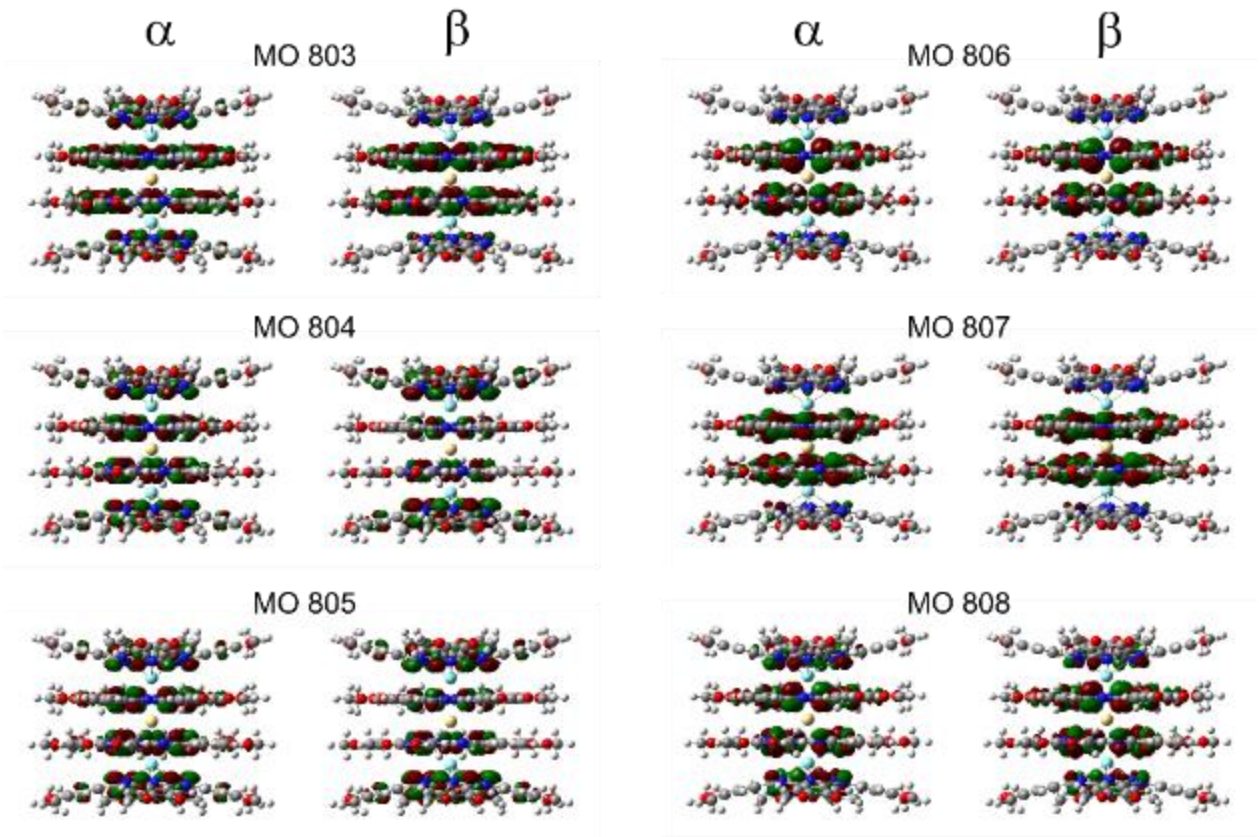

Fig. S260. Molecular orbitals of the quadruple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the triplet +2 state. MO 804α and MO 805α are SOMO.

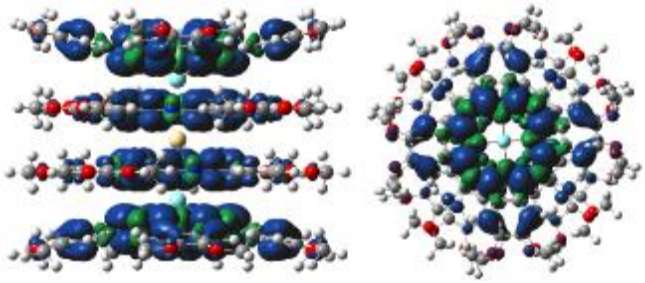

Fig. S261. Spin density (isosurface value 0.0004) of the organic radical of the quadruple-decker, from the DFT optimized Y^{III} analogue in the triplet +2 state.

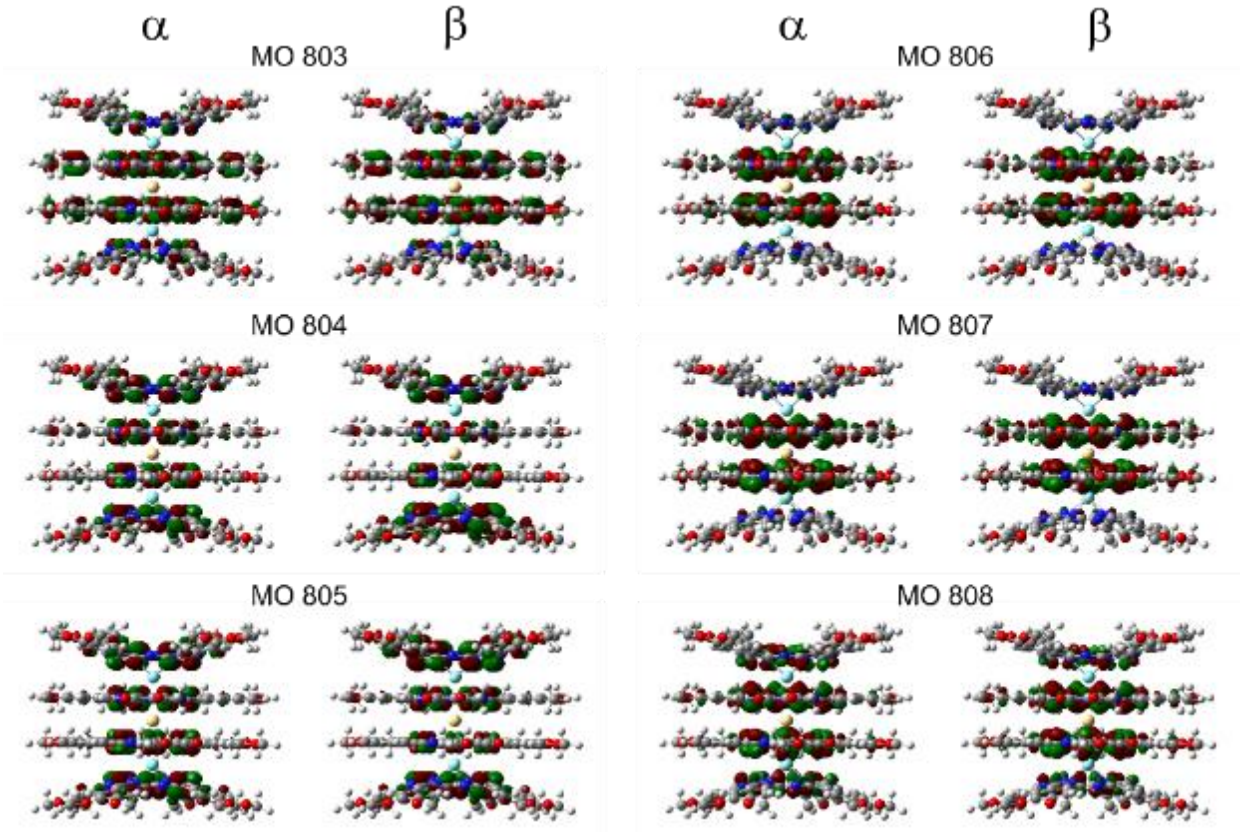

Fig. S262. Molecular orbitals of the quadruple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +3 state. MO 804α is SOMO.

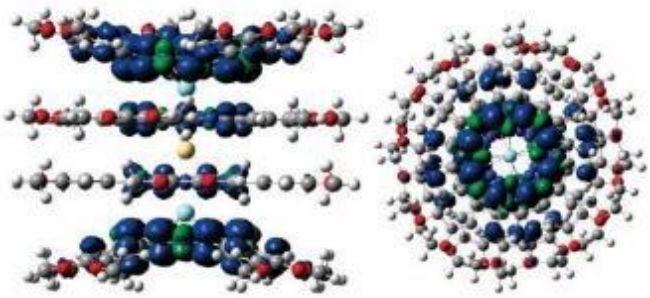

Fig. S263. Spin density (isosurface value 0.0004) of the organic radical of the quadruple-decker, from the DFT optimized Y^{III} analogue in the +3 state.

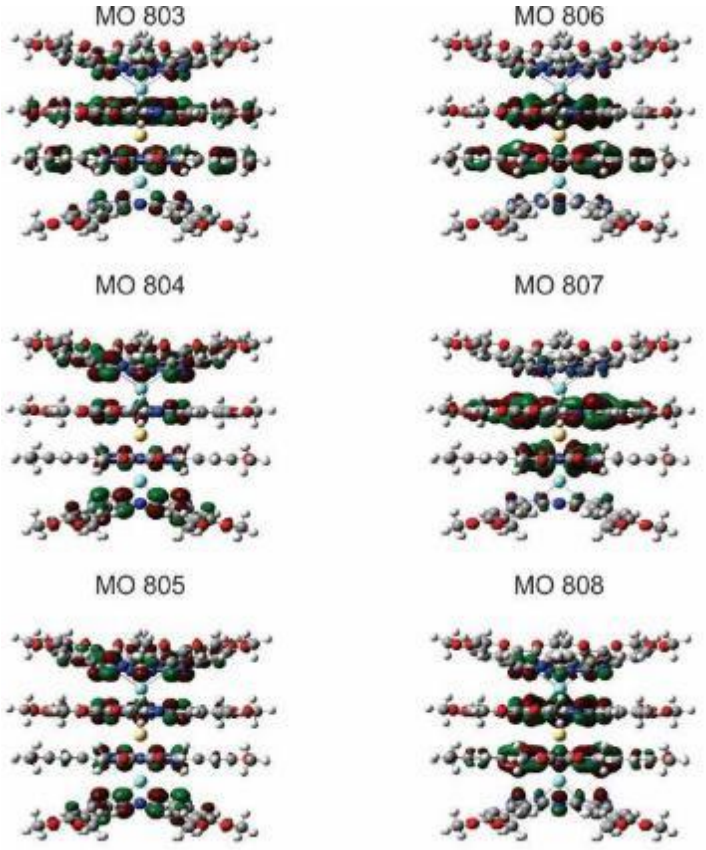

Fig. S264. Molecular orbitals of the quadruple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +4 state. MO 803 is HOMO.

4.4. Quintuple-Deckers **[5]**

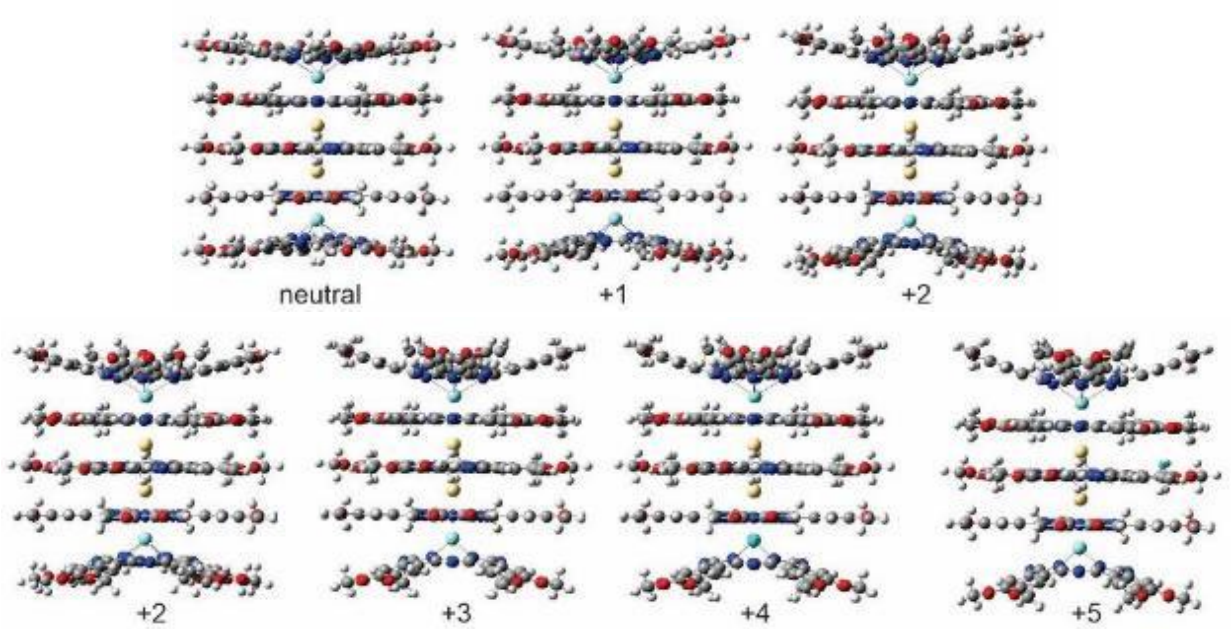

Fig. S265. Comparison of DFT optimized structures of the quintuple-decker (Y^{III} analogue) in various oxidation states.

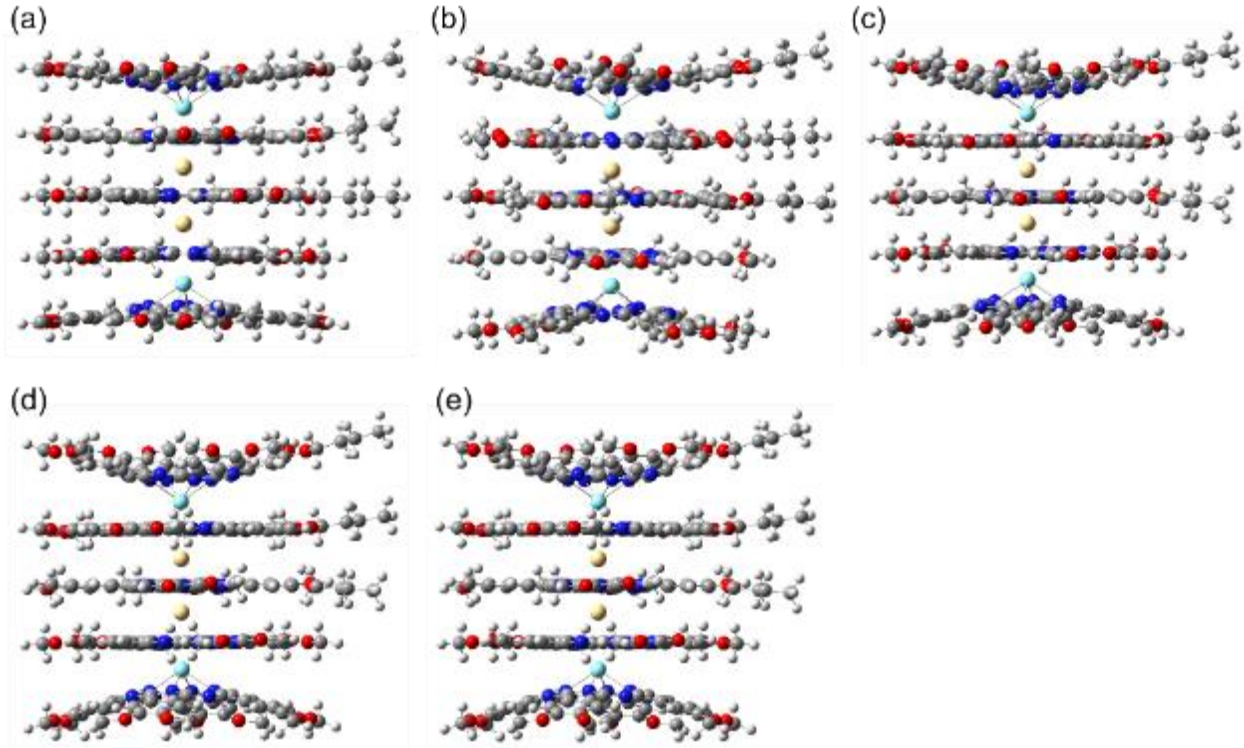

Fig. S266. Optimized structures of (a) $\mathbf{[5]^0}$, (b) $\mathbf{[5]^+}$, (c) $\mathbf{[5]^{2+}}$, (d) $\mathbf{[5]^{3+}}$ and (e) $\mathbf{[5]^{4+}}$. The parts of the methoxy groups of the optimized structures shown in Fig. S254 were replaced to butoxy ones, followed by the optimization of butoxy chains.

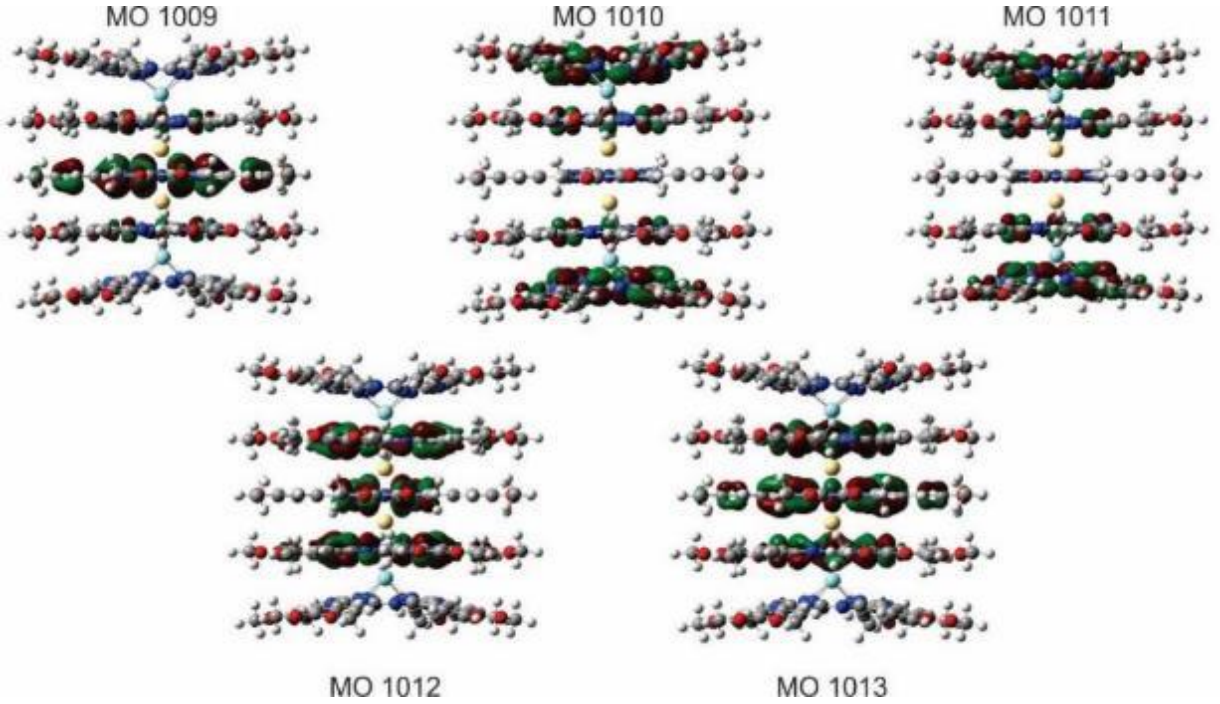

Fig. S267. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the neutral state. MO 1011 is HOMO.

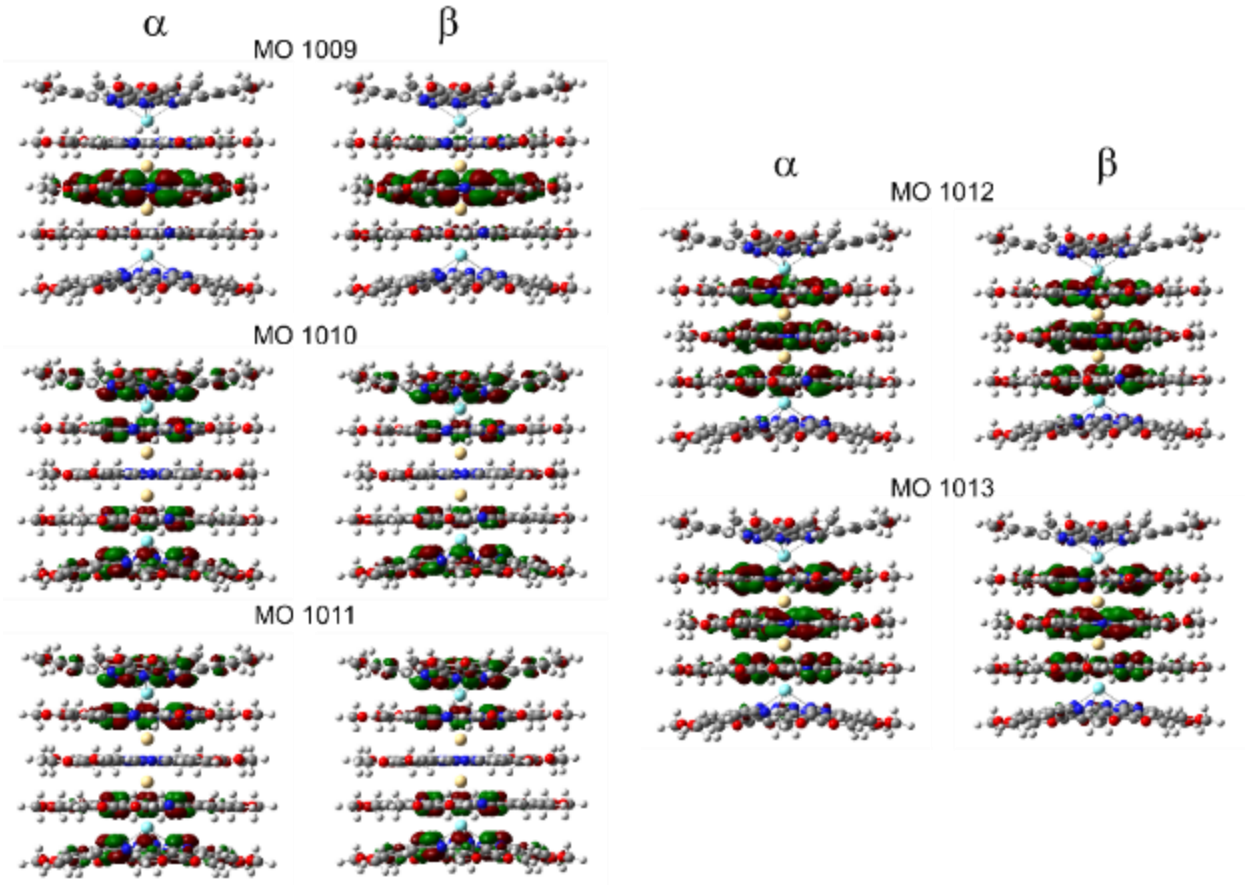

Fig. S268. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the neutral state. MO 1011α is SOMO.

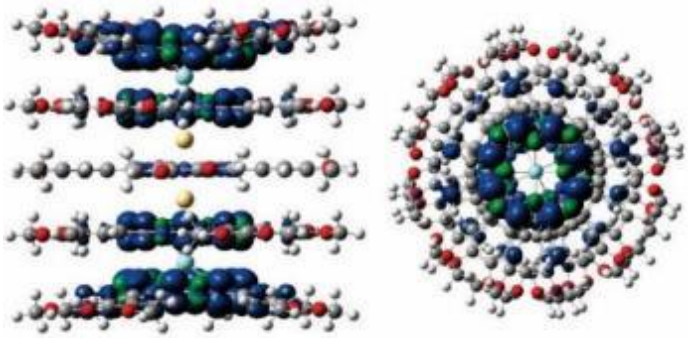

Fig. S269. Spin density (isosurface value 0.0004) of the organic radical of the quintuple-decker, from the DFT optimized Y^{III} analogue in the +1 state.

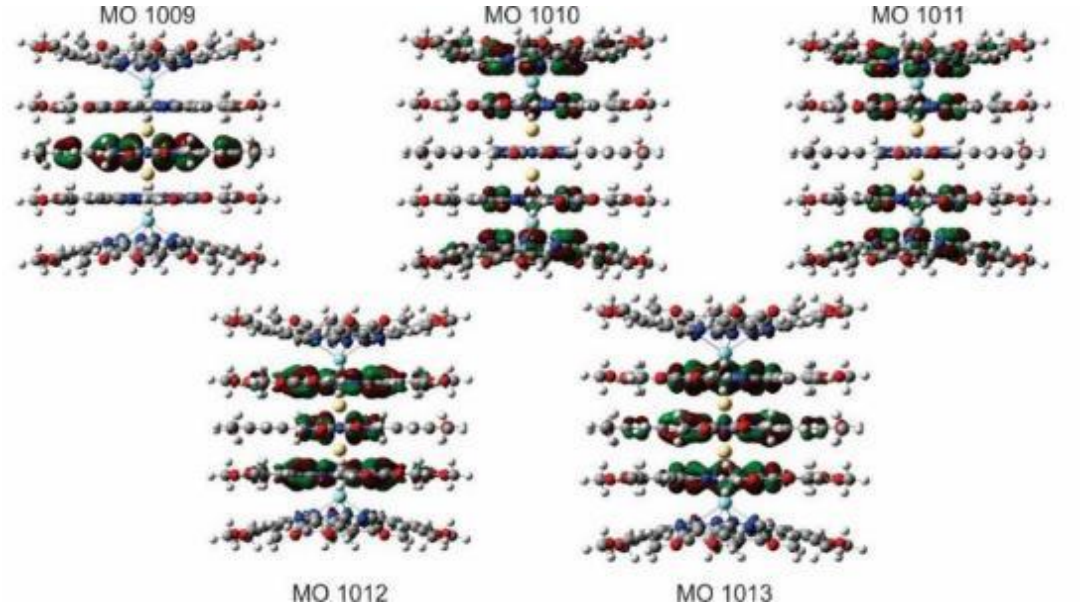

Fig. S270. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +2 state. MO 1010 is HOMO.

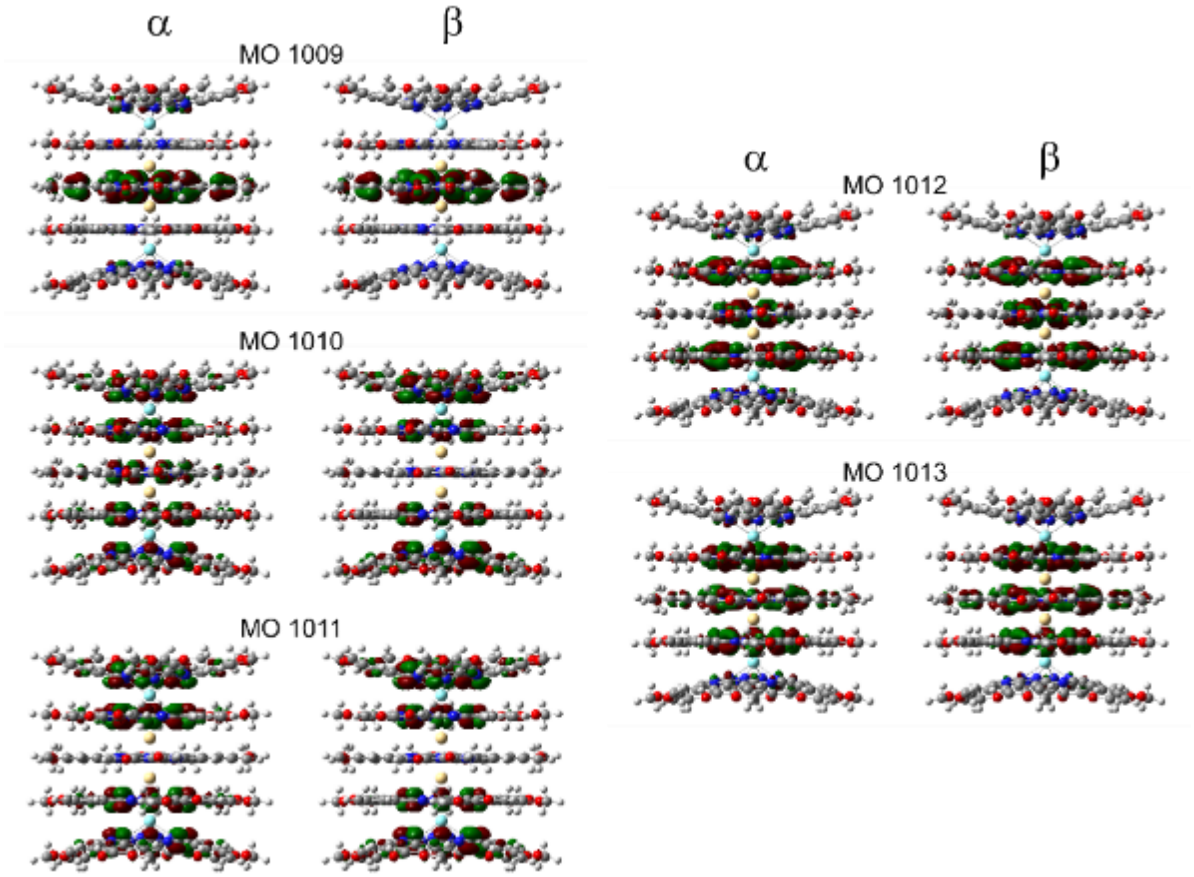

Fig. S271. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the triplet +2 state. MO 1011α and MO 1010α are SOMO.

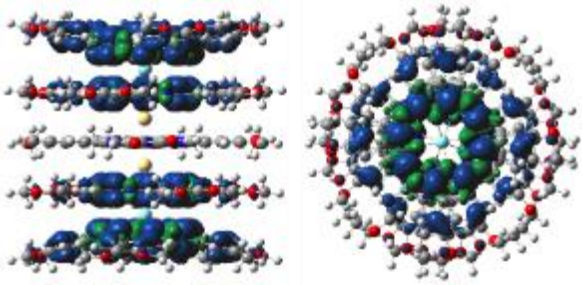

Fig. S272. Spin density (isosurface value 0.0004) of the organic radical of the quintuple-decker, from the DFT optimized Y^{III} analogue in the +2 state.

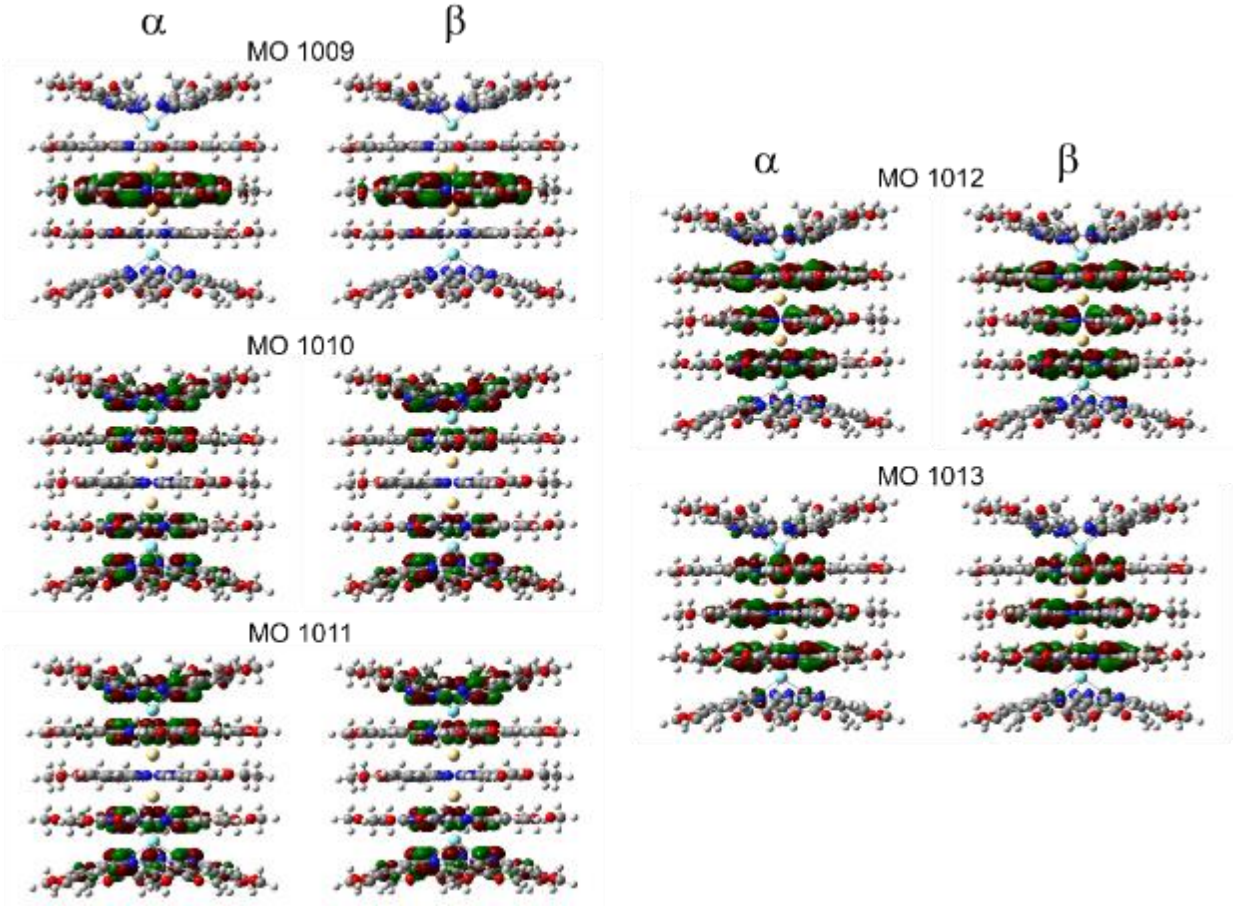

Fig. S273. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +3 state. MO 1010α is SOMO.

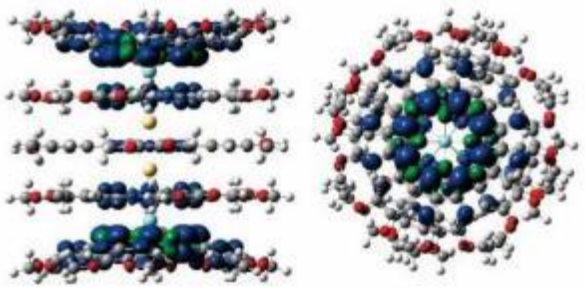

Fig. S274. Spin density (isosurface value 0.0004) of the organic radical of the quintuple-decker, from the DFT optimized Y^{III} analogue in the +3 state.

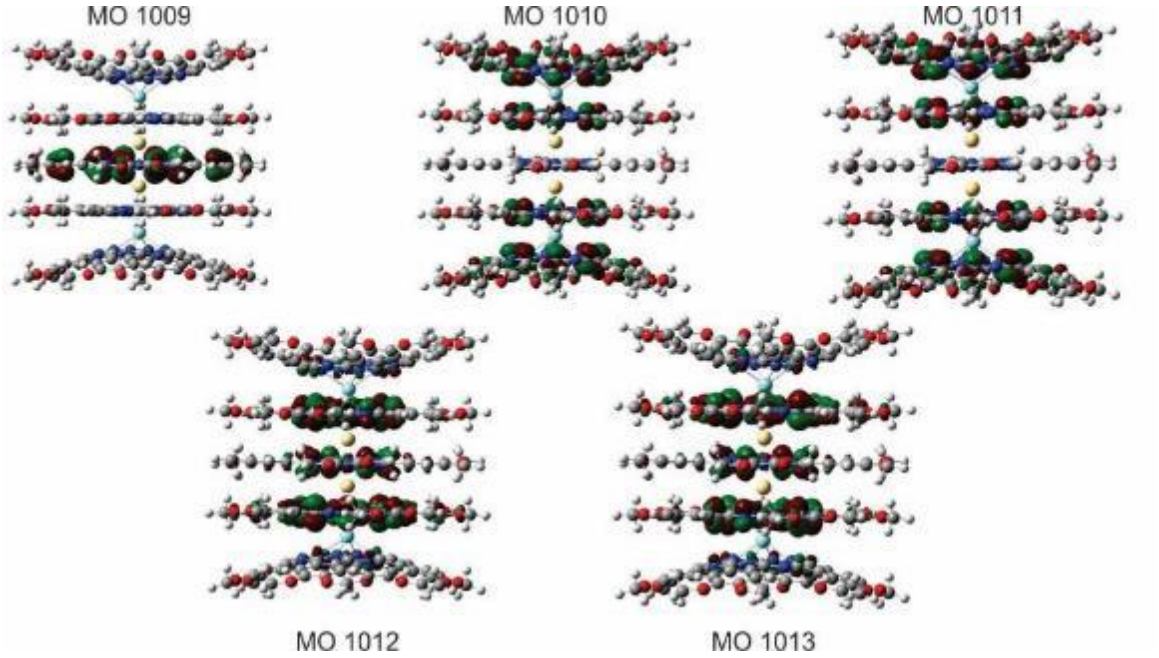

Fig. S275. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +4 state. MO 1009 is HOMO.

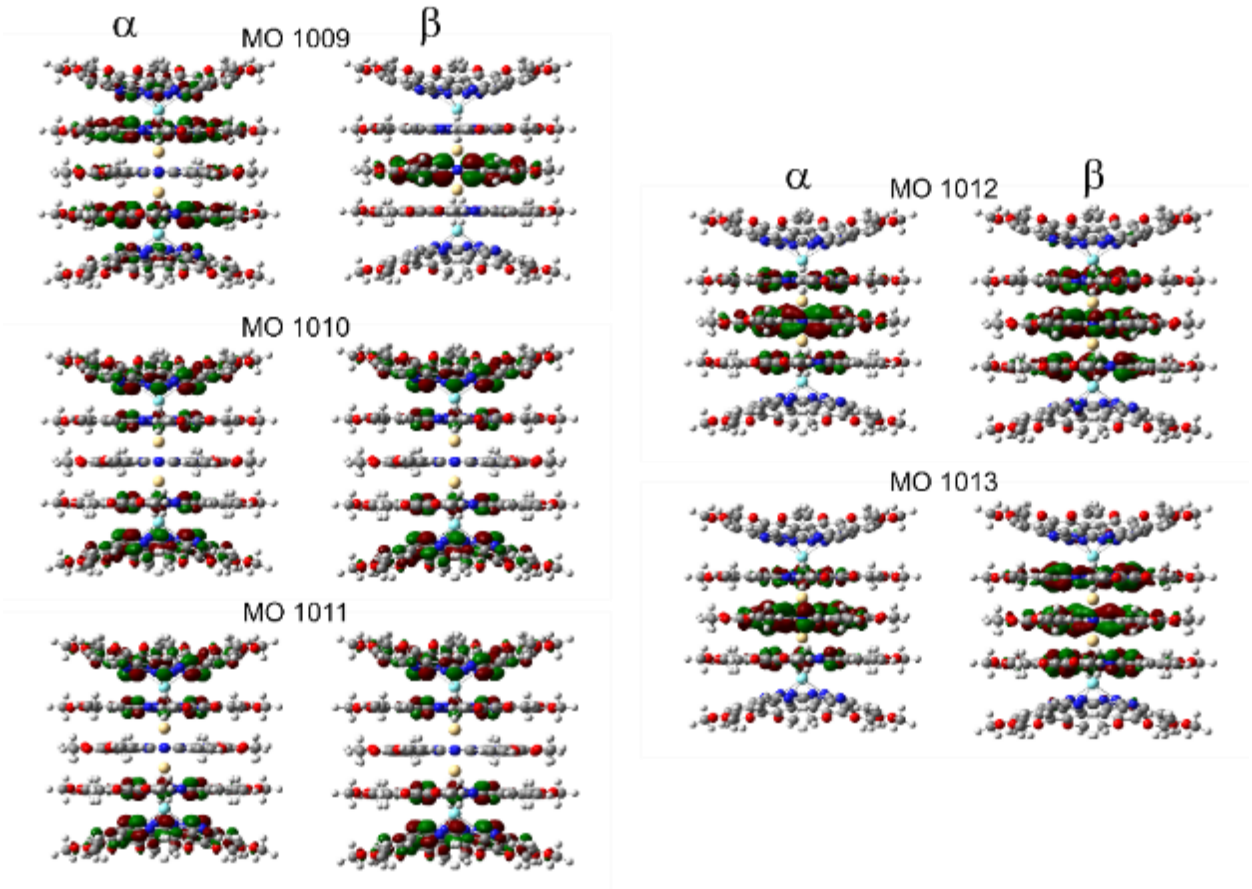

Fig. S276. Molecular orbitals of the quintuple-decker (isosurface value 0.02), from the DFT optimized Y^{III} analogue in the +5 state. MO 1009α is SOMO.

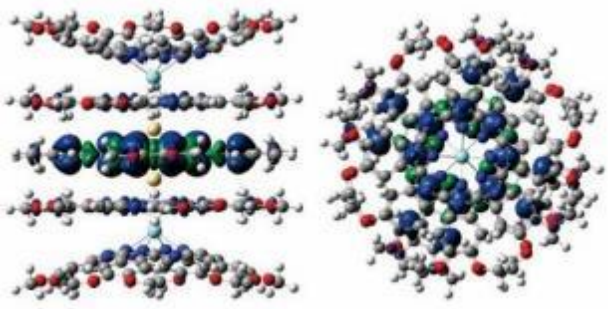

Fig. S277. Spin density (isosurface value 0.0004) of the organic radical of the quintuple-decker, from the DFT optimized Y^{III} analogue in the +5 state.

4.5. Summary from optimized structures

Although the Y(III) to Y(III) distance decreases with each successive oxidation, the distances between the ligands show the following trend: with increasing total oxidation number, the distance between the two outer ligands decreses, whereas the distance between the inner ligands increases. This can be imagined as the sequential formation of double-decker moieties upon oxidation, i.e. oxidation eventually leads to the decomposition. This may clarify why some highly oxidized species were not possible to isolate.

Table S29. Summary of all relevant interligand, intermetal or metal-ligand distances (in Å) for the DFT optimized Y(III) analogues of the double-, triple-and quadruple-deckers in various oxidation states. For distance determination, the planes of the ligands were defined to be the planes formed by the 4 coordinated N-atoms.

	Y^{III}-Y^{III}	Y^{III}-Pc(out)	Y^{III}-Pc (inner)	Pc(outer)-Pc(inner)	Pc(inner1)-Pc(inner2)	Y^{III}-Cd^{II}	Cd^{II}-Pc (inner)	Cd^{II}-Cd^{II}
$[3]^0$	3.580	1.271	1.790	3.061	/	/	/	/
$[3]^+$	3.490	1.245	1.745	2.990	/	/	/	/
$[3]^{2+}$	3.466	1.233	1.733	2.966	/	/	/	/
$[3]^{3+}$	3.451	1.245	1.725	2.970	/	/	/	/
$[4]^0$	6.798	1.300	1.721	3.021	3.340	3.399	1.670	/
$[4]^+$	6.719	1.288	1.682	2.970	3.357	3.360	1.679	/
$[4]^{2+}$	6.685	1.285	1.662	2.947	3.361	3.343	1.681	/
$[4]^{3+}$	6.662	1.284	1.631	2.915	3.399	3.331	1.699	/
$[4]^{4+}$	6.649	1.280	1.619	2.899	3.411	3.324	1.706	/
$[5]^0$	10.088	1.309	1.715	3.024	3.329	3.428	1.713	3.233
$[5]^+$	10.018	1.307	1.695	2.966	3.350	3.405	1.747	3.207
$[5]^{2+}$	9.977	1.299	1.627	2.926	3.361	3.396	1.796	3.184
$[5]^{3+}$	9.961	1.299	1.597	2.896	3.383	3.396	1.799	3.169
$[5]^{4+}$	9.955	1.296	1.582	2.878	3.396	3.398	1.817	3.158
$[5]^{5+}$	9.988	1.288	1.608	2.896	3.386	3.365	1.756	3.259

4.6. XYZ coordinates of the optimized structures

Given below in 3 columns per page.

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[3]^0

Y	0.000000	0.000000	-1.789800
O	5.478600	5.665200	-3.835700
O	7.124600	-3.366500	-3.805700
O	-5.665200	5.478600	-3.835700
O	-5.478600	-5.665200	-3.835700
O	-7.124600	3.366500	-3.805700
O	5.665200	-5.478600	-3.835700
O	-3.366500	-7.124600	-3.805600
O	3.366500	7.124600	-3.805600
N	-3.316700	-0.598800	-3.301300
N	1.635500	-1.138600	-3.060700
N	1.138600	1.635500	-3.060700
N	-0.598800	3.316700	-3.301300
N	0.598800	-3.316700	-3.301300
N	-1.138600	-1.635500	-3.060700
N	3.316700	0.598800	-3.301300
N	-1.635500	1.138600	-3.060700
C	-2.914900	0.668400	-3.251400
C	-0.668400	-2.914900	-3.251400
C	2.914900	-0.668400	-3.251400
C	-1.647100	2.500400	-3.254600
C	1.794800	3.817800	-3.464300
C	0.668400	2.914900	-3.251400
C	-2.500300	-1.647100	-3.254600
C	1.647100	-2.500400	-3.254600
C	-3.817800	1.794800	-3.464400
C	-2.948200	-3.019600	-3.467500
C	1.868700	5.210400	-3.610900
H	0.958300	5.808400	-3.595600
C	3.817800	-1.794800	-3.464400
C	3.131700	5.790900	-3.723400
C	-3.131700	-5.790900	-3.723400
C	3.585200	-4.222100	-3.624700
H	2.945200	-5.104000	-3.630400
C	5.210300	-1.868700	-3.611000
H	5.808300	-0.958200	-3.595700
C	2.500300	1.647100	-3.254600
C	-3.585200	4.222100	-3.624700
H	-2.945200	5.104000	-3.630400
C	4.222100	3.585200	-3.624700
H	5.104000	2.945200	-3.630400
C	3.019600	-2.948200	-3.467600
C	-1.794800	-3.817800	-3.464300
C	-5.790900	3.131700	-3.723400
C	4.313300	4.972900	-3.734800
C	-5.210300	1.868700	-3.611000
H	-5.808300	0.958200	-3.595700
C	-1.868700	-5.210400	-3.610900
H	-0.958300	-5.808400	-3.595600
C	-3.019600	2.948200	-3.467600
C	4.972900	-4.313200	-3.734800
C	2.948200	3.019600	-3.467500
C	-4.972900	4.313200	-3.734800
C	-4.313300	-4.972900	-3.734800
C	5.790900	-3.131700	-3.723400
C	-4.222100	-3.585200	-3.624700
H	-5.104000	-2.945200	-3.630400
C	2.259100	8.005400	-3.741300
H	2.671400	9.016400	-3.853600
H	1.542500	7.813200	-4.559100
H	1.740700	7.929800	-2.770200
C	8.005400	-2.259000	-3.741500
H	7.813100	-1.542500	-4.559300
H	7.929800	-1.740600	-2.770400
H	9.016400	-2.671400	-3.853800
C	4.931500	-6.683400	-3.896200
H	4.337800	-6.845100	-2.977800
H	4.251900	-6.701000	-4.766500
H	5.671300	-7.488100	-3.995900
C	-2.259100	-8.005400	-3.741300
H	-1.542500	-7.813200	-4.559100
H	-1.740700	-7.929800	-2.770200
H	-2.671400	-9.016400	-3.853600
C	-6.683400	-4.931500	-3.896200
H	-6.845200	-4.337800	-2.977800
H	-6.701000	-4.251800	-4.766600
H	-7.488100	-5.671300	-3.995900
C	-8.005400	2.259000	-3.741500
H	-9.016400	2.671400	-3.853800
H	-7.813100	1.542500	-4.559300
H	-7.929800	1.740600	-2.770400
C	-4.931500	6.683400	-3.896200
H	-4.337800	6.845100	-2.977800
H	-4.251900	6.701000	-4.766500
H	-5.671300	7.488100	-3.995900
C	6.683400	4.931500	-3.896200
H	6.845200	4.337800	-2.977800
H	6.701000	4.251800	-4.766600
H	7.488100	5.671300	-3.995900
O	7.892200	0.031200	-0.000400
O	2.496600	7.480800	-0.000100
O	7.480800	-2.496600	-0.000300
O	-0.031200	7.892200	-0.000200
N	0.297600	1.915300	-0.000000
N	1.915300	-0.297600	-0.000000
N	2.728300	1.986500	-0.000000
N	-1.986500	2.728300	-0.000100
C	1.528800	2.555500	-0.000000
C	-0.671200	2.907900	-0.000100
C	-0.572000	5.515600	-0.000200
H	-1.651200	5.663300	-0.000200
C	5.056700	-2.257200	-0.000200
H	4.856400	-3.327300	-0.000200
C	2.257200	5.056700	-0.000100
H	3.327300	4.856400	-0.000100
C	6.580800	-0.326000	-0.000200
C	3.994400	-1.341500	-0.000100
C	6.352200	-1.747100	-0.000200
C	1.747100	6.352200	-0.000200
C	1.341500	3.994400	-0.000100
C	5.515600	0.572000	-0.000100
H	5.663300	1.651200	-0.000200
C	2.907900	0.671200	-0.000000
C	0.326000	6.580800	-0.000200
C	-2.555500	1.528800	-0.000100
C	-0.043700	4.216300	-0.000100
C	4.216300	0.043700	-0.000100
O	-7.892200	-0.031200	-0.000400
O	-2.496600	-7.480800	-0.000100
O	-7.480800	2.496600	-0.000300
O	0.031200	-7.892200	-0.000200
N	-0.297600	-1.915300	-0.000000
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N	-2.728300	-1.986500	-0.000000
N	1.986500	-2.728300	-0.000100
C	-1.528800	-2.555500	-0.000000
C	0.671200	-2.907900	-0.000100
C	0.572000	-5.515600	-0.000200
H	1.651200	-5.663300	-0.000200
C	-5.056700	2.257200	-0.000200
H	-4.856400	3.327300	-0.000200
C	-2.257200	-5.056700	-0.000100
H	-3.327300	-4.856400	-0.000100
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C	-3.994400	1.341500	-0.000100
C	-6.352200	1.747100	-0.000200
C	-1.747100	-6.352200	-0.000200
C	-1.341500	-3.994400	-0.000100
C	-5.515600	-0.572000	-0.000100
H	-5.663300	-1.651200	-0.000200
C	-2.907900	-0.671200	-0.000000
C	-0.326000	-6.580800	-0.000200
C	0.043700	-4.216300	-0.000100
C	-4.216300	-0.043700	-0.000100
C	2.555500	-1.528800	-0.000100
C	-1.409500	8.205100	-0.000200
H	-1.914900	7.807400	-0.898300
H	-1.914800	7.807400	0.898100
H	-1.474600	9.300700	-0.000200
C	3.912600	7.353700	-0.000500
H	4.265000	6.832100	-0.905800
H	4.302400	8.379400	-0.000500
H	4.265500	6.832000	0.904600
C	8.205100	1.409500	-0.000300
H	7.807300	1.914900	-0.898400
H	7.807500	1.914800	0.898000
H	9.300700	1.474600	-0.000400
C	7.353700	-3.912600	-0.000600
H	8.379400	-4.302400	-0.000600
H	6.832000	-4.265500	0.904400
H	6.832100	-4.265000	-0.905900
C	1.409500	-8.205100	-0.000200
H	1.914900	-7.807400	-0.898300
H	1.914800	-7.807400	0.898100
H	1.474600	-9.300700	-0.000200
C	-3.912600	-7.353700	-0.000500
H	-4.302400	-8.379400	-0.000500
H	-4.265500	-6.832000	0.904600
H	-4.265000	-6.832100	-0.905800
C	-8.205100	-1.409500	-0.000300
H	-7.807300	-1.914900	-0.898400
H	-7.807500	-1.914800	0.898000
H	-9.300700	-1.474600	-0.000400
C	-7.353700	3.912600	-0.000600
H	-6.832100	4.265000	-0.905900
H	-8.379400	4.302400	-0.000600
H	-6.832000	4.265500	0.904400
Y	0.000000	0.000000	1.789700
O	-5.481700	-5.662200	3.836200
O	-7.122700	3.370400	3.806000
O	5.662100	-5.481700	3.836300
O	5.481700	5.662200	3.836200
O	7.122700	-3.370400	3.806000
O	-5.662100	5.481700	3.836300
O	3.370400	7.122700	3.805900
O	-3.370400	-7.122700	3.805900
N	3.317100	0.596900	3.301200
N	-1.634900	1.139600	3.060600
N	-1.139600	-1.634900	3.060600
N	0.596800	-3.317100	3.301200
N	-0.596800	3.317100	3.301200
N	1.139600	1.634900	3.060600
N	-3.317100	-0.596900	3.301200
N	1.634900	-1.139600	3.060600
C	2.914500	-0.670100	3.251300
C	0.670100	2.914500	3.251300
C	-2.914500	0.670100	3.251300
C	1.645700	-2.501300	3.254500
C	-1.797000	-3.816800	3.464300
C	-0.670100	-2.914500	3.251300
C	2.501300	1.645700	3.254500
C	-1.645700	2.501300	3.254500
C	3.816800	-1.797000	3.464300
C	2.950000	3.017900	3.467500
C	-1.871500	-5.209300	3.611000
H	-0.961400	-5.807700	3.595700
C	-3.816800	1.797000	3.464300
C	-3.134900	-5.789100	3.723600
C	3.134900	5.789100	3.723600
C	-3.582800	4.224200	3.624900
H	-2.942400	5.105700	3.630700
C	-5.209300	1.871600	3.611000
H	-5.807700	0.961500	3.595600
C	-2.501300	-1.645700	3.254500
C	3.582800	-4.224200	3.624900
H	2.942400	-5.105700	3.630700
C	-4.224200	-3.582900	3.624900
H	-5.105700	-2.942400	3.630600
C	-3.017900	2.950000	3.467500
C	1.797000	3.816800	3.464300
C	5.789100	-3.134900	3.723600
C	-4.316000	-4.970500	3.735100
C	5.209300	-1.871600	3.611000
H	5.807700	-0.961500	3.595600
C	1.871500	5.209300	3.611000
H	0.961400	5.807700	3.595700
C	3.017900	-2.950000	3.467500
C	-4.970500	4.316000	3.735100
C	-2.950000	-3.017900	3.467500

C	4.970500	-4.316000	3.735100
C	4.316000	4.970500	3.735100
C	-5.789100	3.134900	3.723600
C	4.224200	3.582900	3.624900
H	5.105700	2.942400	3.630600
C	-4.927800	6.686100	3.896800
H	-4.248000	6.703300	4.767000
H	-4.334200	6.847600	2.978300
H	-5.667200	7.491200	3.996700
C	-8.004100	2.263300	3.742000
H	-7.928900	1.744800	2.770900
H	-7.812000	1.546800	4.559800
H	-9.014800	2.676200	3.854400
C	-6.686100	-4.927900	3.896600
H	-6.703400	-4.248100	4.766800
H	-6.847600	-4.334200	2.978100
H	-7.491200	-5.667200	3.996400
C	-2.263300	-8.004100	3.742000
H	-1.546800	-7.812000	4.559800
H	-2.676200	-9.014800	3.854400
H	-1.744800	-7.928900	2.770900
C	4.927800	-6.686100	3.896800
H	4.248000	-6.703300	4.767000
H	4.334200	-6.847600	2.978300
H	5.667200	-7.491200	3.996700
C	8.004100	-2.263300	3.742000
H	7.812000	-1.546800	4.559800
H	9.014800	-2.676200	3.854400
H	7.928900	-1.744800	2.770900
C	6.686100	4.927900	3.896600
H	6.703400	4.248100	4.766800
H	6.847600	4.334200	2.978100
H	7.491200	5.667200	3.996400
C	2.263300	8.004100	3.742000
H	1.744800	7.928900	2.770900
H	1.546800	7.812000	4.559800
H	2.676200	9.014800	3.854400

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Y	0.000000	0.000000	1.754500
O	0.050600	7.809900	4.246800
O	-7.379800	2.579200	4.170800
O	7.809900	-0.050600	4.246800
O	-0.050600	-7.809900	4.246800
O	7.379800	-2.579200	4.170800
O	-7.809900	0.050600	4.246800
O	-2.579200	-7.379800	4.170800
O	2.579200	7.379800	4.170800
N	1.949500	-2.745700	3.279200
N	-1.970200	0.330900	3.004200
N	0.330900	1.970200	3.004200
N	2.745700	1.949500	3.279300
N	-2.745700	-1.949500	3.279300
N	-0.330900	-1.970200	3.004200
N	-1.949500	2.745700	3.279200
N	1.970200	-0.330900	3.004200
C	2.549900	-1.561100	3.223100
C	-1.561100	-2.549900	3.223100
C	-2.549900	1.561100	3.223100
C	2.925400	0.632200	3.230300
C	1.387300	3.973400	3.495100
C	1.561100	2.549900	3.223100
C	0.632200	-2.925400	3.230300
C	-2.925400	-0.632200	3.230300
C	3.973400	-1.387300	3.495100
C	-0.006000	-4.210500	3.505300
C	2.309300	4.999400	3.737800
H	3.377500	4.786500	3.729500
C	-3.973400	1.387300	3.495100
C	1.813300	6.284300	3.966400
C	-1.813300	-6.284300	3.966400
C	-5.486400	-0.510200	3.772800
H	-5.645400	-1.587800	3.799800
C	-4.999500	2.309300	3.737800
H	-4.786500	3.377500	3.729500
C	-0.632200	2.925400	3.230300
C	5.486400	0.510200	3.772800
H	5.645400	1.587800	3.799800
C	-0.510200	5.486500	3.772700
H	-1.587800	5.645400	3.799800
C	-4.210500	0.006000	3.505300
C	-1.387300	-3.973400	3.495100
C	6.284300	-1.813300	3.966400
C	0.395400	6.527200	3.994600
C	4.999500	-2.309300	3.737800
H	4.786500	-3.377500	3.729500
C	-2.309300	-4.999400	3.737800
H	-3.377500	-4.786500	3.729500
C	4.210500	-0.006000	3.505300
C	-6.527200	0.395400	3.994600
C	0.006000	4.210500	3.505300
C	6.527200	-0.395400	3.994600
C	-0.395400	-6.527200	3.994600
C	-6.284300	1.813300	3.966400
C	0.510200	-5.486500	3.772700
H	1.587800	-5.645400	3.799800
C	3.986200	7.217100	4.231900
H	4.397100	8.213500	4.435600
H	4.274200	6.528300	5.044500
H	4.391700	6.841300	3.276100
C	-7.217100	3.986200	4.231800
H	-6.528300	4.274200	5.044500
H	-6.841300	4.391700	3.276000
H	-8.213500	4.397100	4.435600
C	-8.130500	-1.323000	4.355200
H	-7.939700	-1.857700	3.407300
H	-7.557000	-1.808300	5.163800
H	-9.201300	-1.368400	4.588800
C	-3.986200	-7.217100	4.231900
H	-4.274200	-6.528300	5.044500
H	-4.391700	-6.841300	3.276100
H	-4.397100	-8.213500	4.435600
C	1.323000	-8.130500	4.355100
H	1.857700	-7.939800	3.407200
H	1.808300	-7.557000	5.163700
H	1.368400	-9.201300	4.588700
C	7.217100	-3.986200	4.231800
H	8.213500	-4.397100	4.435600
H	6.528300	-4.274200	5.044500
H	6.841300	-4.391700	3.276000
C	8.130500	1.323000	4.355200
H	7.939700	1.857700	3.407300
H	7.557000	1.808300	5.163800
H	9.201300	1.368400	4.588800
C	-1.323000	8.130500	4.355100
H	-1.857700	7.939800	3.407200
H	-1.808300	7.557000	5.163700
H	-1.368400	9.201300	4.588700
O	-4.634800	6.388700	0.001000
O	4.558500	6.431200	0.001000
O	-6.431200	4.558500	0.001000
O	6.388700	4.634800	0.001100
N	1.374300	1.367900	-0.000200
N	-1.367900	1.374300	-0.000200
N	0.000000	3.376800	-0.000000
N	3.376800	0.000000	-0.000000
C	1.165000	2.742500	-0.000100
C	2.748000	1.171700	-0.000000
C	4.796700	2.793000	0.000400
H	5.556600	2.012700	0.000500
C	-4.802500	2.752700	0.000300
H	-5.545600	1.957000	0.000400
C	2.752700	4.802500	0.000400
H	1.957000	5.545600	0.000400
C	-4.149000	5.127900	0.000700
C	-3.437300	2.439500	0.000100
C	-5.160000	4.100200	0.000600
C	4.100200	5.160000	0.000700
C	2.439500	3.437300	0.000100
C	-2.793000	4.796700	0.000400
H	-2.012700	5.556600	0.000400
C	-1.171700	2.748000	-0.000100
C	5.127900	4.149000	0.000700
C	2.742500	-1.165000	-0.000100
C	3.436600	2.450700	0.000100
C	-2.450700	3.436600	0.000100
O	4.634800	-6.388700	0.001000
O	-4.558500	-6.431200	0.001000
O	6.431200	-4.558500	0.001000
O	-6.388700	-4.634800	0.001100
N	-1.374300	-1.367900	-0.000200
N	1.367900	-1.374300	-0.000200
N	-0.000000	-3.376800	-0.000000
N	-3.376800	0.000000	-0.000000
C	-1.165000	-2.742500	-0.000100
C	-2.748000	-1.171700	-0.000000
C	-4.796700	-2.793000	0.000400
H	-5.556600	-2.012700	0.000500
C	4.802500	-2.752700	0.000300
H	5.545600	-1.957000	0.000400
C	-2.752700	-4.802500	0.000400
H	-1.957000	-5.545600	0.000400
C	4.149000	-5.127900	0.000700
C	3.437300	-2.439500	0.000100
C	5.160000	-4.100200	0.000600
C	-4.100200	-5.160000	0.000700
C	-2.439500	-3.437300	0.000100
C	2.793000	-4.796700	0.000400
H	2.012700	-5.556600	0.000400
C	1.171700	-2.748000	-0.000100
C	-5.127900	-4.149000	0.000700
C	-3.436600	-2.450700	0.000100
C	2.450700	-3.436600	0.000100
C	-2.742500	1.165000	-0.000100
C	7.465900	3.716600	0.001200
H	7.447700	3.075100	0.899700
H	7.448100	3.075400	-0.897500
H	8.381200	4.321000	0.001500
C	3.612700	7.492400	0.001100
H	2.977100	7.461700	0.902100
H	4.201300	8.417900	0.001100
H	2.977100	7.461800	-0.899900
C	-3.716600	7.465900	0.001100
H	-3.075100	7.447700	0.899500
H	-3.075400	7.448000	-0.897600
H	-4.321000	8.381200	0.001400
C	-7.492400	3.612700	0.001100
H	-8.417900	4.201300	0.001100
H	-7.461800	2.977000	-0.899900
H	-7.461700	2.977100	0.902100
C	-7.465900	-3.716600	0.001200
H	-7.447700	-3.075100	0.899700
H	-7.448100	-3.075400	-0.897500
H	-8.381200	-4.321000	0.001500
C	-3.612700	-7.492400	0.001100
H	-4.201300	-8.417900	0.001100
H	-2.977100	-7.461800	-0.899900
H	-2.977100	-7.461700	0.902100
C	3.716600	-7.465900	0.001100
H	3.075100	-7.447700	0.899500
H	3.075400	-7.448000	-0.897600
H	4.321000	-8.381200	0.001400
C	7.492400	-3.612700	0.001100
H	7.461700	-2.977100	0.902100
H	8.417900	-4.201300	0.001100
H	7.461800	-2.977000	-0.899900
Y	0.000000	0.000000	-1.754300
O	-0.045200	-7.809700	-4.247900
O	7.381400	-2.574200	-4.171800
O	-7.809700	0.045200	-4.247700
O	0.045200	7.809700	-4.247900
O	-7.381400	2.574200	-4.171800
O	7.809700	-0.045200	-4.247700
O	2.574200	7.381400	-4.171900
O	-2.574200	-7.381400	-4.171900
N	-1.951400	2.744400	-3.279200
N	1.970500	-0.329600	-3.004200
N	-0.329600	-1.970500	-3.004200
N	-2.744400	-1.951400	-3.279200
N	2.744400	1.951400	-3.279200
N	0.329600	1.970500	-3.004200
N	1.951400	-2.744400	-3.279200
N	-1.970500	0.329600	-3.004200
C	-2.550900	1.559300	-3.223100
C	1.559300	2.550900	-3.223100
C	2.550900	-1.559300	-3.223100
C	-2.924900	-0.634200	-3.230300
C	-1.384600	-3.974300	-3.495200
C	-1.559300	-2.550900	-3.223100

C	-0.634200	2.924900	-3.230300
C	2.924900	0.634200	-3.230300
C	-3.974300	1.384600	-3.495200
C	0.003100	4.210500	-3.505400
C	-2.305900	-5.000900	-3.738100
H	-3.374200	-4.788700	-3.729900
C	3.974300	-1.384600	-3.495200
C	-1.809000	-6.285400	-3.967100
C	1.809000	6.285400	-3.967100
C	5.486000	0.513900	-3.773100
H	5.644200	1.591600	-3.800100
C	5.000900	-2.305900	-3.738100
H	4.788700	-3.374200	-3.729900
C	0.634200	-2.924900	-3.230300
C	-5.486000	-0.513900	-3.773100
H	-5.644200	-1.591600	-3.800100
C	0.513900	-5.486000	-3.773100
H	1.591600	-5.644200	-3.800200
C	4.210500	-0.003100	-3.505400
C	1.384600	3.974300	-3.495200
C	-6.285400	1.809000	-3.967000
C	-0.390900	-6.527300	-3.995300
C	-5.000900	2.305900	-3.738100
H	-4.788700	3.374200	-3.729900
C	2.305900	5.000900	-3.738100
H	3.374200	4.788700	-3.729900
C	-4.210500	0.003100	-3.505400
C	6.527400	-0.390900	-3.995200
C	-0.003100	-4.210500	-3.505400
C	-6.527400	0.390900	-3.995200
C	0.390900	6.527300	-3.995300
C	6.285400	-1.809000	-3.967000
C	-0.513900	5.486000	-3.773100
H	-1.591600	5.644200	-3.800200
C	8.129400	1.328600	-4.356100
H	7.555300	1.813500	-5.164500
H	7.938500	1.863100	-3.408100
H	9.200100	1.374600	-4.590000
C	7.219600	-3.981200	-4.233100
H	6.844100	-4.387200	-3.277400
H	6.530800	-4.269500	-5.045700
H	8.216200	-4.391500	-4.437100
C	1.328600	-8.129400	-4.356200
H	1.813500	-7.555300	-5.164600
H	1.863100	-7.938500	-3.408300
H	1.374700	-9.200100	-4.590100
C	-3.981200	-7.219600	-4.233200
H	-4.269500	-6.530800	-5.045800
H	-4.391500	-8.216200	-4.437200
H	-4.387200	-6.844100	-3.277400
C	-8.129400	-1.328600	-4.356100
H	-7.555300	-1.813500	-5.164500
H	-7.938500	-1.863100	-3.408100
H	-9.200100	-1.374600	-4.590000
C	-7.219600	3.981200	-4.233100
H	-6.530800	4.269500	-5.045700
H	-8.216200	4.391500	-4.437100
H	-6.844100	4.387200	-3.277400
C	-1.328600	8.129400	-4.356200
H	-1.813500	7.555300	-5.164600
H	-1.863100	7.938500	-3.408300
H	-1.374700	9.200100	-4.590100
C	3.981200	7.219600	-4.233200
H	4.387200	6.844100	-3.277400
H	4.269500	6.530800	-5.045800
H	4.391500	8.216200	-4.437200

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Y	0.000000	0.000000	1.738400
O	2.042700	7.483100	4.441800
O	-6.418500	4.369600	4.381600
O	7.483100	-2.042700	4.442000
O	-2.042700	-7.483100	4.441800
O	6.418500	-4.369600	4.381600
O	-7.483100	2.042700	4.442000
O	-4.369600	-6.418500	4.381500
O	4.369600	6.418500	4.381500
N	1.175600	-3.154200	3.261600
N	-1.820100	0.828600	2.971200
N	0.828600	1.820100	2.971200
N	3.154200	1.175600	3.261600
N	-3.154200	-1.175600	3.261600
N	-0.828600	-1.820100	2.971200
N	-1.175600	3.154200	3.261600
N	1.820100	-0.828600	2.971200
C	2.061700	-2.165600	3.204300
C	-2.165600	-2.061700	3.204300
C	-2.061700	2.165600	3.204300
C	2.988600	-0.144200	3.211100
C	2.362300	3.476300	3.507800
C	2.165600	2.061700	3.204300
C	-0.144200	-2.988600	3.211100
C	-2.988600	0.144200	3.211100
C	3.476300	-2.362300	3.507800
C	-1.088900	-4.061000	3.517300
C	3.512100	4.215700	3.808800
H	4.488600	3.733000	3.813300
C	-3.476300	2.362300	3.507800
C	3.359000	5.574800	4.099800
C	-3.359000	-5.574800	4.099800
C	-5.413300	0.911300	3.839300
H	-5.843100	-0.089300	3.872200
C	-4.215600	3.512100	3.808900
H	-3.733000	4.488600	3.813400
C	0.144200	2.988600	3.211100
C	5.413300	-0.911300	3.839300
H	5.843100	0.089300	3.872200
C	0.911300	5.413300	3.839200
H	-0.089300	5.843100	3.872100
C	-4.061000	1.088900	3.517400
C	-2.362300	-3.476300	3.507800
C	5.574800	-3.359000	4.099900
C	2.050000	6.175400	4.123200
C	4.215600	-3.512100	3.808900
H	3.733000	-4.488600	3.813400
C	-3.512100	-4.215700	3.808800
H	-4.488600	-3.733000	3.813300
C	4.061000	-1.088900	3.517400
C	-6.175400	2.050000	4.123300
C	1.088900	4.061000	3.517300
C	6.175400	-2.050000	4.123300
C	-2.050000	-6.175400	4.123200
C	-5.574800	3.359000	4.099900
C	-0.911300	-5.413300	3.839200
H	0.089300	-5.843100	3.872100
C	5.685300	5.897000	4.496700
H	6.323900	6.747300	4.763500
H	5.740600	5.131600	5.288800
H	6.031100	5.461900	3.542900
C	-5.897000	5.685300	4.496900
H	-5.131500	5.740600	5.289000
H	-5.461900	6.031100	3.543100
H	-6.747200	6.323900	4.763700
C	-8.148000	0.798400	4.583100
H	-8.160400	0.240300	3.630400
H	-7.673900	0.178400	5.362600
H	-9.176300	1.036800	4.879300
C	-5.685300	-5.897000	4.496700
H	-5.740600	-5.131600	5.288800
H	-6.031100	-5.461900	3.542900
H	-6.323900	-6.747300	4.763500
C	-0.798400	-8.148100	4.583000
H	-0.240300	-8.160400	3.630200
H	-0.178400	-7.674000	5.362500
H	-1.036800	-9.176400	4.879000
C	5.897000	-5.685300	4.496900
H	6.747200	-6.323900	4.763700
H	5.131500	-5.740600	5.289000
H	5.461900	-6.031100	3.543100
C	8.148000	-0.798400	4.583100
H	8.160400	-0.240300	3.630400
H	7.673900	-0.178400	5.362600
H	9.176300	-1.036800	4.879300
C	0.798400	8.148100	4.583000
H	0.240300	8.160400	3.630200
H	0.178400	7.674000	5.362500
H	1.036800	9.176400	4.879000
O	-2.400100	7.514700	0.073000
O	6.343700	4.675100	0.093100
O	-4.675100	6.343700	0.092800
O	7.514700	2.400100	0.073100
N	1.731500	0.871400	-0.004500
N	-0.871400	1.731500	-0.004500
N	1.054300	3.209300	0.003200
N	3.209300	-1.054300	0.003100
C	1.964100	2.243900	0.002100
C	2.976200	0.255800	0.000900
C	5.428600	1.150600	0.029700
H	5.905800	0.171700	0.026900
C	-3.702300	4.118200	0.037200
H	-4.658400	3.597300	0.043100
C	4.118200	3.702300	0.037400
H	3.597300	4.658400	0.043300
C	-2.334200	6.171000	0.053300
C	-2.505000	3.393400	0.014500
C	-3.618300	5.512000	0.060400
C	5.512000	3.618300	0.060600
C	3.393400	2.505000	0.014600
C	-1.150600	5.428600	0.029600
H	-0.171700	5.905800	0.027000
C	-0.255800	2.976200	0.000900
C	6.171000	2.334300	0.053400
C	2.243900	-1.964100	0.002100
C	4.031100	1.255400	0.012200
C	-1.255400	4.031100	0.012200
O	2.400100	-7.514700	0.073000
O	-6.343700	-4.675100	0.093100
O	4.675100	-6.343700	0.092800
O	-7.514700	-2.400100	0.073100
N	-1.731500	-0.871400	-0.004500
N	0.871400	-1.731500	-0.004500
N	-1.054300	-3.209300	0.003200
N	-3.209300	1.054300	0.003100
C	-1.964100	-2.243900	0.002100
C	-2.976200	-0.255800	0.000900
C	-5.428600	-1.150600	0.029700
H	-5.905800	-0.171700	0.026900
C	3.702300	-4.118200	0.037200
H	4.658400	-3.597300	0.043100
C	-4.118200	-3.702300	0.037400
H	-3.597300	-4.658400	0.043300
C	2.334200	-6.171000	0.053300
C	2.505000	-3.393400	0.014500
C	3.618300	-5.512000	0.060400
C	-5.512000	-3.618300	0.060600
C	-3.393400	-2.505000	0.014600
C	1.150600	-5.428600	0.029600
H	0.171700	-5.905800	0.027000
C	0.255800	-2.976200	0.000900
C	-6.171000	-2.334300	0.053400
C	-4.031100	-1.255400	0.012200
C	1.255400	-4.031100	0.012200
C	-2.243900	1.964100	0.002100
C	8.259800	1.192900	0.065400
H	8.035200	0.579400	0.954700
H	8.053900	0.602000	-0.843500
H	9.315400	1.488800	0.080200
C	5.789500	5.984500	0.081400
H	5.161200	6.160300	0.970800
H	6.643500	6.671800	0.093900
H	5.190600	6.155200	-0.829000
C	-1.192900	8.259800	0.065300
H	-0.579500	8.035200	0.954700
H	-0.601900	8.053900	-0.843500
H	-1.488800	9.315400	0.080100
C	-5.984500	5.789500	0.081000
H	-6.671800	6.643600	0.093400
H	-6.155100	5.190600	-0.829500
H	-6.160400	5.161200	0.970400
C	-8.259800	-1.192900	0.065400
H	-8.035200	-0.579400	0.954700
H	-8.053900	-0.602000	-0.843500
H	-9.315400	-1.488800	0.080200
C	-5.789500	-5.984500	0.081400
H	-6.643500	-6.671800	0.093900
H	-5.190600	-6.155200	-0.829000
H	-5.161200	-6.160300	0.970800
C	1.192900	-8.259800	0.065300
H	0.579500	-8.035200	0.954700

H	0.601900	-8.053900	-0.843500
H	1.488800	-9.315400	0.080100
C	5.984500	-5.789500	0.081000
H	6.160400	-5.161200	0.970400
H	6.671800	-6.643600	0.093400
H	6.155100	-5.190600	-0.829500
Y	0.000000	0.000000	-1.727700
O	-1.659600	-7.554800	-4.515300
O	6.604500	-4.034200	-4.487200
O	-7.554700	1.659700	-4.515400
O	1.659600	7.554800	-4.515300
O	-6.604500	4.034200	-4.487200
O	7.554700	-1.659700	-4.515400
O	4.034100	6.604500	-4.487300
O	-4.034100	-6.604500	-4.487300
N	-1.325700	3.093600	-3.257500
N	1.859000	-0.742000	-2.961200
N	-0.742000	-1.859000	-2.961200
N	-3.093600	-1.325700	-3.257600
N	3.093600	1.325700	-3.257600
N	0.742000	1.859000	-2.961200
N	1.325700	-3.093600	-3.257500
N	-1.859000	0.742000	-2.961200
C	-2.164400	2.063800	-3.201100
C	2.063800	2.164400	-3.201100
C	2.164400	-2.063800	-3.201100
C	-2.991400	0.000000	-3.204900
C	-2.190400	-3.584900	-3.518300
C	-2.063800	-2.164400	-3.201100
C	0.000000	2.991400	-3.204800
C	2.991400	-0.000000	-3.204900
C	-3.584900	2.190400	-3.518300
C	0.890000	4.106400	-3.523300
C	-3.298200	-4.375400	-3.847400
H	-4.297400	-3.941500	-3.859700
C	3.584900	-2.190400	-3.518300
C	-3.073400	-5.719200	-4.164100
C	3.073400	5.719200	-4.164100
C	5.442500	-0.641000	-3.862700
H	5.821000	0.380300	-3.889200
C	4.375400	-3.298300	-3.847300
H	3.941500	-4.297400	-3.859600
C	-0.000000	-2.991400	-3.204800
C	-5.442500	0.641000	-3.862700
H	-5.821000	-0.380300	-3.889200
C	-0.641000	-5.442500	-3.862600
H	0.380300	-5.821000	-3.889100
C	4.106300	-0.890000	-3.523300
C	2.190400	3.584900	-3.518300
C	-5.719200	3.073400	-4.164100
C	-1.736400	-6.255000	-4.175400
C	-4.375400	3.298300	-3.847300
H	-3.941500	4.297400	-3.859600
C	3.298200	4.375400	-3.847400
H	4.297400	3.941500	-3.859700
C	-4.106300	0.890000	-3.523300
C	6.255000	-1.736500	-4.175500
C	-0.890000	-4.106400	-3.523300
C	-6.255000	1.736500	-4.175500
C	1.736400	6.255000	-4.175400
C	5.719200	-3.073400	-4.164100
C	0.641000	5.442500	-3.862600
H	-0.380300	5.821000	-3.889100
C	8.155800	-0.381800	-4.645700
H	7.641100	0.225300	-5.409500
H	8.153700	0.162300	-3.684900
H	9.190300	-0.564900	-4.959000
C	6.150200	-5.373400	-4.606800
H	5.761000	-5.753600	-3.646300
H	5.366400	-5.459900	-5.378000
H	7.025000	-5.962900	-4.905600
C	-0.381700	-8.155800	-4.645500
H	0.225300	-7.641200	-5.409300
H	0.162200	-8.153700	-3.684700
H	-0.564900	-9.190400	-4.958800
C	-5.373300	-6.150200	-4.607000
H	-5.459800	-5.366400	-5.378300
H	-5.962800	-7.025000	-4.905800
H	-5.753600	-5.760900	-3.646500
C	-8.155800	0.381800	-4.645700
H	-7.641100	-0.225300	-5.409500
H	-8.153700	-0.162300	-3.684900
H	-9.190300	0.564900	-4.959000
C	-6.150200	5.373400	-4.606800
H	-5.366400	5.459900	-5.378000
H	-7.025000	5.962900	-4.905600
H	-5.761000	5.753600	-3.646300
C	0.381700	8.155800	-4.645500
H	-0.225300	7.641200	-5.409300
H	-0.162200	8.153700	-3.684700
H	0.564900	9.190400	-4.958800
C	5.373300	6.150200	-4.607000
H	5.753600	5.760900	-3.646500
H	5.459800	5.366400	-5.378300
H	5.962800	7.025000	-4.905800

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Y	0.000000	0.000000	-1.725500
O	7.672600	0.006700	-4.733900
O	2.521400	-7.246300	-4.734500
O	-0.006700	7.672500	-4.734100
O	-7.672600	-0.006700	-4.733900
O	-2.521400	7.246300	-4.734500
O	0.006700	-7.672500	-4.734100
O	-7.246300	-2.521400	-4.734500
O	7.246300	2.521400	-4.734500
N	-2.741900	1.947100	-3.295400
N	0.334600	-1.974000	-2.970400
N	1.974000	0.334600	-2.970400
N	1.947100	2.741900	-3.295400
N	-1.947100	-2.741900	-3.295400
N	-1.974000	-0.334600	-2.970400
N	2.741900	-1.947100	-3.295400
N	-0.334600	1.974000	-2.970400
C	-1.557500	2.549200	-3.238800
C	-2.549200	-1.557500	-3.238800
C	1.557500	-2.549200	-3.238800
C	0.630500	2.920000	-3.238700
C	3.956000	1.380600	-3.593100
C	2.549200	1.557500	-3.238800
C	-2.920000	0.630500	-3.238600
C	-0.630500	-2.920000	-3.238700
C	-1.380600	3.956000	-3.593100
C	-4.190000	0.000000	-3.592900
C	4.946300	2.291500	-3.978600
H	4.733900	3.359700	-4.002600
C	1.380600	-3.956000	-3.593100
C	6.198900	1.781700	-4.347100
C	-6.198900	-1.781700	-4.347100
C	-0.533800	-5.425100	-3.978300
H	-1.612400	-5.576600	-4.002000
C	2.291500	-4.946300	-3.978600
H	3.359800	-4.733900	-4.002500
C	2.920000	-0.630500	-3.238600
C	0.533800	5.425100	-3.978300
H	1.612400	5.576600	-4.002000
C	5.425100	-0.533800	-3.978200
H	5.576600	-1.612400	-4.001800
C	0.000000	-4.190000	-3.593000
C	-3.956000	-1.380600	-3.593100
C	-1.781700	6.198900	-4.347200
C	6.439900	0.360200	-4.346900
C	-2.291500	4.946300	-3.978600
H	-3.359800	4.733900	-4.002500
C	-4.946300	-2.291500	-3.978600
H	-4.733900	-3.359700	-4.002600
C	0.000000	4.190000	-3.593000
C	0.360200	-6.439900	-4.347000
C	4.190000	-0.000000	-3.592900
C	-0.360200	6.439900	-4.347000
C	-6.439900	-0.360200	-4.346900
C	1.781700	-6.198900	-4.347200
C	-5.425100	0.533800	-3.978200
H	-5.576600	1.612400	-4.001800
C	7.095700	3.928800	-4.871800
H	8.063600	4.300600	-5.226500
H	6.313200	4.171900	-5.609400
H	6.851500	4.399200	-3.903900
C	3.928800	-7.095700	-4.871700
H	4.172000	-6.313200	-5.609300
H	4.399200	-6.851600	-3.903800
H	4.300600	-8.063600	-5.226300
C	-1.371700	-7.994000	-4.871100
H	-1.896200	-7.918200	-3.903200
H	-1.859100	-7.335500	-5.608800
H	-1.403900	-9.030500	-5.225400
C	-7.095700	-3.928800	-4.871800
H	-6.313200	-4.171900	-5.609400
H	-6.851500	-4.399200	-3.903900
H	-8.063600	-4.300600	-5.226500
C	-7.994100	1.371700	-4.870800
H	-7.918200	1.896100	-3.902900
H	-7.335600	1.859100	-5.608600
H	-9.030600	1.403900	-5.225200
C	-3.928800	7.095700	-4.871700
H	-4.300600	8.063600	-5.226300
H	-4.172000	6.313200	-5.609300
H	-4.399200	6.851600	-3.903800
C	1.371700	7.994000	-4.871100
H	1.896200	7.918200	-3.903200
H	1.859100	7.335500	-5.608800
H	1.403900	9.030500	-5.225400
C	7.994100	-1.371700	-4.870800
H	7.918200	-1.896100	-3.902900
H	7.335600	-1.859100	-5.608600
H	9.030600	-1.403900	-5.225200
O	7.086600	-3.453400	-0.000200
O	5.535700	5.612800	0.000200
O	5.612800	-5.535700	-0.000300
O	3.453400	7.086600	0.000300
N	1.119100	1.580800	-0.000100
N	1.580800	-1.119100	-0.000100
N	3.330600	0.569600	-0.000100
N	-0.569600	3.330600	-0.000100
C	2.511000	1.615400	-0.000100
C	0.689100	2.905000	-0.000000
C	1.922600	5.200200	0.000100
H	1.020600	5.810500	0.000200
C	3.541800	-4.265700	-0.000100
H	2.894000	-5.141100	-0.000200
C	4.265700	3.541800	0.000100
H	5.141100	2.894000	0.000100
C	5.770100	-3.198900	-0.000100
C	2.990900	-2.977300	-0.000100
C	4.935000	-4.378700	-0.000200
C	4.378700	4.935000	0.000200
C	2.977300	2.990900	0.000000
C	5.200200	-1.922600	-0.000100
H	5.810500	-1.020600	-0.000100
C	2.905000	-0.689100	-0.000100
C	3.198900	5.770100	0.000200
C	-1.615400	2.511000	-0.000100
C	1.831400	3.802000	0.000000
C	3.802000	-1.831400	-0.000100
O	-7.086600	3.453400	-0.000200
O	-5.535700	-5.612800	0.000200
O	-5.612800	5.535700	-0.000300
O	-3.453400	-7.086600	0.000300
N	-1.119100	-1.580800	-0.000100
N	-1.580800	1.119100	-0.000100
N	-3.330600	-0.569600	-0.000100
N	0.569600	-3.330600	-0.000100
C	-2.511000	-1.615400	-0.000100
C	-0.689100	-2.905000	-0.000000
C	-1.922600	-5.200200	0.000100
H	-1.020600	-5.810500	0.000200
C	-3.541800	4.265700	-0.000100
H	-2.894000	5.141100	-0.000200
C	-4.265700	-3.541800	0.000100
H	-5.141100	-2.894000	0.000100
C	-5.770100	3.198900	-0.000100
C	-2.990900	2.977300	-0.000100
C	-4.935000	4.378700	-0.000200
C	-4.378700	-4.935000	0.000200
C	-2.977300	-2.990900	0.000000
C	-5.200200	1.922600	-0.000100
H	-5.810500	1.020600	-0.000100
C	-2.905000	0.689100	-0.000100
C	-3.198900	-5.770100	0.000200

C	-1.831400	-3.802000	0.000000
C	-3.802000	1.831400	-0.000100
C	1.615400	-2.511000	-0.000100
C	2.366600	8.003300	0.000400
H	1.741300	7.877900	-0.899600
H	1.741400	7.877800	0.900500
H	2.816400	9.002800	0.000500
C	6.761600	4.892800	0.000200
H	6.851200	4.261400	-0.899800
H	7.554700	5.649300	0.000300
H	6.851200	4.261300	0.900200
C	8.003300	-2.366600	-0.000200
H	7.877800	-1.741400	-0.900200
H	7.877900	-1.741400	0.899900
H	9.002800	-2.816400	-0.000200
C	4.892800	-6.761600	-0.000400
H	5.649300	-7.554700	-0.000400
H	4.261400	-6.851300	0.899600
H	4.261400	-6.851100	-0.900400
C	-2.366600	-8.003300	0.000400
H	-1.741300	-7.877900	-0.899600
H	-1.741400	-7.877800	0.900500
H	-2.816400	-9.002800	0.000500
C	-6.761600	-4.892800	0.000200
H	-7.554700	-5.649300	0.000300
H	-6.851200	-4.261300	0.900200
H	-6.851200	-4.261400	-0.899800
C	-8.003300	2.366600	-0.000200
H	-7.877800	1.741400	-0.900200
H	-7.877900	1.741400	0.899900
H	-9.002800	2.816400	-0.000200
C	-4.892800	6.761600	-0.000400
H	-4.261400	6.851100	-0.900400
H	-5.649300	7.554700	-0.000400
H	-4.261400	6.851300	0.899600
Y	0.000000	0.000000	1.725500
O	-7.672500	-0.006800	4.734100
O	-2.521400	7.246200	4.734600
O	0.006700	-7.672500	4.733900
O	7.672500	0.006800	4.734100
O	2.521400	-7.246200	4.734600
O	-0.006700	7.672500	4.733900
O	7.246200	2.521400	4.734700
O	-7.246200	-2.521400	4.734700
N	2.741900	-1.947100	3.295400
N	-0.334600	1.974000	2.970400
N	-1.974000	-0.334600	2.970400
N	-1.947100	-2.741900	3.295400
N	1.947100	2.741900	3.295400
N	1.974000	0.334600	2.970400
N	-2.741900	1.947100	3.295400
N	0.334600	-1.974000	2.970400
C	1.557500	-2.549200	3.238700
C	2.549200	1.557500	3.238700
C	-1.557500	2.549200	3.238700
C	-0.630500	-2.920000	3.238600
C	-3.956000	-1.380600	3.593100
C	-2.549200	-1.557500	3.238700
C	2.920000	-0.630500	3.238600
C	0.630500	2.920000	3.238600
C	1.380600	-3.956000	3.593000
C	4.190000	0.000000	3.592900
C	-4.946200	-2.291500	3.978600
H	-4.733900	-3.359800	4.002600
C	-1.380600	3.956000	3.593000
C	-6.198900	-1.781700	4.347200
C	6.198900	1.781700	4.347200
C	0.533800	5.425100	3.978200
H	1.612400	5.576600	4.001800
C	-2.291500	4.946200	3.978600
H	-3.359700	4.733900	4.002600
C	-2.920000	0.630500	3.238600
C	-0.533800	-5.425100	3.978200
H	-1.612400	-5.576600	4.001800
C	-5.425100	0.533800	3.978300
H	-5.576600	1.612400	4.001900
C	0.000000	4.190000	3.592900
C	3.956000	1.380600	3.593100
C	1.781700	-6.198900	4.347200
C	-6.439800	-0.360200	4.347000
C	2.291500	-4.946200	3.978600
H	3.359700	-4.733900	4.002600
C	4.946200	2.291500	3.978600
H	4.733900	3.359800	4.002600
C	0.000000	-4.190000	3.592900
C	-0.360200	6.439900	4.346900
C	-4.190000	-0.000000	3.592900
C	0.360200	-6.439900	4.346900
C	6.439800	0.360200	4.347000
C	-1.781700	6.198900	4.347200
C	5.425100	-0.533800	3.978300
H	5.576600	-1.612400	4.001900
C	1.371700	7.994100	4.870800
H	1.859200	7.335600	5.608500
H	1.896100	7.918300	3.902800
H	1.403900	9.030600	5.225100
C	-3.928800	7.095600	4.871900
H	-4.399200	6.851500	3.904100
H	-4.171800	6.313100	5.609500
H	-4.300500	8.063500	5.226600
C	-7.994000	1.371700	4.871100
H	-7.335500	1.859100	5.608800
H	-7.918200	1.896100	3.903100
H	-9.030500	1.403900	5.225500
C	-7.095600	-3.928800	4.871900
H	-6.313100	-4.171900	5.609500
H	-8.063500	-4.300600	5.226600
H	-6.851500	-4.399200	3.904000
C	-1.371700	-7.994100	4.870800
H	-1.859200	-7.335600	5.608500
H	-1.896100	-7.918300	3.902800
H	-1.403900	-9.030600	5.225100
C	3.928800	-7.095600	4.871900
H	4.171800	-6.313100	5.609500
H	4.300500	-8.063500	5.226600
H	4.399200	-6.851500	3.904100
C	7.994000	-1.371700	4.871100
H	7.335500	-1.859100	5.608800
H	7.918200	-1.896100	3.903100
H	9.030500	-1.403900	5.225500
C	7.095600	3.928800	4.871900
H	6.851500	4.399200	3.904000
H	6.313100	4.171900	5.609500
H	8.063500	4.300600	5.226600

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Y	0.000000	0.000000	-3.399600
C	-1.434200	2.620900	-4.901100
C	-2.761400	3.183700	-5.129100
C	-3.207600	4.502300	-5.295100
H	-2.492700	5.324200	-5.285000
C	-4.579800	4.717800	-5.420900
C	-2.851800	0.905400	-4.902600
C	-3.655100	2.103100	-5.129000
C	-5.033300	2.300700	-5.297400
H	-5.708900	1.445700	-5.299000
C	-5.495600	3.611000	-5.423700
C	-2.620900	-1.434200	-4.901100
C	-3.183700	-2.761400	-5.129100
C	-4.502300	-3.207600	-5.295100
H	-5.324200	-2.492700	-5.285000
C	-4.717800	-4.579800	-5.420900
C	-0.905400	-2.851800	-4.902600
C	-2.103100	-3.655100	-5.128900
C	-2.300700	-5.033300	-5.297400
H	-1.445700	-5.708900	-5.299000
C	-3.611000	-5.495700	-5.423600
C	1.434200	-2.620900	-4.901100
C	2.761400	-3.183700	-5.129100
C	3.207600	-4.502300	-5.295100
H	2.492700	-5.324200	-5.285000
C	4.579800	-4.717800	-5.420900
C	2.851800	-0.905400	-4.902600
C	3.655100	-2.103100	-5.129000
C	5.033300	-2.300700	-5.297400
H	5.708900	-1.445700	-5.299000
C	5.495600	-3.611000	-5.423700
C	2.620900	1.434200	-4.901100
C	3.183700	2.761400	-5.129100
C	4.502300	3.207600	-5.295100
H	5.324200	2.492700	-5.285000
C	4.717800	4.579800	-5.420900
C	0.905400	2.851800	-4.902600
C	2.103100	3.655100	-5.128900
C	2.300700	5.033300	-5.297400
H	1.445700	5.708900	-5.299000
C	3.611000	5.495700	-5.423600
N	-0.324800	3.352900	-4.953200
N	-1.540300	1.264200	-4.699700
N	-3.352900	-0.324800	-4.953200
N	-1.264200	-1.540300	-4.699700
N	0.324800	-3.352900	-4.953200
N	1.540300	-1.264200	-4.699700
N	3.352900	0.324800	-4.953200
N	1.264200	1.540300	-4.699700
O	-5.165900	5.938200	-5.521800
O	-6.805700	3.961100	-5.531400
O	-5.938200	-5.165900	-5.521700
O	-3.961100	-6.805700	-5.531300
O	5.165900	-5.938200	-5.521800
O	6.805700	-3.961100	-5.531400
O	5.938200	5.165900	-5.521700
O	3.961100	6.805700	-5.531300
C	-2.927100	-7.765600	-5.588800
H	-2.262400	-7.593800	-6.453800
H	-2.318000	-7.764400	-4.666400
H	-3.419700	-8.740700	-5.696700
C	-7.085300	-4.335900	-5.473800
H	-7.079500	-3.592800	-6.290400
H	-7.946400	-5.004700	-5.601200
H	-7.167400	-3.817700	-4.503200
C	-7.765600	2.927100	-5.588900
H	-7.593700	2.262400	-6.453900
H	-7.764400	2.318000	-4.666400
H	-8.740600	3.419700	-5.696800
C	-4.335900	7.085300	-5.473800
H	-3.592800	7.079500	-6.290400
H	-5.004700	7.946400	-5.601200
H	-3.817700	7.167400	-4.503200
C	2.927100	7.765600	-5.588800
H	2.262400	7.593800	-6.453800
H	2.318000	7.764400	-4.666400
H	3.419700	8.740700	-5.696700
C	7.085300	4.335900	-5.473800
H	7.079500	3.592800	-6.290400
H	7.946400	5.004700	-5.601200
H	7.167400	3.817700	-4.503200
C	7.765600	-2.927100	-5.588900
H	8.740600	-3.419700	-5.696800
H	7.593700	-2.262400	-6.453900
H	7.764400	-2.318000	-4.666400
C	4.335900	-7.085300	-5.473800
H	3.817700	-7.167400	-4.503200
H	3.592800	-7.079500	-6.290400
H	5.004700	-7.946400	-5.601200
Y	0.000000	0.000000	3.398800
C	2.139400	-2.091700	4.902200
C	3.574100	-2.237900	5.128700
C	4.396300	-3.361500	5.297300
H	3.959100	-4.359600	5.298800
C	5.770100	-3.153800	5.423700
C	2.987400	-0.034100	4.900800
C	4.108000	-0.941100	5.128900
C	5.481500	-0.715300	5.295100
H	5.871000	0.302000	5.285000
C	6.316600	-1.825200	5.421000
C	2.091700	2.139400	4.902200
C	2.237900	3.574100	5.128700
C	3.361500	4.396300	5.297200
H	4.359600	3.959100	5.298800
C	3.153800	5.770100	5.423600
C	0.034100	2.987400	4.900800
C	0.941100	4.108000	5.128900
C	0.715300	5.481600	5.295000
H	-0.302000	5.871000	5.284900
C	1.825200	6.316600	5.420900
C	-2.139400	2.091700	4.902200
C	-3.574100	2.237900	5.128700
C	-4.396300	3.361500	5.297300

H	-3.959100	4.359600	5.298800	C	6.219400	2.187300	-1.757300	C	0.878800	-4.128000	1.677300
C	-5.770100	3.153800	5.423700	C	2.014500	2.198500	-1.656000	C	1.657000	-5.293400	1.724300
C	-2.987400	0.034100	4.900800	C	3.449000	2.428600	-1.666300	H	2.743800	-5.223800	1.732200
C	-4.108000	0.941100	5.128900	C	4.209100	3.606600	-1.690700	C	0.992100	-6.517700	1.757800
C	-5.481500	0.715300	5.295100	H	3.712100	4.575700	-1.693800	C	2.811400	-0.993800	1.655600
H	-5.871000	-0.302000	5.285000	C	5.595800	3.483200	-1.736400	C	4.185700	-0.522800	1.666000
C	-6.316600	1.825200	5.421000	C	-0.189100	2.978400	-1.664000	C	5.410200	-1.205400	1.690800
C	-2.091700	-2.139400	4.902200	C	-1.164300	4.056700	-1.677500	H	5.427000	-2.294300	1.693900
C	-2.237900	-3.574100	5.128700	C	-1.025100	5.451100	-1.724200	C	6.576300	-0.444800	1.736900
C	-3.361500	-4.396300	5.297200	H	-0.033100	5.900400	-1.732000	C	2.717800	1.232900	1.663600
H	-4.359600	-3.959100	5.298800	C	-2.187300	6.219400	-1.757300	C	4.128000	0.878800	1.677300
C	-3.153800	-5.770100	5.423600	C	-2.198500	2.014500	-1.656000	C	5.293400	1.657000	1.724300
C	-0.034100	-2.987400	4.900800	C	-2.428600	3.449000	-1.666200	H	5.223800	2.743800	1.732200
C	-0.941100	-4.108000	5.128900	C	-3.606600	4.209100	-1.690700	C	6.517700	0.992100	1.757800
C	-0.715300	-5.481600	5.295000	H	-4.575700	3.712100	-1.693700	C	0.993800	2.811400	1.655600
H	0.302000	-5.871000	5.284900	C	-3.483200	5.595800	-1.736400	C	0.522800	4.185700	1.666000
C	-1.825200	-6.316600	5.420900	C	-2.978400	-0.189100	-1.664000	C	1.205400	5.410200	1.690800
N	1.289100	-3.112200	4.952900	C	-4.056700	-1.164300	-1.677500	H	2.294300	5.427000	1.694000
N	1.839800	-0.765400	4.699300	C	-5.451100	-1.025100	-1.724100	C	0.444800	6.576300	1.736900
N	3.112200	1.289100	4.952900	H	-5.900400	-0.033100	-1.731900	C	-1.232900	2.717800	1.663600
N	0.765400	1.839800	4.699300	C	-6.219400	-2.187300	-1.757300	C	-0.878800	4.128000	1.677300
N	-1.289100	3.112200	4.952900	C	-2.014500	-2.198500	-1.656000	C	-1.657000	5.293400	1.724300
N	-1.839800	0.765400	4.699300	C	-3.449000	-2.428600	-1.666300	H	-2.743800	5.223800	1.732200
N	-3.112200	-1.289100	4.952900	C	-4.209100	-3.606600	-1.690700	C	-0.992100	6.517700	1.757800
N	-0.765400	-1.839800	4.699300	H	-3.712100	-4.575700	-1.693800	C	-2.811400	0.993800	1.655600
O	6.694800	-4.145500	5.531600	C	-5.595800	-3.483200	-1.736400	C	-4.185700	0.522800	1.666000
O	7.669300	-1.769000	5.521900	N	-1.122900	-3.181500	-1.661400	C	-5.410200	1.205400	1.690800
O	4.145500	6.694800	5.531500	N	0.837300	-1.755100	-1.670400	H	-5.427000	2.294300	1.693900
O	1.769000	7.669300	5.521800	N	3.181500	-1.122900	-1.661400	C	-6.576300	0.444800	1.736900
O	-6.694800	4.145500	5.531600	N	1.755100	0.837300	-1.670400	C	-2.717800	-1.232900	1.663600
O	-7.669300	1.769000	5.521900	N	1.122900	3.181500	-1.661400	C	-4.128000	-0.878800	1.677300
O	-4.145500	-6.694800	5.531500	N	-0.837300	1.755100	-1.670400	C	-5.293400	-1.657000	1.724300
O	-1.769000	-7.669300	5.521800	N	-3.181500	1.122900	-1.661400	H	-5.223800	-2.743800	1.732200
C	0.497200	8.291800	5.473800	N	-1.755100	-0.837300	-1.670400	C	-6.517700	-0.992100	1.757800
H	0.001300	8.120700	4.503100	O	2.218400	-7.575600	-1.811600	N	-2.280500	-2.486400	1.661000
H	-0.156100	7.937400	6.290300	O	4.526400	-6.465700	-1.766100	N	0.085800	-1.942700	1.670000
H	0.682800	9.366100	5.601200	O	7.575600	2.218400	-1.811600	N	2.486400	-2.280500	1.661000
C	-6.233300	5.478800	5.589300	O	6.465700	4.526400	-1.766200	N	1.942700	0.085800	1.670000
H	-7.126200	6.107900	5.697300	O	-2.218400	7.575600	-1.811600	N	2.280500	2.486400	1.661000
H	-5.565600	5.639400	6.454200	O	-4.526400	6.465700	-1.766100	N	-0.085800	1.942700	1.670000
H	-5.695100	5.764200	4.666800	O	-7.575600	-2.218400	-1.811600	N	-2.486400	2.280500	1.661000
C	-8.291800	0.497200	5.473900	O	-6.465700	-4.526400	-1.766200	N	-1.942700	-0.085800	1.670000
H	-8.120700	0.001300	4.503200	C	-5.938900	-5.840100	-1.852500	O	-0.956800	-7.834300	1.767000
H	-7.937400	-0.156100	6.290400	H	-5.284500	-6.069500	-0.992800	O	1.602000	-7.729500	1.812500
H	-9.366100	0.682800	5.601300	H	-6.805700	-6.513000	-1.836900	O	7.834300	-0.956800	1.767000
C	5.478800	6.233300	5.589200	H	-5.382100	-5.987400	-2.792400	O	7.729500	1.602000	1.812500
H	5.639400	5.565700	6.454100	C	-8.280400	-0.988900	-1.764700	O	0.956800	7.834300	1.767000
H	5.764100	5.695100	4.666700	H	-7.994600	-0.329200	-2.603000	O	-1.602000	7.729500	1.812500
H	6.107900	7.126300	5.697200	H	-9.343000	-1.248500	-1.854600	O	-7.834300	0.956800	1.767000
C	8.291800	-0.497200	5.473900	H	-8.113900	-0.467700	-0.807700	O	-7.729500	-1.602000	1.812500
H	7.937400	0.156100	6.290400	C	-5.840100	5.938900	-1.852300	C	-7.773900	-3.018500	1.765500
H	9.366100	-0.682800	5.601300	H	-6.069500	5.284600	-0.992700	H	-7.211400	-3.466600	2.603700
H	8.120700	-0.001300	4.503200	H	-6.513000	6.805700	-1.836800	H	-8.833900	-3.288600	1.855800
C	6.233300	-5.478800	5.589300	H	-5.987500	5.382100	-2.792300	H	-7.382300	-3.400300	0.808500
H	5.565600	-5.639400	6.454200	C	-0.988900	8.280400	-1.764700	C	-7.986600	2.364100	1.852900
H	5.695100	-5.764200	4.666800	H	-0.329200	7.994600	-2.603100	H	-7.517200	2.873800	0.992900
H	7.126200	-6.107900	5.697300	H	-1.248500	9.343000	-1.854700	H	-9.068000	2.550600	1.837700
C	-0.497200	-8.291800	5.473800	H	-0.467700	8.113900	-0.807900	H	-7.564100	2.756000	2.792600
H	0.156100	-7.937400	6.290300	C	5.938900	5.840100	-1.852500	C	-3.018500	7.773900	1.765500
H	-0.682800	-9.366100	5.601200	H	5.284500	6.069500	-0.992800	H	-3.466600	7.211400	2.603600
H	-0.001300	-8.120700	4.503100	H	6.805700	6.513000	-1.836900	H	-3.288600	8.833900	1.855700
C	-5.478800	-6.233300	5.589200	H	5.382100	5.987400	-2.792400	H	-3.400200	7.382300	0.808400
H	-5.639400	-5.565700	6.454100	C	8.280400	0.988900	-1.764700	C	2.364100	7.986600	1.853000
H	-5.764100	-5.695100	4.666700	H	7.994600	0.329200	-2.603000	H	2.873900	7.517200	0.993100
H	-6.107900	-7.126300	5.697200	H	9.343000	1.248500	-1.854600	H	2.550600	9.068000	1.837800
Cd	0.000000	0.000000	-0.000500	H	8.113900	0.467700	-0.807700	H	2.756000	7.564100	2.792700
C	0.189100	-2.978400	-1.664000	C	5.840100	-5.938900	-1.852300	C	7.773900	3.018500	1.765500
C	1.164300	-4.056700	-1.677500	H	6.069500	-5.284600	-0.992700	H	7.211400	3.466600	2.603700
C	1.025100	-5.451100	-1.724200	H	6.513000	-6.805700	-1.836800	H	8.833900	3.288600	1.855800
H	0.033100	-5.900400	-1.732000	H	5.987500	-5.382100	-2.792300	H	7.382300	3.400300	0.808500
C	2.187300	-6.219400	-1.757300	C	0.988900	-8.280400	-1.764700	C	7.986600	-2.364100	1.852900
C	2.198500	-2.014500	-1.656000	H	0.329200	-7.994600	-2.603100	H	7.517200	-2.873800	0.992900
C	2.428600	-3.449000	-1.666200	H	1.248500	-9.343000	-1.854700	H	9.068000	-2.550600	1.837700
C	3.606600	-4.209100	-1.690700	H	0.467700	-8.113900	-0.807900	H	7.564100	-2.756000	2.792600
H	4.575700	-3.712100	-1.693700	C	-0.993800	-2.811400	1.655600	C	3.018500	-7.773900	1.765500
C	3.483200	-5.595800	-1.736400	C	-0.522800	-4.185700	1.666000	H	3.466600	-7.211400	2.603600
C	2.978400	0.189100	-1.664000	C	-1.205400	-5.410200	1.690800	H	3.288600	-8.833900	1.855700
C	4.056700	1.164300	-1.677500	H	-2.294300	-5.427000	1.694000	H	3.400200	-7.382300	0.808400
C	5.451100	1.025100	-1.724100	C	-0.444800	-6.576300	1.736900	C	-2.364100	-7.986600	1.853000
H	5.900400	0.033100	-1.731900	C	1.232900	-2.717800	1.663600	H	-2.756000	-7.564100	2.792700

H	-2.873900	-7.517200	0.993100	H	-5.768100	5.720200	4.980100	H	0.072300	8.146900	-5.102200
H	-2.550600	-9.068000	1.837800	H	-7.098800	6.009500	6.152000	H	0.114200	7.748800	-6.854800
				C	-8.214100	0.395000	6.052600	H	-0.675000	9.262800	-6.295400
355				H	-7.746700	-0.202100	6.854700	C	-6.151800	-5.468500	-5.938500
[4]$^+$				H	-9.269600	0.569800	6.295600	H	-5.409500	-5.593300	-6.745700
Y	0.000000	0.000000	3.359100	H	-8.145600	-0.164900	5.102200	H	-5.703000	-5.785400	-4.980700
C	-0.007900	2.990100	4.882600	C	-5.398300	-6.213200	5.938200	H	-7.030300	-6.089700	-6.152600
C	0.882500	4.112700	5.169900	H	-6.009500	-7.098700	6.152200	C	0.488200	-8.209300	-6.052600
C	0.642700	5.465800	5.448000	H	-5.531500	-5.472400	6.745400	H	-0.114200	-7.748800	-6.854800
H	-0.378300	5.845300	5.473200	H	-5.720200	-5.768000	4.980400	H	0.675000	-9.262800	-6.295400
C	1.744500	6.292500	5.682300	C	-0.395000	-8.214100	6.052600	H	-0.072300	-8.146900	-5.102200
C	2.055800	2.166200	4.876400	H	0.164900	-8.145600	5.102300	C	5.468500	-6.151700	-5.938800
C	2.183300	3.592500	5.161600	H	0.202100	-7.746600	6.854800	H	5.593200	-5.409400	-6.746000
C	3.297800	4.401300	5.418000	H	-0.569800	-9.269600	6.295700	H	5.785400	-5.702900	-4.981000
H	4.297900	3.969700	5.411000	Y	0.000000	0.000000	-3.360100	H	6.089700	-7.030300	-6.152800
C	3.079900	5.759300	5.657300	C	2.080200	-2.142700	-4.877600	C	8.209300	0.488200	-6.052500
C	2.990100	0.007900	4.882600	C	2.223900	-3.567600	-5.162700	H	7.748900	-0.114200	-6.854800
C	4.112700	-0.882500	5.169800	C	3.347600	-4.363600	-5.418800	H	9.262800	0.675000	-6.295300
C	5.465800	-0.642800	5.448000	H	4.342700	-3.920700	-5.411800	H	8.146900	-0.072300	-5.102200
H	5.845300	0.378300	5.473200	C	3.145100	-5.724100	-5.657900	C	6.151800	5.468500	-5.938500
C	6.292600	-1.744500	5.682200	C	0.026000	-2.990000	-4.883700	H	5.409500	5.593300	-6.745700
C	2.166200	-2.055800	4.876400	C	0.929100	-4.102400	-5.170800	H	5.703000	5.785400	-4.980700
C	3.592500	-2.183300	5.161600	C	0.704800	-5.458200	-5.448700	H	7.030300	6.089700	-6.152600
C	4.401300	-3.297800	5.417900	H	-0.311900	-5.849400	-5.473700	Cd	0.000000	0.000000	-0.000300
H	3.969700	-4.298000	5.410900	C	1.815800	-6.272500	-5.682800	C	2.445400	-1.707100	1.667200
C	5.759300	-3.079900	5.657200	C	-2.142700	-2.080200	-4.877600	C	2.863200	-3.099800	1.675100
C	0.007900	-2.990100	4.882600	C	-3.567600	-2.223900	-5.162600	C	4.131700	-3.693000	1.720100
C	-0.882500	-4.112700	5.169900	C	-4.363700	-3.347600	-5.418700	H	5.025900	-3.072500	1.746200
C	-0.642700	-5.465800	5.448000	H	-3.920700	-4.342700	-5.411700	C	4.198100	-5.085700	1.736300
H	0.378300	-5.845300	5.473200	C	-5.724100	-3.145100	-5.657800	C	0.580900	-2.930500	1.657700
C	-1.744500	-6.292500	5.682300	C	-2.990000	-0.026000	-4.883700	C	1.690100	-3.869100	1.655800
C	-2.055800	-2.166200	4.876400	C	-4.102400	-0.929200	-5.170800	C	1.740300	-5.270500	1.657000
C	-2.183300	-3.592500	5.161600	C	-5.458200	-0.704800	-5.448700	H	0.817600	-5.849000	1.636200
C	-3.297800	-4.401300	5.418000	H	-5.849400	0.311900	-5.473700	C	2.995800	-5.876600	1.689500
H	-4.297900	-3.969700	5.411000	C	-6.272500	-1.815800	-5.682700	C	-1.707100	-2.445400	1.667200
C	-3.079900	-5.759300	5.657300	C	-2.080200	2.142700	-4.877600	C	-3.099800	-2.863200	1.675000
C	-2.990100	-0.007900	4.882600	C	-2.223900	3.567600	-5.162700	C	-3.693000	-4.131700	1.720000
C	-4.112700	0.882500	5.169800	C	-3.347600	4.363600	-5.418800	H	-3.072500	-5.025900	1.746100
C	-5.465800	0.642800	5.448000	H	-4.342700	3.920700	-5.411800	C	-5.085700	-4.198100	1.736200
H	-5.845300	-0.378300	5.473200	C	-3.145100	5.724100	-5.657900	C	-2.930500	-0.580900	1.657700
C	-6.292600	1.744500	5.682200	C	-0.026000	2.990000	-4.883700	C	-3.869100	-1.690100	1.655800
C	-2.166200	2.055800	4.876400	C	-0.929100	4.102400	-5.170800	C	-5.270500	-1.740300	1.657000
C	-3.592500	2.183300	5.161600	C	-0.704800	5.458200	-5.448700	H	-5.849000	-0.817600	1.636100
C	-4.401300	3.297800	5.417900	H	0.311900	5.849400	-5.473700	C	-5.876600	-2.995800	1.689400
H	-3.969700	4.298000	5.410900	C	-1.815800	6.272500	-5.682800	C	-2.445400	1.707100	1.667200
C	-5.759300	3.079900	5.657200	C	2.142700	2.080200	-4.877600	C	-2.863200	3.099800	1.675100
N	-1.333100	3.090300	4.934200	C	3.567600	2.223900	-5.162600	C	-4.131700	3.693000	1.720100
N	0.734400	1.857500	4.647400	C	4.363700	3.347600	-5.418700	H	-5.025900	3.072500	1.746200
N	3.090300	1.333100	4.934200	H	3.920700	4.342700	-5.411700	C	-4.198100	5.085700	1.736300
N	1.857500	-0.734400	4.647400	C	5.724100	3.145100	-5.657800	C	-0.580900	2.930500	1.657700
N	1.333100	-3.090300	4.934200	C	2.990000	0.026000	-4.883700	C	-1.690100	3.869100	1.655800
N	-0.734400	-1.857500	4.647400	C	4.102400	0.929200	-5.170800	C	-1.740300	5.270500	1.657000
N	-3.090300	-1.333100	4.934200	C	5.458200	0.704800	-5.448700	H	-0.817600	5.849000	1.636200
N	-1.857500	0.734400	4.647400	H	5.849400	-0.311900	-5.473700	C	-2.995800	5.876600	1.689500
O	1.672700	7.618600	5.944400	C	6.272500	1.815800	-5.682700	C	1.707100	2.445400	1.667200
O	4.058000	6.669300	5.875100	N	3.105200	-1.297900	-4.935400	C	3.099800	2.863200	1.675000
O	7.618600	-1.672700	5.944400	N	0.755500	-1.849100	-4.648600	C	3.693000	4.131700	1.720000
O	6.669400	-4.058000	5.874900	N	-1.297900	-3.105200	-4.935400	H	3.072500	5.025900	1.746100
O	-1.672700	-7.618600	5.944400	N	-1.849100	-0.755500	-4.648600	C	5.085700	4.198100	1.736200
O	-4.058000	-6.669300	5.875100	N	-3.105200	1.297900	-4.935400	C	2.930500	0.580900	1.657700
O	-7.618600	1.672700	5.944400	N	-0.755500	1.849100	-4.648600	C	3.869100	1.690100	1.655800
O	-6.669400	4.058000	5.874900	N	1.297900	3.105200	-4.935400	C	5.270500	1.740300	1.657000
C	6.213300	-5.398300	5.937900	N	1.849100	0.755500	-4.648600	H	5.849000	0.817600	1.636100
H	5.472400	-5.531500	6.745100	O	4.133500	-6.623000	-5.875500	C	5.876600	2.995800	1.689400
H	5.768100	-5.720200	4.980100	O	1.759100	-7.599300	-5.944700	N	3.302700	-0.694800	1.661500
H	7.098800	-6.009500	6.152000	O	-6.623000	-4.133500	-5.875400	N	1.060500	-1.630700	1.677600
C	8.214100	-0.395000	6.052600	O	-7.599300	-1.759100	-5.944600	N	-0.694800	-3.302700	1.661500
H	7.746700	0.202100	6.854700	O	-4.133500	6.623000	-5.875500	N	-1.630700	-1.060500	1.677600
H	9.269600	-0.569800	6.295600	O	-1.759100	7.599300	-5.944700	N	-3.302700	0.694800	1.661500
H	8.145600	0.164900	5.102200	O	6.623000	4.133500	-5.875400	N	-1.060500	1.630700	1.677600
C	5.398300	6.213200	5.938200	O	7.599300	1.759100	-5.944600	N	0.694800	3.302700	1.661500
H	5.531500	5.472400	6.745400	C	-8.209300	-0.488200	-6.052500	N	1.630700	1.060500	1.677600
H	5.720200	5.768000	4.980400	H	-8.146900	0.072300	-5.102200	O	5.342200	-5.804600	1.785400
H	6.009500	7.098700	6.152200	H	-7.748900	0.114200	-6.854800	O	3.207200	-7.215800	1.670700
C	0.395000	8.214100	6.052600	H	-9.262800	-0.675000	-6.295300	O	-5.804600	-5.342200	1.785100
H	-0.202100	7.746600	6.854800	C	-5.468500	6.151700	-5.938800	O	-7.215800	-3.207200	1.670600
H	0.569800	9.269600	6.295700	H	-6.089700	7.030300	-6.152800	O	-5.342200	5.804600	1.785400
H	-0.164900	8.145600	5.102200	H	-5.593200	5.409400	-6.746000	O	-3.207200	7.215800	1.670700
C	-6.213300	5.398300	5.937900	H	-5.785400	5.702900	-4.981000	O	5.804600	5.342200	1.785100
H	-5.472400	5.531500	6.745100	C	-0.488200	8.209300	-6.052600	O	7.215800	3.207200	1.670600

C	8.072800	2.081700	1.659700
H	7.914600	1.461500	0.759400
H	9.096000	2.477100	1.654800
H	7.924300	1.455200	2.556700
C	5.112500	6.585200	1.772200
H	4.436200	6.675000	2.638800
H	5.889000	7.357300	1.836400
H	4.548300	6.715700	0.834900
C	-2.081600	8.072800	1.659800
H	-1.461500	7.914700	0.759500
H	-2.477100	9.096000	1.654900
H	-1.455200	7.924300	2.556800
C	-6.585200	5.112500	1.772500
H	-6.674900	4.436200	2.639200
H	-7.357300	5.889000	1.836700
H	-6.715700	4.548300	0.835200
C	-8.072800	-2.081700	1.659700
H	-7.914600	-1.461500	0.759400
H	-9.096000	-2.477100	1.654800
H	-7.924300	-1.455200	2.556700
C	-5.112500	-6.585200	1.772200
H	-4.436200	-6.675000	2.638800
H	-5.889000	-7.357300	1.836400
H	-4.548300	-6.715700	0.834900
C	2.081600	-8.072800	1.659800
H	1.461500	-7.914700	0.759500
H	2.477100	-9.096000	1.654900
H	1.455200	-7.924300	2.556800
C	6.585200	-5.112500	1.772500
H	6.674900	-4.436200	2.639200
H	7.357300	-5.889000	1.836700
H	6.715700	-4.548300	0.835200
C	2.937200	-0.545500	-1.658700
C	3.889100	-1.643300	-1.656300
C	5.291100	-1.676600	-1.656300
H	5.858300	-0.746900	-1.635000
C	5.912400	-2.924600	-1.687800
C	1.736500	-2.424700	-1.668400
C	3.134100	-2.825600	-1.675600
C	3.742700	-4.086800	-1.719700
H	3.133100	-4.988600	-1.745800
C	5.136100	-4.136400	-1.734800
C	-0.545500	-2.937200	-1.658700
C	-1.643300	-3.889100	-1.656300
C	-1.676600	-5.291100	-1.656400
H	-0.746900	-5.858300	-1.635100
C	-2.924600	-5.912400	-1.687900
C	-2.424700	-1.736500	-1.668400
C	-2.825600	-3.134100	-1.675700
C	-4.086800	-3.742700	-1.719800
H	-4.988600	-3.133100	-1.745900
C	-4.136400	-5.136100	-1.734900
C	-2.937200	0.545500	-1.658700
C	-3.889100	1.643300	-1.656300
C	-5.291100	1.676600	-1.656300
H	-5.858300	0.746900	-1.635000
C	-5.912400	2.924600	-1.687800
C	-1.736500	2.424700	-1.668400
C	-3.134100	2.825600	-1.675600
C	-3.742700	4.086800	-1.719700
H	-3.133100	4.988600	-1.745800
C	-5.136100	4.136400	-1.734800
C	0.545500	2.937200	-1.658700
C	1.643300	3.889100	-1.656300
C	1.676600	5.291100	-1.656400
H	0.746900	5.858300	-1.635100
C	2.924600	5.912400	-1.687900
C	2.424700	1.736500	-1.668400
C	2.825600	3.134100	-1.675700
C	4.086800	3.742700	-1.719800
H	4.988600	3.133100	-1.745900
C	4.136400	5.136100	-1.734900
N	3.294100	0.734500	-1.662500
N	1.643300	-1.040800	-1.679000
N	0.734500	-3.294100	-1.662500
N	-1.040800	-1.643300	-1.679100
N	-3.294100	-0.734500	-1.662500
N	-1.643300	1.040800	-1.679000
N	-0.734500	3.294100	-1.662500
N	1.040800	1.643300	-1.679100
O	7.254000	-3.119800	-1.667600
O	5.868700	-5.271800	-1.782800
O	-3.119800	-7.254000	-1.667800
O	-5.271800	-5.868800	-1.783100
O	-7.254000	3.119800	-1.667600
O	-5.868700	5.271800	-1.782800
O	3.119800	7.254000	-1.667800
O	5.271800	5.868800	-1.783100
C	6.523000	5.191700	-1.770300
H	6.621000	4.516900	-2.637200
H	7.285700	5.977500	-1.834100
H	6.660200	4.628700	-0.833200
C	1.984000	8.097300	-1.656200
H	1.365700	7.930900	-0.756200
H	2.367100	9.125300	-1.650400
H	1.359500	7.942100	-2.553500
C	-5.191700	6.523000	-1.769900
H	-4.516900	6.621100	-2.636800
H	-5.977500	7.285800	-1.833700
H	-4.628700	6.660100	-0.832800
C	-8.097300	1.984000	-1.656100
H	-7.930800	1.365700	-0.756100
H	-9.125300	2.367100	-1.650300
H	-7.942100	1.359500	-2.553400
C	-6.523000	-5.191700	-1.770300
H	-6.621000	-4.516900	-2.637200
H	-7.285700	-5.977500	-1.834100
H	-6.660200	-4.628700	-0.833200
C	-1.984000	-8.097300	-1.656200
H	-1.365700	-7.930900	-0.756200
H	-2.367100	-9.125300	-1.650400
H	-1.359500	-7.942100	-2.553500
C	5.191700	-6.523000	-1.769900
H	4.516900	-6.621100	-2.636800
H	5.977500	-7.285800	-1.833700
H	4.628700	-6.660100	-0.832800
C	8.097300	-1.984000	-1.656100
H	7.942100	-1.359500	-2.553400
H	7.930800	-1.365700	-0.756100
H	9.125300	-2.367100	-1.650300

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Y	0.001300	-0.001200	3.341700
C	-1.266700	2.700300	4.863500
C	-0.939300	4.092600	5.160700
C	-1.743700	5.203100	5.440500
H	-2.828700	5.107100	5.441100
C	-1.109300	6.420700	5.703900
C	0.949400	2.832500	4.868900
C	0.458600	4.177000	5.168800
C	1.113200	5.378900	5.468800
H	2.201600	5.418300	5.498100
C	0.327100	6.507300	5.727400
C	2.704200	1.266900	4.861000
C	4.096800	0.939400	5.156800
C	5.207600	1.743800	5.435500
H	5.111600	2.828900	5.436200
C	6.425500	1.109400	5.697700
C	2.836400	-0.949300	4.866200
C	4.181300	-0.458400	5.164800
C	5.383400	-1.113100	5.463600
H	5.422800	-2.201500	5.492900
C	6.512100	-0.327000	5.721100
C	1.270800	-2.704100	4.859900
C	0.943600	-4.096700	5.156000
C	1.748300	-5.207500	5.433800
H	2.833300	-5.111500	5.433500
C	1.114100	-6.425400	5.696600
C	-0.945400	-2.836300	4.867200
C	-0.454200	-4.181100	5.165300
C	-1.108600	-5.383300	5.464800
H	-2.197000	-5.422700	5.495100
C	-0.322200	-6.511900	5.721400
C	-2.700200	-1.270700	4.862400
C	-4.092500	-0.943500	5.159900
C	-5.203000	-1.748200	5.438800
H	-5.107000	-2.833200	5.438500
C	-6.420600	-1.114000	5.702800
C	-2.832300	0.945500	4.869800
C	-4.176900	0.454300	5.169200
C	-5.378800	1.108700	5.469800
H	-5.418200	2.197100	5.500100
C	-6.507200	0.322400	5.727600
N	-2.510600	2.235600	4.922000
N	-0.110100	1.991400	4.628000
N	2.239500	2.510700	4.919900
N	1.995100	0.110300	4.626200
N	2.514700	-2.239400	4.917600
N	0.114000	-1.995000	4.626100
N	-2.235400	-2.514600	4.919700
N	-1.991200	-0.113900	4.628000
O	-1.749000	7.582300	5.951300
O	0.809100	7.732900	6.015900
O	7.587300	1.749100	5.943800
O	7.738000	-0.809000	6.008300
O	1.754000	-7.587200	5.942100
O	-0.804000	-7.737900	6.009200
O	-7.582200	-1.753900	5.949600
O	-7.732800	0.804100	6.016500
C	7.906700	-2.209800	6.138900
H	7.259100	-2.619000	6.932900
H	7.690600	-2.730700	5.189200
H	8.958300	-2.364700	6.408200
C	7.575800	3.164400	6.051500
H	6.899300	3.496400	6.857100
H	8.604400	3.456600	6.294200
H	7.272900	3.638800	5.101700
C	2.209900	7.901500	6.146700
H	2.619100	7.253100	6.940000
H	2.730800	7.686400	5.196800
H	2.364800	8.952800	6.417100
C	-3.164300	7.570600	6.059000
H	-3.496200	6.893400	6.864000
H	-3.456500	8.599000	6.302800
H	-3.638700	7.268700	5.108900
C	-7.901400	2.204800	6.148600
H	-7.253000	2.613300	6.942300
H	-7.686200	2.726600	5.199200
H	-8.952700	2.359500	6.419100
C	-7.570500	-3.169300	6.055900
H	-6.893300	-3.502000	6.860600
H	-8.598900	-3.461700	6.299400
H	-7.268600	-3.642800	5.105400
C	-2.204700	-7.906500	6.141100
H	-2.359400	-8.958100	6.410600
H	-2.613100	-7.259000	6.935500
H	-2.726500	-7.690500	5.192000
C	3.169400	-7.575700	6.048300
H	3.642900	-7.272900	5.098000
H	3.502300	-6.899300	6.853500
H	3.461900	-8.604400	6.290700
Y	-0.001300	0.001300	-3.342900
C	1.434200	-2.618900	-4.870600
C	1.189900	-4.029500	-5.169600
C	2.047500	-5.096100	-5.469500
H	3.125600	-4.941400	-5.499600
C	1.474300	-6.346400	-5.726800
C	-0.770200	-2.882800	-4.863300
C	-0.200600	-4.194900	-5.160300
C	-0.795100	-5.430900	-5.438800
H	-1.879900	-5.529200	-5.438300
C	0.045500	-6.516500	-5.702200
C	-2.622800	-1.434300	-4.868200
C	-4.033700	-1.190100	-5.166000
C	-5.100500	-2.047700	-5.464900
H	-4.945900	-3.125800	-5.494900
C	-6.351000	-1.474500	-5.721200
C	-2.886700	0.770100	-4.860900
C	-4.199100	0.200500	-5.156800
C	-5.435300	0.794900	-5.434300
H	-5.533600	1.879800	-5.433900
C	-6.521100	-0.045700	-5.696700
C	-1.438200	2.622700	-4.867200
C	-1.194200	4.033500	-5.165300
C	-2.052100	5.100300	-5.463600
H	-3.130200	4.945700	-5.492800
C	-1.479100	6.350800	-5.720500
C	0.766200	2.886600	-4.861800
C	0.196300	4.198900	-5.157200

C	0.790500	5.435100	-5.435300	H	-5.705000	-1.435900	1.702700	C	-0.388700	-2.956700	-1.669000
H	1.875400	5.533400	-5.435800	C	-5.518000	-3.606600	1.738300	C	-1.432100	-3.967900	-1.675600
C	-0.050300	6.520900	-5.697100	C	-2.627300	1.423400	1.674000	C	-1.368500	-5.366300	-1.700700
C	2.618800	1.438100	-4.869400	C	-3.196900	2.762000	1.684200	H	-0.402600	-5.869100	-1.703100
C	4.029400	1.194100	-5.168600	C	-4.519600	3.228000	1.721500	C	-2.572000	-6.069600	-1.738400
C	5.096000	2.051900	-5.467700	H	-5.350700	2.524300	1.724700	C	-2.334500	-1.866300	-1.672900
H	4.941300	3.130100	-5.496800	C	-4.724000	4.609000	1.748500	C	-2.658000	-3.284700	-1.682400
C	6.346300	1.479000	-5.725500	C	-0.905400	2.841200	1.668500	C	-3.877300	-3.977600	-1.718300
C	2.882700	-0.766300	-4.864100	C	-2.111400	3.651500	1.676500	H	-4.819800	-3.432200	-1.720700
C	4.194800	-0.196500	-5.160600	C	-2.296500	5.039100	1.701900	C	-3.833900	-5.373000	-1.745000
C	5.430800	-0.790700	-5.439500	H	-1.434800	5.705000	1.703600	C	-2.957800	0.388700	-1.666400
H	5.529100	-1.875500	-5.440000	C	-3.605500	5.518100	1.741000	C	-3.969000	1.432100	-1.672200
C	6.516400	0.050100	-5.702100	C	1.424400	2.627300	1.672600	C	-5.367500	1.368500	-1.696000
N	2.646500	-2.072900	-4.922700	C	2.763100	3.196900	1.681700	H	-5.870200	0.402500	-1.697900
N	0.242100	-1.979500	-4.629100	C	3.229100	4.519600	1.718700	C	-6.070800	2.572000	-1.733300
N	-2.076900	-2.646600	-4.920800	H	2.525400	5.350700	1.722300	C	-1.867500	2.334600	-1.671400
N	-1.983200	-0.242300	-4.627300	C	4.610100	4.724000	1.744600	C	-3.285900	2.658000	-1.679700
N	-2.650600	2.076700	-4.918700	C	2.842300	0.905400	1.665900	C	-3.978800	3.877300	-1.715200
N	-0.246000	1.983100	-4.627200	C	3.652600	2.111400	1.673300	H	-3.433400	4.819800	-1.718100
N	2.072800	2.650400	-4.920600	C	5.040200	2.296500	1.697600	C	-5.374300	3.833800	-1.740600
N	1.979400	0.245900	-4.628900	H	5.706100	1.434800	1.698800	C	0.387600	2.957800	-1.666900
O	2.166300	-7.467000	-6.015000	C	5.519200	3.605500	1.736400	C	1.430900	3.969000	-1.673700
O	-0.377700	-7.773400	-5.948500	N	3.361600	-0.314400	1.666500	C	1.367300	5.367500	-1.697400
O	-7.472000	-2.166600	-6.008400	N	1.244400	-1.495500	1.678400	H	0.401300	5.870200	-1.698500
O	-7.778200	0.377500	-5.942000	N	-0.313300	-3.361600	1.667000	C	2.570700	6.070800	-1.735700
O	-2.171400	7.471700	-6.007200	N	-1.494400	-1.244400	1.679800	C	2.333400	1.867500	-1.673600
O	0.372700	7.778000	-5.942900	N	-3.360500	0.313400	1.669900	C	2.656800	3.285900	-1.682100
O	7.466900	2.171300	-6.013000	N	-1.243300	1.494500	1.680900	C	3.876100	3.978900	-1.718600
O	7.773300	-0.372900	-5.948700	N	0.314400	3.360600	1.669500	H	4.818600	3.433500	-1.722300
C	-8.018300	1.772400	-6.049100	N	1.495500	1.243300	1.679400	C	3.832600	5.374300	-1.744000
H	-7.804200	2.292800	-5.099200	O	5.929200	-5.216000	1.762300	N	3.251700	0.905000	-1.670500
H	-7.411900	2.219600	-6.854800	O	3.946400	-6.827600	1.754800	N	1.691100	-0.958700	-1.682300
H	-9.082600	1.877400	-6.291300	O	-5.214900	-5.929200	1.766800	N	0.903800	-3.251700	-1.671100
C	-3.580000	7.388800	-6.137400	O	-6.826600	-3.946300	1.760400	N	-0.959900	-1.691100	-1.681300
H	-3.919300	8.396300	-6.406200	O	-5.928000	5.215000	1.771500	N	-3.252900	-0.903800	-1.668200
H	-3.867800	6.679200	-6.931600	O	-3.945100	6.826600	1.763300	N	-1.692300	0.959900	-1.679800
H	-4.053800	7.083200	-5.187700	O	5.216100	5.928000	1.767100	N	-0.905000	3.252900	-1.667600
C	1.767500	8.018100	-6.051100	O	6.827700	3.945100	1.757700	N	0.958700	1.692300	-1.680800
H	2.288700	7.804100	-5.101600	C	7.798700	2.909000	1.772400	O	7.417600	-2.673300	-1.762500
H	2.214000	7.411600	-6.857000	H	7.720000	2.274700	0.872500	O	6.182700	-4.910300	-1.770900
H	1.872300	9.082400	-6.293500	H	8.774100	3.410100	1.782200	O	-2.674500	-7.417600	-1.760200
C	-7.389100	-3.575000	-6.139700	H	7.698600	2.280000	2.672800	O	-4.911500	-6.182700	-1.766700
H	-6.679500	-3.862200	-6.934200	C	4.418900	7.103200	1.723600	O	-7.418800	2.674400	-1.753900
H	-7.083400	-4.049600	-5.190400	H	3.712200	7.136600	2.570500	O	-6.184000	4.911500	-1.761700
H	-8.396600	-3.914200	-6.408700	H	5.120300	7.942600	1.801100	O	2.673200	7.418800	-1.756400
C	-1.772700	-8.013500	-6.055500	H	3.870100	7.174500	0.770900	O	4.910200	6.184000	-1.766100
H	-2.220000	-7.406400	-6.860500	C	-2.909000	7.797500	1.778600	C	6.208000	5.607500	-1.723000
H	-1.877600	-9.077600	-6.298700	H	-2.274800	7.719500	0.878600	H	6.366100	4.918300	-2.570300
H	-2.292800	-7.800200	-5.105300	H	-3.410100	8.772900	1.789200	H	6.909900	6.446500	-1.800200
C	3.574700	-7.384000	-6.146500	H	-2.279900	7.696800	2.678900	H	6.375500	5.079600	-0.770600
H	3.861800	-6.673800	-6.940500	C	-7.103200	4.417700	1.727400	C	1.481500	8.190900	-1.771000
H	4.049500	-7.079200	-5.197000	H	-7.136600	3.710400	2.573800	H	0.871100	8.000900	-0.871100
H	3.913900	-8.391300	-6.416400	H	-7.942600	5.119100	1.805500	H	1.801800	9.239600	-1.780600
C	8.013400	-1.767700	-6.056800	H	-7.174500	3.869700	0.774300	H	0.880000	7.981100	-2.671500
H	7.406400	-2.214400	-6.862200	C	-7.797500	-2.910200	1.776800	C	-5.607500	6.209300	-1.717500
H	9.077500	-1.872400	-6.300000	H	-7.719600	-2.275200	0.877300	H	-4.918300	6.368000	-2.564600
H	7.800100	-2.288600	-5.107000	H	-8.772900	-3.411300	1.787000	H	-6.446500	6.911200	-1.794100
C	7.384000	3.579800	-6.143300	H	-7.696700	-2.281900	2.677600	H	-5.079600	6.376000	-0.764900
H	6.673800	3.867600	-6.937000	C	-4.417600	-7.104300	1.721700	C	-8.190900	1.482700	-1.769400
H	7.079000	4.053700	-5.193400	H	-3.710300	-7.138400	2.568000	H	-8.000800	0.871600	-0.870000
H	8.391200	3.919200	-6.412800	H	-5.119000	-7.943700	1.799200	H	-9.239600	1.803100	-1.778700
Cd	-0.000000	-0.000000	-0.000400	H	-3.869700	-7.174900	0.768500	H	-7.981200	0.882100	-2.670400
C	2.628400	-1.424400	1.670300	C	2.910400	-7.798600	1.770600	C	-6.209300	-5.606200	-1.721900
C	3.198000	-2.763100	1.679000	H	2.275200	-7.720100	0.871300	H	-6.368100	-4.916300	-2.568500
C	4.520700	-3.229000	1.714800	H	3.411500	-8.774000	1.780100	H	-6.911200	-6.445100	-1.799200
H	5.351800	-2.525200	1.717700	H	2.282100	-7.698500	2.671600	H	-6.375900	-5.079100	-0.768900
C	4.725200	-4.610000	1.740700	C	7.104400	-4.418700	1.717900	C	-1.482800	-8.189600	-1.776700
C	0.906500	-2.842300	1.665200	H	7.138400	-3.712000	2.564900	H	-0.871500	-8.000400	-0.877300
C	2.112500	-3.652600	1.671600	H	7.943800	-5.120000	1.794900	H	-1.803200	-9.238300	-1.786900
C	2.297600	-5.040200	1.695900	H	7.175100	-3.869900	0.765200	H	-0.882300	-7.979100	-2.677500
H	1.436000	-5.706100	1.698000	C	2.956700	-0.387600	-1.669400	C	5.606100	-6.208100	-1.727000
C	3.606700	-5.519100	1.733600	C	3.967900	-1.430900	-1.677000	H	4.916200	-6.366300	-2.573600
C	-1.423400	-2.628300	1.671700	C	5.366300	-1.367300	-1.701900	H	6.445100	-6.910000	-1.804800
C	-2.762000	-3.198000	1.681600	H	5.869100	-0.401400	-1.703500	H	5.079000	-6.375400	-0.774100
C	-3.227900	-4.520700	1.717800	C	6.069600	-2.570800	-1.740700	C	8.189600	-1.481600	-1.777700
H	-2.524200	-5.351800	1.720100	C	1.866300	-2.333400	-1.675100	H	7.979300	-0.880300	-2.678000
C	-4.608900	-4.725100	1.744700	C	3.284700	-2.656800	-1.684800	H	8.000200	-0.871200	-0.877700
C	-2.841200	-0.906500	1.667800	C	3.977600	-3.876100	-1.721700	H	9.238400	-1.802000	-1.788000
C	-3.651500	-2.112500	1.674800	H	3.432100	-4.818600	-1.724800				
C	-5.039100	-2.297600	1.700200	C	5.373000	-3.832700	-1.748300	355			

[4]$^{3+}$				H	4.807900	6.856600	-7.742200	H	0.881000	-7.106300	-7.631800
Y	0.062100	3.330000	0.058000	H	3.680400	5.564000	-7.207700	H	1.078400	-5.392400	-8.150600
C	2.737200	4.802600	1.463200	C	-2.839900	6.662000	-7.443300	H	1.931000	-6.704700	-9.032800
C	3.320900	5.117200	2.766700	H	-3.338300	7.034700	-8.345600	C	-5.246600	-6.258100	-6.402100
C	4.622100	5.458100	3.152500	H	-2.075500	7.386900	-7.117600	H	-4.454600	-7.023300	-6.345600
H	5.426700	5.476300	2.418300	H	-2.358500	5.693000	-7.662100	H	-6.010900	-6.573500	-7.121700
C	4.842400	5.786500	4.496300	C	-6.912500	6.666100	-3.932500	H	-4.808000	-5.298600	-6.727100
C	1.056700	4.809800	2.909000	H	-7.199900	5.701700	-3.479100	C	-8.055700	-6.296400	-1.817500
C	2.260100	5.122700	3.679800	H	-6.700000	7.397700	-3.135300	H	-7.639900	-7.061000	-1.140300
C	2.452000	5.471100	5.021800	H	-7.732600	7.034600	-4.559600	H	-8.156500	-5.340400	-1.275100
H	1.607300	5.500100	5.709300	Y	-0.062100	-3.329800	-0.057900	H	-9.040000	-6.619500	-2.175400
C	3.750800	5.794300	5.436200	C	-3.033500	-4.813400	-0.583500	C	-6.410900	-6.439400	5.014400
C	-1.288000	4.854800	2.732100	C	-3.987600	-5.125300	-1.647800	H	-6.354700	-7.175100	4.194900
C	-2.579100	5.216600	3.315900	C	-5.342500	-5.475800	-1.621700	H	-7.131000	-6.782000	5.766400
C	-2.952000	5.572200	4.617000	H	-5.884800	-5.507900	-0.677400	H	-6.734900	-5.464300	4.611100
H	-2.217400	5.564500	5.421300	C	-5.960200	-5.797100	-2.837500	C	-1.827400	-6.583800	7.821900
C	-4.283000	5.949000	4.837400	C	-1.877300	-4.800100	-2.474900	H	-1.150600	-7.333200	7.378800
C	-2.733200	4.912800	1.052100	C	-3.257300	-5.115900	-2.841700	H	-1.284400	-5.632400	7.957800
C	-3.491800	5.254300	2.255400	C	-3.847200	-5.454900	-4.064600	H	-2.186000	-6.942300	8.793700
C	-4.820300	5.650900	2.447400	H	-3.252200	-5.470100	-4.977000	Cd	0.000100	0.000100	0.000000
H	-5.506500	5.704100	1.602900	C	-5.208500	-5.785300	-4.066300	C	-2.846100	1.731800	0.831800
C	-5.222400	5.989900	3.746000	C	0.408300	-4.834600	-3.028000	C	-4.186100	1.768500	0.266000
C	-2.555500	4.949200	-1.292800	C	1.460100	-5.186100	-3.982000	C	-5.456500	1.810000	0.857400
C	-3.126300	5.330500	-2.584100	C	1.420800	-5.537000	-5.336500	H	-5.560400	1.805900	1.941300
C	-4.413800	5.732300	-2.957000	H	0.475700	-5.535300	-5.878400	C	-6.568100	1.849000	0.011800
H	-5.217700	5.754500	-2.222100	C	2.623800	-5.903300	-5.954200	C	-2.596700	1.758000	-1.385500
C	-4.621000	6.115400	-4.288300	C	2.299300	-4.888800	-1.872400	C	-4.026800	1.775600	-1.128600
C	-0.875000	4.944800	-2.738500	C	2.653900	-5.219400	-3.252100	C	-5.128600	1.810200	-1.992700
C	-2.065500	5.328700	-3.497100	C	3.863400	-5.603400	-3.842100	H	-4.978700	1.813700	-3.071400
C	-2.243500	5.730600	-4.826100	H	4.774900	-5.651200	-3.247300	C	-6.401500	1.843000	-1.421200
H	-1.397800	5.752500	-5.512600	C	3.852500	-5.935400	-5.202900	C	-0.770000	1.758200	-2.848500
C	-3.529200	6.115800	-5.228100	C	2.851600	-4.940900	0.413100	C	-0.203700	1.772500	-4.188800
C	1.469700	4.896500	-2.561600	C	3.792700	-5.325500	1.465000	C	-0.793500	1.833700	-5.459100
C	2.773800	5.230300	-3.133300	C	5.133600	-5.725200	1.425800	H	-1.877000	1.869000	-5.562800
C	3.160500	5.616900	-4.421400	H	5.675000	-5.744000	0.480500	C	0.052600	1.840200	-6.571000
H	2.426500	5.664700	-5.225100	C	5.738100	-6.112100	2.629100	C	1.446900	1.704100	-2.599800
C	4.504700	5.951400	-4.629400	C	1.695400	-4.951200	2.304500	C	1.190300	1.729000	-4.029900
C	2.914900	4.841900	-0.881600	C	3.062500	-5.331100	2.659000	C	2.054800	1.730500	-5.131900
C	3.686500	5.196800	-2.072700	C	3.638500	-5.734900	3.868800	H	3.132900	1.694900	-4.982300
C	5.029000	5.550300	-2.251600	H	3.042700	-5.760100	4.780500	C	1.484400	1.782100	-6.404700
H	5.716100	5.548500	-1.406200	C	4.986500	-6.115700	3.857900	C	2.909500	1.653000	-0.773500
C	5.444200	5.919200	-3.537900	C	-0.590200	-4.919900	2.857600	C	4.249700	1.619500	-0.207700
N	3.443600	4.867500	0.338700	C	-1.655100	-5.265300	3.799300	C	5.521100	1.634300	-0.798000
N	1.388700	4.562400	1.597500	C	-1.629900	-5.665000	5.140500	H	5.625500	1.664700	-1.881500
N	-0.161600	4.879800	3.438100	H	-0.685800	-5.717700	5.681600	C	6.632900	1.601900	0.047700
N	-1.431200	4.618600	1.383800	C	-2.846200	-6.007700	5.745700	C	2.659800	1.610100	1.443500
N	-3.259700	5.000800	-0.166200	C	-2.481200	-4.862600	1.702000	C	4.089800	1.583300	1.186400
N	-1.216700	4.664100	-1.436200	C	-2.848800	-5.228300	3.069400	C	5.191500	1.546300	2.050500
N	0.345500	4.988000	-3.265600	C	-4.072200	-5.587500	3.646100	H	5.041100	1.517400	3.128800
N	1.603200	4.608000	-1.222600	H	-4.984400	-5.580200	3.050600	C	6.465100	1.551600	1.479700
O	6.031600	6.126200	5.019600	C	-4.074600	-5.967500	4.994400	C	0.833400	1.626500	2.906700
O	4.095100	6.143100	6.686200	N	-3.359300	-4.886800	0.703900	C	0.267200	1.615100	4.247100
O	-4.793400	6.308200	6.026400	N	-1.792900	-4.562900	-1.121900	C	0.858100	1.610100	5.518300
O	-6.458900	6.383900	4.090500	N	-0.881100	-4.861600	-3.353300	H	1.942100	1.601300	5.622300
O	-5.796500	6.516700	-4.798700	N	0.955800	-4.602500	-1.787800	C	0.012100	1.609500	6.630300
O	-3.859600	6.520600	-6.464900	N	3.175400	-4.980900	-0.876400	C	-1.383800	1.663800	2.657700
O	5.028800	6.332700	-5.805500	N	1.620900	-4.663400	0.960700	C	-1.127300	1.629100	4.087700
O	6.694700	6.278900	-3.869100	N	0.697100	-5.006400	3.180900	C	-1.991800	1.624700	5.189600
C	-7.436700	6.563400	3.076200	N	-1.127900	-4.623800	1.626800	H	-3.070500	1.634600	5.039600
H	-7.109700	7.315100	2.338600	O	-7.248800	-6.147700	-2.976800	C	-1.420800	1.610700	6.463000
H	-7.656500	5.612800	2.560000	O	-5.916000	-6.123600	-5.156400	N	-2.604800	1.696100	2.138600
H	-8.338700	6.919100	3.587400	O	2.749700	-6.260200	-7.242400	N	-1.900200	1.738600	-0.183600
C	-3.927400	6.416400	7.147400	O	4.929300	-6.314100	-5.910400	N	-2.077100	1.770300	-2.606700
H	-3.129200	7.154200	6.961600	O	7.012600	-6.515100	2.755000	N	0.245300	1.729400	-1.903000
H	-4.554300	6.755900	7.980000	O	5.680100	-6.518500	4.934900	N	2.667900	1.672600	-2.080600
H	-3.475300	5.441600	7.400100	O	-2.986200	-6.404900	7.020500	N	1.964000	1.659200	0.242100
C	3.080700	6.288000	7.669600	O	-5.165300	-6.330500	5.688700	N	2.140300	1.598600	2.664700
H	2.343800	7.051600	7.369700	C	6.169600	-6.492900	-5.241200	N	-0.181700	1.668500	1.961400
H	2.563700	5.330500	7.854800	H	6.529400	-5.545400	-4.804100	O	-7.849300	1.879100	0.417600
H	3.592000	6.610500	8.584000	H	6.085500	-7.254500	-4.448200	O	-7.556800	1.856200	-2.116200
C	7.152900	6.264600	4.158500	H	6.876800	-6.835400	-6.005400	O	-0.352200	1.883200	-7.852100
H	6.968000	7.030900	3.387400	C	7.814200	-6.652700	1.590600	O	2.179200	1.768200	-7.560200
H	7.985500	6.580500	4.797500	H	8.785500	-7.024700	1.936400	O	7.914500	1.598500	-0.357500
H	7.404900	5.306600	3.671500	H	7.370600	-7.376800	0.887100	O	7.619600	1.497300	2.174000
C	7.677800	6.386400	-2.849800	H	7.951000	-5.682500	1.082400	O	0.417400	1.592800	7.911900
H	7.378600	7.123700	-2.086300	C	5.005300	-6.671700	6.175600	O	-2.116200	1.582800	7.617800
H	7.861700	5.410900	-2.367100	H	4.602700	-5.708600	6.534500	C	-3.534700	1.622500	7.565100
H	8.592800	6.725800	-3.349000	H	4.185400	-7.404300	6.092700	H	-3.939500	0.742500	7.035700
C	4.168300	6.511900	-6.921500	H	5.756900	-7.040600	6.883100	H	-3.876300	1.612600	8.606800
H	3.397900	7.272000	-6.709700	C	1.585400	-6.367500	-8.048700	H	-3.888900	2.541300	7.067900

C	1.810200	1.556800	8.203300
H	2.331800	2.417700	7.752100
H	1.886600	1.613900	9.295400
H	2.261300	0.614200	7.855300
C	7.566400	1.486300	3.593100
H	7.036100	0.592900	3.965900
H	8.608000	1.463100	3.934300
H	7.070000	2.392300	3.979600
C	8.206300	1.612200	-1.750600
H	7.756200	2.491600	-2.241100
H	9.298500	1.670900	-1.824600
H	7.857500	0.686600	-2.235200
C	3.598100	1.752900	-7.507000
H	3.969200	0.840500	-7.008700
H	3.939800	1.766400	-8.548600
H	3.986100	2.640000	-6.978500
C	-1.745200	1.909100	-8.143700
H	-2.234800	2.772500	-7.662500
H	-1.818700	2.007100	-9.233100
H	-2.231000	0.972300	-7.828500
C	-7.503100	1.892400	-3.534800
H	-7.006200	0.993200	-3.938700
H	-8.544600	1.919900	-3.876000
H	-6.973100	2.792000	-3.890200
C	-8.141100	1.854700	1.810500
H	-7.658800	2.699000	2.331200
H	-9.230400	1.951500	1.887400
H	-7.827400	0.900400	2.262100
C	-2.398700	-1.671900	1.790400
C	-3.851400	-1.639500	1.767000
C	-4.800200	-1.638500	2.797300
H	-4.478900	-1.650100	3.837800
C	-6.148800	-1.625600	2.438100
C	-3.000600	-1.631000	-0.357900
C	-4.232700	-1.623000	0.416200
C	-5.582300	-1.618900	0.037100
H	-5.859100	-1.608200	-1.016000
C	-6.544100	-1.622000	1.050700
C	-1.849800	-1.608100	-2.395600
C	-1.825800	-1.578400	-3.848300
C	-2.855700	-1.541300	-4.796700
H	-3.895800	-1.514800	-4.475000
C	-2.496900	-1.543400	-6.145500
C	0.298400	-1.645900	-2.998300
C	-0.475400	-1.611500	-4.230100
C	-0.097000	-1.623000	-5.579900
H	0.955700	-1.650900	-5.857100
C	-1.110400	-1.590600	-6.541200
C	2.336000	-1.695900	-1.848100
C	3.788800	-1.718800	-1.824600
C	4.737600	-1.717400	-2.854800
H	4.416800	-1.680600	-3.894900
C	6.085500	-1.767900	-2.496400
C	2.937600	-1.753300	0.300000
C	4.169600	-1.764200	-0.474200
C	5.518200	-1.824000	-0.096200
H	5.794600	-1.860700	0.956500
C	6.479800	-1.827500	-1.109900
C	1.787000	-1.759600	2.338000
C	1.763200	-1.780000	3.790800
C	2.793200	-1.814600	4.739300
H	3.833800	-1.815700	4.418100
C	2.433600	-1.850400	6.087500
C	-0.361500	-1.738700	2.940300
C	0.412300	-1.776100	4.172100
C	0.032800	-1.820700	5.520900
H	-1.020400	-1.819100	5.797600
C	1.046000	-1.859600	6.482200
N	-1.690100	-1.705400	2.912100
N	-1.904500	-1.673200	0.492100
N	-2.971700	-1.600100	-1.686600
N	-0.552100	-1.655800	-1.901900
N	1.627300	-1.663300	-2.969800
N	1.841300	-1.724400	-0.550300
N	2.908900	-1.768300	1.628900
N	0.488900	-1.742000	1.843700
O	-7.177000	-1.600700	3.310100
O	-7.874100	-1.606700	0.856500
O	-3.367800	-1.488500	-7.173400
O	-0.916300	-1.584100	-7.871300
O	7.114400	-1.751300	-3.367700
O	7.809300	-1.868700	-0.916300
O	3.305300	-1.864000	7.116100
O	0.851400	-1.892300	7.811800
C	-0.476500	-1.870800	8.323700
H	-1.066700	-2.715500	7.930100
H	-0.377200	-1.969100	9.411100
H	-0.974100	-0.916900	8.088100
C	4.696800	-1.897800	6.835100
H	5.014400	-0.997300	6.281200
H	5.201000	-1.926200	7.808200
H	4.963600	-2.796200	6.253400
C	8.320900	-1.895700	0.411700
H	7.926000	-2.760500	0.971000
H	9.408100	-1.991700	0.309100
H	8.086300	-0.960000	0.943300
C	6.833900	-1.734700	-4.759600
H	6.281400	-0.822600	-5.044800
H	7.807200	-1.746300	-5.264200
H	6.251100	-2.622100	-5.058700
C	0.411800	-1.594300	-8.383200
H	0.969900	-2.473400	-8.019300
H	0.309500	-1.651200	-9.473200
H	0.944400	-0.668300	-8.115000
C	-4.759800	-1.479900	-6.892800
H	-5.043800	-0.587900	-6.307800
H	-5.264100	-1.455600	-7.866000
H	-5.060400	-2.387300	-6.342400
C	-8.385300	-1.568400	-0.471400
H	-8.022600	-2.427400	-1.060600
H	-9.475500	-1.627200	-0.371600
H	-8.115500	-0.624300	-0.970200
C	-6.897100	-1.643700	4.701600
H	-6.348100	-2.562400	4.968800
H	-6.311000	-0.763700	5.018500
H	-7.870400	-1.636700	5.206000

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Y	3.321800	-0.134900	-0.000800
C	4.751300	-3.134300	-0.519900
C	5.063600	-4.393300	0.156400
C	5.413100	-5.657000	-0.331900
H	5.433500	-5.848800	-1.404100
C	5.756700	-6.648500	0.599400
C	4.769600	-2.682500	1.648800
C	5.074700	-4.107900	1.526600
C	5.435300	-5.072200	2.473700
H	5.472300	-4.819900	3.532800
C	5.767500	-6.354500	2.010900
C	4.850900	-0.716500	2.937300
C	5.241800	-0.055600	4.182400
C	5.622700	-0.559700	5.430700
H	5.607300	-1.632200	5.621600
C	6.044200	0.355300	6.407300
C	4.938700	1.450300	2.485100
C	5.297000	1.313500	3.896700
C	5.735000	2.243600	4.845500
H	5.804700	3.300800	4.591800
C	6.100400	1.765600	6.113000
C	4.991400	2.737800	0.517500
C	5.404900	3.967200	-0.159000
C	5.856400	5.198200	0.329100
H	5.892700	5.387800	1.401300
C	6.279200	6.158400	-0.602400
C	4.971800	2.286000	-1.651200
C	5.392200	3.681800	-1.529100
C	5.829800	4.613600	-2.476500
H	5.845700	4.359000	-3.535600
C	6.265500	5.864500	-2.013900
C	4.891900	0.320000	-2.939700
C	5.227100	-0.370600	-4.185000
C	5.647400	0.100900	-5.433300
H	5.719600	1.171000	-5.624100
C	5.992600	-0.845400	-6.410000
C	4.802800	-1.846800	-2.487500
C	5.170400	-1.739600	-3.899300
C	5.530800	-2.702300	-4.848200
H	5.514100	-3.761700	-4.594500
C	5.933500	-2.255700	-6.115900
N	4.812200	-3.010200	-1.842900
N	4.521200	-2.143300	0.406800
N	4.852900	-2.040700	2.810800
N	4.618200	0.220400	1.956600
N	5.042600	2.609100	1.840500
N	4.680800	1.768900	-0.409100
N	5.001900	1.639600	-2.813200
N	4.583900	-0.594800	-1.958900
O	6.110500	-7.901500	0.292400
O	6.129000	-7.381800	2.787700
O	6.436300	0.032100	7.644800
O	6.534900	2.525400	7.124600
O	6.734100	7.378500	-0.295600
O	6.709100	6.858900	-2.790900
O	6.409500	-0.555200	-7.647600
O	6.304300	-3.048300	-7.127600
C	6.748300	3.917400	6.918300
H	7.488100	4.087600	6.119200
H	5.804500	4.431100	6.667800
H	7.136300	4.304200	7.867300
C	6.538000	-1.338200	8.015300
H	7.248000	-1.870900	7.361800
H	6.911600	-1.342600	9.045400
H	5.553000	-1.834000	7.977000
C	6.294000	-7.182200	4.187300
H	7.058400	-6.413700	4.387300
H	5.341200	-6.892300	4.662200
H	6.626700	-8.145600	4.589400
C	6.252600	-8.278200	-1.072600
H	7.009900	-7.655200	-1.576000
H	6.583500	-9.322700	-1.061800
H	5.291000	-8.200400	-1.608100
C	6.403400	-4.453200	-6.921500
H	7.127100	-4.683200	-6.122600
H	5.420900	-4.888000	-6.670600
H	6.758200	-4.870200	-7.870600
C	6.622700	0.802200	-8.018200
H	7.374000	1.275100	-7.364900
H	6.995100	0.776000	-9.048400
H	5.681400	1.376800	-7.979600
C	6.856600	6.646500	-4.190500
H	7.266500	7.579600	-4.592900
H	7.555800	5.818300	-4.390900
H	5.883200	6.435200	-4.664900
C	6.907100	7.742300	1.069300
H	5.942600	7.743200	1.605300
H	7.611300	7.059600	1.572300
H	7.322100	8.756400	1.058300
Y	-3.321700	0.134900	0.000800
C	-4.769200	2.672100	1.666600
C	-5.074300	4.098200	1.553400
C	-5.434700	5.056700	2.506600
H	-5.471500	4.797700	3.564200
C	-5.767100	6.341800	2.052000
C	-4.751300	3.137500	-0.499100
C	-5.063500	4.392300	0.185100
C	-5.413100	5.658900	-0.295200
H	-5.433800	5.857400	-1.366200
C	-5.756600	6.644600	0.642400
C	-4.803300	1.862300	-2.474700
C	-5.171300	1.763900	-3.887100
C	-5.531900	2.732600	-4.829900
H	-5.515100	3.790300	-4.569600
C	-5.934900	2.293900	-6.100200
C	-4.892500	-0.301600	-2.940500
C	-5.228000	0.396800	-4.181300
C	-5.648700	-0.066900	-5.432500
H	-5.720900	-1.135800	-5.630000
C	-5.994000	0.885500	-6.403200
C	-4.972100	-2.275600	-1.664200
C	-5.392500	-3.672100	-1.550800
C	-5.830300	-4.598000	-2.503900
H	-5.846500	-4.336700	-3.561400
C	-6.265900	-5.851800	-2.049100
C	-4.991200	-2.741000	0.501500
C	-5.404900	-3.966100	-0.182500
C	-5.856300	-5.200200	0.298000
H	-5.892300	-5.396500	1.369000
C	-6.279300	-6.154500	-0.639500
C	-4.938100	-1.465800	2.477100

C	-5.296000	-1.337800	3.889700	C	1.574300	-3.733100	-4.165400	C	-1.446500	5.942800	-2.997800
C	-5.733700	-2.273900	4.832700	H	1.616600	-3.114400	-5.060500	C	-1.631700	1.770400	-2.453800
H	-5.803500	-3.329400	4.572400	C	1.512800	-5.128500	-4.237900	C	-1.574100	3.162800	-2.874200
C	-6.098800	-1.803800	6.103400	C	1.571900	-2.991500	-0.608200	C	-1.575400	3.758800	-4.141800
C	-4.850200	0.698100	2.942900	C	1.525100	-3.920500	-1.724500	H	-1.617900	3.145600	-5.040700
C	-5.240800	0.029400	4.184000	C	1.458900	-5.319300	-1.775900	C	-1.513900	5.154500	-4.205800
C	-5.621300	0.525700	5.435400	H	1.419800	-5.901900	-0.856500	C	-1.716200	-0.520700	-2.928800
H	-5.605800	1.597000	5.633000	C	1.445700	-5.924200	-3.034800	C	-1.752800	-1.630700	-3.865800
C	-6.042600	-0.395300	6.406400	C	1.600600	-2.531500	1.687400	C	-1.745600	-1.673800	-5.266400
N	-4.852200	2.023100	2.824600	C	1.582400	-2.960200	3.078400	H	-1.692800	-0.752200	-5.844400
N	-4.521000	2.140800	0.421300	C	1.555800	-4.231300	3.666000	C	-1.808200	-2.927500	-5.879100
N	-4.812500	3.021600	-1.822900	H	1.536400	-5.126400	3.046100	C	-1.801000	-2.383300	-1.702500
N	-4.584300	0.607000	-1.954000	C	1.548600	-4.303600	5.062700	C	-1.817200	-2.803500	-3.096200
N	-5.002500	-1.622000	-2.822200	C	1.667300	-0.675800	2.925100	C	-1.893600	-4.069000	-3.691600
N	-4.680900	-1.766300	-0.419000	C	1.613300	-1.790800	3.855200	H	-1.947000	-4.966500	-3.077200
N	-5.042200	-2.620500	1.825300	C	1.602300	-1.841700	5.255600	C	-1.891700	-4.133100	-5.088700
N	-4.617700	-0.232600	1.956300	H	1.624200	-0.922500	5.839300	C	-1.810700	-2.858300	0.590100
O	-6.128400	7.364200	2.835200	C	1.562900	-3.100100	5.860500	C	-1.839700	-3.794900	1.700700
O	-6.110500	7.899500	0.343200	N	1.719000	0.595200	3.310600	C	-1.887500	-5.194700	1.743400
O	-6.305900	3.092800	-7.106900	N	1.770700	1.547500	1.076700	H	-1.895900	-5.772800	0.820400
O	-6.411200	0.603100	-7.642500	N	1.826000	3.239800	-0.664700	C	-1.923800	-5.806400	2.998500
O	-6.709700	-6.841300	-2.832100	N	1.748000	1.007300	-1.618300	C	-1.769300	-1.632700	2.454600
O	-6.734200	-7.376500	-0.340200	N	1.663500	-0.732100	-3.311500	C	-1.824900	-3.025300	2.875100
O	-6.533100	-2.569900	7.110300	N	1.637900	-1.685500	-1.077600	C	-1.873600	-3.619200	4.142700
O	-6.434400	-0.079900	7.646000	N	1.556400	-3.376800	0.663800	H	-1.865500	-3.004600	5.041600
C	-6.624500	-0.752000	-8.021500	N	1.660800	-1.145300	1.617400	C	-1.926000	-5.015300	4.206600
H	-5.683300	-1.326800	-7.986800	O	1.967400	5.703000	5.371000	N	-1.718200	-0.615700	3.307300
H	-7.375600	-1.229000	-7.370900	O	1.945900	7.114700	3.251700	N	-1.660400	1.135300	1.624900
H	-6.997200	-0.719400	-9.051400	O	1.947100	5.297100	-5.778300	N	-1.556200	3.372600	0.685100
C	-6.857600	-6.620100	-4.230400	O	1.782500	3.182700	-7.188000	N	-1.638100	1.692100	-1.066700
H	-7.267500	-7.550700	-4.638500	O	1.494800	-5.843000	-5.372000	N	-1.664300	0.752600	-3.306500
H	-7.556800	-5.790700	-4.425400	O	1.359100	-7.248400	-3.252700	N	-1.748300	-0.997300	-1.624100
H	-5.884200	-6.405800	-4.703700	O	1.514000	-5.437200	5.777500	N	-1.826200	-3.235700	-0.684200
C	-6.906900	-7.748800	1.022500	O	1.521700	-3.316400	7.187200	N	-1.770400	-1.554100	1.067600
H	-5.942300	-7.753100	1.558200	C	1.584900	-2.206500	8.072900	O	-1.519900	3.272000	7.207900
H	-7.610900	-7.069300	1.529900	H	0.720500	-1.535100	7.931800	O	-1.512600	5.401400	5.811300
H	-7.321900	-8.762800	1.005200	H	1.562300	-2.626600	9.085000	O	-1.360000	7.268400	-3.207500
C	-6.404900	4.496400	-6.892000	H	2.518500	-1.637600	7.928100	O	-1.496300	5.876100	-5.335400
H	-7.128400	4.721400	-6.091400	C	1.485300	-6.694700	5.106100	O	-1.784400	-3.138300	-7.207100
H	-5.422400	4.929700	-6.638600	H	2.354600	-6.803700	4.436700	O	-1.948800	-5.261300	-5.810400
H	-6.759900	4.919400	-7.838400	H	1.532600	-7.452900	5.896100	O	-1.945300	-7.134600	3.208200
C	-6.252900	8.284700	-1.019400	H	0.548900	-6.815400	4.539400	O	-1.966300	-5.736000	5.336200
H	-7.010200	7.664900	-1.526400	C	1.341100	-8.134200	-2.141100	C	-1.961400	-5.072100	6.598000
H	-6.583800	9.329200	-1.001900	H	0.456700	-7.956800	-1.505200	H	-2.806700	-4.368300	6.676000
H	-5.291300	8.210300	-1.555500	H	1.294200	-9.145200	-2.561800	H	-2.071400	-5.862900	7.348800
C	-6.293100	7.155800	4.233600	H	2.256100	-8.026600	-1.534900	H	-1.008600	-4.544400	6.759800
H	-7.057500	6.386100	4.429000	C	1.544600	-5.173200	-6.629600	C	-1.999300	-8.012000	2.091200
H	-5.340200	6.863000	4.706400	H	2.444300	-4.540100	-6.703300	H	-1.103400	-7.903200	1.456100
H	-6.625700	8.116700	4.641800	H	1.590200	-5.965700	-7.385300	H	-2.034800	-9.026100	2.505600
C	-6.536000	1.288100	8.025100	H	0.637800	-4.568800	-6.788200	H	-2.902500	-7.826600	1.486100
H	-7.246100	1.824800	7.375200	C	1.755400	2.071300	-8.073800	C	-2.022400	-6.521200	-5.146800
H	-6.909300	1.286000	9.055300	H	0.839500	1.472000	-7.932300	H	-2.897800	-6.563500	-4.477900
H	-5.551000	1.784100	7.989700	H	1.766400	2.491900	-9.085800	H	-2.130800	-7.268100	-5.941400
C	-6.746600	-3.960600	6.895300	H	2.640000	1.428800	-7.929200	H	-1.099000	-6.720900	-4.581000
H	-7.486600	-4.125700	6.095300	C	2.020800	6.552800	-5.107000	C	-1.757500	-2.021500	-8.086000
H	-5.802900	-4.472700	6.641300	H	2.896400	6.591100	-4.438000	H	-0.841600	-1.423100	-7.941100
H	-7.134300	-4.353300	7.842000	H	2.128900	7.304700	-5.897000	H	-1.768900	-2.435800	-9.100600
Cd	0.000000	-0.000000	-0.000200	H	1.097500	6.749000	-4.539700	H	-2.642000	-1.379800	-7.937200
C	1.770000	1.617500	2.464200	C	1.999700	7.999000	2.140100	C	-1.546600	5.214000	-6.597200
C	1.825600	3.007400	2.893300	H	1.103600	7.894000	1.504500	H	-2.446300	4.581400	-6.674400
C	1.874600	3.593600	4.164500	H	2.035200	9.010500	2.560800	H	-1.592400	6.011200	-7.347900
H	1.866600	2.973500	5.059600	H	2.902700	7.817300	1.533700	H	-0.639900	4.610600	-6.759800
C	1.926900	4.989300	4.237000	C	1.962900	5.031300	6.628700	C	-1.341700	8.147300	-2.090500
C	1.810800	2.854600	0.607300	H	2.808100	4.327100	6.702200	H	-0.457100	7.966000	-1.456000
C	1.840100	3.784300	1.723600	H	2.073000	5.817500	7.384300	H	-1.294800	9.160900	-2.504900
C	1.887900	5.183800	1.774900	H	1.010000	4.502600	6.787500	H	-2.256500	8.035900	-1.484700
H	1.896000	5.767600	0.855500	C	-1.666500	0.657700	2.929600	C	-1.484100	6.663100	5.147700
C	1.924400	5.787800	3.033900	C	-1.612300	1.766900	3.866600	H	-2.353600	6.776200	4.479300
C	1.800600	2.393800	-1.688200	C	-1.600900	1.809200	5.267200	H	-1.531200	7.416300	5.942400
C	1.816400	2.822600	-3.079300	H	-1.622700	0.886400	5.845300	H	-0.547900	6.787300	4.581500
C	1.892600	4.091700	-3.666900	C	-1.561400	3.063800	5.879900	C	-1.582800	2.156600	8.086800
H	1.946200	4.985400	-3.047000	C	-1.600100	2.521000	1.703400	H	-2.516500	1.588600	7.938700
C	1.890400	4.164400	-5.063600	C	-1.581600	2.941100	3.097100	H	-0.718500	1.486100	7.941300
C	1.715600	0.538800	-2.926000	C	-1.554900	4.208600	3.692500	H	-1.559900	2.570400	9.101500
C	1.751900	1.654600	-3.856100	H	-1.535600	5.107500	3.078100				
C	1.744300	1.706300	-5.256400	C	-1.547300	4.272300	5.089600	444			
H	1.691300	0.788300	-5.840100	C	-1.572000	2.995200	-0.589300	**[5]^{0}**			
C	1.806700	2.963700	-5.861300	C	-1.525500	3.931100	-1.699800	Y	-5.044000	-0.000500	-0.000900
C	1.631200	-1.755200	-2.465100	C	-1.459300	5.330200	-1.742600	C	-6.559400	-1.114500	-2.777500
C	1.573400	-3.145000	-2.894100	H	-1.419900	5.907100	-0.819600	C	-6.791500	-2.367500	-3.489600

C	-6.966700	-2.666100	-4.848700	H	-6.352400	2.886100	7.571200	H	-4.479500	-5.566700	5.805700
H	-6.968200	-1.863500	-5.585700	H	-7.391500	4.052800	8.458600	H	-2.679100	-5.654900	5.731900
C	-7.100100	-4.006500	-5.212100	C	-7.163300	7.383200	3.794300	H	-3.538000	-5.983600	7.273800
C	-6.558200	-2.719700	-1.237300	H	-6.191200	7.430500	3.274500	C	-3.498700	-0.362400	8.328200
C	-6.792200	-3.378900	-2.518400	H	-7.977300	7.318400	3.051000	H	-4.337100	0.267200	7.980800
C	-6.965700	-4.726100	-2.864900	H	-7.296700	8.291300	4.396400	H	-3.602900	-0.540700	9.406100
H	-6.956500	-5.492600	-2.090800	Cd	-1.616400	-0.001000	-0.000200	H	-2.542800	0.151700	8.135900
C	-7.098200	-5.042300	-4.216700	C	-3.315900	-2.174300	-2.040700	C	-3.546400	6.359200	5.376300
C	-6.559900	-2.777000	1.112600	C	-3.331300	-3.622400	-2.162900	H	-2.680700	5.732100	5.654300
C	-6.792500	-3.489100	2.365600	C	-3.363700	-4.468800	-3.280300	H	-3.539600	7.274100	5.982500
C	-6.967700	-4.848200	2.664200	H	-3.364200	-4.046100	-4.284000	H	-4.481000	5.806000	5.565300
H	-6.969000	-5.585200	1.861500	C	-3.423400	-5.841800	-3.052800	C	-3.498000	8.328300	0.361300
C	-7.101600	-5.211500	4.004500	C	-3.326200	-2.984000	0.034700	H	-4.336200	7.981000	-0.268500
C	-6.559200	-1.236800	2.717800	C	-3.346300	-4.133200	-0.856600	H	-3.602200	9.406300	0.539500
C	-6.793400	-2.517900	3.376900	C	-3.409100	-5.512400	-0.613000	H	-2.542000	8.135800	-0.152400
C	-6.967400	-2.864300	4.724100	H	-3.423600	-5.885500	0.410000	C	-0.006400	-1.221000	-2.722400
H	-6.958400	-2.090300	5.490600	C	-3.452700	-6.365600	-1.714100	C	-0.011900	-0.862400	-4.132900
C	-7.100000	-4.216200	5.040200	C	-3.316700	-2.040600	2.173400	C	-0.038800	-1.638300	-5.300000
C	-6.560800	1.113100	2.775100	C	-3.332400	-2.162800	3.621500	H	-0.058500	-2.725000	-5.231700
C	-6.793400	2.366200	3.487200	C	-3.364800	-3.280100	4.467800	C	-0.024900	-0.971600	-6.523700
C	-6.969100	2.664700	4.846100	H	-3.365200	-4.283800	4.045100	C	0.007700	1.005400	-2.808400
H	-6.970800	1.862100	5.583200	C	-3.424900	-3.052700	5.840800	C	0.013500	0.539000	-4.187100
C	-7.102900	4.005100	5.209500	C	-3.327200	0.034900	2.983200	C	0.040600	1.222600	-5.410500
C	-6.559300	2.718400	1.234900	C	-3.347500	-0.856400	4.132300	H	0.060300	2.311400	-5.426200
C	-6.793800	3.377500	2.515900	C	-3.410500	-0.612800	5.511600	C	0.026800	0.463500	-6.579100
C	-6.967700	4.724700	2.862300	H	-3.425200	0.410200	5.884700	C	-0.007000	2.721600	-1.220100
H	-6.958200	5.491200	2.088300	C	-3.454300	-1.714000	6.364700	C	-0.012900	4.132100	-0.861500
C	-7.100700	5.040800	4.214200	C	-3.317200	2.173600	2.039700	C	-0.040100	5.299100	-1.637400
C	-6.560100	2.775700	-1.115000	C	-3.332800	3.621700	2.161900	H	-0.059600	5.230700	-2.724200
C	-6.792300	3.487700	-2.368100	C	-3.365600	4.468000	3.279200	C	-0.026700	6.522900	-0.970800
C	-6.967800	4.846700	-2.666700	H	-3.366400	4.045400	4.282900	C	0.006800	2.807700	1.006400
H	-6.969600	5.583800	-1.864100	C	-3.425400	5.841000	3.051700	C	0.012200	4.186300	0.540000
C	-7.101200	5.210100	-4.007100	C	-3.327000	2.983300	-0.035800	C	0.038900	5.409800	1.223500
C	-6.558300	1.235400	-2.720300	C	-3.347500	4.132500	0.855500	H	0.058300	5.425500	2.312300
C	-6.792600	2.516500	-3.379400	C	-3.410200	5.511700	0.611900	C	0.024900	6.578400	0.464400
C	-6.966000	2.862900	-4.726700	H	-3.424500	5.884800	-0.411100	N	0.000000	1.945500	-0.075200
H	-6.956500	2.088900	-5.493200	C	-3.454300	6.364900	1.713000	N	0.000500	2.289900	-2.475000
C	-7.098900	4.214700	-5.042900	C	-3.316300	2.039900	-2.174400	N	0.000500	-0.076100	-1.946300
N	-6.352500	-1.375500	-1.443800	C	-3.331600	2.162100	-3.622600	N	0.000700	-2.475900	-2.290800
N	-6.611700	-3.367800	-0.077000	C	-3.364000	3.279300	-4.469000	N	-0.000500	2.474200	2.290900
N	-6.353200	-1.443300	1.373700	H	-3.364900	4.283100	-4.046300	O	0.055400	7.836800	0.978000
N	-6.612800	-0.076500	3.365900	C	-3.423600	3.051900	-5.842000	O	-0.057900	7.737900	-1.580000
N	-6.353500	1.374200	1.441500	C	-3.326000	-0.035600	-2.984200	O	0.057900	0.977200	-7.837500
N	-6.612400	3.366500	0.074600	C	-3.346200	0.855700	-4.133400	O	-0.055700	-1.580800	-7.738800
N	-6.352900	1.442000	-1.376000	C	-3.408600	0.612000	-5.512600	C	0.007500	-2.809400	-1.006300
N	-6.611400	0.075100	-3.368400	H	-3.422900	-0.411000	-5.885700	C	0.013200	-4.188100	-0.539800
O	-7.214800	-4.452300	-6.492400	C	-3.452400	1.713100	-6.365900	C	0.040400	-5.411600	-1.223300
O	-7.206800	-6.302600	-4.710200	N	-3.328500	-1.813700	-0.703600	H	0.060200	-5.427300	-2.312100
O	-7.216400	-6.491900	4.450300	N	-3.324100	-3.088100	1.358400	C	0.026500	-6.580200	-0.464200
O	-7.209100	-4.709600	6.300600	N	-3.329300	-0.703400	1.812800	C	-0.007000	-2.723300	1.220200
O	-7.218100	4.450800	6.489800	N	-3.325000	1.358600	3.087200	C	-0.012400	-4.133900	0.861600
O	-7.209700	6.301200	4.707600	N	-3.329500	1.813000	0.702500	C	-0.039400	-5.300900	1.637500
O	-7.216200	6.490400	-4.452900	N	-3.324300	3.087400	-1.359500	H	-0.059200	-5.232600	2.724300
O	-7.207600	4.708100	-6.303200	N	-3.328700	0.702700	-1.813900	C	-0.025400	-6.524700	0.970900
C	-7.160600	-7.384600	-3.796900	N	-3.323500	-1.359300	-3.088300	C	0.006700	-1.007200	2.808600
H	-6.188800	-7.431800	-3.276700	O	-3.461800	-6.787600	-4.028200	C	0.012100	-0.540800	4.187200
H	-7.974900	-7.320000	-3.053900	O	-3.525900	-7.719900	-1.642600	C	0.038900	-1.224200	5.410700
H	-7.293600	-8.292800	-4.399000	O	-3.463400	-4.028100	6.786700	H	0.058700	-2.313000	5.426500
C	-7.273300	-3.491800	-7.525500	O	-3.527800	-1.642500	7.719000	C	0.024800	-0.465100	6.579300
H	-8.135100	-2.812700	-7.399400	O	-3.464300	6.786900	4.027100	C	-0.007600	1.219200	2.722500
H	-6.348800	-2.887500	-7.573500	O	-3.527700	7.719200	1.641500	C	-0.013500	0.860600	4.133000
H	-7.387500	-4.054300	-8.461300	O	-3.462100	4.027200	-6.787900	C	-0.040900	1.636600	5.300000
C	-7.161000	3.794900	-7.385200	O	-3.525600	1.641600	-7.720100	H	-0.060600	2.723400	5.231600
H	-7.294100	4.396900	-8.293400	C	-3.544200	5.376500	-6.360200	C	-0.027100	0.970000	6.523800
H	-6.189000	3.275000	-7.432300	H	-2.678600	5.654300	-5.732900	N	-0.000300	0.074300	1.946400
H	-7.975000	3.051600	-7.320600	H	-3.537100	5.982600	-7.275100	N	-0.000100	-2.291700	2.475100
C	-7.275100	7.523500	-3.492400	H	-4.478900	5.565600	-5.807300	N	0.000100	-1.947300	0.075300
H	-8.136900	7.397100	-2.813400	C	-3.496100	0.361400	-8.329200	O	-0.058200	1.579300	7.738800
H	-6.350700	7.571700	-2.888000	H	-4.334500	-0.268200	-7.982000	O	0.055600	-0.978700	7.837700
H	-7.389500	8.459200	-4.054900	H	-3.600100	0.539700	-9.407200	O	-0.056300	-7.739700	1.580100
C	-7.274600	-7.525000	3.489700	H	-2.540200	-0.152500	-8.136700	O	0.057600	-7.838600	-0.977800
H	-8.136200	-7.398900	2.810400	C	-3.543500	-6.360000	-5.377400	C	0.027900	2.386500	-7.991000
H	-6.349900	-7.573000	2.885700	H	-2.677800	-5.732800	-5.655100	H	0.885800	2.864900	-7.485800
H	-7.388900	-8.460700	4.052200	H	-3.536400	-7.274900	-5.983600	H	0.094500	2.572300	-9.070700
C	-7.163300	-3.796300	7.382600	H	-4.478100	-5.806900	-5.566800	H	-0.913800	2.811700	-7.607800
H	-7.977500	-3.053300	7.317600	C	-3.496800	-8.329000	-0.362400	C	-0.024800	-2.997700	-7.783200
H	-7.296700	-4.398400	8.290700	H	-4.335200	-7.981700	0.267100	H	-0.882200	-3.436400	-7.242600
H	-6.191500	-3.276100	7.430200	H	-3.600900	-9.407000	-0.540700	H	-0.091300	-3.266100	-8.845400
C	-7.276900	3.490300	7.522900	H	-2.540900	-8.136600	0.151700	H	0.917400	-3.391400	-7.368500
H	-8.138600	2.811100	7.396400	C	-3.545000	-5.377300	6.359000	C	0.027200	-7.992100	-2.387200

H	0.884900	-7.486800	-2.865800	C	7.162300	-7.067000	4.356600	N	3.324600	-3.182600	-1.115700
H	0.093900	-9.071800	-2.572900	H	6.190600	-7.154600	3.841400	O	3.464100	-4.539100	-6.455300
H	-0.914700	-7.609000	-2.812100	H	7.976800	-7.059700	3.611100	O	3.528000	-2.232700	-7.569100
C	-0.025600	-7.784000	2.997100	H	7.295500	-7.925800	5.027200	O	3.462300	6.456800	-4.539500
H	-0.883100	-7.243400	3.435500	C	7.275700	-7.770600	-2.897200	O	3.525600	7.570600	-2.233000
H	-0.092200	-8.846200	3.265600	H	8.137400	-7.592200	-2.229800	O	3.460900	4.540900	6.456400
H	0.916500	-7.369300	3.390900	H	6.351100	-7.771800	-2.291200	O	3.524700	2.234500	7.570200
C	0.025300	-2.388000	7.991400	H	7.390200	-8.747000	-3.385600	O	3.462700	-6.454900	4.540500
H	0.091800	-2.573600	9.071100	C	7.163700	-4.354300	-7.066900	O	3.527000	-7.568600	2.234100
H	-0.916500	-2.813000	7.608100	H	6.191900	-3.839400	-7.154600	C	3.495400	1.005100	8.276300
H	0.883100	-2.866500	7.486300	H	7.977900	-3.608500	-7.059600	H	4.333800	0.350700	7.978800
C	-0.028200	2.996200	7.783100	H	7.297100	-5.024900	-7.925700	H	3.599300	1.266200	9.337300
H	-0.885800	3.434300	7.242300	C	7.276400	2.899700	-7.770400	H	2.539500	0.477800	8.124000
H	-0.095000	3.264700	8.845200	H	8.138100	2.232500	-7.591800	C	3.542900	5.853100	5.925900
H	0.913800	3.390500	7.368500	H	6.351900	2.293500	-7.771800	H	2.677400	6.081500	5.278700
C	0.024900	7.990400	2.387300	H	7.390900	3.388200	-8.746800	H	3.535300	6.528100	6.791200
H	0.882600	7.485300	2.866000	C	7.162900	7.069400	-4.354100	H	4.477700	5.999200	5.360200
H	0.091300	9.070100	2.573000	H	7.977100	7.062200	-3.608300	C	3.496200	8.276600	-1.003600
H	-0.917000	7.607100	2.812100	H	7.296100	7.928200	-5.024600	H	4.334700	7.979200	-0.349200
C	-0.027100	7.782300	-2.997000	H	6.191000	7.156800	-3.839200	H	3.599900	9.337700	-1.264600
H	-0.094100	8.844400	-3.265400	C	7.274200	7.772800	2.899800	H	2.540300	8.124100	-0.476300
H	0.915200	7.368000	-3.390800	H	8.136000	7.594500	2.232700	C	3.544700	5.926200	-5.851700
H	-0.884300	7.241200	-3.435500	H	6.349700	7.774100	2.293500	H	4.479500	5.360600	-5.997500
Y	5.044100	0.001100	0.000800	H	7.388400	8.749300	3.388300	H	2.679200	5.279100	-6.080300
C	6.560500	-2.853000	-0.894600	C	7.160800	4.356500	7.069500	H	3.537300	6.791600	-6.526700
C	6.793100	-3.659900	-2.088700	H	6.189000	3.841500	7.156700	C	3.498800	-1.003400	-8.275200
C	6.968500	-5.037900	-2.281300	H	7.975100	3.610800	7.062400	H	4.337200	-0.348900	-7.977400
H	6.969900	-5.710700	-1.424000	H	7.293800	5.027100	7.928300	H	3.603000	-1.264400	-9.336200
C	7.102300	-5.503900	-3.589500	C	7.273800	-2.897400	7.773000	H	2.542900	-0.476000	-8.123100
C	6.559500	-1.441600	-2.614200	H	8.135500	-2.230000	7.594700	C	3.546100	-5.851300	-5.924700
C	6.793800	-2.769800	-3.172200	H	6.349200	-2.291400	7.774100	H	2.680400	-6.079900	-5.277900
C	6.967700	-3.219400	-4.488600	H	7.388000	-3.385800	8.749400	H	3.538900	-6.526400	-6.790100
H	6.958500	-2.507100	-5.312600	Cd	1.616700	-0.000400	0.000400	H	4.480800	-5.997200	-5.358800
C	7.100500	-4.591700	-4.699100	C	3.317100	-2.201200	-2.009200	C	3.498500	-8.274700	1.004700
C	6.560800	0.896800	-2.853000	C	3.332900	-2.435000	-3.443600	H	4.337000	-7.976800	0.350600
C	6.793300	2.091100	-3.659800	C	3.365500	-3.614300	-4.201100	H	3.602700	-9.335700	1.265700
C	6.968900	2.283600	-5.037800	H	3.366000	-4.582400	-3.702200	H	2.542700	-8.122800	0.477000
H	6.970600	1.426400	-5.710600	C	3.425400	-3.493600	-5.587600	C	3.544300	-5.924300	5.852800
C	7.102400	3.591900	-5.503800	C	3.327400	-0.194600	-2.976900	H	2.678600	-5.277500	6.081100
C	6.559100	2.616400	-1.441500	C	3.347800	-1.172000	-4.053800	H	3.537000	-6.789700	6.527800
C	6.793600	3.174500	-2.769700	C	3.410700	-1.035600	-5.447700	H	4.478900	-5.358400	5.998900
C	6.967300	4.490900	-3.219300	H	3.425300	-0.044500	-5.898700				
H	6.957800	5.315000	-2.506900	C	3.454500	-2.199300	-6.213300	444			
C	7.100200	4.701500	-4.591500	C	3.317100	2.010600	-2.201600	**[5]**$^{+}$			
C	6.559800	2.855300	0.896900	C	3.332200	3.445000	-2.435400	Y	4.986800	-0.469800	0.001000
C	6.792000	3.662100	2.091100	C	3.364600	4.202600	-3.614700	C	6.718400	1.502700	2.102500
C	6.967300	5.040200	2.283700	H	3.365400	3.703600	-4.582800	C	7.011300	1.645700	3.527700
H	6.969000	5.712900	1.426500	C	3.423900	5.589000	-3.494000	C	7.377200	2.745900	4.315900
C	7.100600	5.506200	3.592000	C	3.326700	2.978300	-0.195000	H	7.494500	3.728800	3.860500
C	6.558200	1.443800	2.616500	C	3.346700	4.055200	-1.172400	C	7.571700	2.537100	5.683800
C	6.792400	2.772100	3.174600	C	3.409000	5.449100	-1.036000	C	6.520000	-0.525800	2.985100
C	6.965800	3.221700	4.491000	H	3.423300	5.900100	-0.044900	C	6.881300	0.366500	4.083300
H	6.956300	2.509300	5.315100	C	3.452700	6.214800	-2.199700	C	7.097900	0.133500	5.447000
C	7.098400	4.593900	4.701600	C	3.316100	2.203000	2.010200	H	6.992100	-0.872300	5.851700
C	6.559600	-0.894600	2.855300	C	3.331200	2.436800	3.444600	C	7.421000	1.225900	6.253900
C	6.792000	-2.088800	3.662200	C	3.363400	3.616100	4.202200	C	6.321500	-2.705800	2.127800
C	6.967100	-2.281300	5.040300	H	3.364100	4.584200	3.703200	C	6.464700	-4.150800	2.297900
H	6.968500	-1.424100	5.713000	C	3.422700	3.495400	5.588700	C	6.650200	-4.959900	3.427700
C	7.100800	-3.589600	5.506300	C	3.326000	0.196400	2.977900	H	6.716800	-4.508700	4.417300
C	6.558700	-2.614200	1.443900	C	3.345900	1.173800	4.054800	C	6.734400	-6.341800	3.238100
C	6.792800	-3.172200	2.772100	C	3.408300	1.037400	5.448800	C	6.232600	-3.583900	0.089700
C	6.966600	-4.488600	3.221700	H	3.422700	0.046300	5.899700	C	6.403900	-4.703100	1.012100
H	6.957600	-5.312700	2.509300	C	3.451700	2.201100	6.214400	C	6.512600	-6.083200	0.800600
C	7.099100	-4.699200	4.594000	C	3.316200	-2.008800	2.202700	H	6.464400	-6.485100	-0.210700
N	6.353500	-1.543500	-1.258000	C	3.331900	-3.443100	2.436400	C	6.654700	-6.906900	1.918600
N	6.612900	-0.334900	-3.350100	C	3.364300	-4.200700	3.615700	C	6.320700	-2.731100	-2.099300
N	6.353500	1.260200	-1.543500	H	3.364700	-3.701800	4.583800	C	6.582500	-2.926500	-3.524300
N	6.612100	3.352300	-0.334800	C	3.424100	-5.587200	3.495000	C	6.736700	-4.075800	-4.312300
N	6.352800	1.545800	1.260200	C	3.326700	-2.976500	0.196000	H	6.667900	-5.063300	-3.856800
N	6.611400	0.337100	3.352400	C	3.347000	-4.053400	1.173400	C	6.967700	-3.907200	-5.680100
N	6.352800	-1.258000	1.545800	C	3.409900	-5.447300	1.037100	C	6.505600	-0.701400	-2.981900
N	6.612300	-3.350100	0.337100	H	3.424700	-5.898300	0.045900	C	6.694300	-1.645600	-4.079900
O	7.217300	-6.814900	-3.934800	C	3.453600	-6.212900	2.200800	C	6.951600	-1.457400	-5.443600
O	7.209500	-5.181200	-5.917500	N	3.329600	-0.840200	-1.753100	H	7.036100	-0.449600	-5.848300
O	7.217500	3.937300	-6.814700	N	3.324900	1.117200	-3.183000	C	7.065300	-2.591000	-6.250200
O	7.209000	5.919900	-5.181000	N	3.329600	1.754500	-0.840600	C	6.717400	1.477400	-2.124600
O	7.215400	6.817200	3.937400	N	3.323900	3.184400	1.116700	C	7.128400	2.870000	-2.294500
O	7.207000	5.183400	5.920100	N	3.328800	0.842000	1.754100	C	7.462700	3.630100	-3.424100
O	7.215500	-3.935000	6.817300	N	3.323600	-1.115300	3.184000	H	7.444600	3.174400	-4.413600
O	7.208000	-5.917600	5.183500	N	3.328800	-1.752600	0.841600	C	7.803600	4.972000	-3.234400

C	6.792700	2.356800	-0.086500	C	3.468900	1.122900	-3.969300	H	0.007700	0.878800	-5.834100
C	7.170900	3.424100	-1.008700	C	3.599000	2.044200	-5.018200	C	0.255400	3.042400	-5.846800
C	7.535500	4.759500	-0.797100	H	3.707600	3.106400	-4.803700	N	0.102500	1.079500	-1.617700
H	7.562500	5.163500	0.214200	C	3.578400	1.552700	-6.323900	N	0.310600	3.295000	-0.654000
C	7.829900	5.542100	-1.914900	C	3.590700	2.597000	-0.594100	N	0.151200	1.611200	1.083700
N	6.362400	0.204200	1.829700	C	3.714400	3.887100	0.063100	N	0.060100	0.651700	3.309000
N	6.454500	-1.845300	3.133200	C	3.855600	5.184500	-0.447000	N	-0.060000	-0.650600	-3.309100
N	6.116100	-2.412500	0.801500	H	3.870000	5.347500	-1.523700	O	0.237000	3.268900	-7.184600
N	6.277600	-3.736900	-1.230100	C	3.995900	6.228900	0.464800	O	0.578600	5.368400	-5.762600
N	6.213600	-1.389000	-1.826700	C	3.560900	2.198300	1.598900	O	0.601100	7.160300	3.276100
N	6.687800	0.607100	-3.130000	C	3.704000	3.638400	1.443500	O	0.610100	5.731300	5.398300
N	6.459800	1.227700	-0.798500	C	3.845200	4.678700	2.372800	C	-0.067300	-0.610700	2.920200
N	6.864700	2.498700	1.233400	H	3.833400	4.464400	3.440500	C	-0.179200	-1.724600	3.848800
O	7.903500	3.503200	6.572800	C	3.992800	5.976200	1.881500	C	-0.218200	-1.780200	5.249100
O	7.607300	1.164400	7.594300	N	3.301300	-0.668000	1.913400	H	-0.159800	-0.863300	5.833900
O	6.889100	-7.249300	4.231300	N	3.060300	-3.080000	1.914000	C	-0.319700	-3.035100	5.846700
O	6.719500	-8.259300	1.874900	N	3.156500	-2.218800	-0.355200	C	-0.223200	-2.456200	1.679400
O	7.113500	-4.918400	-6.568900	N	3.143300	-2.218200	-2.779200	C	-0.257000	-2.887900	3.067900
O	7.260600	-2.565500	-7.590500	N	3.369900	0.039700	-1.912800	C	-0.343300	-4.158100	3.655100
O	8.126000	5.834500	-4.227400	N	3.582800	2.454300	-1.913500	H	-0.399100	-5.046900	3.028300
O	8.146300	6.858600	-1.871100	N	3.514700	1.590500	0.355800	C	-0.367200	-4.230000	5.046700
C	7.543300	-0.104200	8.223000	N	3.500000	1.592600	2.779800	C	-0.282000	-2.906100	-0.615000
H	6.540800	-0.556100	8.122700	O	3.385800	-0.443900	7.890500	C	-0.375700	-3.830000	-1.734400
H	8.296300	-0.795800	7.807400	O	3.182700	-2.958000	7.440100	C	-0.540200	-5.221000	-1.793500
H	7.758600	0.073000	9.284100	O	2.659200	-8.175600	-0.124400	H	-0.622700	-5.800600	-0.875200
C	8.132300	4.811500	6.088100	O	2.735400	-7.730300	-2.646400	C	-0.579300	-5.817500	-3.052500
H	8.951700	4.831000	5.348600	O	3.413600	-0.196100	-7.889900	C	-0.147900	-1.672400	-2.467000
H	7.222700	5.237000	5.627000	O	3.683100	2.311700	-7.439400	C	-0.271100	-3.055400	-2.899900
H	8.413500	5.415200	6.960000	O	4.139300	7.535300	0.124800	C	-0.292900	-3.643100	-4.172600
C	8.260000	7.479400	-0.602200	O	4.130200	7.083700	2.646800	H	-0.206500	-3.021600	-5.062700
H	8.556700	8.517300	-0.798700	C	4.179400	7.869600	-1.252300	C	-0.439900	-5.027000	-4.246500
H	7.299000	7.469500	-0.058500	H	3.250400	7.566600	-1.766900	N	-0.151200	-1.610000	-1.083800
H	9.031700	6.989200	0.016100	H	4.280000	8.961300	-1.295800	N	-0.310300	-3.293900	0.653800
C	8.185400	5.342000	-5.551300	H	5.042800	7.401900	-1.755200	N	-0.102300	-1.078400	1.617600
H	8.926300	4.529300	-5.647300	C	4.110000	6.942400	4.058800	O	-0.467400	-5.743400	-5.398500
H	7.200800	4.971700	-5.889800	H	4.911300	6.265400	4.403300	O	-0.744200	-7.145600	-3.276400
H	8.489900	6.189000	-6.178700	H	4.285400	7.947400	4.462600	O	-0.435800	-5.380600	5.762600
C	7.038600	-6.776500	5.555300	H	3.132800	6.574900	4.411400	O	-0.380600	-3.254200	7.184400
H	7.918200	-6.116500	5.651900	C	3.523400	0.926400	8.227200	C	0.697400	8.031000	2.159600
H	6.140300	-6.228800	5.893100	H	2.679100	1.522700	7.838200	H	-0.176900	7.926900	1.493100
H	7.178900	-7.665500	6.182900	H	3.525000	0.969900	9.323500	H	0.718800	9.047100	2.573100
C	6.716300	-8.890500	0.606000	H	4.470000	1.342400	7.842600	H	1.624600	7.850600	1.592400
H	7.566600	-8.553200	-0.011400	C	3.043000	-4.363100	7.297500	C	0.530700	5.036300	6.633100
H	6.813600	-9.965500	0.802700	H	3.868100	-4.787100	6.698900	H	1.323500	4.271900	6.714800
H	5.774500	-8.701100	0.061500	H	3.084800	-4.772600	8.314500	H	0.676200	5.794000	7.413200
C	7.093300	-6.246400	-6.084100	H	2.075600	-4.625800	6.839800	H	-0.457500	4.566700	6.763300
H	7.894000	-6.418600	-5.344100	C	2.635900	-8.511600	1.252700	C	-0.262700	-2.143900	8.060300
H	6.119800	-6.494100	-5.623600	H	3.571300	-8.213400	1.755800	H	-1.057400	-1.400100	7.874300
H	7.257200	-6.892100	-6.955900	H	1.779700	-8.040400	1.767200	H	-0.375200	-2.548600	9.073900
C	7.435100	-1.307400	-8.219300	H	2.530700	-9.602900	1.296100	H	0.726200	-1.666700	7.968000
H	6.534700	-0.676100	-8.119600	C	2.741800	-7.587500	-4.058400	C	-0.564600	-6.608700	5.063200
H	8.303900	-0.768700	-7.803200	H	3.655500	-7.072300	-4.402900	H	0.285200	-6.770400	4.376700
H	7.614200	-1.521800	-9.280300	H	2.726200	-8.607500	-4.462200	H	-0.564100	-7.392300	5.831200
Cd	1.596500	-0.149900	0.000200	H	1.850500	-7.043800	-4.410800	H	-1.512300	-6.650700	4.502800
C	3.371100	0.279500	2.922600	C	3.293100	-1.568000	-8.226700	C	-0.812500	-8.019100	-2.160000
C	3.311700	-0.375000	4.218600	H	2.352100	-1.996200	-7.838200	H	-0.981500	-9.021200	-2.573700
C	3.378000	0.131100	5.523500	H	3.287200	-1.611000	-9.323000	H	0.132000	-8.015400	-1.592700
H	3.477800	1.203200	5.687100	H	4.145200	-2.153400	-7.841600	H	-1.652000	-7.753400	-1.493600
C	3.334000	-0.780500	6.576500	C	3.808100	3.718200	-7.296600	C	-0.415200	-5.045800	-6.633300
C	3.174100	-1.904600	2.522800	H	4.697500	3.980600	-6.697500	H	0.506300	-4.442900	-6.714700
C	3.195600	-1.750500	3.969900	H	3.926100	4.112700	-8.313500	H	-0.413600	-5.817300	-7.413400
C	3.151100	-2.679800	5.019000	H	2.906500	4.156800	-6.839300	H	-1.298400	-4.400000	-6.763700
H	3.059600	-3.743600	4.804600	C	0.165000	1.672000	2.466900	C	0.146000	2.156100	-8.060500
C	3.222000	-2.192900	6.324600	C	0.302100	3.053700	2.899800	H	-0.773600	1.573600	-7.874700
C	3.042400	-3.221700	0.594600	C	0.389700	3.635300	4.172500	H	0.111200	2.574700	-9.074100
C	2.923400	-4.512300	-0.062600	H	0.358000	3.008600	5.062600	H	1.028500	1.502900	-7.968000
C	2.819400	-5.813200	0.447500	C	0.503800	5.022300	4.246300	C	0.680400	6.599000	-5.063300
H	2.802500	-5.976000	1.524100	C	0.265000	2.908900	0.614800	H	0.827200	7.368700	-5.831300
C	2.762500	-6.865400	-0.464400	C	0.344700	3.834100	1.734300	H	-0.243300	6.816800	-4.503400
C	3.089200	-2.824600	-1.598200	C	0.443000	5.231300	1.793300	H	1.545000	6.599700	-4.376300
C	2.960300	-4.266000	-1.442900	H	0.470800	5.816100	0.875000	Y	-4.987000	0.469500	-0.000900
C	2.904900	-5.314300	-2.372300	C	0.515200	5.824800	3.052200	C	-6.629900	-0.547300	2.750700
H	2.933800	-5.101600	-3.440000	C	0.240600	2.455800	-1.679500	C	-6.871400	-0.137500	4.133000
C	2.807200	-6.616600	-1.881000	C	0.288400	2.886100	-3.068000	C	-7.201600	-0.854300	5.291800
C	3.262100	-0.904200	-2.922000	C	0.440600	4.150100	-3.655200	H	-7.327800	-1.935700	5.247500
C	3.326400	-0.250100	-4.218000	H	0.551100	5.033700	-3.028300	C	-7.349300	-0.141200	6.484500
C	3.297600	-0.759700	-5.523000	C	0.431200	4.225200	-5.046800	C	-6.415000	1.662900	2.790800
H	3.195600	-1.831500	-5.686700	C	0.050300	0.613500	-2.920400	C	-6.731100	1.256000	4.157300
C	3.425000	0.144200	-6.575800	C	0.148400	1.728600	-3.848900	C	-6.901200	1.989900	5.337700
C	3.475900	1.278200	-2.522200	C	0.121000	1.790500	-5.249300	H	-6.788400	3.073300	5.326900

C	-7.187900	1.287200	6.509300	C	-3.265100	0.871900	2.928400	C	-3.915700	-4.859000	6.529000
C	-6.262100	3.353800	1.164700	C	-3.164600	1.968100	3.877100	H	-4.709100	-4.096600	6.619600
C	-6.409500	4.756300	0.779200	C	-3.181400	1.994600	5.277900	H	-4.069500	-5.634900	7.289200
C	-6.561000	5.934500	1.523600	H	-3.267800	1.065100	5.838900	H	-2.929300	-4.392000	6.681000
H	-6.589800	5.892700	2.612100	C	-3.106700	3.236800	5.904700	C	-4.166100	-7.728300	1.970700
C	-6.661400	7.142000	0.827500	C	-3.097200	2.740400	1.724500	H	-3.258000	-7.649300	1.347000
C	-6.250700	3.393100	-1.056000	C	-3.066900	3.146100	3.122000	H	-4.260600	-8.754400	2.347600
C	-6.397500	4.779500	-0.621300	C	-2.992000	4.403200	3.738500	H	-5.050000	-7.479700	1.359200
C	-6.523200	5.977100	-1.336200	H	-2.915400	5.305800	3.134000				
H	-6.513000	5.965300	-2.425400	C	-3.013500	4.447800	5.132900	444			
C	-6.631800	7.164200	-0.609700	C	-3.041800	3.228100	-0.562100	**[5]**$^{2+}$			
C	-6.409300	1.774600	-2.753800	C	-2.955200	4.172800	-1.662900	Y	0.629500	4.948600	-0.001000
C	-6.722000	1.416900	-4.136300	C	-2.842800	5.569200	-1.687600	C	0.640200	6.501000	2.977700
C	-6.911800	2.182700	-5.295300	H	-2.789300	6.127600	-0.754200	C	1.488800	6.708400	4.149100
H	-6.834000	3.268600	-5.251000	C	-2.825600	6.197300	-2.931400	C	1.189900	7.053600	5.472300
C	-7.189100	1.509600	-6.488100	C	-3.162400	2.030300	-2.438200	H	0.154200	7.187800	5.781900
C	-6.610600	-0.436900	-2.793900	C	-3.038800	3.422300	-2.845000	C	2.254900	7.212800	6.363800
C	-6.844100	0.021800	-4.160600	C	-3.023700	4.040100	-4.103500	C	2.731900	6.241200	2.284700
C	-7.147300	-0.667700	-5.341200	H	-3.088600	3.439100	-5.009300	C	2.809500	6.548800	3.712500
H	-7.238600	-1.753100	-5.330300	C	-2.918300	5.430700	-4.145800	C	3.891400	6.737400	4.582500
C	-7.297100	0.076200	-6.512900	C	-3.368100	-0.247200	-2.929000	H	4.912700	6.636700	4.216500
C	-6.777000	-2.126500	-1.167700	C	-3.473500	-1.342900	-3.877600	C	3.613400	7.061300	5.914700
C	-7.183700	-3.476800	-0.782400	C	-3.494300	-1.365800	-5.278400	C	3.778900	6.101600	0.183800
C	-7.551900	-4.606200	-1.527000	H	-3.405200	-0.436700	-5.839400	C	4.980500	6.263600	-0.632000
H	-7.571700	-4.559800	-2.615500	C	-3.652600	-2.600200	-5.905300	C	6.331500	6.398900	-0.292100
C	-7.876300	-5.773700	-0.831000	C	-3.552800	-2.114100	-1.725100	H	6.639100	6.362600	0.752300
C	-6.774600	-2.167100	1.052900	C	-3.597800	-2.518500	-3.122500	C	7.252800	6.575700	-1.328600
C	-7.177200	-3.501800	0.618100	C	-3.758700	-3.767400	-3.739000	C	3.092100	6.194600	-1.924000
C	-7.524600	-4.654900	1.332800	H	-3.852300	-4.668400	-3.134500	C	4.548300	6.326600	-1.962200
H	-7.513100	-4.645000	2.422000	C	-3.787500	-3.807200	-5.133400	C	5.452100	6.537200	-3.011900
C	-7.852300	-5.800900	0.606300	C	-3.591100	-2.603400	0.561600	H	5.092600	6.611700	-4.037700
N	-6.293000	0.548400	1.993600	C	-3.682600	-3.547600	1.662400	C	6.809800	6.652900	-2.695300
N	-6.353600	2.939600	2.425300	C	-3.832300	-4.940600	1.687100	C	1.007300	6.453500	-2.980200
N	-6.101200	2.578200	0.042300	H	-3.883100	-5.499200	0.753600	C	0.237400	6.866400	-4.151700
N	-6.343000	3.034600	-2.332800	C	-3.933200	-5.560800	2.930900	C	0.613000	7.125900	-5.474900
N	-6.283300	0.635400	-1.996600	C	-3.487600	-1.404000	2.437600	H	1.649400	6.996900	-5.784600
N	-6.788800	-1.702600	-2.428400	C	-3.625700	-2.794600	2.844400	C	-0.378300	7.546200	-6.366400
N	-6.474900	-1.394500	-0.045200	C	-3.726800	-3.404400	4.102900	C	-1.083000	6.725200	-2.287200
N	-6.799400	-1.797600	2.329700	H	-3.679200	-2.801800	5.008800	C	-1.081200	7.042200	-3.715100
O	-7.642600	-0.696000	7.684500	C	-3.882300	-4.790300	4.145200	C	-2.081700	7.495300	-4.585000
O	-7.327300	1.853400	7.732000	N	-3.237300	1.366100	1.633800	H	-3.095700	7.653200	-4.219000
O	-6.787600	8.359300	1.407200	N	-3.012700	3.596800	0.712400	C	-1.731500	7.739200	-5.917200
O	-6.707400	8.399500	-1.160500	N	-3.181800	1.940900	-1.056800	C	-2.131600	6.852500	-0.186300
O	-7.372900	2.109300	-7.688300	N	-3.253500	1.022200	-3.298800	C	-3.254300	7.310300	0.629400
O	-7.538900	-0.454200	-7.735800	N	-3.433800	-0.737800	-1.634300	C	-4.528600	7.779200	0.289400
O	-8.227100	-6.946100	-1.410900	N	-3.630400	-2.971200	-0.712900	H	-4.835500	7.820600	-0.755000
O	-8.157500	-7.000300	1.156900	N	-3.489300	-1.312700	1.056200	C	-5.376200	8.181400	1.325700
C	-8.222300	-7.093000	2.569600	N	-3.389700	-0.396500	3.298200	C	-1.443200	6.771500	1.921500
H	-7.242900	-6.884000	3.034900	O	-3.109800	3.423500	7.249400	C	-2.820100	7.263700	1.959600
H	-8.975400	-6.399800	2.982500	O	-2.940300	5.578100	5.873300	C	-3.642400	7.694300	3.009100
H	-8.518300	-8.125900	2.791800	O	-2.719800	7.537900	-3.116900	H	-3.275500	7.677000	4.034900
C	-7.879200	-2.088800	7.740300	O	-2.881600	6.171100	-5.278000	C	-4.927900	8.145900	2.692400
H	-8.724000	-2.381400	7.092800	O	-3.689800	-2.783100	-7.249900	N	1.417400	6.157900	1.895200
H	-6.983400	-2.663500	7.443000	O	-3.926400	-4.931400	-5.873900	N	3.811400	6.157600	1.511300
H	-8.125200	-2.315000	8.785300	O	-4.079300	-6.897600	3.116300	N	2.674400	5.997800	-0.630400
C	-7.250300	3.265200	7.830300	O	-3.985000	-5.524500	5.277400	N	2.331600	6.344900	-3.005400
H	-6.255200	3.638700	7.531000	C	-4.036600	-6.178100	-5.204800	N	0.168900	6.315900	-1.897700
H	-8.022400	3.752700	7.210400	H	-4.902500	-6.187800	-4.519800	N	-2.149100	6.914400	-1.513800
H	-7.427000	3.504900	8.886300	H	-4.187900	-6.927500	-5.991700	N	-1.088100	6.475900	0.628000
C	-6.887500	8.424800	2.816000	H	-3.116400	-6.417300	-4.647700	N	-0.669300	6.727200	3.002900
H	-7.758700	7.856700	3.186100	C	-3.591100	-1.641800	-8.085200	O	2.123000	7.515900	7.672300
H	-5.974300	8.039800	3.304700	H	-2.640100	-1.104700	-7.921400	O	4.545200	7.263500	6.869700
H	-7.012000	9.486200	3.064200	H	-3.624100	-2.017300	-9.115600	O	8.586700	6.692200	-1.159700
C	-6.753100	8.502600	-2.573200	H	-4.433200	-0.948400	-7.920700	O	7.797300	6.847500	-3.594400
H	-7.622100	7.962000	-2.986500	C	-2.936800	5.504200	-6.529600	O	-0.174900	7.806600	-7.674900
H	-6.851100	9.572500	-2.795400	H	-3.858200	4.902900	-6.620600	O	-2.583200	8.167900	-6.872200
H	-5.829700	8.114600	-3.038000	H	-2.942900	6.295200	-7.289900	O	-6.638500	8.627900	1.156700
C	-7.345500	3.521700	-7.744100	H	-2.054500	4.861700	-6.681200	O	-5.835200	8.581900	3.591300
H	-8.121300	3.966800	-7.097200	C	-2.650900	8.370400	-1.971400	C	5.912700	7.224700	6.503900
H	-6.358400	3.919300	-7.446200	H	-3.566000	8.291000	-1.360500	H	6.202100	6.225600	6.132000
H	-7.544300	3.789800	-8.789300	H	-1.773900	8.123600	-1.347200	H	6.143400	7.978500	5.731900
C	-7.726600	-1.855500	-7.834100	H	-2.552200	9.396000	-2.348400	H	6.477600	7.450900	7.416300
H	-6.818900	-2.408100	-7.534000	C	-2.815600	6.823400	5.204200	C	0.827000	7.791400	8.178100
H	-8.576500	-2.190300	-7.214700	H	-3.664200	6.994600	4.519000	H	0.367500	8.645900	7.652600
H	-7.944100	-2.058200	-8.890200	H	-2.824500	7.587900	5.991100	H	0.163800	6.912900	8.091900
C	-8.336400	-6.991900	-2.819700	H	-1.866800	6.886500	4.647300	H	0.963100	8.043600	9.236600
H	-9.086000	-6.271300	-3.190500	C	-3.226100	2.283800	8.084600	C	-5.455400	8.668900	4.952800
H	-7.367000	-6.784100	-3.307700	H	-2.391900	1.578700	7.921200	H	-6.323300	9.077200	5.484600
H	-8.656600	-8.011500	-3.068000	H	-3.188900	2.658900	9.115000	H	-5.206600	7.675200	5.366000
Cd	-1.596600	0.150800	-0.000200	H	-4.182700	1.759800	7.919700	H	-4.591700	9.342500	5.086400

C	-7.126500	8.800600	-0.163800	H	-4.956500	4.887000	5.856100	N	1.928400	-0.244700	-0.094900
H	-6.505700	9.517800	-0.727300	C	0.186600	3.434500	8.341600	O	-1.630700	0.283000	-7.719700
H	-7.161400	7.842200	-0.710700	H	0.889800	4.215500	8.006600	O	0.876000	-0.190000	-7.843900
H	-8.142900	9.199100	-0.060500	H	0.020300	3.533500	9.421100	O	7.667000	-0.898300	-1.652800
C	9.102400	6.737700	0.160700	H	0.599200	2.435900	8.127600	O	7.771000	-1.065100	0.893500
H	8.681000	7.587600	0.724000	C	6.811000	2.480200	5.290700	C	-2.293000	0.218900	8.027100
H	8.896400	5.801200	0.708000	H	6.102600	1.669100	5.536000	H	-2.868000	-0.579600	7.526200
H	10.186300	6.869100	0.057300	H	7.726600	2.357000	5.882000	H	-2.462100	0.163600	9.109400
C	7.451300	7.026200	-4.955900	H	6.343700	3.450400	5.532800	H	-2.617900	1.204900	7.658400
H	6.783600	7.894400	-5.089900	C	8.708500	2.348500	0.247600	C	3.056800	-0.312100	7.764700
H	8.393700	7.204100	-5.487900	H	8.485400	3.247300	-0.351600	H	3.580900	0.492800	7.220100
H	6.961700	6.126100	-5.368700	H	9.789100	2.288600	0.425000	H	3.329800	-0.269500	8.826200
C	1.148800	7.749000	-8.180800	H	8.377400	1.444400	-0.287400	H	3.344300	-1.293300	7.354600
H	1.807500	8.461400	-7.655500	C	5.668100	2.623500	-6.443900	C	7.953200	-1.084700	2.301900
H	1.571000	6.732500	-8.094700	H	6.022400	3.489100	-5.858100	H	7.346800	-1.878700	2.772000
H	1.080000	8.027200	-9.239400	H	5.798400	1.705700	-5.843400	H	9.017200	-1.297300	2.462700
C	-3.917000	8.472200	-6.506500	H	6.253800	2.541900	-7.367700	H	7.706200	-0.108200	2.748100
H	-4.446900	7.577200	-6.134400	C	0.679200	3.368800	-8.342900	C	7.711500	-0.907000	-3.072300
H	-3.951900	9.259800	-5.734500	H	0.194000	4.301100	-8.008100	H	7.280400	0.019200	-3.491000
H	-4.407500	8.832400	-7.418900	H	0.864900	3.422700	-9.422400	H	8.774200	-0.965200	-3.337700
Cd	0.200400	1.579400	-0.000200	H	0.029600	2.505300	-8.128600	H	7.186200	-1.785000	-3.480900
C	2.604100	3.034800	2.018900	C	-5.972900	4.103300	-5.292100	C	2.273400	-0.365100	-8.027000
C	4.041900	2.842600	2.122200	H	-5.490100	3.140600	-5.537100	H	2.423300	-0.461500	-9.109300
C	4.898500	2.726300	3.225200	H	-6.890200	4.212900	-5.883400	H	2.834900	0.508300	-7.658700
H	4.494000	2.754700	4.236100	H	-5.277600	4.925500	-5.534500	H	2.630100	-1.281800	-7.525600
C	6.263400	2.578300	2.976000	C	-7.842600	4.453600	-0.249100	C	-3.039300	0.458800	-7.764900
C	3.381900	2.947200	-0.068500	H	-7.401400	5.268200	0.349600	H	-3.345700	1.369200	-7.220700
C	4.534400	2.801400	0.809500	H	-8.903800	4.666200	-0.426500	H	-3.293000	0.567600	-8.826500
C	5.902300	2.666200	0.541400	H	-7.748600	3.495700	0.286600	H	-3.562600	-0.419500	-7.354400
H	6.260900	2.644800	-0.486400	C	1.239300	-0.147600	2.711700	C	-7.973000	0.938500	-2.301700
C	6.771700	2.562600	1.628800	C	0.898300	-0.096600	4.123800	H	-7.584900	0.017600	-2.771100
C	2.425000	3.056700	-2.200700	C	1.684600	-0.160500	5.283100	H	-9.056400	0.999200	-2.462500
C	2.526300	3.034300	-3.651200	H	2.765700	-0.266900	5.205800	H	-7.489300	1.821700	-2.748600
C	3.619500	2.887700	-4.515700	C	1.033700	-0.095300	6.513800	C	-7.694100	1.051800	3.072500
H	4.619400	2.737500	-4.110800	C	-0.972600	0.114900	2.820300	H	-8.737600	1.261200	3.337900
C	3.375500	2.944100	-5.888400	C	-0.496700	0.047300	4.192200	H	-7.405200	0.070300	3.481100
C	0.355700	3.331100	-2.983300	C	-1.167300	0.097100	5.422700	H	-7.045100	1.840800	3.491100
C	1.226700	3.220900	-4.145000	H	-2.250700	0.203700	5.451700	Y	-0.629200	-4.948700	0.001000
C	0.965600	3.292800	-5.519100	C	-0.400500	0.017700	6.584000	C	2.099900	-6.848600	-0.473300
H	-0.051000	3.446300	-5.877400	C	-2.689500	0.351100	1.248600	C	3.296000	-7.315400	0.224400
C	2.045200	3.162200	-6.394600	C	-4.089500	0.536400	0.903900	C	4.531200	-7.779500	-0.242800
C	-1.761000	3.588500	-2.020300	C	-5.235000	0.717600	1.692000	H	4.735600	-7.808300	-1.312400
C	-3.201100	3.762300	-2.123600	H	-5.154600	0.738200	2.777900	C	5.474900	-8.193400	0.701800
C	-4.059600	3.863700	-3.226500	C	-6.458200	0.855200	1.038100	C	1.618800	-6.793200	1.692000
H	-3.660900	3.789500	-4.237500	C	-2.799700	0.346500	-0.978800	C	2.992600	-7.284900	1.590900
C	-5.418100	4.062100	-2.977400	C	-4.161500	0.512200	-0.498100	C	3.912300	-7.727400	2.550800
C	-2.535900	3.698900	0.067100	C	-5.386700	0.632200	-1.169600	H	3.646400	-7.722500	3.607400
C	-3.688200	3.846000	-0.810900	H	-5.419300	0.605500	-2.257900	C	5.160900	-8.174400	2.105800
C	-5.046400	4.057700	-0.542800	C	-6.536400	0.796100	-0.398900	C	-0.352500	-6.536500	2.948000
H	-5.398800	4.127200	0.485000	N	-1.929600	0.245200	0.094800	C	-1.084000	-6.758300	4.193500
C	-5.914100	4.174700	-1.630200	N	-2.248800	0.286100	2.498700	C	-0.658800	-7.119200	5.477300
C	-1.581900	3.566500	2.199400	N	0.093600	-0.011500	1.944400	H	0.401900	-7.256400	5.683700
C	-1.685500	3.570800	3.649900	N	2.478300	-0.314200	2.266200	C	-1.632600	-7.289600	6.465700
C	-2.780600	3.702700	4.514300	N	-2.479500	0.314900	-2.266300	C	-2.501400	-6.269800	2.463700
H	-3.786300	3.807100	4.109300	O	-7.791600	0.912900	-0.893300	C	-2.440600	-6.594500	3.888500
C	-2.530200	3.697000	5.886900	O	-7.649000	1.049000	1.652900	C	-3.433500	-6.794100	4.856800
C	0.490400	3.315100	2.982000	O	-0.896300	0.038400	7.843800	H	-4.485300	-6.689700	4.592400
C	-0.380500	3.426700	4.143600	O	1.648900	-0.130600	7.719500	C	-3.028100	-7.133600	6.151800
C	-0.109700	3.431700	5.517700	C	2.796200	-0.364000	0.978700	C	-3.746600	-6.105800	0.475800
H	0.913000	3.326500	5.876200	C	4.156100	-0.544600	0.498100	C	-5.021500	-6.258900	-0.221900
C	-1.187600	3.575700	6.393200	C	5.372400	-0.734900	1.169700	C	-6.333400	-6.399200	0.245400
N	2.230400	3.105600	0.687300	H	5.397200	-0.768700	2.257900	H	-6.538500	-6.375600	1.315000
N	3.472500	2.928600	-1.392300	C	6.526500	-0.864300	0.399000	C	-7.350700	-6.564300	-0.699200
N	1.106900	3.247600	-1.821000	C	2.690600	-0.332700	-1.248700	C	-3.266900	-6.173000	-1.689600
N	-0.958400	3.491200	-3.075600	C	4.092400	-0.503600	-0.903900	C	-4.720100	-6.305600	-1.588400
N	-1.381400	3.563600	-0.688700	C	5.246900	-0.615100	-1.692100	C	-5.721200	-6.504300	-2.548200
N	-2.628200	3.704100	1.391000	H	5.174200	-0.575400	-2.777900	H	-5.462600	-6.566300	-3.604800
N	-0.258000	3.421500	1.819600	C	6.465600	-0.787800	-1.038100	C	-7.042000	-6.624800	-2.103200
N	1.802800	3.141600	3.074200	C	0.969100	-0.132600	-2.820400	C	-1.294200	-6.417800	-2.945600
O	7.209600	2.426700	3.932900	C	0.491400	-0.079600	-4.192300	C	-0.641400	-6.815900	-4.190900
O	8.111300	2.428400	1.537000	C	1.153100	-0.199700	-5.422800	C	-1.143400	-7.059400	-5.474700
O	4.320800	2.792300	-6.846100	H	2.228800	-0.367300	-5.451700	H	-2.204800	-6.927200	-5.681100
O	1.958600	3.209400	-7.740300	C	0.390800	-0.085300	-6.584000	C	-0.243100	-7.468300	-6.462900
O	-6.372100	4.151800	-3.934300	C	-1.238200	0.166200	-2.711800	C	0.853200	-6.696600	-2.461300
O	-7.244500	4.380400	-1.538400	C	-0.895300	0.129900	-4.123900	C	0.713100	-6.996300	-3.886000
O	-3.483400	3.787100	6.844600	C	-1.672600	0.264100	-5.283300	C	1.624500	-7.438200	-4.854100
O	-1.092000	3.600500	7.738900	H	-2.746000	0.431500	-5.206200	H	2.669000	-7.600000	-4.589700
C	-4.830100	3.960500	6.442400	C	-1.026100	0.163900	-6.514000	C	1.147000	-7.666100	-6.149000
H	-5.185900	3.104300	5.842300	N	-0.094800	0.011800	-1.944600	N	1.140300	-6.482400	0.442600
H	-5.417500	4.028600	7.366200	N	2.247600	-0.285800	-2.498800	N	0.953100	-6.762100	2.843700

N	-1.230700	-6.181000	1.949900	H	3.232400	-3.736600	-4.616000	C	3.653700	2.865600	6.585700
N	-3.650600	-6.177700	1.799400	C	5.103000	-4.023400	-3.535000	C	4.514800	3.945900	6.809600
N	-2.726000	-5.991400	-0.440200	C	2.528700	-3.698000	-0.222100	H	5.510900	3.955300	6.368700
N	-2.614700	-6.309800	-2.841200	C	3.590700	-3.834000	-1.209000	C	4.057900	4.990400	7.622800
N	-0.355000	-6.292800	-1.947500	C	4.968300	-4.048200	-1.076000	C	1.816700	1.514300	6.787600
N	1.988900	-6.894500	-1.796900	H	5.418300	-4.129900	-0.088000	C	2.382800	2.808800	7.168700
O	6.714700	-8.637100	0.406200	C	5.726700	-4.151800	-2.243500	C	1.914800	3.829800	8.003900
O	6.150700	-8.620500	2.907500	N	0.430900	-3.442900	1.745500	H	0.934200	3.751000	8.471900
O	-1.375000	-7.608100	7.751600	N	-1.498800	-3.179000	3.196600	C	2.751000	4.931400	8.224200
O	-3.863400	-7.347900	7.190000	N	-2.154900	-3.114400	0.862700	C	0.242500	-0.187900	7.180000
O	-8.662000	-6.683700	-0.403500	N	-3.592200	-2.913800	-1.084900	C	-0.867600	-0.705700	7.980100
O	-8.111900	-6.809400	-2.904800	N	-1.279200	-3.226000	-1.743900	C	-1.719100	-0.095900	8.908200
O	-0.572300	-7.712700	-7.748700	N	0.655200	-3.453500	-3.195000	H	-1.641000	0.972400	9.106700
O	1.902100	-8.082700	-7.187100	N	1.306600	-3.554400	-0.861100	C	-2.650400	-0.903700	9.572700
C	3.264800	-8.390800	-6.955700	N	2.748400	-3.718900	1.086500	C	0.159000	-2.367000	6.785200
H	3.828900	-7.500300	-6.625700	O	4.126700	-3.865600	6.430500	C	-0.920100	-2.081900	7.731500
H	3.373600	-9.187800	-6.200400	O	1.833100	-3.691200	7.553900	C	-1.826400	-2.912100	8.401200
H	3.664500	-8.739700	-7.915500	O	-6.797100	-2.478800	4.582100	H	-1.829600	-3.985500	8.214900
C	7.072500	-8.793700	-0.957300	O	-7.926000	-2.452500	2.284700	C	-2.703500	-2.319900	9.318500
H	6.399900	-9.504600	-1.466700	O	-4.963500	-2.713600	-6.429100	N	2.535700	-3.084500	5.242100
H	7.054700	-7.828700	-1.493600	O	-2.699000	-3.118200	-7.552400	N	4.813100	-3.415600	4.470800
H	8.094000	-9.192600	-0.957600	O	5.960000	-4.101300	-4.580600	N	4.427500	-1.036700	4.769100
C	5.904400	-8.723900	4.298200	O	7.059700	-4.358000	-2.283200	N	4.992300	1.258600	5.320000
H	5.697200	-7.735300	4.745300	C	-1.483800	-3.268900	-8.277600	N	2.685500	0.847100	5.957300
H	5.057300	-9.399500	4.506800	H	-0.968600	-4.204600	-8.002500	N	0.672300	1.065100	7.295300
H	6.819500	-9.137900	4.738700	H	-1.773000	-3.310200	-9.334800	N	0.793700	-1.200600	6.430200
C	-0.036200	-7.888700	8.126400	H	-0.816600	-2.407400	-8.116900	N	0.492900	-3.609000	6.445700
H	0.369900	-8.736600	7.548900	C	-6.265600	-2.550800	-5.896700	O	1.858400	-8.931800	6.278300
H	0.615800	-7.008700	7.987000	H	-6.337100	-1.640400	-5.275500	O	4.185500	-8.829600	5.223600
H	-0.069500	-8.153500	9.190100	H	-6.937800	-2.458800	-6.758500	O	10.158200	-2.371600	3.720200
C	-5.259800	-7.305700	6.958600	H	-6.561800	-3.423700	-5.289700	O	10.258400	0.140900	4.184300
H	-5.564300	-8.050400	6.203600	C	-8.645100	-2.358000	1.060100	O	4.762500	6.095100	7.924200
H	-5.733900	-7.543200	7.918600	H	-8.481000	-3.249300	0.431400	O	2.442600	5.989700	8.994200
H	-5.583300	-6.302500	6.628300	H	-9.703500	-2.301300	1.341800	O	-3.537500	-0.465500	10.482900
C	-9.047600	-6.745500	0.960000	H	-8.367200	-1.447200	0.506400	O	-3.630500	-2.981000	10.033700
H	-8.574100	-7.601900	1.469600	C	-6.269200	-2.548300	5.894300	C	5.522800	-8.872000	4.750500
H	-8.789200	-5.815500	1.496000	H	-5.781000	-3.520900	6.078400	H	5.593000	-8.502900	3.712400
H	-10.136400	-6.876400	0.960300	H	-5.540100	-1.739600	6.079800	H	6.192000	-8.278200	5.395500
C	-7.899300	-6.971600	-4.295400	H	-7.123300	-2.432900	6.572700	H	5.821400	-9.926300	4.784500
H	-7.451400	-6.066300	-4.742800	C	0.618700	-3.533700	8.279200	C	0.632000	-9.085900	6.976800
H	-7.248000	-7.837600	-4.503700	H	-0.113700	-4.311300	8.004400	H	0.642800	-8.525100	7.926400
H	-8.888800	-7.143800	-4.735800	H	0.888500	-3.645500	9.336400	H	-0.223700	-8.752600	6.364200
C	-1.938700	-7.649800	-8.123500	H	0.187500	-2.533000	8.118100	H	0.536800	-10.157900	7.185200
H	-2.543900	-8.368900	-7.545700	C	5.428100	-4.033400	5.898000	C	-3.693500	-4.395600	9.939700
H	-2.349900	-6.634600	-7.984600	H	5.724700	-3.169900	5.276500	H	-4.485600	-4.708800	10.629800
H	-1.972700	-7.914900	-9.187100	H	6.102100	-4.112000	6.759800	H	-3.949000	-4.718700	8.915300
Cd	-0.201500	-1.579500	0.000100	H	5.496800	-4.952800	5.291300	H	-2.738200	-4.857300	10.240900
C	1.785200	-3.591600	1.993700	C	7.779600	-4.445800	-1.058700	C	-3.492100	0.893600	10.890800
C	2.028500	-3.612900	3.427300	H	7.398000	-5.267600	-0.429700	H	-2.510500	1.144800	11.326200
C	3.202000	-3.754300	4.180200	H	8.818600	-4.655700	-1.340400	H	-3.703500	1.573400	10.047200
H	4.163800	-3.853300	3.678700	H	7.738400	-3.494300	-0.505300	H	-4.271000	1.005100	11.654100
C	3.085400	-3.764900	5.570600	C	5.431400	-4.036800	-5.892800	C	10.229700	-3.780800	3.563400
C	-0.201500	-3.350700	2.975900	H	4.927900	-3.071500	-6.078600	H	9.872800	-4.299600	4.468900
C	0.777500	-3.475500	4.046500	H	6.287200	-4.139000	-6.571300	H	9.641900	-4.118300	2.692100
C	0.640800	-3.496900	5.440200	H	4.715400	-4.856400	-6.076700	H	11.288900	-4.012500	3.401700
H	-0.342400	-3.396400	5.897100					C	10.439400	1.505100	4.531000
C	1.798200	-3.650500	6.205600	444				H	10.105700	1.700700	5.563900
C	-2.398300	-3.060100	2.224900	**[5]**$^{3+}$				H	11.515900	1.696300	4.451100
C	-3.819300	-2.870300	2.469000	Y	2.070700	-0.887400	4.441500	H	9.895000	2.170700	3.838400
C	-4.565300	-2.768000	3.650800	C	1.606800	-3.933900	5.796200	C	6.105700	6.199200	7.476400
H	-4.065000	-2.808200	4.617500	C	2.069400	-5.317900	5.690500	H	6.719900	5.370800	7.867500
C	-5.947800	-2.618100	3.536500	C	1.512200	-6.528200	6.118400	H	6.162100	6.208200	6.374000
C	-3.374100	-2.948100	0.223700	H	0.532000	-6.544400	6.593600	H	6.481300	7.151100	7.869400
C	-4.436300	-2.813700	1.210600	C	2.259500	-7.697200	5.928400	C	1.223100	5.981600	9.720100
C	-5.823700	-2.676400	1.077600	C	3.621200	-3.844400	4.876700	H	0.352600	5.954900	9.041600
H	-6.279800	-2.643000	0.089500	C	3.341700	-5.261700	5.110500	H	1.176000	5.121600	10.409000
C	-6.583900	-2.586600	2.245000	C	4.116100	-6.414000	4.932700	H	1.208900	6.914100	10.296300
C	-2.627700	-3.031600	-1.992200	H	5.116600	-6.343600	4.507200	Cd	0.658500	-0.282100	1.412900
C	-2.868700	-2.992000	-3.425800	C	3.569300	-7.639500	5.333300	C	2.410900	-3.224600	1.999100
C	-4.040300	-2.835900	-4.178700	C	5.194300	-2.141700	4.482000	C	3.553500	-3.824000	1.327900
H	-4.996300	-2.691300	-3.677300	C	6.590700	-1.746600	4.296300	C	3.818100	-5.138100	0.921000
C	-3.930100	-2.875900	-5.569100	C	7.745900	-2.486600	4.020000	H	3.079400	-5.921300	1.086200
C	-0.643900	-3.295300	-2.974300	H	7.683600	-3.561800	3.856000	C	5.045400	-5.394100	0.307100
C	-1.623000	-3.171800	-4.045000	C	8.967600	-1.803300	3.979000	C	3.877400	-1.580500	1.656100
C	-1.496000	-3.227200	-5.438600	C	5.278700	0.037000	4.878800	C	4.482900	-2.793500	1.122500
H	-0.518900	-3.375800	-5.895400	C	6.644500	-0.371000	4.547400	C	5.724100	-3.033900	0.520300
C	-2.655000	-3.087000	-6.204100	C	7.857100	0.328000	4.535100	H	6.431500	-2.219300	0.373100
C	1.555800	-3.563000	-2.223400	H	7.880000	1.393000	4.763500	C	6.009200	-4.340400	0.114900
C	2.979100	-3.734700	-2.467400	C	9.023500	-0.388300	4.239000	C	3.916300	0.720200	2.085400
C	3.726900	-3.822600	-3.649300	C	3.829900	1.604300	5.865600	C	4.563500	2.021300	2.024700

C	5.800100	2.429600	1.508600	C	-1.673800	-6.365500	-0.448100	C	-7.540800	-0.147300	3.595700
H	6.460800	1.705700	1.033500	C	-1.909900	-2.255700	0.428800	H	-8.482100	-0.031900	4.146400
C	6.141300	3.778000	1.628000	C	-2.053400	-3.683700	0.201400	H	-7.756500	-0.508900	2.577900
C	2.515500	2.168900	3.039600	C	-3.101500	-4.576600	0.468600	H	-6.893000	-0.868100	4.124500
C	3.689100	2.932100	2.636000	H	-4.021400	-4.220100	0.929800	Y	-2.070700	0.887600	-4.441900
C	4.020000	4.285600	2.776600	C	-2.914100	-5.917100	0.134600	C	-0.185700	0.339800	-7.176300
H	3.327200	4.974600	3.257100	C	-2.711900	-0.209900	1.233400	C	0.326800	-0.742100	-8.017400
C	5.253100	4.710100	2.274900	C	-3.733200	0.596600	1.879700	C	1.384700	-0.798300	-8.931700
C	0.382700	2.027000	3.993400	C	-4.977200	0.266500	2.437300	H	2.028900	0.067500	-9.080800
C	-0.773900	2.632500	4.634600	H	-5.323600	-0.766000	2.432200	C	1.569800	-1.987700	-9.647400
C	-1.054100	3.953300	5.007800	C	-5.741300	1.299300	2.978500	C	-1.556900	-1.375900	-6.881000
H	-0.332200	4.743700	4.806400	C	-1.939600	1.883100	1.269300	C	-0.539300	-1.825500	-7.831600
C	-2.274400	4.206400	5.636400	C	-3.257200	1.918000	1.881100	C	-0.387600	-3.015300	-8.553100
C	-1.074700	0.379100	4.355800	C	-4.022400	2.970700	2.404100	H	-1.091600	-3.835300	-8.415200
C	-1.687000	1.595000	4.875000	H	-3.637100	3.989200	2.388300	C	0.678000	-3.102000	-9.457800
C	-2.910000	1.827700	5.516000	C	-5.269600	2.661300	2.944800	C	-3.693500	-1.653300	-5.939000
H	-3.602800	1.006900	5.694900	N	-1.634200	0.587700	0.879300	C	-4.951400	-2.398700	-5.887500
C	-3.203700	3.138000	5.902900	N	-2.837700	-1.513800	1.020500	C	-5.316200	-3.657600	-6.378100
C	-1.122500	-1.917700	3.907400	N	-0.681100	-1.822800	-0.046500	H	-4.578400	-4.290800	-6.869600
C	-1.783600	-3.212800	3.938200	N	1.167900	-2.954900	-1.135100	C	-6.649700	-4.057900	-6.228300
C	-3.035900	-3.614500	4.420800	N	-1.168300	2.954700	1.135000	C	-5.171700	-0.307100	-4.983000
H	-3.713300	-2.883400	4.860100	O	-6.130800	3.559900	3.472300	C	-5.885200	-1.548700	-5.284500
C	-3.370100	-4.965800	4.316400	O	-6.949900	1.145200	3.564300	C	-7.228100	-1.918200	-5.145700
C	0.287100	-3.370200	2.972200	O	-3.829100	-6.896200	0.312900	H	-7.944800	-1.228700	-4.700900
C	-0.893100	-4.130700	3.361700	O	-1.621200	-7.695300	-0.685500	C	-7.611200	-3.182900	-5.609600
C	-1.205700	-5.491900	3.260200	C	1.930900	-1.879800	-1.287100	C	-5.250900	1.990000	-4.486500
H	-0.498300	-6.187300	2.811300	C	3.241600	-1.911800	-1.913500	C	-6.049900	3.194600	-4.260100
C	-2.447500	-5.912800	3.743600	C	3.974400	-2.950700	-2.505900	C	-7.411800	3.381000	-3.998000
N	2.632200	-1.870100	2.192800	H	3.559700	-3.956600	-2.552900	H	-8.072000	2.522000	-3.883500
N	4.467600	-0.391900	1.609600	C	5.237500	-2.648200	-3.012600	C	-7.887600	4.694800	-3.905800
N	2.683500	0.832900	2.708700	C	2.719600	0.206200	-1.215900	C	-3.880700	3.706200	-4.784000
N	1.460400	2.716000	3.631700	C	3.747900	-0.603300	-1.847300	C	-5.185000	4.278500	-4.448400
N	0.181000	0.664200	3.841600	C	5.024500	-0.287300	-2.335000	C	-5.643200	5.599500	-4.384500
N	-1.671500	-0.806700	4.388300	H	5.400500	0.732500	-2.266900	H	-4.958900	6.428000	-4.564600
N	0.129700	-2.038800	3.325600	C	5.772900	-1.313500	-2.909700	C	-6.998400	5.810300	-4.101200
N	1.335600	-3.914600	2.365900	C	1.901200	2.259000	-0.446500	C	-1.742900	3.983000	-5.723500
O	5.434800	-6.599000	-0.163400	C	2.038100	3.689800	-0.233500	C	-0.771300	4.851000	-6.389200
O	7.149000	-4.732000	-0.484500	C	3.054000	4.596500	-0.569600	C	-0.710100	6.239800	-6.550200
O	7.281700	4.328500	1.157700	H	3.944900	4.252400	-1.092900	H	-1.463800	6.879800	-6.092800
O	5.713000	5.974200	2.323100	C	2.882500	5.930300	-0.201800	C	0.333000	6.764500	-7.323300
O	-2.699800	5.426800	6.029800	C	0.036500	2.929300	0.579100	C	-0.265800	2.637300	-6.681900
O	-4.335900	3.526400	6.518400	C	0.874400	4.107500	0.433100	C	0.161200	4.001400	-6.995000
O	-4.546400	-5.501000	4.709800	C	0.695800	5.441800	0.826700	C	1.197700	4.502100	-7.791300
O	-2.899700	-7.180100	3.711700	H	-0.211200	5.742500	1.349200	H	1.894600	3.821100	-8.278600
C	-5.502500	-4.659900	5.334200	C	1.705600	6.351500	0.516600	C	1.291600	5.890700	-7.948200
H	-5.837000	-3.857500	4.653300	N	0.680600	1.822700	0.046500	N	-1.278000	-0.096400	-6.463500
H	-6.353300	-5.303600	5.587400	N	2.837100	1.513600	-1.020700	N	-2.628400	-2.109000	-6.591700
H	-5.095300	-4.207000	6.254100	N	1.633600	-0.588000	-0.879500	N	-3.847900	-0.428800	-5.332100
C	-2.077400	-8.197600	3.150100	O	1.692400	7.664500	0.838300	N	-5.797800	0.779000	-4.538600
H	-1.104100	-8.250500	3.666300	O	3.758400	6.926000	-0.464200	N	-3.943000	2.333800	-4.736700
H	-2.622800	-9.136600	3.301400	O	7.021200	-1.176500	-3.410300	N	-2.856500	4.459500	-5.174800
H	-1.926000	-8.034000	2.071500	O	6.059400	-3.530000	-3.624500	N	-1.373100	2.666200	-5.868000
C	4.577700	-7.713100	0.024800	C	-5.065400	-6.578500	0.938600	N	0.312800	1.571500	-7.228200
H	3.613400	-7.570200	-0.494000	H	-5.609800	-5.802600	0.372600	O	2.542000	-2.197500	-10.552200
H	5.101100	-8.574800	-0.406300	H	-5.648500	-7.507200	0.936100	O	0.956900	-4.175800	-10.217400
H	4.388100	-7.894300	1.096500	H	-4.910000	-6.249000	1.978000	O	-7.149700	-5.236300	-6.639500
C	8.166200	-3.769300	-0.739700	C	-0.468800	-8.237600	-1.316900	O	-8.858100	-3.681600	-5.543000
H	8.485000	-3.272900	0.192200	H	0.441200	-8.034700	-0.725800	O	-9.163600	5.034700	-3.652700
H	9.007900	-4.331900	-1.160600	H	-0.637000	-9.320100	-1.366000	O	-7.585300	7.016000	-4.002000
H	7.827100	-3.019300	-1.471600	H	-0.352900	-7.840600	-2.337700	O	0.529500	8.072700	-7.563200
C	8.245700	3.484100	0.550400	C	5.659300	-4.890400	-3.724100	O	2.230800	6.521100	-8.675100
H	8.594700	2.707500	1.252100	H	4.706800	-4.985700	-4.273900	C	3.158900	5.748500	-9.420500
H	7.840800	2.998200	-0.354700	H	6.455100	-5.395300	-4.284700	H	3.787500	5.127700	-8.758300
H	9.085400	4.132600	0.273300	H	5.568000	-5.350300	-2.727400	H	2.642900	5.099800	-10.148000
C	4.909500	6.983700	2.924900	C	7.622900	0.111400	-3.418900	H	3.790400	6.468100	-9.954400
H	4.663700	6.724900	3.968500	H	7.697300	0.522600	-2.397200	C	3.404800	-1.124400	-10.898000
H	5.517700	7.895800	2.908100	H	8.630400	-0.032600	-3.827500	H	2.835100	-0.272200	-11.304800
H	3.986100	7.151000	2.348300	H	7.063600	0.805500	-4.066000	H	3.996000	-0.788200	-10.028500
C	-1.834600	6.537400	5.858900	C	4.984200	6.612700	-1.112200	H	4.078700	-1.516200	-11.668700
H	-1.609600	6.710700	4.791800	H	5.501500	7.569600	-1.251100	C	0.076300	-5.288300	-10.187700
H	-2.369200	7.403900	6.265800	H	5.604500	5.950900	-0.487300	H	0.040900	-5.745200	-9.183300
H	-0.888900	6.395000	6.409100	H	4.805900	6.146400	-2.096800	H	-0.942800	-4.997300	-10.492900
C	-5.333900	2.555500	6.815300	C	0.550600	8.202500	1.492200	H	0.480900	-6.012400	-10.904500
H	-4.925300	1.746500	7.444000	H	0.363100	7.689600	2.451600	C	-6.312600	-6.124800	-7.364300
H	-6.113100	3.091400	7.370100	H	0.784800	9.256700	1.682800	H	-5.937200	-5.652500	-8.287500
H	-5.766100	2.137000	5.892700	H	-0.341100	8.138300	0.848700	H	-5.458400	-6.461600	-6.751700
C	-0.028700	-2.933000	-0.561500	C	-5.741400	4.924900	3.549200	H	-6.939600	-6.986300	-7.622200
C	-0.859700	-4.114100	-0.400700	H	-5.511500	5.329900	2.548300	C	-9.904000	-2.858500	-5.050300
C	-0.648500	-5.462300	-0.724700	H	-6.603100	5.458000	3.968400	H	-10.009700	-1.943600	-5.657100
H	0.287700	-5.775500	-1.184500	H	-4.874600	5.052300	4.216800	H	-10.819600	-3.456500	-5.126300

H	-9.732600	-2.580300	-3.995700
C	-10.143400	4.011800	-3.558000
H	-10.198600	3.427200	-4.491600
H	-9.935100	3.333200	-2.712600
H	-11.097900	4.523800	-3.389100
C	-6.822300	8.178900	-4.284000
H	-5.986600	8.292900	-3.571500
H	-6.424800	8.154300	-5.312500
H	-7.511300	9.024900	-4.177500
C	-0.424400	9.011200	-7.089200
H	-1.424400	8.806200	-7.506800
H	-0.479700	9.005700	-5.986700
H	-0.077800	9.992800	-7.432900
Cd	-0.659100	0.282100	-1.413300
C	-0.342900	-2.005400	-4.007900
C	-0.691600	-3.413900	-4.107900
C	-0.000800	-4.515600	-4.628900
H	0.997200	-4.388300	-5.046000
C	-0.635300	-5.758400	-4.590500
C	-2.374900	-2.219200	-3.115300
C	-1.975200	-3.548500	-3.558300
C	-2.632600	-4.784500	-3.523200
H	-3.630100	-4.865500	-3.094100
C	-1.962200	-5.893800	-4.045500
C	-3.899900	-0.761500	-2.101400
C	-5.166900	-0.495100	-1.438800
C	-6.234400	-1.331200	-1.086800
H	-6.186800	-2.398400	-1.299400
C	-7.339400	-0.747900	-0.464400
C	-3.936100	1.423800	-1.660300
C	-5.197300	0.881700	-1.171800
C	-6.302400	1.486500	-0.560300
H	-6.305700	2.557700	-0.364800
C	-7.380400	0.669600	-0.209000
C	-2.451200	3.203600	-1.985400
C	-2.088600	4.606100	-1.855400
C	-2.763600	5.701100	-1.300600
H	-3.744800	5.566600	-0.847300
C	-2.135800	6.946700	-1.353300
C	-0.428100	3.421200	-2.896900
C	-0.821200	4.747600	-2.439800
C	-0.181800	5.991300	-2.513600
H	0.801000	6.078600	-2.974100
C	-0.843400	7.096900	-1.972400
C	1.106000	1.959600	-3.891500
C	2.387100	1.687200	-4.523700
C	3.470600	2.516400	-4.841400
H	3.439900	3.576300	-4.592500
C	4.569000	1.935800	-5.477900
C	1.133200	-0.221800	-4.351800
C	2.401100	0.317300	-4.825800
C	3.488400	-0.279800	-5.475600
H	3.476800	-1.344700	-5.702700
C	4.575400	0.533200	-5.807600
N	-1.377800	-1.302400	-3.411200
N	-3.533700	-1.970000	-2.516700
N	-3.176400	0.413600	-2.230300
N	-3.604000	2.704700	-1.550700
N	-1.435800	2.508900	-2.623800
N	0.737300	3.169100	-3.481500
N	0.362900	0.792800	-3.804500
N	0.807600	-1.505500	-4.447700
O	-0.090800	-6.915000	-5.027000
O	-2.451300	-7.147300	-4.077800
O	-8.430700	-1.422700	-0.041900
O	-8.507700	1.094000	0.391500
O	-2.644200	8.087900	-0.839500
O	-0.361500	8.353500	-1.955700
O	5.696500	2.595100	-5.822800
O	5.695700	0.111800	-6.423200
C	0.916700	8.615400	-2.525200
H	0.950000	8.306500	-3.583500
H	1.055000	9.700900	-2.456700
H	1.714000	8.110200	-1.957700
C	-3.935700	8.055400	-0.254500
H	-3.963200	7.382900	0.620800
H	-4.149700	9.082100	0.065700
H	-4.696400	7.730000	-0.984400
C	-8.649400	2.474800	0.707600
H	-8.548900	3.100500	-0.195200
H	-9.661000	2.583000	1.116500
H	-7.914500	2.784600	1.467100
C	-8.509800	-2.816100	-0.293800
H	-8.467500	-3.029100	-1.375500
H	-7.696400	-3.363000	0.214700
H	-9.476800	-3.142400	0.107100
C	-3.748400	-7.401200	-3.548800
H	-4.509600	-6.780300	-4.050400
H	-3.949100	-8.459900	-3.751300
H	-3.773700	-7.227200	-2.461500
C	1.192900	-6.879100	-5.628900
H	1.959800	-6.523500	-4.918500
H	1.418200	-7.910700	-5.924800
H	1.197500	-6.229700	-6.520700
C	5.818300	-1.260900	-6.780200
H	4.990600	-1.574900	-7.438100
H	6.767600	-1.342400	-7.322800
H	5.854500	-1.901200	-5.884700
C	5.767700	3.991900	-5.587900
H	5.693300	4.222300	-4.510600
H	6.746200	4.313300	-5.964300
H	4.969600	4.528700	-6.128300

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Y	-1.558300	-4.727500	-0.002900
C	-0.438400	-6.740200	2.451100
C	-0.639900	-7.046900	3.867800
C	0.156900	-7.714600	4.803600
H	1.150800	-8.067200	4.530400
C	-0.374800	-7.929100	6.083400
C	-2.489400	-6.064700	2.943000
C	-1.936100	-6.621000	4.178600
C	-2.497400	-6.844200	5.440500
H	-3.520800	-6.536000	5.651600
C	-1.710100	-7.492200	6.403300
C	-4.378800	-5.438300	1.690900
C	-5.835100	-5.330300	1.595400
C	-6.844500	-5.402400	2.561000
H	-6.592700	-5.511200	3.615300
C	-8.175800	-5.352200	2.123100
C	-4.845800	-5.283800	-0.468600
C	-6.130500	-5.233500	0.231000
C	-7.450300	-5.205600	-0.232300
H	-7.659200	-5.165200	-1.300800
C	-8.480400	-5.254200	0.718100
C	-3.656000	-5.673700	-2.459100
C	-3.676100	-6.038200	-3.876200
C	-4.713500	-6.098700	-4.812600
H	-5.722100	-5.790500	-4.539300
C	-4.413600	-6.585800	-6.092900
C	-1.605900	-6.352100	-2.951000
C	-2.381200	-6.467600	-4.187100
C	-2.062700	-6.979400	-5.449600
H	-1.056900	-7.340900	-5.660800
C	-3.080600	-7.029600	-6.412900
C	0.284200	-6.976200	-1.698800
C	1.518500	-7.756600	-1.603900
C	2.287100	-8.414000	-2.570200
H	2.020600	-8.349800	-3.624500
C	3.386500	-9.166800	-2.132800
C	0.750400	-7.133300	0.460600
C	1.812900	-7.856700	-0.239500
C	2.889700	-8.620600	0.223100
H	3.081200	-8.714200	1.291500
C	3.688900	-9.271500	-0.727900
N	-1.544800	-6.098300	1.944800
N	-3.765400	-5.701900	2.841100
N	-3.815300	-5.346800	0.439200
N	-4.766300	-5.367700	-1.794000
N	-2.385100	-5.817800	-1.952400
N	-0.364900	-6.821000	-2.849200
N	-0.114600	-6.569100	-0.446700
N	0.636000	-7.155000	1.785900
O	0.263300	-8.546900	7.086800
O	-2.102300	-7.775200	7.653100
O	-9.250000	-5.405300	2.922300
O	-9.789800	-5.233800	0.434100
O	-5.293700	-6.700700	-7.096900
O	-2.933600	-7.488600	-7.663400
O	4.218400	-9.847800	-2.932700
O	4.753100	-10.035000	-0.444500
C	-3.440500	-7.498100	8.045000
H	-3.651400	-6.415500	8.004600
H	-4.159000	-8.038700	7.407000
H	-3.529500	-7.850600	9.078800
C	1.538700	-9.129800	6.850000
H	1.482600	-9.892100	6.055600
H	2.283000	-8.362700	6.575300
H	1.831500	-9.603500	7.793900
C	5.076400	-10.306600	0.913000
H	5.944800	-10.974600	0.886700
H	5.339100	-9.380600	1.452900
H	4.239400	-10.808600	1.425700
C	3.945700	-9.918500	-4.326700
H	2.959100	-10.373700	-4.512900
H	3.986200	-8.918800	-4.792200
H	4.730000	-10.553800	-4.753500
C	-9.073800	-5.626800	4.316100
H	-8.552100	-6.580200	4.501000
H	-8.511400	-4.800200	4.783300
H	-10.082400	-5.671000	4.742300
C	-10.210600	-5.257700	-0.923700
H	-9.836600	-6.158600	-1.437400
H	-11.306100	-5.277600	-0.897900
H	-9.870300	-4.356500	-1.462200
C	-6.665600	-6.410100	-6.860100
H	-7.074600	-7.057300	-6.066800
H	-6.807200	-5.351200	-6.583900
H	-7.182600	-6.615000	-7.804500
C	-1.693200	-8.062100	-8.055700
H	-0.879300	-7.318000	-8.013800
H	-1.438100	-8.925200	-7.419000
H	-1.831300	-8.396600	-9.090100
Cd	-0.494600	-1.499800	-0.000900
C	-1.624100	-3.021400	2.924900
C	-2.676200	-2.656000	3.860800
C	-2.716400	-2.623400	5.260700
H	-1.836000	-2.895400	5.841500
C	-3.912200	-2.233500	5.868500
C	-3.392200	-2.446600	1.694300
C	-3.793800	-2.305400	3.088400
C	-5.004700	-1.925100	3.678300
H	-5.860400	-1.659000	3.059600
C	-5.066900	-1.892500	5.075100
C	-3.834500	-2.288300	-0.599700
C	-4.717500	-1.977600	-1.713200
C	-6.040800	-1.520300	-1.761500
H	-6.586700	-1.321400	-0.840200
C	-6.619100	-1.333200	-3.019200
C	-2.668700	-2.682700	-2.458800
C	-3.989600	-2.236400	-2.884400
C	-4.555200	-2.067900	-4.153500
H	-3.972600	-2.276600	-5.049500
C	-5.877700	-1.618000	-4.222700
C	-0.487500	-3.392900	-2.928400
C	0.575800	-3.724200	-3.864400
C	0.628400	-3.719100	-5.264200
H	-0.240500	-3.412300	-5.845000
C	1.821700	-4.116500	-5.872100
C	1.274300	-3.986600	-1.697800
C	1.681900	-4.109500	-3.092000
C	2.881700	-4.523400	-3.681900
H	3.727300	-4.820100	-3.063400
C	2.952100	-4.531300	-5.078800
C	1.722800	-4.126100	0.596200
C	2.617200	-4.402500	1.709700
C	3.952800	-4.822200	1.758200
H	4.510200	-4.986600	0.837000
C	4.528700	-5.016600	3.016000
C	0.550900	-3.750400	2.455200
C	1.877900	-4.178200	2.880900
C	2.432400	-4.379900	4.150000
H	1.839800	-4.201400	5.045900
C	3.763000	-4.805200	4.219300
N	-2.079800	-2.889900	1.622100
N	-4.197200	-2.171600	0.674800
N	-2.603400	-2.714800	-1.073500
N	-1.698200	-2.994600	-3.309400
N	-0.044200	-3.561400	-1.625800

N	2.084200	-4.246700	-0.678400	H	-5.588600	1.749600	0.753200	H	3.423000	6.568800	-5.674000
N	0.479500	-3.736800	1.070000	C	-5.627400	1.815200	2.928400	C	5.569700	6.218000	-5.510300
N	-0.414700	-3.423500	3.305800	C	-2.307000	0.773900	-1.732300	C	0.605300	6.685200	-2.563600
O	-4.101300	-2.125800	7.198400	C	-2.686200	0.908200	-3.128300	C	-0.543200	7.437100	-3.070600
O	-6.147300	-1.541600	5.791200	C	-3.871500	1.339700	-3.742100	C	-0.845400	7.941800	-4.339800
O	-7.868100	-0.874500	-3.232500	H	-4.719700	1.656000	-3.136800	H	-0.182800	7.748300	-5.182600
O	-6.559100	-1.397500	-5.358500	C	-3.920200	1.337300	-5.135900	C	-2.007300	8.714700	-4.478500
O	2.038500	-4.139900	-7.201900	C	-0.527800	0.166800	-2.935300	C	-0.678000	7.109200	-0.809000
O	4.029600	-4.890700	-5.795000	C	-1.573800	0.504100	-3.885400	C	-1.353800	7.705900	-1.962100
O	5.805500	-5.391000	3.229300	C	-1.613300	0.477400	-5.287300	C	-2.504900	8.493600	-2.070400
O	4.441500	-5.034000	5.355300	H	-0.742200	0.153500	-5.855200	H	-3.103400	8.720100	-1.188700
C	6.632100	-5.684300	2.112800	C	-2.791300	0.885400	-5.912600	C	-2.841300	8.993000	-3.336900
H	6.767400	-4.796300	1.471100	N	-0.995200	0.330700	-1.638900	N	0.807200	6.339100	1.587600
H	7.600700	-5.989900	2.525400	N	-3.129200	1.034700	-0.723600	N	2.475500	6.123500	3.337400
H	6.210100	-6.507100	1.511400	N	-1.556400	0.514000	1.049000	N	3.468300	5.460500	1.222600
C	3.789700	-4.856100	6.610200	O	-2.995300	0.903300	-7.246500	N	5.230300	5.216500	-0.428900
H	2.886200	-5.484700	6.678100	O	-4.976200	1.735700	-5.875700	N	3.122300	5.576900	-1.579900
H	4.515100	-5.174100	7.368000	O	-6.909000	2.187900	3.127800	N	1.654500	6.399500	-3.329300
H	3.530700	-3.798300	6.773600	O	-5.554600	1.917900	5.270000	N	0.461300	6.455600	-1.214800
C	-3.047500	-2.495300	8.075200	C	6.234600	-1.947900	5.218700	N	-1.100300	7.306500	0.437100
H	-2.160400	-1.855300	7.926300	H	6.586000	-1.144800	4.548000	O	-2.831300	9.387600	5.217100
H	-3.435400	-2.354200	9.090800	H	6.971600	-2.107000	6.014600	O	-0.909100	8.760600	6.774000
H	-2.762700	-3.551200	7.931300	H	6.101500	-2.883200	4.652500	O	7.463400	5.987300	5.634700
C	-7.349900	-1.181200	5.116500	C	1.866000	-0.732500	8.116600	O	8.944800	5.508200	3.612900
H	-7.689800	-1.994800	4.454400	H	0.981400	-1.359400	7.910000	O	7.862400	5.863800	-5.206900
H	-8.093200	-1.015700	5.905000	H	2.228700	-0.936400	9.130900	O	5.945400	6.506700	-6.763800
H	-7.215700	-0.252300	4.540300	H	1.603200	0.333700	8.030700	O	-2.433200	9.262500	-5.624800
C	-8.707200	-0.619200	-2.115900	C	-4.923600	1.731100	6.531400	O	-3.909400	9.757300	-3.602900
H	-8.857400	-1.532000	-1.515100	H	-4.013200	2.349400	6.614600	C	-4.739100	10.194400	-2.534400
H	-8.287700	0.174600	-1.473600	H	-5.654600	2.055400	7.281400	H	-5.220000	9.339800	-2.028100
H	-9.667500	-0.288400	-2.528400	H	-4.677600	0.670300	6.696800	H	-4.162300	10.781600	-1.801100
C	-5.928900	-1.640700	-6.613600	C	-7.741600	2.440900	2.002000	H	-5.506900	10.829200	-2.991200
H	-5.576200	-2.683200	-6.682500	H	-7.818500	1.548400	1.357400	C	-3.890700	9.899600	4.418300
H	-6.701100	-1.464400	-7.371400	H	-8.730000	2.682100	2.410500	H	-3.502200	10.553000	3.619900
H	-5.091800	-0.944000	-6.776200	H	-7.368600	3.298100	1.419600	H	-4.484600	9.083300	3.972600
C	0.972200	-3.808100	-8.078700	C	-6.167700	2.150600	-5.218000	H	-4.522100	10.484200	5.096900
H	0.640000	-2.766200	-7.928100	H	-6.854700	2.461600	-6.013800	C	0.154200	8.573000	7.698900
H	1.368400	-3.923800	-9.094300	H	-6.616900	1.318900	-4.652700	H	0.333800	7.500400	7.887200
H	0.115000	-4.487500	-7.936400	H	-5.972900	3.004700	-4.546500	H	1.081900	9.044900	7.335600
C	5.210500	-5.317100	-5.120300	C	-1.933000	0.530200	-8.116400	H	-0.166400	9.059400	8.627200
H	4.999600	-6.174600	-4.459900	H	-1.595400	-0.500200	-7.910400	C	6.752600	6.383300	6.801200
H	5.906900	-5.624700	-5.909000	H	-2.345800	0.582900	-9.130700	H	6.226900	7.338300	6.637400
H	5.654500	-4.491500	-4.542500	H	-1.087300	1.230500	-8.030000	H	6.028200	5.609700	7.108800
C	0.521900	-0.185000	2.935600	C	4.990300	-1.530100	-6.530800	H	7.508800	6.509700	7.584300
C	1.562800	-0.537500	3.885700	H	4.626200	-0.491400	-6.612600	C	9.872100	5.366800	2.544600
C	1.578400	-0.583200	5.287600	H	5.771300	-1.703000	-7.280600	H	9.758500	6.182900	1.812100
H	0.685500	-0.325200	5.855400	H	4.161900	-2.236400	-6.697600	H	10.866700	5.419200	3.001800
C	2.767600	-0.956900	5.913000	C	7.675200	-2.642400	-2.001600	H	9.749900	4.394400	2.037000
C	2.313100	-0.755900	1.732700	H	8.613700	-3.035400	-2.410100	C	9.018000	5.643600	-4.407700
C	2.697400	-0.874600	3.128700	H	7.884500	-1.732100	-1.417800	H	9.094500	6.399000	-3.608400
C	3.906600	-1.233500	3.742600	H	7.206200	-3.406700	-1.358200	H	9.009000	4.633600	-3.963100
H	4.776600	-1.483900	3.137300	Y	1.558300	4.727400	0.002900	H	9.873600	5.738200	-5.085800
C	3.944000	-1.265100	5.136400	C	-0.391400	7.011300	1.523000	C	4.979900	6.990200	-7.688600
C	2.784400	-0.929800	-0.553400	C	-0.762300	7.505500	2.849500	H	4.197000	6.235700	-7.878200
C	3.684500	-1.234100	-1.652400	C	-1.847400	8.267800	3.294900	H	4.515500	7.921300	-7.324400
C	5.004000	-1.709300	-1.681500	H	-2.640200	8.554800	2.605100	H	5.527500	7.191200	-8.616400
H	5.532100	-1.920900	-0.752900	C	-1.863600	8.661700	4.640700	C	-1.626100	9.158600	-6.791200
C	5.603900	-1.887000	-2.928000	C	1.274900	6.461700	2.874400	H	-0.635100	9.612600	-6.626800
C	1.648700	-0.532900	-2.433300	C	0.290700	7.159100	3.703500	H	-1.504700	8.106000	-7.099700
C	2.977000	-0.962400	-2.835400	C	0.308900	7.560100	5.043700	H	-2.158200	9.711100	-7.573900
C	3.572300	-1.117400	-4.096200	H	1.154700	7.309900	5.683000	Cd	0.494600	1.499800	0.001200
H	3.008500	-0.894000	-5.000800	C	-0.778700	8.306600	5.519900	C	0.406000	3.419100	2.909300
C	4.890300	-1.571000	-4.141700	C	3.488800	5.729100	2.571700	C	0.987800	3.207400	4.225700
N	1.556500	-0.514000	-1.048700	C	4.859000	5.648800	3.079100	C	0.466000	3.358600	5.517000
N	3.129300	-1.034700	0.723900	C	5.401800	5.872900	4.348700	H	-0.565100	3.679900	5.658100
N	0.995300	-0.330800	1.639200	H	4.753900	6.111000	5.191500	C	1.309600	3.083800	6.596000
N	-0.688000	0.224600	3.296000	C	6.795400	5.802000	4.488000	C	2.501700	2.737500	2.571200
N	0.688100	-0.224700	-3.295700	C	4.773000	5.307800	0.817100	C	2.310600	2.789900	4.015400
O	5.608000	-1.757000	-5.269300	C	5.670700	5.383400	1.970600	C	3.175400	2.522600	5.082800
O	6.855900	-2.349400	-3.127300	C	7.064500	5.330900	2.079400	H	4.199100	2.201600	4.896700
O	5.029700	-1.573600	5.876300	H	7.680600	5.157500	1.197700	C	2.675000	2.673800	6.380100
O	2.941900	-1.064500	7.246800	C	7.631600	5.530300	3.346400	C	3.816900	2.294300	0.685300
C	-1.642700	0.550900	2.433600	C	4.485500	5.403000	-1.514900	C	5.061600	1.865300	0.066400
C	-2.965900	0.995600	2.835800	C	5.078400	5.580800	-2.840900	C	6.281500	1.441600	0.609300
C	-3.537300	1.222800	4.096600	C	6.404200	5.547700	-3.285800	H	6.409500	1.379100	1.689100
H	-2.951800	1.065100	5.001300	H	7.211700	5.305200	-2.595800	C	7.307700	1.108000	-0.277900
C	-4.866500	1.642400	4.142200	C	6.652400	5.856100	-4.631000	C	3.499500	2.411600	-1.518500
C	-2.790300	0.911700	0.553700	C	2.820100	5.955500	-2.866400	C	4.867900	1.949700	-1.320600
C	-3.695500	1.200600	1.652800	C	4.026500	5.930700	-3.694900	C	5.887400	1.632800	-2.225600
C	-5.038800	1.603600	1.681900	C	4.251300	6.265400	-5.034600	H	5.716000	1.707300	-3.298300

C	7.115200	1.213700	-1.703000
C	1.705900	2.994900	-2.906300
C	1.112900	3.172400	-4.222700
C	1.622300	2.983700	-5.513900
H	2.641900	2.627600	-5.655100
C	0.781300	3.265900	-6.593000
C	-0.383500	3.695400	-2.568100
C	-0.198400	3.624600	-4.012300
C	-1.052100	3.925400	-5.079800
H	-2.065800	4.277100	-4.893800
C	-0.559800	3.749600	-6.377100
C	-1.704900	4.119900	-0.682200
C	-2.960900	4.514700	-0.063400
C	-4.193300	4.900800	-0.606200
H	-4.332900	4.928600	-1.686000
C	-5.217000	5.241700	0.281100
C	-1.381300	4.021400	1.521500
C	-2.755800	4.464900	1.323700
C	-3.764200	4.815200	2.228700
H	-3.582600	4.771200	3.301500
C	-5.000100	5.209700	1.706300
N	1.339200	3.131700	1.925000
N	3.638500	2.354400	2.002100
N	2.888600	2.622100	-0.290900
N	2.956900	2.583600	-2.718000
N	0.785100	3.319300	-1.922000
N	-1.525100	4.063700	-1.999000
N	-0.764400	3.829500	0.294000
N	-0.843700	3.834300	2.721000
O	0.950200	3.155300	7.892800
O	3.370700	2.448600	7.506400
O	8.525200	0.659300	0.085800
O	8.186400	0.865800	-2.434100
O	1.112900	3.110100	-7.889800
O	-1.252500	3.983400	-7.503400
O	-6.462400	5.606000	-0.082600
O	-6.068500	5.566100	2.437500
C	-2.592400	4.461800	-7.417000
H	-2.638900	5.403300	-6.844900
H	-2.908300	4.645000	-8.450500
H	-3.252100	3.706600	-6.961800
C	2.430900	2.696400	-8.217900
H	2.647300	1.692300	-7.813300
H	2.475500	2.668200	-9.312900
H	3.178500	3.411600	-7.835500
C	8.115600	0.927100	-3.856400
H	7.848100	1.941900	-4.194600
H	9.120600	0.674700	-4.213700
H	7.393900	0.192800	-4.247200
C	8.842600	0.574300	1.467000
H	8.766000	1.561100	1.953800
H	8.180500	-0.140300	1.986300
H	9.878300	0.218600	1.518100
C	4.732200	2.036000	7.419800
H	5.329800	2.765500	6.848100
H	5.095100	1.994900	8.453300
H	4.813300	1.036800	6.964100
C	-0.355300	3.606900	8.220900
H	-1.126600	2.929100	7.815600
H	-0.408100	3.609900	9.315900
H	-0.530300	4.626900	7.839300
C	-5.975600	5.570800	3.859800
H	-5.157200	6.227100	4.199500
H	-6.933900	5.965000	4.217400
H	-5.832200	4.550600	4.249000
C	-6.767500	5.728700	-1.463800
H	-6.660100	4.761300	-1.984600
H	-7.811500	6.059100	-1.514800
H	-6.118500	6.477200	-1.949000

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Y	-4.993900	0.001500	0.001200
C	-6.563400	2.166200	-2.050600
C	-6.943200	2.362700	-3.449500
C	-7.366800	3.494900	-4.153800
H	-7.396500	4.469600	-3.668000
C	-7.774900	3.325000	-5.486000
C	-6.563700	0.155600	-2.977200
C	-6.943400	1.091700	-4.035200
C	-7.367300	0.891800	-5.353500
H	-7.397400	-0.110800	-5.778900
C	-7.775200	2.015000	-6.089600
C	-6.563400	-2.050700	-2.163300
C	-6.942900	-3.449700	-2.359600
C	-7.366700	-4.154100	-3.491700
H	-7.396900	-3.668200	-4.466400
C	-7.774500	-5.486300	-3.321700
C	-6.562900	-2.977400	-0.152700
C	-6.942600	-4.035500	-1.088600
C	-7.366200	-5.353800	-0.888600
H	-7.395900	-5.779200	0.113900
C	-7.774300	-6.090000	-2.011800
C	-6.562300	-2.163400	2.053600
C	-6.941500	-2.359800	3.452700
C	-7.364800	-3.492100	4.157200
H	-7.394800	-4.466800	3.671400
C	-7.772300	-3.322200	5.489600
C	-6.562200	-0.152800	2.980300
C	-6.941400	-1.088900	4.038500
C	-7.364600	-0.889000	5.357000
H	-7.394500	0.113600	5.782400
C	-7.772200	-2.012200	6.093300
C	-6.562300	2.053500	2.166400
C	-6.941600	3.452500	2.362900
C	-7.364600	4.157000	3.495300
H	-7.394200	3.671200	4.470000
C	-7.772200	5.489400	3.325500
C	-6.562900	2.980200	0.155800
C	-6.942000	4.038300	1.091900
C	-7.365400	5.356800	0.892200
H	-7.395700	5.782200	-0.110400
C	-7.772700	6.093000	2.015600
N	-6.282300	0.839000	-1.816000
N	-6.620300	-1.161900	-3.151100
N	-6.282000	-1.816100	-0.836200
N	-6.619100	-3.151300	1.164900
N	-6.281400	-0.836200	1.818900
N	-6.618700	1.164800	3.154300
N	-6.281800	1.818800	0.839100
N	-6.619800	3.154100	-1.161800
O	-8.203800	4.303200	-6.289000
O	-8.204500	1.990200	-7.354900
O	-8.203600	-6.289400	-4.299700
O	-8.203300	-7.355400	-1.986800
O	-8.200900	-4.300300	6.292800
O	-8.200900	-1.987400	7.358700
O	-8.200600	6.292500	4.303800
O	-8.201500	7.358500	1.990800
C	-8.372700	0.742500	-8.020200
H	-7.408700	0.216100	-8.124700
H	-9.090200	0.103400	-7.480400
H	-8.769200	0.984300	-9.012600
C	-8.371600	5.619800	-5.772900
H	-9.089200	5.624800	-4.936500
H	-7.407400	6.040900	-5.440800
H	-8.767800	6.217000	-6.601600
C	-8.369800	8.023900	0.743200
H	-8.765800	9.016400	0.985100
H	-7.405800	8.128000	0.216600
H	-9.087600	7.484300	0.104300
C	-8.368200	5.776500	5.620500
H	-9.086100	4.940300	5.625600
H	-7.404000	5.444000	6.041300
H	-8.763900	6.605300	6.217800
C	-8.372100	-5.773300	-5.616300
H	-9.089900	-4.937100	-5.620900
H	-7.408200	-5.440900	-6.037800
H	-8.768300	-6.602100	-6.213400
C	-8.370900	-8.020700	-0.739000
H	-9.088300	-7.481100	-0.099700
H	-8.767200	-9.013200	-0.980700
H	-7.406700	-8.125100	-0.213000
C	-8.369100	-5.616900	5.776700
H	-9.087100	-5.621800	4.940600
H	-7.405200	-6.038200	5.444100
H	-8.765000	-6.214100	6.605600
C	-8.368700	-0.739700	8.024200
H	-7.404500	-0.213400	8.128200
H	-9.086400	-0.100600	7.484800
H	-8.764600	-0.981500	9.016800
Cd	-1.629100	0.000500	0.000300
C	-3.371400	0.088800	-2.985600
C	-3.361400	-0.780900	-4.150200
C	-3.352000	-0.506700	-5.524800
H	-3.340700	0.522800	-5.880300
C	-3.362100	-1.591300	-6.404800
C	-3.380600	-2.003500	-2.212500
C	-3.378800	-2.098900	-3.665600
C	-3.405300	-3.199400	-4.531600
H	-3.427900	-4.213800	-4.136000
C	-3.398400	-2.946600	-5.907000
C	-3.370500	-2.984900	-0.086300
C	-3.360100	-4.149500	0.783400
C	-3.350300	-5.524100	0.509200
H	-3.339100	-5.879500	-0.520300
C	-3.360000	-6.404100	1.593700
C	-3.379800	-2.211800	2.006000
C	-3.377500	-3.664800	2.101500
C	-3.403600	-4.530900	3.201900
H	-3.426100	-4.135400	4.216300
C	-3.396200	-5.906300	2.949100
C	-3.370200	-0.085500	2.987400
C	-3.359200	0.784100	4.152000
C	-3.348400	0.510000	5.526600
H	-3.336900	-0.519600	5.882000
C	-3.357500	1.594500	6.406600
C	-3.380200	2.006700	2.214300
C	-3.377000	2.102200	3.667400
C	-3.402400	3.202700	4.533500
H	-3.425200	4.217100	4.138000
C	-3.394000	2.949800	5.908900
C	-3.371100	2.988100	0.088000
C	-3.360500	4.152800	-0.781600
C	-3.350000	5.527400	-0.507500
H	-3.338500	5.882800	0.522000
C	-3.359400	6.407400	-1.592000
C	-3.381000	2.215100	-2.004200
C	-3.378300	3.668100	-2.099700
C	-3.404100	4.534200	-3.200200
H	-3.426800	4.138600	-4.214600
C	-3.396000	5.909600	-2.947400
N	-3.385300	-0.671000	-1.823700
N	-3.369100	-3.064500	-1.413500
N	-3.384800	-1.823000	0.673500
N	-3.368400	-1.412700	3.067100
N	-3.385400	0.674200	1.825600
N	-3.369100	3.067800	1.415200
N	-3.386100	1.826300	-0.671700
N	-3.369800	1.416000	-3.065300
O	-3.329900	-1.497000	-7.746000
O	-3.410200	-3.884400	-6.865100
O	-3.327500	-7.745300	1.499300
O	-3.407500	-6.864500	3.886800
O	-3.324100	1.500100	7.747800
O	-3.404700	3.887600	6.867000
O	-3.326300	7.748600	-1.497700
O	-3.407000	6.867700	-3.885200
C	-3.374100	8.355200	-0.213000
H	-2.492000	8.079900	0.390700
H	-3.375500	9.436900	-0.389700
H	-4.291500	8.066200	0.326300
C	-3.467000	6.506800	-5.263500
H	-4.352100	5.882100	-5.467900
H	-3.548700	7.451200	-5.813600
H	-2.549700	5.981200	-5.572300
C	-3.378100	-0.212200	-8.352600
H	-2.495600	0.391300	-8.077900
H	-3.380200	-0.388900	-9.434300
H	-4.295200	0.327200	-8.063000
C	-3.470200	-5.262700	-6.504200
H	-4.354700	-5.467000	-5.878700
H	-3.552800	-5.812900	-7.448500
H	-2.552500	-5.571700	-5.979400
C	-3.375800	-8.351800	0.214600
H	-4.293100	-8.062400	-0.324600
H	-2.493600	-8.077000	-0.389200
H	-3.377700	-9.433500	0.391300
C	-3.467100	-6.503700	5.265200
H	-4.351800	-5.878500	5.469800

H	-3.549200	-7.448000	5.815300	H	-0.159300	-8.307200	-4.501500	H	9.086400	-5.409000	-5.176900
H	-2.549400	-5.978600	5.573800	H	0.862800	-7.475100	-3.285800	H	7.404200	-5.803000	-5.697300
C	-3.372100	0.215400	8.354400	C	0.073100	-7.580500	3.540300	H	8.763800	-5.929500	-6.865500
H	-2.490100	-0.388400	8.078900	H	0.154500	-8.490000	4.146400	C	8.368700	-0.399400	-8.048800
H	-3.373300	0.392100	9.436100	H	-0.865700	-7.606500	2.965900	H	7.404700	0.131100	-8.130200
H	-4.289600	-0.323700	8.065500	H	0.938800	-7.512400	2.860100	H	9.086600	0.215900	-7.482500
C	-3.464500	5.266000	6.506200	C	-0.073700	-3.857500	7.424200	H	8.764600	-0.598700	-9.050800
H	-4.349600	5.470700	5.881700	H	-0.938600	-3.174200	7.384700	C	8.369000	6.008200	-5.368700
H	-3.545800	5.816000	7.450600	H	-0.155900	-4.501400	8.307200	H	9.086900	5.173000	-5.409500
H	-2.547200	5.574500	5.980500	H	0.865700	-3.285700	7.474600	H	7.404900	5.693900	-5.803500
C	-0.008200	1.227000	-2.717500	C	0.076200	3.540400	7.580400	H	8.764700	6.861800	-5.930100
C	-0.014700	2.520200	-3.387500	H	0.941700	2.860000	7.511800	C	8.370600	8.045300	-0.400000
C	-0.044500	2.873600	-4.741500	H	0.158300	4.146500	8.489800	H	9.088400	7.478900	0.215200
H	-0.071600	2.104900	-5.512500	H	-0.862700	2.966200	7.607000	H	8.766800	9.047200	-0.599400
C	-0.030800	4.236300	-5.059100	C	-0.072000	7.424200	3.857300	H	7.406700	8.127000	0.130700
C	0.007100	2.766900	-1.111200	H	-0.153600	8.307200	4.501300	C	8.371600	5.365400	6.007500
C	0.013600	3.490800	-2.375000	H	0.867000	7.474400	3.285000	H	9.089300	5.406000	5.172200
C	0.043400	4.858500	-2.671000	H	-0.937400	7.384900	3.174500	H	7.407500	5.800300	5.693500
H	0.070500	5.596500	-1.870600	Y	4.994300	-0.001500	-0.001200	H	8.767600	5.926700	6.861000
C	0.029600	5.233300	-4.019100	C	6.562700	-2.076600	-2.144300	C	8.372500	0.396600	8.044700
C	-0.007500	2.717400	1.227000	C	6.941700	-2.213100	-3.550500	H	7.408500	-0.133800	8.126600
C	-0.013400	3.387400	2.520200	C	7.364700	-3.314300	-4.302800	H	9.090100	-0.218700	7.478200
C	-0.043000	4.741400	2.873600	H	7.394700	-4.308900	-3.859000	H	8.768900	0.595900	9.046500
H	-0.070200	5.512500	2.105000	C	7.772000	-3.087700	-5.626800	C	8.370500	-6.011300	5.364800
C	-0.028800	5.059000	4.236300	C	6.562600	-0.028300	-2.984300	H	9.088600	-5.176300	5.405400
C	0.008200	1.111200	2.766800	C	6.941700	-0.918300	-4.081500	H	7.406600	-5.696900	5.799900
C	0.015000	2.375000	3.490800	C	7.364800	-0.662300	-5.390300	H	8.766300	-6.865000	5.926100
C	0.045200	2.670900	4.858500	H	7.394700	0.357500	-5.772500	Cd	1.629400	-0.000600	-0.000500
H	0.072300	1.870400	5.596400	C	7.772100	-1.753200	-6.173900	C	3.370200	0.038600	-2.988200
C	0.031500	4.019000	5.233300	C	6.562700	2.141300	-2.076800	C	3.359800	0.957200	-4.114700
N	-0.000100	1.341700	1.399600	C	6.942100	3.547400	-2.213400	C	3.349900	0.741900	-5.499700
N	-0.000200	3.371500	0.071200	C	7.365100	4.299500	-3.314700	H	3.338600	-0.271600	-5.898600
N	-0.000700	1.399600	-1.341800	H	7.394800	3.855800	-4.309200	C	3.359400	1.862900	-6.332700
N	-0.000500	0.071200	-3.371600	C	7.772800	5.623400	-3.088200	C	3.379900	2.096100	-2.126600
N	0.001100	-0.071200	3.371500	C	6.563200	2.981300	-0.028500	C	3.377300	2.253400	-3.574200
O	0.071900	4.469300	6.498000	C	6.942400	4.078400	-0.918600	C	3.403200	3.389800	-4.392600
O	-0.068500	6.303500	4.739700	C	7.365900	5.387100	-0.662700	H	3.425700	4.386400	-3.954200
O	0.069600	6.498000	-4.469500	H	7.396100	5.769300	0.357100	C	3.395500	3.195800	-5.777600
O	-0.070900	4.739600	-6.303600	C	7.773200	6.170600	-1.753700	C	3.370800	2.985900	0.039600
C	0.007300	-1.111200	-2.766900	C	6.563700	2.073800	2.141000	C	3.360800	4.112400	0.958100
C	0.013200	-2.375000	-3.490900	C	6.943500	2.210300	3.547100	C	3.351000	5.497400	0.742700
C	0.042000	-2.670900	-4.858600	C	7.366900	3.311500	4.299100	H	3.339400	5.896300	-0.270700
H	0.068700	-1.870400	-5.596600	H	7.396700	4.306100	3.855300	C	3.360900	6.330400	1.863700
C	0.027600	-4.018900	-5.233400	C	7.774900	3.084900	5.622900	C	3.381100	2.124300	2.097000
C	-0.007200	-2.717500	-1.227100	C	6.564000	0.025500	2.981000	C	3.378700	3.571900	2.254300
C	-0.014600	-3.387500	-2.520300	C	6.943600	0.915500	4.078100	C	3.405000	4.390400	3.390600
C	-0.045100	-4.741400	-2.873700	C	7.367400	0.659500	5.386700	H	3.427800	3.952000	4.387300
H	-0.071900	-5.512500	-2.105100	H	7.397400	-0.360200	5.768900	C	3.397300	5.775300	3.196700
C	-0.032300	-5.059000	-4.236400	C	7.775100	1.750400	6.170100	C	3.372000	-0.041900	2.986700
C	0.008500	-2.766900	1.111100	C	6.563700	-2.144000	2.073600	C	3.361500	-0.960400	4.113300
C	0.014700	-3.490900	2.374900	C	6.943000	-3.550200	2.210000	C	3.351600	-0.745100	5.498200
C	0.043900	-4.858600	2.670800	C	7.366300	-4.302400	3.311100	H	3.340400	0.268400	5.897200
H	0.070700	-5.596500	1.870400	H	7.396400	-3.858700	4.305700	C	3.360800	-1.866100	6.331300
C	0.029800	-5.233400	4.018900	C	7.773700	-5.626400	3.084500	C	3.381600	-2.099300	2.125200
C	-0.006500	-1.227000	2.717400	C	6.563300	-2.984000	0.025300	C	3.378900	-2.256600	3.572800
C	-0.013300	-2.520300	3.387400	C	6.942700	-4.081200	0.915200	C	3.404300	-3.393000	4.391200
C	-0.043400	-2.873700	4.741400	C	7.365800	-5.390000	0.659200	H	3.426700	-4.389600	3.952900
H	-0.070300	-2.105100	5.512400	H	7.395600	-5.772200	-0.360600	C	3.396500	-3.199000	5.776200
C	-0.030100	-4.236400	5.058900	C	7.773500	-6.173600	1.749900	C	3.371500	-2.989100	-0.041000
N	0.001200	-1.399600	1.341700	N	6.281800	-0.760600	-1.853100	C	3.360400	-4.115600	-0.959500
N	0.000700	-3.371600	-0.071300	N	6.619100	1.295500	-3.101800	C	3.350200	-5.500600	-0.744200
N	0.000500	-1.341800	-1.399700	N	6.281900	1.850200	-0.760800	H	3.339300	-5.899600	0.269200
O	-0.070400	-4.739800	6.303400	N	6.620100	3.098700	1.295300	C	3.358900	-6.333600	-1.865300
O	0.069300	-6.498100	4.469300	N	6.282600	0.757800	1.850000	C	3.380400	-2.127500	-2.098400
O	-0.073000	-6.303500	-4.739800	N	6.620600	-1.298300	3.098500	C	3.377500	-3.575200	-2.255800
O	0.066700	-4.469300	-6.498200	N	6.282500	-1.852900	0.757700	C	3.402400	-4.393600	-3.392100
C	0.074300	7.580400	-3.540600	N	6.619500	-3.101500	-1.298500	H	3.424500	-3.955200	-4.388800
H	0.940000	7.511700	-2.860500	O	8.200300	-4.030700	-6.471100	C	3.394400	-5.778500	-3.198200
H	0.156200	8.489800	-4.146700	O	8.200600	-1.674300	-7.437200	N	3.384700	0.748200	-1.795000
H	-0.864400	7.607100	-2.966100	O	8.201200	6.467600	-4.031300	N	3.368800	3.122100	-1.283000
C	-0.074600	3.857200	-7.424300	O	8.202100	7.433800	-1.674900	N	3.385400	1.792700	0.749100
H	-0.939800	3.174200	-7.384700	O	8.203600	4.027900	6.467000	N	3.370200	1.280700	3.123000
H	-0.156600	4.501100	-8.307300	O	8.204300	1.671600	7.433200	N	3.386600	-0.751400	1.793600
H	0.864600	3.285000	-7.474700	O	8.202200	-6.470700	4.027400	N	3.370100	-3.125300	1.281500
C	0.070800	-3.540300	-7.580500	O	8.202100	-7.436800	1.671000	N	3.386000	-1.795900	-0.750500
H	0.936700	-2.860400	-7.512500	C	8.370000	-8.048400	0.396000	N	3.368700	-1.283900	-3.124400
H	0.151800	-4.146400	-8.490000	H	7.405800	-8.129900	-0.134200	O	3.326700	1.825800	-7.676700
H	-0.867800	-2.965500	-7.606400	H	9.087600	-7.482100	-0.219400	O	3.406500	4.173600	-6.694800
C	-0.076600	-7.424200	-3.857500	H	8.766000	-9.050400	0.595200	O	3.328400	7.674400	1.826600
H	-0.941400	-7.384400	-3.174100	C	8.368200	-5.368200	-6.011800	O	3.408700	6.692600	4.174400

O	3.328100	-1.829000	7.675300	C	3.468300	6.273400	5.536100	C	3.375100	0.568100	-8.337400
O	3.407000	-4.176800	6.693500	H	4.353000	5.640100	5.714000	H	2.493000	-0.046900	-8.088400
O	3.325900	-7.677600	-1.828200	H	3.550300	7.193400	6.125900	H	3.376800	0.790800	-9.410600
O	3.404500	-6.695800	-4.176000	H	2.550700	5.735600	5.822100	H	4.292500	0.017200	-8.071400
C	3.465700	-5.538500	6.274200	C	3.376700	8.335100	0.568800	C	3.463300	-6.276500	-5.537700
H	4.350500	-5.717000	5.641200	H	4.293900	8.068800	0.017700	H	4.348300	-5.643700	-5.716200
H	3.547100	-6.128500	7.194300	H	2.494300	8.086300	-0.046000	H	3.544400	-7.196600	-6.127700
H	2.548000	-5.823800	5.736200	H	3.378700	9.408300	0.791400	H	2.545800	-5.738200	-5.823000
C	3.377000	-0.571200	8.336000	C	3.466000	5.535300	-6.275500	C	3.374800	-8.338400	-0.570500
H	2.495100	0.044100	8.087100	H	4.350700	5.713200	-5.642300	H	2.493100	-8.089200	0.045100
H	3.378700	-0.793900	9.409200	H	3.547900	6.125200	-7.195500	H	3.376200	-9.411600	-0.793100
H	4.294600	-0.020700	8.069900	H	2.548400	5.821200	-5.737600	H	4.292600	-8.072500	-0.020100

XYZ coordinates from structures with added butoxy chains are given below in 2 columns per page. These are relevant for the analysis of NMR data. One butoxy chain was added per ligand to the structure optimized with methoxy groups as bubstitutes, and the chains were positioned close to each other in neighboring ligands. These were optimized with the same basis set and functional as described above. Only the butoxy chains were optimized, whereas the rest of the molecules was helf unmodified (i.e. “frozen”).

284				C	5.492900	4.475200	3.412500	C	-3.561300	-1.412700	0.301300
[3]^0 with butoxy				C	3.850400	-5.659200	3.688900	C	-0.064600	-5.523500	0.180300
Y	0.501600	0.035300	1.834500	C	4.102900	4.356700	3.384000	H	-1.138800	-5.690200	0.244900
O	-4.930200	-5.506300	4.301100	H	3.447200	5.226700	3.409800	C	-0.214000	-2.918300	0.138800
O	4.114600	-6.986900	3.782400	C	-7.333800	-2.332200	4.282300	C	-6.163300	-0.445400	0.431400
O	-4.960600	5.637100	4.088900	H	-8.328500	-2.760400	4.460600	C	-1.176300	2.527100	0.089300
O	6.166800	5.655400	3.452500	H	-7.109300	-1.597200	5.074900	C	-3.809800	-0.032200	0.289000
O	-2.881400	7.134800	3.911200	H	-7.324400	-1.831600	3.299400	C	0.437200	-4.214300	0.126500
O	6.197200	-5.488100	3.664600	C	3.023000	-7.888100	3.797000	O	0.277300	7.890800	-0.096800
O	7.663400	3.569300	3.376900	H	2.351200	-7.693600	4.651100	O	7.818400	2.634200	-0.426900
O	-6.430200	-3.421400	4.316700	H	2.449100	-7.841200	2.856100	O	-2.238100	7.433600	0.055800
N	1.121400	3.391100	3.248400	H	3.460300	-8.889000	3.904400	O	8.277700	0.114600	-0.404800
N	1.742700	-1.554900	3.067300	C	7.388200	-4.731200	3.642100	N	2.305200	0.334000	-0.067600
N	-1.036900	-1.108900	3.217700	H	7.486000	-4.153000	2.705800	N	0.064800	1.909900	0.030200
N	-2.734800	0.602300	3.522300	H	7.442600	-4.035400	4.497200	N	2.328900	2.764400	-0.115600
N	3.910400	-0.473700	3.163100	H	8.211800	-5.454200	3.709100	N	3.161000	-1.934300	-0.073000
N	2.185000	1.228200	2.988600	C	8.559500	2.477600	3.281500	C	2.920100	1.576300	-0.126600
N	0.054200	-3.262500	3.437100	H	8.428400	1.774000	4.122000	C	3.315100	-0.616500	-0.107100
N	-0.594600	1.674200	3.139000	H	8.439300	1.939800	2.325900	C	5.916500	-0.469700	-0.258600
C	-0.138400	2.965000	3.278500	H	9.567100	2.910100	3.328800	H	6.084100	-1.545600	-0.247600
C	3.481700	0.784500	3.113400	C	5.414200	6.846700	3.532700	C	-1.951500	5.014900	0.085900
C	1.308200	-2.838400	3.307200	H	4.766700	6.980200	2.647500	H	-3.015700	4.794400	0.150900
C	-1.942200	1.664000	3.410600	H	4.785800	6.868900	4.440800	C	5.403500	2.349900	-0.283400
C	-3.179200	-1.796900	3.757100	H	6.142900	7.666900	3.575500	H	5.182100	3.415800	-0.291200
C	-2.311800	-0.657900	3.472200	C	-1.797200	8.033500	3.766900	C	-0.053600	6.573700	-0.052600
C	2.180700	2.592700	3.157100	H	-2.221600	9.038800	3.885100	C	-1.016600	3.969000	0.052500
C	3.112500	-1.537200	3.183100	H	-1.032100	7.870400	4.545800	C	-1.467600	6.318800	0.033200
C	-1.268700	3.851200	3.539500	H	-1.334100	7.949400	2.769300	C	6.706000	1.863800	-0.348500
C	3.554600	3.069700	3.281700	C	-6.144700	4.882500	4.231200	C	4.360200	1.414700	-0.205800
C	-4.558800	-1.893600	3.985100	H	-6.347300	4.269100	3.334900	C	0.863400	5.525600	-0.084900
H	-5.174300	-0.994100	3.988000	H	-6.099900	4.220100	5.112900	H	1.937600	5.692300	-0.149500
C	2.462800	-3.716400	3.471400	H	-6.956900	5.609400	4.363800	C	1.012800	2.920300	-0.043400
C	-5.107900	-3.164600	4.153100	C	-4.170800	-6.695300	4.340600	C	6.962100	0.447500	-0.336000
C	6.331600	3.309400	3.374900	H	-3.628100	-6.864000	3.393100	C	4.608600	0.034300	-0.193500
C	4.890100	-3.435900	3.488600	H	-3.442900	-6.684200	5.171300	C	0.361600	4.216300	-0.031000
H	5.758400	-2.779900	3.431400	H	-4.888100	-7.511700	4.497400	C	1.975200	-2.525100	0.006100
C	2.572100	-5.103700	3.639100	O	0.521500	-7.888800	0.192200	C	-6.865300	-4.045300	0.541700
H	1.673500	-5.718500	3.687200	O	-7.019600	-2.632200	0.522300	H	-6.285800	-4.370300	1.421400
C	-1.010400	-2.465900	3.436600	O	3.036900	-7.431600	0.039600	H	-7.880900	-4.453000	0.607500
C	-3.677600	3.576900	3.843700	N	-1.506300	-0.332000	0.163000	H	-6.389100	-4.406000	-0.386300
H	-4.545300	2.921000	3.910900	N	0.734000	-1.907800	0.065200	C	-0.848900	-8.226900	0.277000
C	-2.890400	-4.215700	3.948300	N	-1.530100	-2.762400	0.211100	H	-1.309500	-7.821100	1.195200
H	-2.234200	-5.085600	3.932500	N	-2.362100	1.936300	0.168400	H	-1.412000	-7.856500	-0.597500
C	3.598500	-2.897500	3.394800	C	-2.121300	-1.574300	0.222000	H	-0.892600	-9.323700	0.300600
C	4.373300	1.931700	3.253800	C	-2.516300	0.618500	0.202500	C	4.447900	-7.278700	-0.043000
C	-2.626700	5.803900	3.839100	C	-5.117700	0.471800	0.354000	H	4.856100	-8.296200	-0.046800
C	-4.267800	-4.330000	4.139400	H	-5.285300	1.547700	0.343000	H	4.738500	-6.767700	-0.976000
C	-1.361200	5.244100	3.665300	C	2.750400	-5.012900	0.009600	H	4.840800	-6.733100	0.830700
H	-0.464300	5.858300	3.587200	H	3.814500	-4.792300	-0.055500	C	8.616800	-1.258200	-0.397900
C	5.769800	2.034000	3.319300	C	-4.604600	-2.347800	0.378800	H	8.280600	-1.753100	0.530500
H	6.383500	1.134000	3.286400	H	-4.383300	-3.413800	0.386700	H	8.178100	-1.787500	-1.262200
C	-2.403900	3.032400	3.624100	C	0.852400	-6.571700	0.148000	H	9.712100	-1.303100	-0.459600
C	5.014100	-4.819600	3.618200	C	1.815400	-3.967000	0.042900	C	7.664200	4.047400	-0.444200
C	-2.360100	-2.934800	3.735100	C	2.266400	-6.316700	0.062300	H	8.679800	4.455000	-0.510100
C	-3.789000	4.964800	3.933600	C	-5.907200	-1.861700	0.444000	H	7.084600	4.373400	-1.325000

H	7.188000	4.407100	0.482700
C	1.647800	8.229000	-0.181600
H	2.210800	7.857600	0.693000
H	2.108300	7.824200	-1.099800
H	1.691400	9.325800	-0.205100
C	-3.649000	7.280800	0.140400
H	-3.938600	6.769800	1.073400
H	-4.057200	8.298300	0.144200
H	-4.042900	6.735100	-0.733300
O	-7.478500	-0.111300	0.499400
C	-7.829200	1.267000	0.485600
H	-7.354200	1.783200	1.341600
H	-7.449200	1.740800	-0.439500
C	-9.344400	1.369700	0.564000
H	-9.779000	0.815100	-0.285400
H	-9.685000	0.856600	1.479500
C	-9.840700	2.819200	0.556000
H	-9.388100	3.366300	1.402900
H	-9.481200	3.324700	-0.358700
C	-11.364300	2.932300	0.633900
H	-11.688100	3.984800	0.625800
H	-11.844800	2.425900	-0.219300
H	-11.750900	2.468400	1.556100
Y	0.297300	-0.033300	-1.739000
O	5.726000	5.511300	-4.205500
O	-3.319700	6.986900	-3.686700
O	5.762300	-5.632100	-3.993700
O	-5.364900	-5.656300	-3.357200
O	3.684200	-7.130700	-3.816100
O	-5.401300	5.487100	-3.569000
O	7.227000	3.427400	-4.221300
N	-0.320500	-3.389000	-3.153100
N	-0.944900	1.555900	-2.971900
N	1.834700	1.111900	-3.122200
N	3.533600	-0.598200	-3.426900
N	-3.111500	0.473800	-3.067700
N	-1.385200	-1.227200	-2.893300
N	0.742700	3.264500	-3.341500
N	1.394400	-1.671200	-3.043600
C	0.939200	-2.962000	-3.183200
C	-2.681800	-0.784400	-3.018000
C	-0.511400	2.839400	-3.211600
C	2.742100	-1.660900	-3.315200
C	3.977000	1.801000	-3.661600
C	3.109600	0.661900	-3.376800
C	-1.380800	-2.591600	-3.061700
C	-2.314700	1.538300	-3.087600
C	2.069500	-3.848100	-3.444200
C	-2.753700	-3.069700	-3.186400
C	5.356600	1.897600	-3.889600
H	5.973000	0.999200	-3.892600
C	-1.666000	3.717400	-3.375900
C	5.904600	3.169600	-4.058600
C	-5.530800	-3.310300	-3.280500
C	-4.093200	3.435900	-3.393000
H	-4.961500	2.778900	-3.336800
C	-1.776200	5.104700	-3.543400
H	-0.878600	5.720500	-3.591500
C	1.808200	2.468900	-3.341100
C	4.478400	-3.572800	-3.748400
H	5.346000	-2.916000	-3.816700
C	3.687200	4.219700	-3.852800
H	3.029900	5.089600	-3.837900
C	-2.801600	2.897500	-3.298200
C	-3.573500	-1.931700	-3.158400
C	3.428500	-5.799900	-3.744900
C	5.064600	4.335000	-4.043900
C	2.163000	-5.241000	-3.570000
H	1.267100	-5.856200	-3.492000
C	-4.969900	-2.033900	-3.223900
H	-5.584600	-1.135000	-3.191000
C	3.204700	-3.028300	-3.527800
C	-4.218200	4.819600	-3.522600
C	3.156900	2.938800	-3.639600
C	4.590800	-4.960700	-3.838400
C	-4.692000	-4.476100	-3.317100
C	-3.054600	5.659200	-3.594200
C	-3.302000	-4.356600	-3.288600
H	-2.645400	-5.226700	-3.315500
C	-6.592300	4.730100	-3.547500
H	-6.645800	4.033400	-4.402600
H	-6.690100	4.151000	-2.610100
H	-7.415900	5.452200	-3.614400
C	-2.228200	7.889000	-3.702300
H	-1.654300	7.842200	-2.761400
H	-1.556400	7.694600	-4.556400
H	-2.666400	8.890000	-3.808700
C	4.966500	6.700300	-4.246000
H	4.237700	6.688200	-5.075700
H	4.422800	6.869000	-3.297500
H	5.682900	7.516600	-4.401800
C	8.131500	2.338200	-4.187900
H	7.907000	1.603200	-4.980500
H	9.126200	2.767400	-4.365200
H	8.122100	1.837600	-3.205000
C	6.946400	-4.877400	-4.137000
H	6.900600	-4.214000	-5.018700
H	7.149100	-4.263100	-3.239700
H	7.758600	-5.603300	-4.269600
C	2.600000	-8.030400	-3.672700
H	1.834900	-7.867300	-4.451600
H	3.025400	-9.035600	-3.789900
H	2.136900	-7.946300	-2.675100
C	-4.612400	-6.847600	-3.438400
H	-3.982900	-6.868800	-4.345600
H	-3.963900	-6.981000	-2.552300
H	-5.340100	-7.667700	-3.480300
O	-6.862200	-3.569300	-3.278400
C	-7.769700	-2.476100	-3.167100
H	-7.576800	-1.925300	-2.228900
H	-7.620800	-1.778600	-4.012800
C	-9.182000	-3.040100	-3.176500
H	-9.328700	-3.613000	-4.108100
H	-9.276300	-3.760000	-2.345600
C	-10.252000	-1.951100	-3.049400
H	-10.081100	-1.381200	-2.118300
H	-10.139100	-1.227900	-3.877400
C	-11.677100	-2.507300	-3.052400
H	-12.422300	-1.701500	-2.959500
H	-11.889000	-3.054700	-3.985600
H	-11.832500	-3.206800	-2.214600

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[3]$^{+1}$ with butoxy

Y	-0.236800	-0.002500	-1.677400
O	-1.734100	7.514200	-4.684100
O	6.535000	4.144300	-3.848700
O	-7.439000	-1.795400	-5.240700
O	1.823600	-7.527400	-4.306600
O	-6.446300	-4.157500	-5.134000
O	4.173800	-6.529000	-4.069200
O	-4.085000	6.515800	-4.913600
N	-1.341700	-3.123000	-3.346000
N	1.725100	0.776500	-2.733700
N	-0.889700	1.842900	-2.996500
N	-3.184900	1.260600	-3.536600
N	3.020500	-1.270000	-2.912800
N	0.663600	-1.851500	-2.835900
N	1.177300	3.113600	-3.103400
N	-1.951200	-0.785100	-3.098800
C	-2.202100	-2.110000	-3.374200
C	2.006600	-2.128900	-2.953600
C	2.026000	2.100700	-2.957800
C	-3.063900	-0.061400	-3.463300
C	-2.300500	3.533800	-3.721900
C	-2.182700	2.119600	-3.378400
C	-0.032000	-2.995300	-3.156000
C	2.887700	0.052100	-2.868700
C	-3.577200	-2.261900	-3.841100
C	0.905700	-4.089600	-3.390400
C	-3.380700	4.305000	-4.173700
H	-4.365200	3.853000	-4.286500
C	3.466300	2.251600	-3.143700
C	-3.145000	5.648400	-4.477700
C	3.166300	-5.660600	-3.830500
C	5.377000	0.734800	-3.295200
H	5.772900	-0.279600	-3.270300
C	4.268200	3.370900	-3.407900
H	3.820100	4.361700	-3.469200
C	-0.144100	2.985900	-3.175900
C	-5.419700	-0.746100	-4.372100
H	-5.812400	0.268300	-4.428900
C	-0.757300	5.419500	-3.915100
H	0.253700	5.815900	-3.830700
C	4.008900	0.961400	-3.087600
C	2.189600	-3.544100	-3.262800
C	-5.616200	-3.178300	-4.711800
C	-1.826500	6.208600	-4.347700
C	-4.311300	-3.382200	-4.255500
H	-3.860200	-4.373000	-4.224000
C	3.337600	-4.316300	-3.489700
H	4.325100	-3.864300	-3.406700
C	-4.119800	-0.971600	-3.897200
C	6.194900	1.841300	-3.539700
C	-1.016600	4.079300	-3.594400
C	-6.173300	-1.853500	-4.770400
C	1.848100	-6.220800	-3.962400
C	5.637600	3.166100	-3.596300
C	0.714600	-5.430800	-3.752200
H	-0.293200	-5.827200	-3.868400
C	-5.392200	6.029500	-5.157100
H	-5.970400	6.885000	-5.526700
H	-5.388300	5.231200	-5.918300
H	-5.859700	5.644000	-4.233400
C	6.062700	5.469100	-4.011400
H	5.344900	5.539800	-4.846100
H	5.581900	5.843800	-3.090200
H	6.945300	6.080700	-4.234700
C	5.503500	-6.043000	-4.050600
H	5.650500	-5.246900	-4.799800
H	5.779000	-5.654700	-3.053800
H	6.143100	-6.899400	-4.295900
C	0.570900	-8.139700	-4.545500
H	-0.060500	-8.138700	-3.639800
H	0.027300	-7.636300	-5.363400
H	0.788200	-9.175500	-4.835800
C	-5.951500	-5.482600	-5.196200
H	-6.772600	-6.095100	-5.587900
H	-5.082700	-5.555500	-5.872100
H	-5.662600	-5.854500	-4.197000
C	-8.036600	-0.525200	-5.416800
H	-8.132700	0.014400	-4.458400
H	-7.459000	0.095900	-6.122800
H	-9.035800	-0.713100	-5.830000
C	-0.458600	8.126200	-4.672100
H	-0.019000	8.127900	-3.659300
H	0.235900	7.620600	-5.364700
H	-0.613900	9.161000	-5.002700
O	7.529400	1.783300	-3.740500
C	8.172100	0.511300	-3.749500
H	7.988400	-0.007200	-2.789400
H	7.744900	-0.115200	-4.554700
C	9.659800	0.739800	-3.963600
H	9.798600	1.287000	-4.911200
H	10.030200	1.402100	-3.162200
C	10.462700	-0.565200	-3.983200
H	10.296100	-1.112800	-3.037400
H	10.078200	-1.219900	-4.785900
C	11.962700	-0.341800	-4.183400
H	12.510000	-1.297000	-4.197000
H	12.164400	0.174600	-5.135900
H	12.384700	0.276500	-3.374100
O	1.364400	7.683300	0.225100
O	-7.080700	4.153200	-0.613800
O	3.723200	6.704200	0.462300
O	-8.055300	1.782500	-0.707700
N	-2.194400	0.739200	-0.120400
N	0.325300	1.793100	0.129900

N	-1.701800	3.118000	-0.074700
N	-3.513000	-1.298300	-0.249300
C	-2.532500	2.086200	-0.156200
C	-3.379200	0.023100	-0.237800
C	-5.879800	0.717100	-0.488700
H	-6.268700	-0.299700	-0.526100
C	2.939600	4.403700	0.387300
H	3.930900	3.962900	0.487000
C	-4.791700	3.366000	-0.383800
H	-4.352900	4.362400	-0.341400
C	1.414300	6.334400	0.232100
C	1.812900	3.577700	0.275900
C	2.740700	5.784200	0.365400
C	-6.165400	3.166000	-0.520800
C	-3.970000	2.233900	-0.300100
C	0.303900	5.496800	0.122300
H	-0.707800	5.887500	0.020600
C	-0.387000	2.983600	0.056900
C	-6.713100	1.832900	-0.573600
C	-2.486500	-2.132900	-0.145400
C	-4.502800	0.937500	-0.351400
C	0.523000	4.113000	0.146200
O	-2.185100	-7.683200	-0.107200
O	6.260000	-4.153200	0.731600
O	-4.543900	-6.704200	-0.344400
N	1.373700	-0.739100	0.238300
N	-1.146100	-1.793000	-0.012000
N	0.881100	-3.117900	0.192500
N	2.692300	1.298400	0.367100
C	1.711700	-2.086100	0.274100
C	2.558400	-0.023100	0.355700
C	5.059100	-0.717000	0.606600
H	5.448000	0.299800	0.644000
C	-3.760300	-4.403600	-0.269400
H	-4.751600	-3.962800	-0.369200
C	3.971000	-3.365900	0.501700
H	3.532200	-4.362300	0.459300
C	-2.235100	-6.334300	-0.114200
C	-2.633700	-3.577600	-0.158100
C	-3.561400	-5.784100	-0.247600
C	5.344700	-3.165900	0.638700
C	3.149300	-2.233800	0.417900
C	-1.124700	-5.496700	-0.004400
H	-0.112900	-5.887500	0.097200
C	-0.433800	-2.983500	0.060900
C	5.892300	-1.832800	0.691500
C	3.682000	-0.937400	0.469300
C	-1.343700	-4.112900	-0.028400
C	1.665800	2.133000	0.263300
C	-8.679600	0.511600	-0.768200
H	-8.322200	-0.071100	-1.634100
H	-8.500800	-0.068500	0.152900
H	-9.754200	0.706300	-0.875900
C	-6.630600	5.496200	-0.570700
H	-5.943000	5.716900	-1.404800
H	-7.528500	6.120300	-0.661400
H	-6.121600	5.719500	0.382300
C	0.099900	8.310500	0.097800
H	-0.389400	8.039700	-0.853100
H	-0.568000	8.042300	0.933900
H	0.293700	9.390500	0.115600
C	5.059400	6.252000	0.596500
H	5.680600	7.154500	0.657300
H	5.191000	5.652100	1.513000
H	5.369600	5.649500	-0.274100
C	5.809800	-5.496100	0.688600
H	6.707700	-6.120200	0.779200
H	5.122300	-5.716800	1.522700
H	5.300900	-5.719400	-0.264400
C	-0.920600	-8.310500	0.020000
H	-0.252700	-8.042200	-0.816100
H	-0.431300	-8.039600	0.971000
H	-1.114400	-9.390500	0.002200
C	-5.880200	-6.252000	-0.478600
H	-6.011700	-5.652000	-1.395100
H	-6.501300	-7.154400	-0.539400
H	-6.190300	-5.649400	0.392000
O	7.234400	-1.782100	0.817900
C	7.877800	-0.508000	0.845700
H	7.614900	0.059800	-0.065900
H	7.516400	0.071300	1.715800
C	9.377600	-0.742200	0.926500
H	9.682300	-1.356200	0.061600
H	9.593200	-1.342400	1.826900
C	10.179500	0.563600	0.956000
H	9.860400	1.170500	1.822300
H	9.937400	1.162500	0.059400
C	11.690800	0.335800	1.022100
H	12.236800	1.291400	1.046300
H	11.969200	-0.233300	1.924100
H	12.046500	-0.232800	0.147300
Y	-0.583900	0.002600	1.795300
O	0.912700	-7.514900	4.801900
O	-7.356700	-4.143600	3.967500
O	6.619000	1.794900	5.358700
O	-2.643800	7.528200	4.424600
O	5.626200	4.156900	5.253000
O	-8.350100	-1.781500	3.867800
O	-4.994000	6.529800	4.188100
O	3.263500	-6.516500	5.032400
N	0.520900	3.123100	3.463900
N	-2.545300	-0.775600	2.851600
N	0.068200	-1.842200	3.114300
N	2.364100	-1.260500	3.654500
N	-3.841200	1.270100	3.030700
N	-1.483600	1.850900	2.953900
N	-1.998000	-3.113500	3.221200
N	1.129800	0.784400	3.216600
C	1.381400	2.110100	3.492100
C	-2.827300	2.129000	3.071400
C	-2.846700	-2.100700	3.075700
C	2.243100	0.061500	3.581200
C	1.479800	-3.533800	3.839800
C	1.362000	-2.119600	3.496300
C	-0.788700	2.995300	3.273900
C	-3.708500	-0.052000	2.986500
C	2.756500	2.262000	3.958900
C	-1.725800	4.090400	3.508300
C	2.559400	-4.305700	4.291500
H	3.544400	-3.852900	4.404400
C	-4.287100	-2.251500	3.261600
C	2.324200	-5.648300	4.595600
C	-3.987100	5.660600	3.948300
C	-6.197700	-0.734700	3.413100
H	-6.593000	0.280500	3.388200
C	-5.089700	-3.370200	3.525700
H	-4.640800	-4.361600	3.587100
C	-0.676600	-2.985900	3.293800
C	4.598900	0.746100	4.490000
H	4.991000	-0.269000	4.546700
C	-0.063400	-5.419400	4.033000
H	-1.075200	-5.815200	3.948500
C	-4.830400	-0.960700	3.205400
C	-3.010400	3.544200	3.380700
C	4.795500	3.178400	4.829700
C	1.004400	-6.208600	4.465500
C	3.491300	3.381600	4.373400
H	3.039400	4.373000	4.341900
C	-4.157800	4.317100	3.607600
H	-5.145800	3.864300	3.524600
C	3.299800	0.971100	4.015100
C	-7.015800	-1.839800	3.657600
C	0.195200	-4.080000	3.712200
C	5.352800	1.852100	4.888300
C	-2.667400	6.221000	4.080400
C	-6.458300	-3.166000	3.714200
C	-1.535400	5.430800	3.870100
H	-0.526800	5.826600	3.986400
C	-8.969800	-0.510200	3.918600
H	-8.542300	0.112400	4.723200
H	-8.874200	0.026600	2.958600
H	-10.030200	-0.697800	4.126500
C	-6.884300	-5.468400	4.129200
H	-6.403400	-5.843100	3.208000
H	-6.166500	-5.539100	4.963900
H	-7.766800	-6.080000	4.352500
C	-0.363500	-8.126300	4.789800
H	-1.057400	-7.619900	5.482500
H	-0.803200	-8.128000	3.777100
H	-0.207600	-9.160300	5.120500
C	4.570800	-6.030200	5.274900
H	4.567000	-5.231900	6.036100
H	5.149000	-6.885700	5.644500
H	5.038300	-5.644700	4.351200
C	7.216000	0.523900	5.534700
H	6.637600	-0.096600	6.240600
H	7.312200	-0.015700	4.576300
H	8.214400	0.712400	5.947800
C	5.131500	5.482000	5.314200
H	4.262800	5.555000	5.990000
H	5.952600	6.094600	5.705900
H	4.842600	5.854000	4.314900
C	-1.390200	8.140000	4.663500
H	-0.847300	7.635700	5.481300
H	-0.758800	8.138900	3.757800
H	-1.608200	9.174900	4.953800
C	-6.323600	6.043800	4.168500
H	-6.599200	5.655600	3.171700
H	-6.470700	5.247700	4.917800
H	-6.963200	6.900300	4.413900

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[3]$^{+2}$ with butoxy

Y	0.246200	-0.010100	-1.665000
O	-4.436900	6.326100	-3.968700
O	2.112400	-7.474200	-4.554300
O	7.399600	2.104800	-5.114600
O	4.418200	-6.378500	-4.735000
O	-2.139600	7.421200	-4.239000
O	6.312000	4.417600	-4.979700
O	-6.330700	-4.470100	-3.723900
N	3.257400	-1.153100	-3.477500
N	-0.721100	1.791800	-2.822400
N	-1.671200	-0.870800	-2.716000
N	-1.025200	-3.188500	-3.057900
N	1.228700	3.150000	-3.310300
N	1.930200	0.835800	-3.068800
N	-3.054000	1.114600	-2.890700
N	0.980000	-1.826800	-2.962500
C	2.291500	-2.052400	-3.323000
C	2.130300	2.174200	-3.333000
C	-2.077300	2.014600	-2.931800
C	0.291200	-3.004800	-3.133000
C	-3.349900	-2.428100	-3.095500
C	-1.916000	-2.212000	-2.921800
C	3.079000	0.164800	-3.417200
C	-0.078000	2.966900	-3.133700
C	2.476300	-3.465200	-3.643500
C	4.103200	1.120300	-3.833800
C	-4.097900	-3.586600	-3.333800
H	-3.605800	-4.556900	-3.382900
C	-2.320700	3.423700	-3.228400
C	-5.478600	-3.450500	-3.507700
C	5.517100	3.401700	-4.594700
C	-0.932000	5.374600	-3.711700
H	0.055800	5.815400	-3.838500
C	-3.502400	4.143900	-3.436800
H	-4.468800	3.649300	-3.349900
C	-2.865800	-0.202700	-2.849500
C	1.023600	-5.420200	-3.833100
H	0.030100	-5.861300	-3.766100
C	-5.326900	-1.001900	-3.255500
H	-5.769300	-0.006700	-3.249500
C	-1.061300	4.024100	-3.359900
C	3.505500	2.386600	-3.776400
C	3.433100	-5.548900	-4.342900
C	-6.096400	-2.149800	-3.474800
C	3.598300	-4.189100	-4.062300

H	4.563200	-3.694700	-4.165100	C	-1.692200	-6.249300	0.296600	O	5.255700	-6.326700	4.090200
C	4.193800	3.541300	-4.165300	C	2.444300	-2.172400	-0.120300	O	-1.289600	7.474600	4.675400
H	3.700200	4.511600	-4.132100	C	-0.694100	-4.072800	0.189600	O	-6.578800	-2.102500	5.235900
C	1.215300	-4.065700	-3.528000	C	-3.645000	1.111900	0.439300	O	-3.595400	6.379900	4.856100
C	-2.101600	6.118100	-3.904300	O	7.972500	-2.133300	-0.647400	O	2.958400	-7.420900	4.360500
C	-3.949100	-1.161900	-3.054100	O	4.835400	6.505300	-0.400700	O	-5.492300	-4.415300	5.101200
C	2.136700	-6.167200	-4.233900	O	6.888800	-4.448500	-0.530400	O	7.152500	4.468500	3.845200
C	6.131500	2.100700	-4.663400	O	2.529900	7.595200	-0.187900	N	-2.436800	1.154400	3.597900
C	-3.394600	5.500100	-3.759500	N	1.214700	1.761700	-0.026900	N	1.541800	-1.791400	2.942700
C	5.418500	0.956400	-4.289400	N	2.164400	-0.808700	-0.101800	N	2.491900	0.871200	2.836400
H	5.855200	-0.039200	-4.355100	N	3.565700	1.167800	-0.247000	N	1.846900	3.188900	3.178200
C	-5.806300	-5.779300	-3.884500	N	-0.753800	3.170400	0.151900	N	-0.409000	-3.149700	3.430700
H	-6.668100	-6.426900	-4.081900	C	2.572000	2.042000	-0.157700	N	-1.109500	-0.835500	3.189200
H	-5.107900	-5.825400	-4.737200	C	0.558300	2.983700	0.028200	N	3.874700	-1.115200	3.011100
H	-5.290300	-6.122100	-2.970200	C	1.360800	5.466300	-0.063000	N	-0.159300	1.827100	3.082900
C	-5.750400	5.788100	-3.959100	H	0.370000	5.908500	0.028600	C	-1.469800	2.052800	3.443300
H	-5.865400	5.007400	-4.730000	C	4.640200	-3.554500	-0.320900	C	-1.309600	-2.172800	3.453300
H	-6.006500	5.366700	-2.970800	H	4.155300	-4.528500	-0.268900	C	2.897000	-2.014300	3.052200
H	-6.420600	6.625600	-4.183600	C	3.946800	4.247000	-0.301600	C	0.530500	3.005200	3.253300
C	-0.921800	8.099300	-4.495500	H	4.916600	3.759400	-0.391000	C	4.170600	2.427400	3.215900
H	-0.283100	8.131000	-3.596100	C	6.632900	-2.115200	-0.520100	C	2.736800	2.211300	3.042200
H	-0.365900	7.624200	-5.321000	C	3.876400	-2.382700	-0.255300	C	-2.258300	-0.163400	3.537600
H	-1.199600	9.120700	-4.781600	C	6.023400	-3.421700	-0.454300	C	0.897700	-2.966600	3.254100
C	5.765200	5.725400	-5.054100	C	3.813700	5.636600	-0.298300	C	-1.654600	3.465600	3.763800
H	4.918600	5.762200	-5.760300	C	2.780500	3.480500	-0.186100	C	-3.282500	-1.118900	3.954100
H	5.430500	6.079600	-4.063000	C	5.852600	-0.957700	-0.451800	C	4.919600	3.586000	3.454100
H	6.573600	6.369600	-5.418100	H	6.292200	0.037300	-0.499500	H	4.427500	4.556300	3.503200
C	8.063200	0.867400	-5.306900	C	3.380600	-0.150200	-0.221500	C	3.140400	-3.423400	3.348900
H	8.180000	0.322500	-4.354400	C	2.512700	6.249600	-0.178200	C	6.300400	3.448900	3.629000
H	7.522100	0.231300	-6.027100	C	1.514800	4.073200	-0.069300	C	-4.697300	-3.399300	4.716100
H	9.052800	1.115100	-5.708900	C	4.465700	-1.111600	-0.318900	C	1.750700	-5.374300	3.832300
C	5.709400	-5.842000	-4.979500	C	-1.623600	2.172700	0.240700	H	0.762900	-5.815100	3.959000
H	6.326100	-6.682900	-5.316400	C	-0.482300	-8.297400	0.193800	C	4.322100	-4.144500	3.557200
H	5.676100	-5.070600	-5.767500	H	0.024200	-8.065800	-0.758900	H	5.288600	-3.650000	3.470400
H	6.146700	-5.409200	-4.062400	H	0.194500	-8.055100	1.031000	C	3.686500	0.202000	2.969900
C	0.868800	-8.153900	-4.568500	H	-0.738200	-9.362700	0.224500	C	-0.200900	5.420600	3.953300
H	0.411200	-8.174200	-3.564500	C	-5.336600	-5.996400	0.641800	H	0.792600	5.861700	3.886300
H	0.166700	-7.688000	-5.280000	H	-5.616500	-5.394600	-0.239300	C	6.147700	1.000200	3.375900
H	1.088900	-9.178900	-4.889700	H	-5.990800	-6.874700	0.709200	H	6.590100	0.005100	3.369900
O	-7.426300	-2.158500	-3.671600	H	-5.446100	-5.383900	1.552600	C	1.881000	-4.023800	3.480300
C	-8.137700	-0.919700	-3.716700	C	-5.562800	5.776300	0.592800	C	-2.684800	-2.385200	3.896800
H	-7.997700	-0.380200	-2.760800	H	-6.437500	6.433900	0.672100	C	-2.610400	5.550300	4.464000
H	-7.725100	-0.288300	-4.524800	H	-4.873200	5.976800	1.430100	C	6.917100	2.148100	3.595200
C	-9.606000	-1.229400	-3.956600	H	-5.043600	5.966100	-0.361800	C	-2.776700	4.190500	4.182600
H	-9.695100	-1.797900	-4.897300	C	1.302800	8.297700	-0.075400	H	-3.741600	3.696000	4.285400
H	-9.959800	-1.896100	-3.151800	H	0.626100	8.055400	-0.912600	C	-3.374100	-3.540000	4.285700
C	-10.473300	0.032900	-4.017500	H	0.796300	8.066100	0.877300	H	-2.880500	-4.510200	4.252600
H	-10.361300	0.601100	-3.075500	H	1.558700	9.363100	-0.106100	C	-0.393600	4.066100	3.648300
H	-10.100600	0.695000	-4.819600	C	6.157100	5.996800	-0.523400	C	2.920300	-6.117800	4.024800
C	-11.953600	-0.271100	-4.255300	H	6.811300	6.875100	-0.590900	C	4.769900	1.161300	3.174500
H	-12.547900	0.654400	-4.296000	H	6.437000	5.394900	0.357700	C	-1.314100	6.167600	4.354100
H	-12.101300	-0.807000	-5.206500	H	6.266600	5.384200	-1.434200	C	-5.310800	-2.098300	4.783800
H	-12.365600	-0.901000	-3.450200	C	8.671200	-0.901000	-0.721200	C	4.213500	-5.500700	3.881100
O	-4.014900	-6.505000	0.519100	H	8.349800	-0.312000	-1.597300	C	-4.597800	-0.954000	4.409700
O	-6.068300	4.448900	0.648800	H	8.520100	-0.301300	0.192600	H	-5.034500	0.041500	4.475500
O	-1.709400	-7.594900	0.306300	H	9.731900	-1.158800	-0.820600	C	1.740600	-8.099900	4.617000
N	-0.394000	-1.761300	0.147200	C	6.383300	-5.776000	-0.474400	H	1.184700	-7.623900	5.442600
N	-1.343700	0.809100	0.222200	H	5.693700	-5.976500	-1.311700	H	1.101800	-8.130700	3.716700
N	-2.745000	-1.167400	0.367300	H	7.258000	-6.433500	-0.553700	H	2.017400	-9.121300	4.903200
N	1.574500	-3.170000	-0.031600	H	5.864100	-5.965800	0.480200	C	6.569200	-5.788800	4.080600
C	-1.751300	-2.041600	0.278000	O	-7.150800	2.133500	0.758500	H	6.825300	-5.368400	3.092400
C	0.262300	-2.983400	0.092100	C	-7.867900	0.896800	0.804900	H	6.684100	-5.008100	4.850500
C	-0.540100	-5.466000	0.183300	H	-7.636700	0.305100	-0.100100	H	7.239400	-6.627300	4.305200
H	0.450700	-5.908200	0.091700	H	-7.534800	0.312600	1.682900	C	8.938000	0.920400	3.878400
C	-3.819500	3.554900	0.441300	C	-9.351600	1.215400	0.885500	H	8.542100	0.293400	4.695300
H	-3.334600	4.528800	0.389300	H	-9.625400	1.829600	0.010900	H	8.872600	0.364100	2.926600
C	-3.126100	-4.246700	0.422000	H	-9.529800	1.841600	1.776000	H	9.985400	1.170700	4.083600
H	-4.095900	-3.759100	0.511300	C	-10.223700	-0.044100	0.940700	C	6.628100	5.777700	4.005800
C	-5.812400	2.115600	0.638500	H	-9.934600	-0.652800	1.816500	H	5.929600	5.823800	4.857500
C	-3.055700	2.383000	0.375600	H	-10.019200	-0.670900	0.053600	H	7.490900	6.425300	4.203100
C	-5.202900	3.422100	0.572700	C	-11.719700	0.268600	1.008600	H	6.113100	6.120500	3.091400
C	-2.993200	-5.636300	0.416700	H	-12.316700	-0.655000	1.051000	C	-0.046000	8.155300	4.689700
C	-1.959900	-3.480100	0.306500	H	-11.961800	0.866600	1.901800	H	0.656100	7.688500	5.401200
C	-5.031900	0.958000	0.572100	H	-12.047300	0.840800	0.125500	H	0.411500	8.174600	3.684700
H	-5.471500	-0.037000	0.619900	Y	0.574500	0.010500	1.785400	H	-0.265100	9.180300	5.010800
C	-2.559900	0.150500	0.341800	O	8.247600	2.156200	3.800100	C	-4.886600	5.843400	5.100700

H	-4.853400	5.072100	5.887700
H	-5.503400	6.685300	5.437600
H	-5.324000	5.411600	4.183500
C	-7.243500	-0.865000	5.428300
H	-6.701400	-0.228900	6.148500
H	-7.359300	-0.320100	4.474800
H	-8.233100	-1.111700	5.830300
C	-4.945500	-5.723100	5.175500
H	-4.611800	-6.077300	4.184600
H	-4.098900	-5.759900	5.880800
H	-5.754900	-6.367300	5.539700

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[3]$^{+3}$ with butoxy

Y	-0.603500	0.002700	1.775500
O	-5.031300	6.480900	4.295500
O	-8.357700	-1.762600	3.935200
O	5.495000	4.126700	5.480100
O	3.153600	-6.466100	5.233900
O	6.480000	1.777400	5.594200
O	-7.372700	-4.111900	4.049300
O	0.818800	-7.457700	4.973500
O	-2.696500	7.472500	4.555900
N	2.317800	-1.260100	3.684000
N	-2.575400	-0.774100	2.807200
N	-1.515800	1.849200	2.922000
N	0.479500	3.121000	3.470900
N	-2.036300	-3.110700	3.198400
N	0.031500	-1.839900	3.101400
N	-3.874600	1.270400	2.985300
N	1.091000	0.783500	3.216100
C	2.196100	0.061800	3.611900
C	-0.716300	-2.981800	3.289900
C	-3.740500	-0.051600	2.946100
C	1.338400	2.106100	3.512500
C	-1.767300	4.083700	3.517200
C	-0.828000	2.992000	3.268100
C	1.315400	-2.118300	3.516500
C	-2.882700	-2.096000	3.045500
C	3.241200	0.968000	4.084000
C	1.426400	-3.527300	3.887400
C	-1.575700	5.408800	3.925100
H	-0.570200	5.804300	4.061400
C	-4.864500	-0.956800	3.177600
C	-2.713400	6.191700	4.166500
C	0.922000	-6.178100	4.593700
C	-5.115600	-3.360600	3.540600
H	-4.669900	-4.351300	3.616300
C	-6.223700	-0.720300	3.413200
H	-6.619200	0.294300	3.391400
C	-2.859800	2.128500	3.041500
C	3.406500	3.373100	4.486200
H	2.955400	4.363800	4.458200
C	-4.199700	4.293400	3.631400
H	-5.186900	3.842000	3.545500
C	-4.322900	-2.247000	3.240400
C	0.144100	-4.072500	3.744400
C	5.251000	1.837000	5.066800
C	-4.033800	5.630400	4.019300
C	4.514400	0.732700	4.615600
H	4.904500	-0.281700	4.685100
C	-0.133600	-5.396400	4.103700
H	-1.144500	-5.791800	4.015100
C	2.699700	2.258300	4.021200
C	-6.484800	-3.152000	3.758000
C	-3.049600	3.538600	3.374200
C	4.693400	3.165600	5.002200
C	2.242400	-5.616800	4.740900
C	-7.042400	-1.823400	3.693400
C	2.490600	-4.280900	4.395400
H	3.472500	-3.829500	4.529000
C	-1.451800	8.103200	4.833400
H	-1.696600	9.119900	5.160500
H	-0.912100	7.574700	5.636400
H	-0.819200	8.147800	3.930200
C	-8.999400	-0.494500	4.000000
H	-8.555200	0.132500	4.790500
H	-8.938000	0.031500	3.032000
H	-10.048800	-0.700700	4.238900
C	-6.920400	-5.447000	4.240000
H	-6.468900	-5.849500	3.317200
H	-6.190300	-5.502200	5.064600
H	-7.811800	-6.030900	4.497100
C	-0.456600	-8.087900	4.970300
H	-1.160700	-7.557200	5.632100
H	-0.873500	-8.135500	3.949500
H	-0.290800	-9.103600	5.346700
C	4.465500	-5.995200	5.518200
H	4.971900	-5.650900	4.600400
H	4.439800	-5.177400	6.256700
H	5.006700	-6.851800	5.936500
C	7.091000	0.509700	5.803600
H	8.061400	0.717000	6.268400
H	6.482400	-0.115000	6.477900
H	7.245400	-0.019300	4.847700
C	5.012200	5.462200	5.561700
H	4.776500	5.861700	4.560500
H	4.117500	5.519700	6.203800
H	5.824700	6.047300	6.008100
C	-6.373700	6.010400	4.283500
H	-6.664300	5.663100	3.277300
H	-6.512600	5.194900	5.011800
H	-6.993900	6.868100	4.568800
O	-7.090100	4.119300	-0.695500
O	1.335800	7.685600	0.244200
O	-8.048400	1.756600	-0.799300
O	3.683700	6.721700	0.509100
N	0.316200	1.793600	0.139000
N	-2.193300	0.731500	-0.140900
N	-1.712600	3.115100	-0.090700
N	2.684800	1.310300	0.405500
C	-0.398800	2.985600	0.056900
C	1.655400	2.142800	0.288700
C	2.919500	4.417100	0.427000
H	3.913300	3.985100	0.539100
C	-5.877900	0.693100	-0.554200
H	-6.265100	-0.323700	-0.596000
C	0.278600	5.501300	0.129000
H	-0.731800	5.890700	0.015000
C	-6.173800	3.145400	-0.591200
C	-4.503400	0.921500	-0.400300
C	-6.716700	1.806900	-0.650000
C	1.385600	6.345500	0.251900
C	0.505400	4.118200	0.156600
C	-4.800000	3.350800	-0.437400
H	-4.370500	4.350900	-0.390800
C	-2.540100	2.079100	-0.181900
C	2.715700	5.799500	0.401900
C	2.555800	-0.011700	0.393100
C	1.797100	3.588000	0.302300
C	-3.976200	2.221400	-0.343200
O	6.268000	-4.119200	0.816000
O	-2.157900	-7.685500	-0.123800
O	-4.505800	-6.721600	-0.388700
N	-1.138300	-1.793500	-0.018600
N	1.371100	-0.731400	0.261300
N	0.890400	-3.115000	0.211100
N	-3.507000	-1.310200	-0.285100
C	-0.423300	-2.985400	0.063500
C	-2.477500	-2.142700	-0.168300
C	-3.741600	-4.417000	-0.306500
H	-4.735500	-3.985000	-0.418700
C	5.055800	-0.693000	0.674600
H	5.443000	0.323800	0.716500
C	-1.100700	-5.501200	-0.008600
H	-0.090300	-5.890600	0.105400
C	5.351700	-3.145300	0.711600
C	3.681300	-0.921400	0.520800
C	5.894600	-1.806800	0.770400
C	-2.207700	-6.345400	-0.131400
C	-1.327500	-4.118100	-0.036200
C	3.977900	-3.350600	0.557800
H	3.548400	-4.350800	0.511200
C	1.718000	-2.079000	0.302300
C	-3.537800	-5.799400	-0.281500
C	-2.619200	-3.587900	-0.181900
C	3.154100	-2.221300	0.463700
C	-3.377900	0.011800	-0.272700
C	5.031300	6.298500	0.660900
H	5.160600	5.704800	1.582000
H	5.361300	5.702000	-0.206800
H	5.629700	7.214700	0.725600
C	0.077600	8.332300	0.102000
H	-0.599900	8.068900	0.932100
H	0.287600	9.407300	0.123900
H	-0.399200	8.066100	-0.856700
C	-6.669300	5.475500	-0.650400
H	-6.178200	5.708000	0.309900
H	-5.977600	5.705300	-1.478800
H	-7.579700	6.077300	-0.753500
C	-8.691200	0.490300	-0.869500
H	-9.759600	0.701400	-0.989700
H	-8.327900	-0.091800	-1.733500
H	-8.528600	-0.089000	0.055300
C	-5.853500	-6.298400	-0.540500
H	-6.183400	-5.701900	0.327200
H	-5.982700	-5.704700	-1.461600
H	-6.451500	-7.214600	-0.607200
C	-0.899700	-8.332100	0.018400
H	-1.109700	-9.407200	-0.003500
H	-0.222200	-8.068800	-0.811600
H	-0.422900	-8.066000	0.977100
C	5.847200	-5.475400	0.770900
H	5.155500	-5.705100	1.599300
H	5.356100	-5.707900	-0.189500
H	6.757600	-6.077200	0.873900
O	7.225000	-1.756200	0.911200
C	7.890300	-0.485300	0.941900
H	7.522900	0.095900	1.807600
H	7.639200	0.077400	0.024200
C	9.385100	-0.738600	1.038900
H	9.691100	-1.360000	0.180200
H	9.584300	-1.336100	1.944300
C	10.201800	0.558800	1.069900
H	9.878700	1.175200	1.928400
H	9.978400	1.153900	0.165600
C	11.708900	0.311600	1.157800
H	12.264900	1.260700	1.180400
H	11.968200	-0.251400	2.068600
H	12.068700	-0.268600	0.292900
Y	-0.218600	-0.002600	-1.655000
O	4.209200	-6.480800	-4.175000
O	-6.317100	-4.126600	-5.359600
O	-3.975800	6.466200	-5.113500
O	-7.302000	-1.777300	-5.474800
O	6.550600	4.112000	-3.928900
O	-1.640800	7.457800	-4.854100
O	1.874500	-7.472300	-4.436400
N	-3.139900	1.260200	-3.563600
N	1.753200	0.774200	-2.686800
N	0.693700	-1.849100	-2.801600
N	-1.301600	-3.120900	-3.350500
N	1.214200	3.110800	-3.078000
N	-0.853600	1.840000	-2.980900
N	3.052500	-1.270300	-2.864900
N	-1.913100	-0.783400	-3.095700
C	-3.018200	-0.061700	-3.491500
C	-0.105800	2.981900	-3.169500
C	2.918300	0.051800	-2.825700
C	-2.160500	-2.106000	-3.392100
C	0.945200	-4.083600	-3.396800
C	0.005900	-2.991900	-3.147700
C	-2.137600	2.118400	-3.396100
C	2.060600	2.096100	-2.925100
C	-4.063300	-0.967900	-3.963600
C	-2.248500	3.527400	-3.767000
C	0.753600	-5.408700	-3.804600
H	-0.252000	-5.804200	-3.941000

C	4.042400	0.956900	-3.057200
C	1.891300	-6.191600	-4.046100
C	-1.744100	6.178200	-4.473300
C	4.293500	3.360800	-3.420200
H	3.847700	4.351400	-3.495900
C	5.401600	0.720400	-3.292800
H	5.797100	-0.294100	-3.271000
C	2.037700	-2.128400	-2.921100
C	-4.228600	-3.373000	-4.365800
H	-3.777500	-4.363700	-4.337800
C	3.377600	-4.293300	-3.511000
H	4.364800	-3.841900	-3.425100
C	3.500800	2.247100	-3.120000
C	-0.966200	4.072600	-3.624000
C	-6.073100	-1.836900	-4.946400
C	3.211700	-5.630300	-3.898800
C	-5.336500	-0.732600	-4.495200
H	-5.726600	0.281800	-4.564700
C	-0.688500	5.396500	-3.983300
H	0.322400	5.791900	-3.894700
C	-3.521800	-2.258200	-3.900800
C	5.662700	3.152100	-3.637600
C	2.227500	-3.538500	-3.253800
C	-5.515600	-3.165400	-4.881800
C	-3.064500	5.617000	-4.620500
C	6.220300	1.823500	-3.573000
C	-3.312700	4.281100	-4.275000
H	-4.294600	3.829600	-4.408600
C	6.098300	5.447100	-4.119600
H	5.369100	5.502800	-4.944100
H	5.646800	5.849600	-3.196800
H	6.989700	6.031100	-4.376700
C	5.551600	-6.010300	-4.163000
H	5.690000	-5.194000	-4.891400
H	5.842200	-5.663000	-3.156900
H	6.171900	-6.868000	-4.449300
C	0.629700	-8.103100	-4.712900
H	0.090000	-7.574600	-5.515900
H	0.874000	-9.119000	-5.041200
H	-0.003000	-8.147700	-3.809800
C	-5.834300	-5.462100	-5.441200
H	-4.940500	-5.520100	-6.083500
H	-5.598700	-5.861600	-4.440100
H	-6.646800	-6.047200	-5.887700
C	-7.913100	-0.509600	-5.683200
H	-7.304500	0.115100	-6.357500
H	-8.882600	-0.716400	-6.148900
H	-8.066700	0.019900	-4.727200
C	-5.287600	5.995300	-5.397800
H	-5.261400	5.176700	-6.136200
H	-5.794000	5.651000	-4.480000
H	-5.828700	6.851900	-5.817100
C	-0.365500	8.088000	-4.849900
H	0.051300	8.135700	-3.829100
H	0.338600	7.557300	-5.511700
H	-0.530600	9.102900	-5.227200
O	7.535900	1.762400	-3.805900
C	8.201800	0.491600	-3.828600
H	8.057900	-0.011200	-2.854000
H	7.745900	-0.141300	-4.611100
C	9.675000	0.738000	-4.105200
H	9.767500	1.272000	-5.065300
H	10.069200	1.415300	-3.328500
C	10.491500	-0.559200	-4.140100
H	10.375100	-1.091900	-3.178000
H	10.078800	-1.230800	-4.914100
C	11.977400	-0.319500	-4.413600
H	12.534400	-1.268200	-4.434200
H	12.127500	0.178900	-5.384500
H	12.428100	0.319200	-3.636800

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Y	1.059000	-0.151100	3.358200
C	-0.417300	-2.579600	5.119300
C	-1.735400	-2.937700	5.633300
C	-2.343100	-4.175700	5.883800
H	-1.790900	-5.098100	5.707300
C	-3.670500	-4.179800	6.311400
C	-1.502400	-0.664800	5.452800
C	-2.420000	-1.731300	5.842300
C	-3.741100	-1.718600	6.312300
H	-4.252200	-0.769400	6.472600
C	-4.371400	-2.944400	6.528400
C	-0.900800	1.607000	5.419100
C	-1.177100	2.994300	5.778400
C	-2.336100	3.634100	6.238500
H	-3.245200	3.057600	6.406400
C	-2.293500	5.016000	6.421300
C	0.980800	2.737700	5.049600
C	0.008100	3.707300	5.544400
C	0.078200	5.090500	5.764100
H	1.011000	5.623700	5.580800
C	-1.079100	5.746600	6.184600
C	3.193100	2.144000	4.523000
C	4.611200	2.481900	4.453500
C	5.291600	3.705000	4.526600
H	4.735000	4.628400	4.683600
C	6.674300	3.698000	4.344600
C	4.279200	0.229000	4.193500
C	5.295800	1.275400	4.244500
C	6.690500	1.247800	4.102000
H	7.202500	0.298400	3.945600
C	7.376500	2.462300	4.133500
C	3.676700	-2.042600	4.223300
C	4.052800	-3.450200	4.308400
C	5.284700	-4.104700	4.171900
H	6.189400	-3.527400	3.984500
C	5.297300	-5.497900	4.234700
C	1.796000	-3.173500	4.596600
C	2.867700	-4.163200	4.542400
C	2.871200	-5.561300	4.650100
H	1.939300	-6.094700	4.837400
C	4.084200	-6.228700	4.477200
N	0.542200	-3.477700	4.916000
N	-0.343000	-1.215200	4.958700
N	-1.773800	0.625000	5.623900
N	0.377900	1.508300	4.920800
N	2.256400	3.037400	4.827700
N	3.030700	0.797500	4.291900
N	4.572400	-1.065200	4.119800
N	2.309900	-1.926100	4.329700
O	-4.410300	-5.296400	6.530400
O	-5.665100	-3.089600	6.922500
O	-3.350000	5.780500	6.797300
O	-1.179700	7.089100	6.378300
O	7.458300	4.805600	4.322500
O	8.717100	2.598000	3.948000
O	6.398000	-6.271400	4.055500
O	4.231700	-7.580700	4.492200
C	-0.016300	7.872000	6.211900
H	0.785100	7.559900	6.904900
H	0.367000	7.815900	5.176200
H	-0.308600	8.906400	6.435600
C	-4.598800	5.143100	6.999800
H	-4.535800	4.372900	7.787700
H	-5.290700	5.932200	7.321700
H	-4.974600	4.688000	6.067300
C	-6.408100	-1.921800	7.202300
H	-5.945100	-1.331100	8.012600
H	-6.509600	-1.280200	6.307400
H	-7.402500	-2.260600	7.521300
C	-3.808500	-6.555800	6.288400
H	-2.914000	-6.703400	6.917700
H	-4.564100	-7.306400	6.554300
H	-3.536300	-6.674600	5.225500
C	3.093700	-8.368800	4.771600
H	2.671400	-8.133600	5.764800
H	2.305800	-8.230600	4.008100
H	3.433400	-9.412800	4.758400
C	7.625800	-5.629700	3.759500
H	7.920500	-4.932100	4.562300
H	8.373300	-6.430100	3.685200
H	7.576000	-5.088200	2.799200
C	9.485500	1.425100	3.781200
H	10.527300	1.754200	3.672800
H	9.401600	0.757300	4.657100
H	9.182400	0.865500	2.876800
C	6.835500	6.069300	4.471000
H	6.137700	6.274400	3.641000
H	6.298700	6.144300	5.432300
H	7.646800	6.808500	4.452600
Y	-0.431100	0.151300	-3.268600
C	1.637000	1.947700	-5.193800
C	2.991600	1.877500	-5.734500
C	3.927900	2.864400	-6.072300
H	3.669300	3.918600	-5.968100
C	5.188400	2.450900	-6.504900
C	2.118900	-0.215500	-5.399800
C	3.294700	0.514200	-5.864800
C	4.542600	0.083900	-6.335400
H	4.754900	-0.981100	-6.421400
C	5.499500	1.053900	-6.635500
C	0.904800	-2.219600	-5.219200
C	0.762500	-3.648200	-5.485300
C	1.672600	-4.627500	-5.907000
H	2.704300	-4.352400	-6.128500
C	1.222500	-5.945200	-5.996200
C	-1.212600	-2.734500	-4.765600
C	-0.572000	-3.972300	-5.200000
C	-1.048900	-5.285300	-5.323000
H	-2.088300	-5.510500	-5.089300
C	-0.144200	-6.277200	-5.701000
C	-3.158100	-1.511500	-4.273400
C	-4.612200	-1.421000	-4.175200
C	-5.622200	-2.393100	-4.164800
H	-5.364400	-3.447000	-4.272900
C	-6.938300	-1.968300	-3.979700
C	-3.639600	0.651700	-4.065400
C	-4.915300	-0.057800	-4.044800
C	-6.235900	0.387300	-3.897900
H	-6.443800	1.451400	-3.792300
C	-7.248100	-0.571500	-3.843300
C	-2.425900	2.655800	-4.247900
C	-2.383100	4.104700	-4.424300
C	-3.366900	5.098800	-4.330100
H	-4.399400	4.824000	-4.112500
C	-2.972400	6.427800	-4.488400
C	-0.308000	3.170600	-4.699600
C	-1.048600	4.428700	-4.709600
C	-0.644400	5.756500	-4.910200
H	0.399400	5.980800	-5.124400
C	-1.604400	6.759600	-4.777900
N	0.973700	3.089400	-5.044900
N	1.178400	0.676100	-4.940400
N	2.013000	-1.538200	-5.489700
N	-0.278800	-1.726100	-4.722300
N	-2.517200	-2.648600	-4.521700
N	-2.610500	-0.258000	-4.131000
N	-3.556400	1.979000	-4.076900
N	-1.153300	2.144300	-4.349100
O	6.215700	3.289900	-6.808500
O	6.769000	0.791700	-7.036600
O	2.003100	-7.008200	-6.331000
O	-0.439800	-7.597900	-5.798400
O	-8.013000	-2.797600	-3.886700
O	-3.800300	7.500500	-4.364200
O	-1.353100	8.089300	-4.877300
C	-1.754200	-8.015800	-5.472700
H	-1.990800	-7.812700	-4.414000
H	-2.503600	-7.527100	-6.119000
H	-1.777500	-9.099000	-5.647100
C	-7.797400	-4.182600	-4.056900
H	-8.782400	-4.658700	-3.967900
H	-7.371300	-4.406300	-5.050400
H	-7.124000	-4.588900	-3.280900
C	3.348000	-6.758300	-6.680600
H	3.420700	-6.086700	-7.553700

H	3.911700	-6.313000	-5.841000
H	3.784500	-7.733000	-6.934000
C	7.172400	-0.562900	-7.139800
H	6.546000	-1.115400	-7.861400
H	8.208000	-0.541700	-7.502100
H	7.140100	-1.068800	-6.159400
C	5.975200	4.679900	-6.749400
H	5.169900	4.980600	-7.442100
H	5.705900	5.004300	-5.728100
H	6.912800	5.165700	-7.048900
C	-0.017600	8.502900	-5.109500
H	0.374100	8.086800	-6.053800
H	-0.050000	9.597400	-5.182600
H	0.644600	8.213500	-4.275400
C	-5.170300	7.255600	-4.125800
H	-5.622100	6.661000	-4.938800
H	-5.329800	6.728400	-3.168000
H	-5.654100	8.239900	-4.082900
O	-8.563700	-0.294100	-3.654400
C	-8.956400	1.069200	-3.516000
H	-8.502400	1.496800	-2.603400
H	-8.595500	1.651500	-4.384300
C	-10.474600	1.115400	-3.439800
H	-10.888300	0.658400	-4.354900
H	-10.805500	0.484900	-2.597100
C	-11.012100	2.539900	-3.268400
H	-10.577900	2.985200	-2.355100
H	-10.663900	3.166400	-4.109500
C	-12.538600	2.599600	-3.189200
H	-12.915900	2.011600	-2.336200
H	-12.893400	3.635000	-3.065900
H	-13.001100	2.192600	-4.103500
Cd	0.314000	0.000100	0.045300
C	1.343900	2.835000	1.649200
C	2.460000	3.746500	1.453200
C	2.562900	5.141600	1.541900
H	1.683200	5.739400	1.775200
C	3.812800	5.716200	1.321000
C	3.119400	1.569800	1.184100
C	3.575900	2.949300	1.154600
C	4.838100	3.513800	0.922200
H	5.690300	2.871700	0.704400
C	4.953900	4.899700	1.005600
C	3.512900	-0.726100	0.999100
C	4.395500	-1.857500	0.762300
C	5.769500	-1.940400	0.497800
H	6.364300	-1.032200	0.413700
C	6.326900	-3.208500	0.348400
C	2.257300	-2.558200	1.189600
C	3.602700	-3.010000	0.876700
C	4.148100	-4.292300	0.721200
H	3.513300	-5.170900	0.827000
C	5.512500	-4.388900	0.456200
C	0.013100	-2.982700	1.683100
C	-1.097300	-3.895400	1.904400
C	-1.179600	-5.294700	1.907300
H	-0.296400	-5.893200	1.689600
C	-2.415000	-5.872200	2.192600
C	-1.765900	-1.716800	2.132600
C	-2.218000	-3.097200	2.181600
C	-3.469300	-3.663900	2.462700
H	-4.320200	-3.022100	2.686400
C	-3.565300	-5.053800	2.467100
C	-2.155900	0.578400	2.333200
C	-3.032800	1.708600	2.595300
C	-4.386200	1.787400	2.951500
H	-4.977500	0.878400	3.051200
C	-4.929200	3.052600	3.165100
C	-0.903800	2.411200	2.127100
C	-2.244900	2.862200	2.459500
C	-2.779300	4.142200	2.663700
H	-2.143200	5.020500	2.563800
C	-4.124000	4.234800	3.016500
N	0.114100	3.241600	1.941200
N	1.770000	1.526600	1.499900
N	3.921500	0.536700	0.961700
N	2.232300	-1.174500	1.272700
N	1.241600	-3.389000	1.385200
N	-0.410400	-1.674900	1.844100
N	-2.565900	-0.684100	2.364800
N	-0.872700	1.026200	2.071300
O	4.075000	7.047800	1.379200
O	6.105100	5.593700	0.809100
O	7.639500	-3.453800	0.098500
O	6.186700	-5.555400	0.282100
O	-2.653100	-7.208700	2.241600
O	-4.703500	-5.750500	2.722000
O	-6.217700	3.292900	3.522300
O	-4.785100	5.398700	3.249000
C	-4.045600	6.608900	3.227200
H	-3.567700	6.770800	2.244800
H	-4.774000	7.409200	3.411100
H	-3.280100	6.625100	4.019200
C	-7.104800	2.192500	3.623300
H	-6.754100	1.459400	4.370800
H	-8.065700	2.610300	3.950800
H	-7.239500	1.695000	2.649000
C	-5.863200	-5.028800	3.103900
H	-6.165600	-4.309500	2.323400
H	-6.654800	-5.778300	3.232300
H	-5.708200	-4.498000	4.057700
C	-1.595300	-8.093500	1.915200
H	-0.730400	-7.952800	2.586900
H	-1.997400	-9.105800	2.051700
H	-1.276900	-7.968600	0.867400
C	5.485400	-6.773400	0.473500
H	4.630600	-6.858800	-0.220500
H	6.206800	-7.572300	0.258400
H	5.131500	-6.873100	1.512000
C	8.506100	-2.349200	-0.094100
H	8.522700	-1.690700	0.791900
H	9.506400	-2.775000	-0.246200
H	8.221200	-1.766600	-0.985400
C	7.302600	4.864400	0.594800
H	7.228500	4.221500	-0.299100
H	8.087600	5.615200	0.437200
H	7.559600	4.250000	1.473400
C	2.996600	7.936800	1.614000
H	2.499000	7.721500	2.575800
H	3.438100	8.941100	1.652900
H	2.258700	7.897000	0.796300
C	-0.549000	3.002800	-1.323700
C	0.125200	4.286300	-1.427000
C	-0.337700	5.601800	-1.288600
H	-1.383300	5.789000	-1.048000
C	0.572800	6.635500	-1.493300
C	1.576700	2.563100	-1.830000
C	1.462200	4.010300	-1.751600
C	2.389600	5.040200	-1.961300
H	3.422400	4.802500	-2.212600
C	1.941300	6.354400	-1.835400
C	2.816700	0.614900	-2.189500
C	4.060900	-0.064400	-2.510500
C	5.343700	0.418200	-2.802600
H	5.536200	1.490200	-2.800100
C	6.332000	-0.512000	-3.114500
C	2.363800	-1.567600	-2.195400
C	3.775000	-1.438200	-2.520200
C	4.759200	-2.386000	-2.833000
H	4.514600	-3.447400	-2.834600
C	6.038300	-1.919900	-3.134200
C	0.450700	-2.855300	-1.815800
C	-0.227900	-4.137900	-1.732000
C	0.224000	-5.451100	-1.919200
H	1.268300	-5.638100	-2.165600
C	-0.706500	-6.480700	-1.804100
C	-1.678500	-2.414900	-1.325100
C	-1.569700	-3.860900	-1.428900
C	-2.517700	-4.886600	-1.310800
H	-3.554000	-4.648200	-1.075100
C	-2.084200	-6.197800	-1.502900
C	-2.915000	-0.467400	-0.950000
C	-4.163500	0.212900	-0.648500
C	-5.457300	-0.267500	-0.405200
H	-5.651200	-1.339200	-0.413500
C	-6.465800	0.666800	-0.183000
C	-2.465600	1.715800	-0.959700
C	-3.882500	1.587600	-0.660300
C	-4.887300	2.539600	-0.439100
H	-4.646100	3.601700	-0.453100
C	-6.181300	2.076500	-0.204200
N	-1.840100	2.883500	-1.044000
N	0.346000	1.978100	-1.586100
N	2.711700	1.934800	-2.110800
N	1.803200	-0.314300	-2.018300
N	1.739600	-2.735500	-2.105300
N	-0.450400	-1.829300	-1.580700
N	-2.812200	-1.786900	-1.038500
N	-1.907600	0.463100	-1.148500
O	0.277900	7.958100	-1.397500
O	2.712700	7.456400	-2.015100
O	7.618900	-0.202300	-3.420500
O	7.092300	-2.708700	-3.463600
O	-0.424800	-7.800700	-1.958400
O	-2.879800	-7.294800	-1.430500
O	-7.259400	2.870300	0.018000
C	-7.062400	4.272400	0.085900
H	-6.631500	4.664600	-0.852800
H	-8.057900	4.709500	0.237400
H	-6.413300	4.545400	0.935300
C	-4.239100	-7.119900	-1.068700
H	-4.763300	-6.456900	-1.780300
H	-4.691700	-8.119400	-1.104800
H	-4.333000	-6.715900	-0.046200
C	0.885100	-8.167900	-2.358000
H	1.640600	-7.822200	-1.629700
H	0.892800	-9.264400	-2.394300
H	1.125000	-7.770000	-3.358200
C	6.915900	-4.115000	-3.439900
H	6.117700	-4.432700	-4.134700
H	7.872000	-4.544200	-3.766800
H	6.686700	-4.473200	-2.421800
C	7.975700	1.165900	-3.526500
H	7.794800	1.704400	-2.578900
H	9.049300	1.180700	-3.751900
H	7.426400	1.660700	-4.344900
C	4.092600	7.277200	-2.285300
H	4.249500	6.688700	-3.207200
H	4.505700	8.284700	-2.424600
H	4.606400	6.788100	-1.440300
C	-1.069800	8.333000	-1.165600
H	-1.721600	8.018700	-1.997800
H	-1.448300	7.910800	-0.217400
H	-1.070900	9.428200	-1.100000
O	-7.763800	0.351800	0.064200
C	-8.156600	-1.016600	-0.036800
H	-7.582800	-1.625400	0.687400
H	-7.932200	-1.387900	-1.051600
C	-9.647300	-1.108000	0.246200
H	-9.843200	-0.771600	1.279200
H	-10.170900	-0.402700	-0.420200
C	-10.191400	-2.524600	0.032900
H	-9.988000	-2.831600	-1.008300
H	-9.638300	-3.232500	0.677300
C	-11.689300	-2.642200	0.319300
H	-12.049500	-3.669500	0.151900
H	-11.919600	-2.371500	1.363100
H	-12.272000	-1.972400	-0.334200

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[4]$^{+1}$ with butoxy

Y	1.244500	0.165200	3.253000
C	4.526800	0.465600	3.884800
C	5.755700	-0.325200	3.872200
C	7.108100	0.025000	3.756500
H	7.392700	1.070900	3.647600
C	8.056500	-1.000100	3.781100
C	3.908000	-1.650800	4.163000

C	5.363100	-1.659500	4.044600	H	-3.527600	5.443900	7.876000	H	-7.066200	5.015500	-3.300800
C	6.301500	-2.698700	4.095600	H	-4.312200	5.523000	6.258500	H	-7.791400	6.257700	-4.377200
H	5.970300	-3.726600	4.235800	C	-5.915100	0.093200	8.112800	C	-6.748000	-6.186100	-3.816600
C	7.649700	-2.371000	3.941600	H	-6.064800	-0.506400	7.195900	H	-6.247800	-6.296200	-4.794700
C	1.921000	-2.737800	4.794900	H	-5.197400	-0.428100	8.769200	H	-6.028100	-6.422100	-3.013000
C	1.241300	-3.907200	5.348300	H	-6.874400	0.202700	8.635000	H	-7.595900	-6.880100	-3.761200
C	1.659700	-5.223900	5.585400	Y	-0.603100	-0.164800	-3.198500	C	-0.190500	-8.438900	-5.698100
H	2.676100	-5.525900	5.335800	C	-2.899400	-2.467300	-4.004100	H	-1.026100	-8.063900	-6.313200
C	0.738500	-6.116300	6.138500	C	-4.330600	-2.728500	-3.877600	H	0.010100	-9.487100	-5.953900
C	-0.126700	-2.067600	5.339800	C	-5.069500	-3.918600	-3.871800	H	-0.470600	-8.371200	-4.630900
C	-0.050600	-3.483300	5.688300	H	-4.560200	-4.877200	-3.961300	C	4.438900	-6.021900	-7.028800
C	-0.980600	-4.357700	6.266000	C	-6.454800	-3.827100	-3.728600	H	4.274700	-5.313300	-7.858500
H	-1.976300	-4.001500	6.525600	C	-3.883900	-0.483200	-3.829900	H	4.968500	-5.504500	-6.209200
C	-0.592600	-5.682900	6.471500	C	-4.952500	-1.477700	-3.771900	H	5.049100	-6.861700	-7.383500
C	-1.199600	0.014500	5.547900	C	-6.346400	-1.366900	-3.667900	O	-8.444200	-2.596800	-3.518300
C	-2.270600	0.833400	6.111600	H	-6.812700	-0.383500	-3.610600	C	-9.179400	-1.378800	-3.475400
C	-3.470200	0.510500	6.761200	C	-7.097600	-2.544300	-3.636200	H	-8.972400	-0.785000	-4.385300
H	-3.741000	-0.532900	6.918100	C	-3.191800	1.744000	-4.135700	H	-8.855900	-0.777500	-2.603700
C	-4.289900	1.558600	7.186000	C	-3.527100	3.139000	-4.407900	C	-10.656400	-1.726300	-3.376000
C	-0.584700	2.130100	5.256200	C	-4.740600	3.837500	-4.362700	H	-10.926400	-2.353700	-4.242100
C	-1.882500	2.166900	5.923900	H	-5.654700	3.324200	-4.067400	H	-10.810600	-2.349200	-2.478200
C	-2.680100	3.231300	6.364500	C	-4.725500	5.195300	-4.685400	C	-11.555800	-0.487000	-3.320900
H	-2.352700	4.258500	6.210900	C	-1.296800	2.736900	-4.735500	H	-11.265500	0.139600	-2.457600
C	-3.896900	2.927100	6.977400	C	-2.333500	3.764800	-4.790100	H	-11.381300	0.132500	-4.218900
C	1.406200	3.217900	4.637700	C	-2.308700	5.118200	-5.155900	C	-13.043200	-0.830800	-3.221600
C	2.243800	4.415400	4.635500	H	-1.374100	5.580400	-5.473200	H	-13.661800	0.079200	-3.185300
C	1.978300	5.759500	4.932300	C	-3.505200	5.836700	-5.093700	H	-13.372000	-1.426100	-4.088800
H	0.975600	6.063900	5.229900	C	0.858300	1.988500	-5.308100	H	-13.256300	-1.419500	-2.314200
C	3.028100	6.674900	4.828500	C	2.132800	2.221600	-5.981900	Cd	0.320800	0.000200	0.027700
C	3.450000	2.546900	4.079400	C	2.730900	3.386700	-6.479400	C	-0.651500	-2.477700	2.169000
C	3.531200	3.990700	4.280200	H	2.225400	4.345900	-6.376400	C	-1.948600	-2.995100	2.575300
C	4.602000	4.890300	4.194100	C	3.984800	3.271700	-7.081500	C	-2.398300	-4.300100	2.817700
H	5.593900	4.533400	3.921000	C	1.839500	0.003800	-5.493900	H	-1.721600	-5.144200	2.694200
C	4.345500	6.238900	4.447500	C	2.750200	0.970100	-6.103000	C	-3.722600	-4.466400	3.222100
N	4.525900	1.795200	3.870200	C	3.991300	0.832000	-6.740900	C	-1.981100	-0.710300	2.450000
N	3.438700	-0.367600	3.993300	H	4.443900	-0.153800	-6.846100	C	-2.788400	-1.883500	2.739200
N	3.212500	-2.738500	4.478200	C	4.613800	1.986500	-7.221900	C	-4.126800	-2.035300	3.131300
N	1.050800	-1.674800	4.744000	C	1.150700	-2.222800	-5.176500	H	-4.763200	-1.159900	3.246900
N	-1.170700	-1.310200	5.660400	C	1.329300	-3.645800	-5.451600	C	-4.593300	-3.328900	3.365400
N	-0.241300	0.824500	4.986200	C	2.402000	-4.369500	-5.988400	C	-1.705200	1.604600	2.262000
N	0.142800	3.223600	5.052400	H	3.319900	-3.855500	-6.270300	C	-2.219700	2.962100	2.348200
N	2.146600	2.131700	4.235500	C	2.255400	-5.750800	-6.124700	C	-3.472300	3.462700	2.728200
O	9.392700	-0.820000	3.662100	C	-0.747500	-3.216300	-4.588300	H	-4.269600	2.780300	3.018500
O	8.663000	-3.268300	3.924400	C	0.131300	-4.272400	-5.084800	C	-3.647500	4.846300	2.724300
O	0.989300	-7.419200	6.406200	C	-0.046400	-5.653100	-5.252800	C	-0.024500	2.958000	1.702000
O	-1.393400	-6.649800	6.977400	H	-0.994700	-6.117800	-4.983500	C	-1.165700	3.812600	1.983100
O	-5.482000	1.404300	7.808200	C	1.021400	-6.394600	-5.764400	C	-1.330400	5.205600	1.960000
O	-4.790200	3.845800	7.413300	N	-2.020100	-3.429700	-4.266000	H	-0.501300	5.847400	1.667900
O	2.921400	8.003500	5.064000	N	-2.665500	-1.114800	-3.901700	C	-2.575200	5.719400	2.323600
O	5.266100	7.227300	4.360300	N	-4.118600	0.824800	-3.882700	C	2.210000	2.641800	1.087700
C	-2.697600	-6.290000	7.398100	N	-1.835200	1.558800	-4.276300	C	3.511500	3.160000	0.696800
H	-2.665900	-5.521900	8.190200	N	-0.052300	2.945300	-5.155700	C	3.985900	4.469400	0.540800
H	-3.306600	-5.917200	6.555700	N	0.750400	0.658500	-4.970700	H	3.323600	5.316100	0.714200
H	-3.150900	-7.206600	7.797700	N	2.046200	-1.309200	-5.539000	C	5.319000	4.637300	0.167100
C	2.293100	-7.913500	6.171600	N	-0.080000	-2.015100	-4.596100	C	3.534600	0.873600	0.789400
H	3.046400	-7.365500	6.763100	O	-7.293100	-4.887400	-3.660300	C	4.340800	2.046500	0.496400
H	2.280500	-8.966300	6.482200	O	-5.806500	6.008300	-4.643400	C	5.679800	2.198400	0.106200
H	2.562300	-7.851800	5.101000	O	-3.633500	7.149800	-5.397000	H	6.304600	1.321000	-0.049700
C	8.355500	-4.633200	4.147900	O	4.703700	4.310600	-7.566500	C	6.164400	3.495300	-0.064500
H	7.878800	-4.781000	5.132400	O	5.817600	2.013400	-7.840900	C	3.263700	-1.440400	0.994700
H	7.692700	-5.033400	3.360500	O	3.217200	-6.585000	-6.583400	C	3.782600	-2.797200	0.923900
H	9.314100	-5.167900	4.123600	O	1.005600	-7.733500	-5.964200	C	5.060000	-3.293400	0.630300
C	9.885800	0.501700	3.566700	C	-2.496700	7.844700	-5.870600	H	5.871500	-2.608500	0.389900
H	9.609200	1.101800	4.450500	H	-1.693700	7.870400	-5.111500	C	5.243900	-4.675400	0.665000
H	10.978700	0.416200	3.511200	H	-2.102200	7.390900	-6.795600	C	1.578000	-2.794800	1.537400
H	9.512400	1.007900	2.657400	H	-2.830400	8.869100	-6.079500	C	2.718100	-3.649600	1.252500
C	6.605000	6.873700	4.060600	C	4.123400	5.603000	-7.533100	C	2.883400	-5.042500	1.277500
H	7.017200	6.184900	4.818200	H	4.853600	6.276000	-7.999500	H	2.042800	-5.686300	1.529300
H	6.687200	6.406800	3.063200	H	3.179400	5.633900	-8.104800	C	4.145800	-5.553100	0.975400
H	7.176000	7.811300	4.072000	H	3.930300	5.933200	-6.497000	N	0.387800	-3.259100	1.905100
C	1.677600	8.508500	5.507900	C	6.478300	0.786400	-8.079800	N	-0.691400	-1.092000	2.121000
H	1.365300	8.039300	6.456600	H	6.727200	0.270700	-7.134300	N	-2.444100	0.533700	2.522100
H	1.823800	9.585100	5.664000	H	5.867400	0.113800	-8.705700	N	-0.369200	1.630200	1.889500
H	0.885400	8.353300	4.752300	H	7.405700	1.037400	-8.610300	N	1.167400	3.422600	1.340100
C	-4.448100	5.216900	7.310800	C	-7.063500	5.438800	-4.320900	N	2.255900	1.257200	1.156800
H	-5.289000	5.772600	7.746100	H	-7.343100	4.651000	-5.041000	N	3.999300	-0.370200	0.723100

N	1.933800	-1.465000	1.388300
O	-4.302200	-5.655900	3.500000
O	-5.863400	-3.637500	3.725100
O	-4.789800	5.481700	3.069900
O	-2.894100	7.037000	2.328700
O	5.925600	5.831700	-0.016700
O	7.424100	3.802000	-0.460700
O	6.413200	-5.306000	0.413400
O	4.454800	-6.872500	0.935700
C	3.445800	-7.808600	1.261000
H	2.591000	-7.740600	0.564000
H	3.908200	-8.799200	1.174100
H	3.079500	-7.661700	2.292600
C	7.542300	-4.525900	0.036600
H	7.810500	-3.803300	0.825800
H	8.364200	-5.240500	-0.095600
H	7.363000	-4.000500	-0.914800
C	8.335800	2.743100	-0.679100
H	7.988500	2.069800	-1.483600
H	9.281300	3.210800	-0.979000
H	8.492200	2.151800	0.240500
C	5.154400	7.018800	0.129900
H	4.737800	7.101800	1.147900
H	5.852000	7.847500	-0.044600
H	4.345600	7.062200	-0.616500
C	-1.891200	7.972000	1.982200
H	-1.531900	7.815500	0.949000
H	-2.356300	8.962100	2.059600
H	-1.031500	7.913300	2.673200
C	-5.926100	4.700300	3.421800
H	-5.717400	4.062900	4.297600
H	-6.712800	5.421300	3.676900
H	-6.262100	4.082900	2.573700
C	-6.781200	-2.579700	3.922400
H	-6.929400	-1.994900	2.996600
H	-7.729400	-3.047900	4.212700
H	-6.444200	-1.900200	4.725300
C	-3.538200	-6.844300	3.328500
H	-2.644800	-6.842200	3.975400
H	-4.200100	-7.666700	3.627800
H	-3.244700	-6.979800	2.275500
C	-0.412000	-3.046600	-1.334300
C	-1.383400	-4.074700	-1.000400
C	-1.298800	-5.473800	-0.953100
H	-0.354900	-5.969900	-1.176100
C	-2.451100	-6.184700	-0.620000
C	-2.315500	-1.987500	-0.852700
C	-2.585000	-3.409700	-0.711100
C	-3.754100	-4.110200	-0.386300
H	-4.676100	-3.569500	-0.177000
C	-3.688800	-5.502200	-0.349500
C	-2.994000	0.247900	-0.763400
C	-3.996700	1.272500	-0.525500
C	-5.342400	1.204400	-0.136700
H	-5.802000	0.237700	0.066300
C	-6.050200	2.400800	-0.028500
C	-2.003200	2.207600	-1.156800
C	-3.377900	2.504900	-0.786600
C	-4.078600	3.714600	-0.693700
H	-3.576800	4.656200	-0.912600
C	-5.421100	3.661300	-0.322100
C	0.141300	2.884000	-1.796200
C	1.114300	3.912400	-2.124300
C	1.029800	5.311500	-2.171700
H	0.097400	5.809600	-1.908300
C	2.164500	6.019300	-2.566100
C	2.039900	1.824000	-2.295000
C	2.305000	3.245400	-2.452000
C	3.449800	3.941700	-2.861300
H	4.357600	3.398400	-3.120500
C	3.376300	5.332100	-2.927000
C	2.723300	-0.410500	-2.367100
C	3.727600	-1.434800	-2.599200
C	5.073300	-1.366700	-2.988100
H	5.544500	-0.398000	-3.150700
C	5.763600	-2.566200	-3.157700
C	1.727500	-2.371000	-1.991000
C	3.097800	-2.669200	-2.376500
C	3.774300	-3.883100	-2.554000
H	3.258300	-4.827300	-2.385000
C	5.108500	-3.831300	-2.954300
N	0.842700	-3.309300	-1.684400
N	-1.000700	-1.794700	-1.250600
N	-3.230100	-1.053400	-0.633400
N	-1.801500	0.835100	-1.155800
N	-1.115600	3.146300	-1.453800
N	0.719000	1.630100	-1.918300
N	2.957200	0.890400	-2.504800
N	1.519800	-0.999700	-2.013100
O	-2.520300	-7.534800	-0.510300
O	-4.728800	-6.317400	-0.059900
O	-6.231200	4.737200	-0.195100
O	2.244600	7.371300	-2.637400
O	4.389900	6.142600	-3.308700
O	7.070800	-2.661800	-3.506300
O	5.892300	-4.912000	-3.173500
C	5.351900	-6.206700	-2.939000
H	4.475200	-6.396100	-3.581200
H	6.150900	-6.912700	-3.198300
H	5.081800	-6.338200	-1.879100
C	7.786600	-1.468300	-3.759900
H	7.823500	-0.820500	-2.866300
H	8.804900	-1.774700	-4.029600
H	7.339000	-0.901100	-4.596000
C	5.648300	5.559900	-3.625700
H	5.560100	4.852000	-4.467200
H	6.295800	6.395200	-3.920600
H	6.084200	5.055000	-2.748900
C	1.089400	8.129000	-2.332900
H	0.758900	7.962800	-1.292400
H	1.372100	9.181200	-2.461400
H	0.257100	7.885000	-3.016200
C	-5.683700	6.033200	-0.404700
H	-5.283800	6.137400	-1.427500
H	-6.517900	6.733000	-0.268200
H	-4.898200	6.256700	0.334800
C	-5.980000	-5.733400	0.282100
H	-6.368700	-5.110700	-0.541400
H	-6.662800	-6.575000	0.454000
H	-5.900600	-5.136500	1.204700
C	-1.358500	-8.291300	-0.791900
H	-1.019500	-8.135400	-1.831100
H	-0.533000	-8.036700	-0.104000
H	-1.637800	-9.342900	-0.651800
O	-7.346300	2.496800	0.354800
C	-8.073100	1.300800	0.620800
H	-7.590800	0.746800	1.448800
H	-8.053100	0.648800	-0.272600
C	-9.499500	1.684800	0.980800
H	-9.926800	2.265300	0.145500
H	-9.474500	2.361900	1.851600
C	-10.381200	0.468700	1.284400
H	-9.935500	-0.109200	2.114500
H	-10.386000	-0.208200	0.410800
C	-11.819800	0.846200	1.642300
H	-12.425400	-0.048000	1.856400
H	-11.851700	1.495300	2.532500
H	-12.305000	1.390700	0.816000

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[4]$^{+2}$ with butoxy

Y	-1.331700	0.218600	3.202500
C	-4.071300	-1.512100	4.050300
C	-5.524700	-1.480800	3.898500
C	-6.491700	-2.490800	3.954500
H	-6.194400	-3.525600	4.119800
C	-7.830200	-2.124400	3.780500
C	-4.621200	0.615500	3.735300
C	-5.873100	-0.138300	3.704300
C	-7.211400	0.252600	3.567600
H	-7.465100	1.305700	3.445500
C	-8.192300	-0.744300	3.595200
C	-3.492400	2.668300	3.945400
C	-3.542200	4.115600	4.141900
C	-4.591000	5.037400	4.038900
H	-5.585700	4.704700	3.745400
C	-4.310300	6.379900	4.311800
C	-1.449900	3.285800	4.557800
C	-2.256200	4.506000	4.532400
C	-1.965100	5.839600	4.848200
H	-0.965500	6.120400	5.177300
C	-2.992800	6.781800	4.727400
C	0.490300	2.149400	5.246000
C	1.764100	2.157600	5.961600
C	2.562700	3.203000	6.436400
H	2.266300	4.237900	6.271400
C	3.741900	2.871700	7.110400
C	1.035600	0.022300	5.572100
C	2.107500	0.816200	6.171900
C	3.264500	0.463300	6.879400
H	3.501100	-0.584700	7.057700
C	4.090800	1.494900	7.340700
C	-0.088400	-2.031100	5.349900
C	-0.217200	-3.439500	5.718600
C	0.661700	-4.324300	6.351900
H	1.656500	-3.991600	6.645400
C	0.223000	-5.632400	6.579400
C	-2.135700	-2.648000	4.749600
C	-1.509300	-3.829000	5.343900
C	-1.981800	-5.123700	5.598700
H	-2.999400	-5.399600	5.325600
C	-1.109000	-6.031100	6.209500
N	-3.417500	-2.616700	4.394700
N	-3.559400	-0.245100	3.878300
N	-4.583100	1.946200	3.710100
N	-2.205300	2.218200	4.138300
N	-0.199600	3.261300	5.011600
N	0.120400	0.851800	4.971000
N	0.966700	-1.300400	5.696300
N	-1.233700	-1.611500	4.711000
O	-8.866500	-2.987200	3.769800
O	-9.516700	-0.526800	3.463200
O	-5.204600	7.384600	4.217500
O	-2.864200	8.099900	4.979900
O	4.630400	3.766700	7.589300
O	5.240800	1.314900	8.021400
O	0.968200	-6.605100	7.142500
O	-1.411500	-7.311900	6.503700
C	-1.627900	8.581800	5.477800
H	-1.362000	8.093000	6.430600
H	-0.812800	8.424800	4.748700
H	-1.765700	9.656300	5.643400
C	-6.556100	7.068800	3.922000
H	-6.980200	6.389100	4.681100
H	-7.100000	8.020400	3.939500
H	-6.654800	6.607500	2.924200
C	-9.982300	0.807900	3.361700
H	-9.694300	1.400600	4.246600
H	-9.593100	1.300800	2.452800
H	-11.075000	0.744500	3.302600
C	-8.618000	-4.354900	4.055800
H	-8.164700	-4.476100	5.054700
H	-9.595600	-4.850900	4.035500
H	-7.957900	-4.812300	3.298000
C	-2.727800	-7.775700	6.256800
H	-3.472500	-7.183500	6.813500
H	-2.969200	-7.743300	5.178900
H	-2.752800	-8.816100	6.603900
C	2.255400	-6.275400	7.640700
H	2.193200	-5.489800	8.413700
H	2.652300	-7.195400	8.085300
H	2.927700	-5.938800	6.831400
C	5.626800	-0.002700	8.373000
H	6.556100	0.096700	8.945600
H	4.859500	-0.491000	8.998500
H	5.812000	-0.620100	7.476200
C	4.317200	5.148300	7.506800
H	4.230800	5.481000	6.457600

H	3.377600	5.375400	8.040100	H	7.084100	5.165000	-3.439300	O	4.137300	-5.659300	3.679400
H	5.147600	5.675900	7.990200	H	8.703800	5.242800	-4.211500	O	-4.592900	-6.803900	0.994900
Y	0.687800	-0.218300	-3.155200	C	1.626200	7.794600	-6.258500	O	-6.475000	-5.230100	0.279500
C	3.321600	1.656700	-4.052800	H	2.402200	7.249900	-6.821100	O	-7.390200	3.884000	-0.630300
C	4.775300	1.710700	-3.908800	H	1.592900	8.838300	-6.595900	O	-5.844400	5.889500	-0.285400
C	5.698400	2.760600	-4.002600	H	1.866300	7.764000	-5.181100	C	-5.067000	7.063900	-0.103900
H	5.356200	3.774600	-4.212200	C	-3.221300	5.997500	-7.767100	H	-4.188100	7.068400	-0.770100
C	7.053000	2.461900	-3.821800	H	-3.114300	5.191400	-8.512900	H	-5.724500	7.902900	-0.359700
C	3.987600	-0.429500	-3.690100	H	-3.892700	5.657900	-6.958400	H	-4.732900	7.163900	0.943000
C	5.193600	0.394300	-3.675300	H	-3.649000	6.885200	-8.247700	C	-8.321900	2.846400	-0.900700
C	6.545800	0.070600	-3.516700	O	8.806100	0.959900	-3.396800	H	-8.474400	2.205900	-0.014800
H	6.844700	-0.963600	-3.349900	C	9.349100	-0.357100	-3.269900	H	-9.263700	3.348300	-1.153500
C	7.477700	1.110300	-3.568000	H	9.061800	-0.958000	-4.152000	H	-7.995900	2.234300	-1.757400
C	2.990700	-2.552800	-3.867100	H	8.927200	-0.848700	-2.373300	C	-7.584800	-4.435000	-0.110800
C	3.123000	-3.999200	-4.039500	C	10.860000	-0.230300	-3.162200	H	-7.361300	-3.859300	-1.025500
C	4.218900	-4.867800	-3.946200	H	11.233000	0.291100	-4.059600	H	-8.402400	-5.137000	-0.312200
H	5.204900	-4.481100	-3.690700	H	11.097800	0.418500	-2.301700	H	-7.883000	-3.742100	0.693400
C	3.999500	-6.227500	-4.192100	C	11.558300	-1.585900	-3.008200	C	-3.610100	-7.774600	1.326400
C	0.981100	-3.295300	-4.447800	H	11.160800	-2.104000	-2.116300	H	-3.198600	-7.596500	2.335700
C	1.853000	-4.465900	-4.401900	H	11.306500	-2.227400	-3.871700	H	-4.127800	-8.741600	1.311000
C	1.618700	-5.817800	-4.675200	C	13.078600	-1.463600	-2.891400	H	-2.796500	-7.785800	0.583700
H	0.624400	-6.153400	-4.968400	H	13.550400	-2.452200	-2.783800	C	3.350600	-6.831600	3.527300
C	2.691400	-6.706300	-4.550000	H	13.508800	-0.981300	-3.783900	H	3.014800	-6.954300	2.482600
C	-1.024800	-2.294200	-5.160300	H	13.363700	-0.858000	-2.015500	H	4.002000	-7.669400	3.802200
C	-2.299000	-2.387300	-5.872300	Cd	-0.322100	0.000200	0.024100	H	2.472500	-6.813200	4.194300
C	-3.039800	-3.476800	-6.347800	C	-0.000300	2.980400	1.678800	C	6.636600	-2.620800	4.226300
H	-2.680900	-4.493900	-6.194600	C	1.138200	3.831000	1.992000	H	6.277000	-1.869300	4.950200
C	-4.239900	-3.211800	-7.017700	C	1.309200	5.223700	1.989100	H	7.531900	-3.112800	4.625500
C	-1.694700	-0.207100	-5.510600	H	0.491900	5.877300	1.687700	H	6.886400	-2.133800	3.269200
C	-2.721500	-1.070400	-6.088300	C	2.551900	5.728500	2.376900	C	5.868100	4.667300	3.535300
C	-3.905400	-0.783000	-6.776600	C	1.654900	1.616900	2.292900	H	6.187900	3.973400	2.738000
H	-4.204200	0.251300	-6.943400	C	2.179300	2.969900	2.374500	H	6.679700	5.371500	3.754600
C	-4.679500	-1.857000	-7.224800	C	3.431600	3.458400	2.764500	H	5.622500	4.092700	4.443900
C	-0.694200	1.915300	-5.345000	H	4.217900	2.766500	3.063800	C	1.925100	8.000100	1.998200
C	-0.645600	3.321900	-5.741200	C	3.616800	4.840400	2.768800	H	1.002400	7.932300	2.600100
C	-1.560600	4.151600	-6.403200	C	1.898800	-0.696400	2.536000	H	2.395600	8.977200	2.162000
H	-2.528800	3.761200	-6.714800	C	2.684300	-1.873200	2.876600	H	1.687000	7.886200	0.928200
C	-1.186800	5.477700	-6.646300	C	3.998000	-2.032600	3.343000	C	-0.021200	2.855000	-1.830400
C	1.311800	2.658700	-4.752900	H	4.638600	-1.164100	3.489400	C	0.761600	4.068400	-1.672900
C	0.619200	3.790700	-5.362800	C	4.444700	-3.329900	3.602100	C	0.441800	5.413200	-1.892800
C	1.021300	5.106500	-5.617200	C	0.563400	-2.456500	2.227600	H	-0.555900	5.689600	-2.231000
H	2.015100	5.440900	-5.325200	C	1.842500	-2.978300	2.677200	C	1.443100	6.361400	-1.680300
C	0.107800	5.959900	-6.242500	C	2.274300	-4.286500	2.930200	C	2.005600	2.221800	-1.149100
N	2.595300	2.713400	-4.410600	H	1.595900	-5.124600	2.775000	C	2.039600	3.673600	-1.248000
N	2.879900	0.371400	-3.850900	C	3.576800	-4.461500	3.396200	C	3.056400	4.614500	-1.028000
N	4.034900	-1.757300	-3.645200	C	-1.654200	-2.761400	1.549700	H	4.042400	4.290900	-0.695600
N	1.682300	-2.177100	-4.055300	C	-2.798400	-3.610800	1.254500	C	2.757100	5.960900	-1.242500
N	-0.267000	-3.357600	-4.901300	C	-2.991800	-4.998700	1.327900	C	3.018100	0.165200	-0.680300
N	-0.727900	-0.977400	-4.903500	H	-2.176300	-5.652000	1.635000	C	4.163900	-0.627300	-0.269200
N	-1.705700	1.113300	-5.666500	C	-4.250200	-5.500100	0.989500	C	5.464900	-0.259300	0.092900
N	0.468800	1.571000	-4.699400	C	-3.306400	-1.398600	0.926100	H	5.750300	0.791600	0.109700
O	8.054400	3.363900	-3.867900	C	-3.834300	-2.750400	0.859100	C	6.363700	-1.277200	0.409300
O	4.948000	-7.184300	-4.127000	C	-5.102600	-3.235000	0.515300	C	2.372900	-1.968500	-0.743800
O	2.610100	-8.039100	-4.742400	H	-5.889900	-2.543800	0.219800	C	3.762700	-1.971500	-0.311200
O	-5.067800	-4.151000	-7.517400	C	-5.310900	-4.613000	0.584300	C	4.654000	-3.007300	0.005100
O	-5.859800	-1.738500	-7.866800	C	-3.553500	0.915400	0.693500	H	4.325500	-4.045700	-0.031500
O	-1.960800	6.397400	-7.257000	C	-4.344800	2.093400	0.370900	C	5.956500	-2.659600	0.367000
O	0.336900	7.260400	-6.518300	C	-5.680600	2.257600	-0.026100	C	0.384500	-3.072700	-1.293000
C	1.386700	-8.587100	-5.206400	H	-6.322700	1.389400	-0.167700	C	-0.394100	-4.287000	-1.463900
H	0.572000	-8.431900	-4.477000	C	-6.143300	3.558300	-0.234800	C	-0.060400	-5.635200	-1.290900
H	1.096000	-8.148500	-6.176300	C	-2.214900	2.674800	0.991400	H	0.938500	-5.911800	-0.956500
H	1.565700	-9.662400	-5.330400	C	-3.498400	3.198500	0.555000	C	-1.037800	-6.588100	-1.575300
C	-4.681300	-5.512400	-7.438100	C	-3.944200	4.509200	0.349900	C	-1.640000	-2.440400	-1.985100
H	-5.475400	-6.081900	-7.934500	H	-3.267900	5.347300	0.508700	C	-1.667300	-3.893200	-1.903900
H	-3.722800	-5.687800	-7.957400	C	-5.270600	4.688900	-0.044100	C	-2.662300	-4.838700	-2.192400
H	-4.591700	-5.844600	-6.389000	N	-1.176400	3.449700	1.269600	H	-3.646500	-4.515500	-2.530500
C	-6.318300	-0.440900	-8.214800	N	0.329400	1.649900	1.883000	C	-2.347300	-6.188600	-2.027300
H	-6.505100	0.175100	-7.318400	N	2.373200	0.545400	2.596600	C	-2.654600	-0.382900	-2.444100
H	-5.594100	0.074400	-8.867400	N	0.617600	-1.070200	2.162600	C	-3.796200	0.408700	-2.868500
H	-7.258600	-0.590000	-8.758000	N	-0.475900	-3.231200	1.952200	C	-5.082400	0.036600	-3.276100
C	6.286800	-6.801600	-3.866400	N	-1.987500	-1.429700	1.360100	H	-5.366900	-1.014500	-3.295800
H	6.658900	-6.098900	-4.631000	N	-4.025300	-0.327000	0.624300	C	-5.958400	1.050500	-3.665000
H	6.384500	-6.337300	-2.868000	N	-2.276800	1.291100	1.080000	C	-2.006000	1.750100	-2.391100
H	6.877600	-7.725300	-3.898200	O	2.881000	7.035200	2.414300	C	-3.390600	1.752000	-2.839800
C	7.746800	4.708300	-4.195400	O	4.767900	5.460400	3.114500	C	-4.259900	2.783100	-3.225500
H	7.269200	4.779400	-5.188000	O	5.678300	-3.652700	4.039500	H	-3.929600	3.821000	-3.194700

C	-5.546700	2.431900	-3.636900
N	-1.284500	2.856800	-2.234200
N	0.758200	1.748000	-1.520600
N	3.046700	1.488500	-0.763800
N	1.948900	-0.670500	-0.975700
N	1.649000	-3.074700	-0.893000
N	-0.386800	-1.967400	-1.628500
N	-2.682200	-1.706400	-2.363500
N	-1.577500	0.451000	-2.173400
O	1.286700	7.694400	-1.843200
O	3.614700	6.985200	-1.064100
O	6.925900	-3.531500	0.711700
O	-0.868700	-7.923800	-1.452300
O	-3.192500	-7.216000	-2.247900
O	-7.230700	0.851200	-4.076800
O	-6.502600	3.300000	-4.023300
C	-6.225300	4.693300	-3.985100
H	-5.356100	4.943900	-4.616600
H	-7.120700	5.186200	-4.384500
H	-6.052900	5.033900	-2.952600
C	-7.719100	-0.479100	-4.156900
H	-7.696800	-0.973300	-3.169600
H	-8.756800	-0.399700	-4.502800
H	-7.135600	-1.077200	-4.876900
C	-4.527400	-6.937600	-2.645000
H	-4.551700	-6.357200	-3.583100
H	-4.999100	-7.914900	-2.808100
H	-5.072300	-6.399600	-1.852900
C	0.395700	-8.413400	-1.032700
H	0.658100	-8.035300	-0.029800
H	0.300700	-9.505600	-0.998700
H	1.189100	-8.135100	-1.746900
C	6.621800	-4.918100	0.757100
H	6.263700	-5.280000	-0.221600
H	7.562900	-5.421300	1.009700
H	5.873500	-5.134900	1.536200
C	4.923900	6.712800	-0.583000
H	5.459600	6.021100	-1.256100
H	5.442400	7.679100	-0.566300
H	4.892600	6.298700	0.437400
C	0.031600	8.182000	-2.292400
H	-0.218000	7.785400	-3.291000
H	-0.774600	7.920900	-1.584400
H	0.132900	9.271900	-2.345200
O	7.647400	-1.080300	0.778800
C	8.170900	0.251400	0.788200
H	7.598700	0.867400	1.507100
H	8.048900	0.699400	-0.214400
C	9.638900	0.179600	1.175400
H	9.723900	-0.282000	2.174000
H	10.152600	-0.498700	0.473100
C	10.316500	1.554600	1.168300
H	10.208500	2.008900	0.166900
H	9.788100	2.227400	1.868400
C	11.798200	1.492100	1.543300
H	12.360300	0.859000	0.837500
H	12.254200	2.493700	1.530700
H	11.937900	1.071300	2.552200

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[4]$^{+3}$ with butoxy

Y	-1.671200	-3.038400	-0.107400
C	-1.363100	-4.963100	2.631200
C	-0.395400	-5.796100	3.345300
C	-0.357300	-6.266100	4.662400
H	-1.127800	-5.972700	5.374700
C	0.686500	-7.129800	5.019300
C	0.149100	-5.579600	1.132500
C	0.558800	-6.186700	2.398600
C	1.596400	-7.066900	2.726500
H	2.310200	-7.383100	1.966600
C	1.668400	-7.532800	4.045900
C	0.270100	-5.548300	-1.216300
C	0.809000	-6.123800	-2.448100
C	1.878900	-6.993600	-2.685700
H	2.511900	-7.323900	-1.863000
C	2.089200	-7.429500	-4.000200
C	-1.081400	-4.895500	-2.847600
C	-0.044600	-5.711800	-3.478800
C	0.131700	-6.154100	-4.794600
H	-0.562300	-5.847700	-5.575700
C	1.210200	-7.008600	-5.060400
C	-3.228900	-3.941300	-2.945200
C	-4.476700	-3.744300	-3.681500
C	-4.815900	-3.953300	-5.023500
H	-4.061700	-4.284300	-5.736800
C	-6.146900	-3.741000	-5.403500
C	-4.742400	-3.327500	-1.446600
C	-5.432900	-3.358200	-2.736100
C	-6.773700	-3.163800	-3.088100
H	-7.508900	-2.893900	-2.330000
C	-7.132300	-3.345200	-4.429600
C	-4.861700	-3.355200	0.902400
C	-5.681200	-3.416600	2.111900
C	-7.050800	-3.225300	2.324800
H	-7.700600	-2.931300	1.500900
C	-7.548800	-3.439400	3.617000
C	-3.511900	-4.011600	2.533500
C	-4.830100	-3.831800	3.142200
C	-5.309600	-4.075300	4.433900
H	-4.635200	-4.428800	5.213600
C	-6.673600	-3.868500	4.676700
N	-2.491300	-4.547500	3.198600
N	-0.970100	-4.802200	1.322500
N	0.751300	-5.866900	-0.018900
N	-0.826000	-4.767200	-1.502200
N	-2.146800	-4.463400	-3.516400
N	-3.409200	-3.621200	-1.619700
N	-5.390100	-3.143600	-0.300000
N	-3.553800	-3.657200	1.205000
O	0.864700	-7.656600	6.242500
O	2.603500	-8.375000	4.513800
O	3.074100	-8.256000	-4.386900
O	1.513000	-7.512000	-6.268100
O	-6.624600	-3.891800	-6.649500
O	-8.372100	-3.192500	-4.922900
O	-8.834100	-3.290200	3.980000
O	-7.281200	-4.054600	5.860100
C	0.650600	-7.248700	-7.365300
H	-0.368100	-7.620500	-7.166200
H	0.611000	-6.170000	-7.593300
H	1.076800	-7.787600	-8.219400
C	3.927200	-8.824800	-3.403600
H	3.350900	-9.415600	-2.672500
H	4.614600	-9.484300	-3.946700
H	4.503800	-8.047200	-2.874500
C	3.557600	-8.921600	3.614700
H	3.062700	-9.489200	2.808600
H	4.189900	-8.130900	3.173900
H	4.179900	-9.598700	4.210600
C	-0.110900	-7.419300	7.247100
H	-1.101600	-7.789600	6.933600
H	0.226300	-7.973100	8.130800
H	-0.182100	-6.344700	7.490900
C	-6.534400	-4.579400	6.947700
H	-6.117000	-5.570700	6.700900
H	-5.716300	-3.897900	7.237700
H	-7.242000	-4.676900	7.779400
C	-9.802200	-2.984300	2.987100
H	-9.831400	-3.763300	2.207800
H	-10.766500	-2.951200	3.508400
H	-9.602400	-2.004100	2.519800
C	-9.440900	-2.907900	-4.032200
H	-10.345500	-2.866800	-4.650600
H	-9.548700	-3.701500	-3.273900
H	-9.294900	-1.936200	-3.528400
C	-5.765400	-4.392500	-7.663700
H	-4.917800	-3.709300	-7.845800
H	-5.380000	-5.392100	-7.399400
H	-6.378900	-4.464300	-8.570200
Y	1.020400	3.052000	0.107400
C	1.545200	4.615700	-2.823200
C	0.839800	5.345400	-3.876400
C	1.182500	5.651500	-5.198900
H	2.115200	5.282400	-5.625000
C	0.302000	6.453400	-5.934900
C	-0.309100	5.400700	-1.895800
C	-0.331400	5.840400	-3.290500
C	-1.215000	6.661900	-3.999800
H	-2.105200	7.059900	-3.514700
C	-0.904700	6.960300	-5.332400
C	-1.083400	5.667500	0.308200
C	-1.929300	6.388400	1.259300
C	-2.996900	7.276900	1.081900
H	-3.364000	7.501700	0.081700
C	-3.552700	7.869700	2.222700
C	-0.261900	5.232000	2.320800
C	-1.411000	6.112400	2.530100
C	-1.935700	6.710200	3.681000
H	-1.496600	6.504300	4.657100
C	-3.020300	7.584000	3.530600
C	1.745100	4.318300	3.137300
C	2.732000	4.224900	4.213000
C	2.692900	4.605600	5.559600
H	1.780700	5.021400	5.987400
C	3.859800	4.451100	6.318700
C	3.598200	3.530500	2.209800
C	3.901800	3.727200	3.627900
C	5.085600	3.585200	4.360900
H	5.991700	3.223900	3.876900
C	5.062900	3.936800	5.716800
C	4.375000	3.266900	0.006100
C	5.501500	3.182900	-0.922800
C	6.872700	2.981100	-0.721100
H	7.261200	2.802500	0.280800
C	7.715200	3.036500	-1.838800
C	3.552300	3.699700	-2.006700
C	4.981500	3.455300	-2.193700
C	5.806800	3.537800	-3.320800
H	5.384400	3.780000	-4.294800
C	7.178700	3.315400	-3.147200
N	2.776300	4.140500	-2.992100
N	0.798500	4.616500	-1.667900
N	-1.200200	5.827400	-1.006600
N	-0.134500	4.935800	0.983400
N	0.560900	4.897200	3.310100
N	2.279100	3.834200	1.965300
N	4.537400	3.210400	1.324600
N	3.212500	3.515800	-0.686000
O	0.486900	6.829400	-7.211200
O	-1.653500	7.725800	-6.143300
O	-4.578500	8.735700	2.217000
O	-3.635400	8.226400	4.535700
O	3.978800	4.764900	7.619200
O	6.111800	3.849900	6.550400
O	8.094000	3.350200	-4.128500
C	-3.117000	8.108600	5.853700
H	-3.165300	7.065000	6.210500
H	-2.074600	8.466100	5.901600
H	-3.751800	8.741000	6.484200
C	2.887000	5.380700	8.285800
H	3.228800	5.574000	9.309600
H	2.612300	6.333300	7.802900
H	2.006700	4.715000	8.311500
C	7.378300	3.465900	6.033000
H	7.350500	2.440800	5.625200
H	7.713700	4.164000	5.248700
H	8.072500	3.503900	6.880400
C	-5.111400	9.171100	0.973500
H	-4.337900	9.665300	0.362600
H	-5.545500	8.329000	0.407300
H	-5.899700	9.892100	1.220200
C	-2.803900	8.372300	-5.617300
H	-2.535200	9.043500	-4.784900
H	-3.222400	8.961200	-6.442000
H	-3.552700	7.639500	-5.270200
C	1.695200	6.474700	-7.869100
H	2.570700	6.884300	-7.337600

H	1.796600	5.379300	-7.955800
H	1.633900	6.918300	-8.869500
C	7.691100	3.731900	-5.437000
H	7.254400	4.744200	-5.437700
H	8.602700	3.725900	-6.045700
H	6.962800	3.016600	-5.856500
O	9.043000	2.851900	-1.809400
C	9.701700	2.632100	-0.556700
H	9.517300	3.495500	0.107900
H	9.276700	1.732600	-0.072900
C	11.185500	2.454200	-0.830900
H	11.557800	3.355200	-1.345900
H	11.313800	1.613900	-1.534400
C	11.994600	2.202600	0.446600
H	11.849500	3.047000	1.144100
H	11.597900	1.308200	0.962000
C	13.488900	2.015100	0.178200
H	13.920900	2.906200	-0.304400
H	14.041100	1.839700	1.113800
H	13.669800	1.154600	-0.486300
Cd	-0.325400	0.006800	0.000000
C	0.063000	-1.917400	-2.817500
C	-0.290400	-1.713200	-4.214200
C	0.385800	-2.001300	-5.408400
H	1.375900	-2.453900	-5.384500
C	-0.249000	-1.682200	-6.610500
C	-1.974300	-1.007900	-2.829300
C	-1.569100	-1.133300	-4.218800
C	-2.220200	-0.801800	-5.413900
H	-3.210800	-0.351700	-5.390500
C	-1.557000	-1.073700	-6.611900
C	-3.524400	-0.390000	-1.187100
C	-4.808000	0.161700	-0.782100
C	-5.901400	0.639200	-1.516900
H	-5.871400	0.650100	-2.606000
C	-7.012300	1.102500	-0.807300
C	-3.560500	-0.443500	1.043500
C	-4.824700	0.135200	0.621300
C	-5.926900	0.598900	1.351300
H	-5.914800	0.568600	2.439700
C	-7.021200	1.086800	0.634400
C	-2.081800	-1.164500	2.708400
C	-1.730300	-1.370100	4.105800
C	-2.429400	-1.134100	5.297200
H	-3.430000	-0.706500	5.272900
C	-1.796700	-1.459900	6.500000
C	-0.037500	-2.058600	2.721100
C	-0.440700	-1.924100	4.110900
C	0.211700	-2.253000	5.305100
H	1.213800	-2.680800	5.283100
C	-0.466000	-2.017300	6.502200
C	1.504600	-2.691500	1.077900
C	2.787400	-3.245000	0.672700
C	3.857700	-3.774600	1.406700
H	3.816800	-3.809100	2.494400
C	4.966500	-4.242500	0.696800
C	1.547800	-2.622500	-1.151900
C	2.816300	-3.192200	-0.729100
C	3.919700	-3.653100	-1.458900
H	3.918200	-3.600200	-2.547000
C	4.998100	-4.175500	-0.744000
N	1.223200	-2.434400	-2.424800
N	-0.974600	-1.495300	-1.997500
N	-3.145000	-0.504000	-2.456000
N	-2.790600	-0.760700	-0.069100
N	-3.236300	-0.632600	2.316400
N	-1.050700	-1.598000	1.888600
N	1.132000	-2.562900	2.347600
N	0.765400	-2.332600	-0.040800
O	0.267100	-1.881600	-7.835500
O	-2.040400	-0.794200	-7.838800
O	-8.131100	1.602100	-1.359900
O	-8.143100	1.586100	1.190400
O	-2.323300	-1.285500	7.724700
O	0.034100	-2.258200	7.731300
O	6.074900	-4.767000	1.248100
O	6.137600	-4.636800	-1.297800
C	6.254100	-4.652200	-2.713500
H	6.197000	-3.631700	-3.129200
H	7.239300	-5.081900	-2.930200
H	5.468900	-5.276200	-3.170700
C	6.174200	-4.855400	2.665400
H	5.342400	-5.446100	3.085400
H	7.123000	-5.366500	2.865600
H	6.197200	-3.853000	3.122100
C	1.322200	-2.845400	7.843000
H	2.098200	-2.192800	7.407800
H	1.505800	-2.966900	8.917300
H	1.355400	-3.830600	7.348200
C	-3.620000	-0.710500	7.850800
H	-4.370900	-1.303000	7.301100
H	-3.850600	-0.731700	8.923100
H	-3.624900	0.332000	7.497200
C	-8.270100	1.578900	2.604700
H	-7.488600	2.197100	3.078600
H	-9.256600	2.005900	2.822300
H	-8.214800	0.552500	3.004100
C	-8.227100	1.700000	-2.776800
H	-8.091200	0.713800	-3.252400
H	-9.238300	2.069200	-2.981800
H	-7.490500	2.417000	-3.172900
C	-3.339000	-0.229700	-7.951900
H	-3.390600	0.756300	-7.458400
H	-3.524700	-0.112700	-9.026400
H	-4.101700	-0.896300	-7.514900
C	1.566700	-2.445800	-7.962200
H	1.621700	-3.430200	-7.468200
H	1.734300	-2.567300	-9.038500
H	2.332000	-1.769300	-7.547900
C	2.288900	0.768000	-2.083400
C	2.439600	0.746300	-3.528000
C	3.487300	0.311900	-4.349600
H	4.387600	-0.115800	-3.909800
C	3.330900	0.449800	-5.730000
C	0.416000	1.634000	-2.932000
C	1.266100	1.299800	-4.064500
C	1.095500	1.454300	-5.446700
H	0.178800	1.887100	-5.844300
C	2.131700	1.029400	-6.283000
C	-1.574000	2.471800	-2.028200
C	-2.895900	3.055600	-2.174600
C	-3.633900	3.420300	-3.308300
H	-3.222400	3.260200	-4.303800
C	-4.892500	3.990100	-3.108700
C	-2.373600	2.761800	0.034400
C	-3.398100	3.247600	-0.877200
C	-4.655900	3.826900	-0.658400
H	-5.027700	3.970000	0.355400
C	-5.404700	4.201200	-1.776300
C	-1.577900	2.325300	2.191900
C	-1.732900	2.338000	3.636900
C	-2.781400	2.770500	4.458500
H	-3.691200	3.175100	4.017500
C	-2.608900	2.667100	5.838800
C	0.301700	1.473800	3.041300
C	-0.547200	1.810700	4.174000
C	-0.353900	1.707500	5.558000
H	0.573600	1.298300	5.957000
C	-1.387600	2.137800	6.394600
C	2.285000	0.621500	2.136700
C	3.603700	0.028200	2.282600
C	4.339900	-0.337800	3.416100
H	3.918700	-0.200800	4.411400
C	5.614000	-0.874100	3.218500
C	3.091700	0.347000	0.075000
C	4.117000	-0.137100	0.986700
C	5.397900	-0.664200	0.769700
H	5.780500	-0.783700	-0.242600
C	6.149600	-1.032200	1.888100
N	3.221800	0.326600	-1.248200
N	1.058500	1.315600	-1.744100
N	-0.796400	2.165100	-3.059200
N	-1.275000	2.308800	-0.680900
N	-2.510800	2.766800	1.356700
N	-0.335300	1.804100	1.853100
N	1.507400	0.928200	3.167600
N	1.998500	0.811700	0.791000
O	4.236100	0.059200	-6.649700
O	2.120400	1.096100	-7.625500
O	-5.728400	4.371400	-4.094700
O	-6.629000	4.754700	-1.738700
O	-3.531800	3.019600	6.757300
O	-1.365000	2.095700	7.737500
O	6.433600	-1.293000	4.202500
C	6.017500	-1.142600	5.552300
H	5.102600	-1.726500	5.754900
H	6.840400	-1.526000	6.166600
H	5.834700	-0.082800	5.796900
C	-0.224200	1.561900	8.400900
H	0.689800	2.110100	8.119600
H	-0.415400	1.693400	9.472200
H	-0.107200	0.489100	8.180100
C	-4.755100	3.590500	6.317200
H	-5.321700	2.882600	5.687500
H	-5.328000	3.813600	7.224300
H	-4.579500	4.520400	5.751000
C	-7.254800	4.980500	-0.480400
H	-6.631500	5.625400	0.161600
H	-8.198600	5.490800	-0.706100
H	-7.468100	4.028300	0.029500
C	-5.302400	4.244900	-5.443300
H	-5.112200	3.189300	-5.704100
H	-6.123500	4.632100	-6.057400
H	-4.389800	4.835600	-5.629000
C	0.974500	1.618900	-8.288500
H	0.756100	2.646800	-7.952700
H	1.227300	1.629700	-9.356000
H	0.097200	0.972800	-8.129400
C	5.470700	-0.487200	-6.208100
H	6.024100	0.233800	-5.584200
H	5.313800	-1.418300	-5.636500
H	6.045300	-0.706600	-7.115000
O	7.384100	-1.558500	1.848400
C	8.024700	-1.775100	0.582200
H	8.041300	-0.825100	0.017400
H	7.444700	-2.516700	0.006800
C	9.434500	-2.274600	0.849100
H	9.962800	-1.529700	1.468400
H	9.372800	-3.198200	1.448400
C	10.216400	-2.539200	-0.442700
H	9.672100	-3.284800	-1.050200
H	10.249400	-1.614600	-1.047900
C	11.642300	-3.030900	-0.187300
H	11.642600	-3.971100	0.387100
H	12.174400	-3.215100	-1.132800
H	12.222700	-2.289700	0.385600

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[4]$^{+4}$ with butoxy

Y	1.815000	-2.953100	-0.057500
C	4.929100	-3.102000	-1.316900
C	5.659100	-3.118500	-2.584500
C	7.003600	-2.886500	-2.894600
H	7.705100	-2.582600	-2.118700
C	7.415600	-3.083600	-4.221400
C	3.488400	-3.794200	-2.851100
C	4.748100	-3.555100	-3.554300
C	5.137600	-3.780200	-4.878400
H	4.421900	-4.154200	-5.609300
C	6.476100	-3.533500	-5.219400
C	1.387000	-4.848900	-2.801800
C	0.416800	-5.729000	-3.453000
C	0.315200	-6.202900	-4.766100
H	1.015600	-5.867900	-5.529700
C	-0.695500	-7.132400	-5.051800
C	0.028100	-5.560800	-1.203500
C	-0.442200	-6.178400	-2.443800
C	-1.443900	-7.122300	-2.698000
H	-2.078300	-7.486100	-1.890600

C	-1.581000	-7.594900	-4.011300	C	-5.181100	3.074900	2.302700	H	-3.398300	6.105500	-8.967900
C	0.089900	-5.575700	1.148200	C	-6.032500	3.074300	3.413000	O	-9.210200	2.381800	1.791200
C	-0.314000	-6.209500	2.402800	H	-5.641800	3.282900	4.408200	C	-9.849000	2.222200	0.514100
C	-1.299700	-7.157100	2.698500	C	-7.396000	2.824900	3.195500	H	-9.673400	3.129500	-0.091100
H	-1.975500	-7.513100	1.921800	C	-1.811300	4.341000	3.068200	H	-9.393900	1.363100	-0.013200
C	-1.367300	-7.646000	4.011400	C	-1.168800	5.047900	4.175600	C	-11.331300	1.995100	0.755200
C	1.530800	-4.883400	2.681000	C	-1.564500	5.271200	5.499300	H	-11.731900	2.855800	1.315700
C	0.595600	-5.771300	3.371700	H	-2.484100	4.832100	5.882400	H	-11.450000	1.112000	1.405900
C	0.563900	-6.260200	4.682900	C	-0.753300	6.092400	6.296500	C	-12.115300	1.801300	-0.548300
H	1.304000	-5.933300	5.412400	C	0.014300	5.274200	2.228900	H	-11.979600	2.688600	-1.192300
C	-0.429400	-7.194700	5.009900	C	-0.015800	5.637400	3.645100	H	-11.690500	0.947500	-1.108300
C	3.633100	-3.829400	2.632500	C	0.797500	6.479100	4.413300	C	-13.608600	1.565600	-0.314100
C	4.929000	-3.598700	3.270700	H	1.670800	6.957200	3.971100	H	-14.067700	2.417400	0.211900
C	5.388700	-3.841900	4.569300	C	0.435000	6.700200	5.749700	H	-14.142300	1.433200	-1.267000
H	4.713500	-4.228000	5.332000	C	0.809900	5.713900	0.059300	H	-13.779500	0.664000	0.296200
C	6.743400	-3.598500	4.842300	C	1.624400	6.546300	-0.825300	Cd	0.325900	0.019000	0.000000
C	4.991100	-3.116800	1.033400	C	2.624800	7.488600	-0.565000	C	-1.410000	-2.733500	-1.108900
C	5.786600	-3.147800	2.260700	H	2.963100	7.667800	0.454400	C	-2.649800	-3.362400	-0.676800
C	7.145300	-2.919200	2.501600	C	3.151400	8.204100	-1.651500	C	-3.721000	-3.912900	-1.394000
H	7.804600	-2.602200	1.693700	C	0.043100	5.370200	-1.989600	H	-3.716800	-3.908700	-2.482800
C	7.627700	-3.133300	3.801900	C	1.139500	6.329000	-2.120900	C	-4.783500	-4.454100	-0.664500
N	5.538500	-2.882200	-0.155100	C	1.632000	7.045200	-3.216800	C	-1.372000	-2.747900	1.122900
N	3.614600	-3.454300	-1.522600	H	1.216000	6.887700	-4.211200	C	-2.629000	-3.359900	0.726800
N	2.446400	-4.368000	-3.446200	C	2.651100	7.980500	-2.985400	C	-3.686200	-3.894200	1.476400
N	1.087700	-4.722100	-1.465000	C	-1.903300	4.411900	-2.898600	H	-3.651100	-3.880300	2.564600
N	-0.469100	-5.896800	-0.016600	C	-2.872000	4.354100	-3.993700	C	-4.769000	-4.435600	0.779400
N	1.161800	-4.740500	1.362600	C	-2.834700	4.845500	-5.303100	C	0.144400	-2.030200	2.755400
N	2.623000	-4.410900	3.274500	H	-1.937900	5.331400	-5.684500	C	0.540400	-1.856400	4.145400
N	3.689400	-3.472400	1.304400	C	-3.990000	4.711600	-6.087000	C	-0.079300	-2.218900	5.348200
O	8.661300	-2.903400	-4.674500	C	-3.729700	3.480500	-2.059300	H	-1.044900	-2.721000	5.341800
O	7.001000	-3.696800	-6.439400	C	-4.025800	3.766400	-3.463200	C	0.580300	-1.905300	6.541200
O	-0.922800	-7.675500	-6.253400	C	-5.197900	3.641500	-4.216300	C	2.135200	-1.021800	2.727600
O	-2.487100	-8.492500	-4.414800	H	-6.097000	3.214300	-3.774100	C	1.788300	-1.212600	4.125800
O	-2.249900	-8.549800	4.451100	C	-5.179500	4.106500	-5.540200	C	2.463100	-0.886600	5.309400
O	-0.593800	-7.750600	6.215700	N	-4.665000	3.057900	-1.213000	H	3.429100	-0.384500	5.272000
O	7.333400	-3.779200	6.029700	N	-3.385100	3.294100	0.838600	C	1.854500	-1.228400	6.519900
O	8.894700	-2.955800	4.191000	N	-3.020100	3.797100	3.186000	C	3.586100	-0.271400	1.050200
C	-3.337300	-9.112000	-3.456000	N	-1.044200	4.445800	1.930200	C	4.825100	0.359300	0.618000
H	-2.747800	-9.650900	-2.696300	N	0.898500	5.796600	1.384000	C	5.917400	0.864500	1.334100
H	-3.989500	-8.369900	-2.964300	N	-0.088600	4.976200	-0.677900	H	5.929100	0.829100	2.423300
H	-3.951500	-9.824600	-4.018000	N	-0.746600	5.057300	-3.013600	C	6.976600	1.414200	0.605400
C	-0.041000	-7.388800	-7.332500	N	-2.428700	3.824900	-1.770100	C	3.539100	-0.241300	-1.180600
H	0.989900	-7.695000	-7.091300	O	-8.332300	2.789900	4.149100	C	4.788900	0.387200	-0.786000
H	-0.408100	-7.974300	-8.183000	O	-0.992800	6.398200	7.576800	C	5.837600	0.937400	-1.533700
H	-0.060500	-6.315200	-7.586800	O	1.107200	7.473200	6.610900	H	5.788700	0.951300	-2.621500
C	6.203800	-4.251000	-7.479500	O	4.109200	9.133400	-1.567100	C	6.930700	1.458200	-0.837200
H	5.843900	-5.255600	-7.206300	O	3.226300	8.740100	-3.925800	C	2.031400	-0.975900	-2.813600
H	5.345000	-3.598200	-7.712600	O	-4.111400	5.125900	-7.353000	C	1.633700	-1.146000	-4.203600
H	6.860900	-4.320600	-8.354200	O	-6.213900	4.056400	-6.387100	C	2.276200	-0.829300	-5.407300
C	9.701400	-2.576200	-3.760300	C	2.228600	8.221400	6.155600	H	3.257100	-0.356400	-5.401800
H	9.807200	-3.356100	-2.989200	H	3.036300	7.553800	5.807700	C	1.613200	-1.133400	-6.600900
H	10.618200	-2.521600	-4.358300	H	1.940500	8.910700	5.345800	C	0.032700	-1.967000	-2.785900
H	9.514900	-1.600300	-3.280100	H	2.575600	8.795500	7.021900	C	0.371300	-1.760200	-4.183600
C	9.885000	-2.615400	3.226600	C	4.596900	9.528100	-0.289700	C	-0.312000	-2.069200	-5.368200
H	9.951700	-3.386200	2.442200	H	5.333500	10.316700	-0.481700	H	-1.291900	-2.543600	-5.328900
H	9.673600	-1.634500	2.769200	H	3.782400	9.926700	0.335900	C	0.306700	-1.749200	-6.578500
H	10.832500	-2.567300	3.776400	H	5.085600	8.683800	0.227500	N	-1.097400	-2.541300	-2.385600
C	6.592800	-4.347600	7.103100	C	2.736400	8.697300	-5.260500	N	-0.648000	-2.377800	-0.003800
H	6.217100	-5.348400	6.835900	H	2.868100	7.693200	-5.699700	N	-1.003900	-2.587700	2.389900
H	7.294800	-4.429400	7.940100	H	1.671900	8.982600	-5.299000	N	1.127800	-1.524900	1.913400
H	5.748300	-3.697300	7.391700	H	3.333100	9.425000	-5.821900	N	3.264900	-0.446700	2.327300
C	0.344300	-7.476100	7.250900	C	-2.197500	5.957100	8.192000	N	2.826700	-0.634700	-0.054400
H	0.019600	-8.070400	8.112700	H	-3.078300	6.344800	7.654600	N	3.171300	-0.400300	-2.448200
H	1.360300	-7.780300	6.951600	H	-2.242300	4.854900	8.234000	N	1.051700	-1.487200	-1.972100
H	0.338600	-6.405200	7.517400	H	-2.179200	6.362300	9.209600	O	-5.883200	-5.006800	-1.196200
C	-3.149500	-9.159100	3.531800	C	-7.984400	3.114000	5.490000	O	-5.867700	-4.961400	1.349800
H	-3.827100	-8.412200	3.085000	H	-7.575600	4.135400	5.553700	O	0.118900	-2.172800	7.771000
H	-2.600900	-9.686500	2.735200	H	-8.915200	3.053900	6.064300	O	2.358700	-0.961900	7.738200
H	-3.731900	-9.880000	4.116300	H	-7.251500	2.394500	5.895800	O	8.086300	1.947200	1.136600
Y	-1.163300	2.991000	0.057600	C	-7.477500	3.590600	-5.927000	O	8.000000	2.042000	-1.406300
C	-4.525000	3.038800	0.109600	H	-7.844600	4.208300	-5.091100	O	2.083800	-0.885900	-7.830500
C	-5.664700	2.856000	1.008000	H	-8.158900	3.682900	-6.779800	O	-0.226900	-1.956500	-7.794700
C	-7.023600	2.627200	0.761200	H	-7.420700	2.534500	-5.612400	C	-1.486600	-2.605500	-7.898300
H	-7.385200	2.494600	-0.257300	C	-3.046400	5.847300	-7.963100	H	-2.279800	-2.016200	-7.406800
C	-7.894200	2.599000	1.861100	H	-2.822100	6.768200	-7.400400	H	-1.698800	-2.684000	-8.970600
C	-3.758900	3.383300	2.159800	H	-2.137800	5.225500	-8.037800	H	-1.450000	-3.612800	-7.452000

C	3.359600	-0.268500	-7.988300
H	4.147100	-0.861100	-7.493400
H	3.544500	-0.242800	-9.068200
H	3.349000	0.759100	-7.593500
C	8.088600	2.094200	-2.824500
H	7.261000	2.684200	-3.253800
H	9.043500	2.583400	-3.048900
H	8.080200	1.080700	-3.258900
C	8.247900	1.974800	2.553300
H	8.185500	0.959200	2.976200
H	9.248500	2.386200	2.728100
H	7.496500	2.630500	3.020200
C	3.635800	-0.344700	7.840400
H	3.630700	0.657300	7.379700
H	3.842200	-0.255500	8.913200
H	4.413200	-0.964200	7.362600
C	-1.136600	-2.830400	7.927800
H	-1.142100	-3.799000	7.402200
H	-1.251800	-2.995800	9.005200
H	-1.959800	-2.193900	7.565900
C	-5.939800	-5.045500	2.767100
H	-5.909600	-4.042800	3.227500
H	-6.900400	-5.524200	2.992000
H	-5.115900	-5.658300	3.169000
C	-6.024100	-5.075600	-2.613800
H	-5.180000	-5.620300	-3.067400
H	-6.954700	-5.625400	-2.791700
H	-6.106500	-4.067200	-3.047700
C	-2.363800	0.605200	-2.054000
C	-3.653000	-0.048700	-2.199700
C	-4.396400	-0.409200	-3.330800
H	-4.008400	-0.212600	-4.329400
C	-5.635600	-1.021600	-3.126800
C	-3.106600	0.202300	0.011600
C	-4.127800	-0.292300	-0.900800
C	-5.373100	-0.893000	-0.674700
H	-5.725100	-1.069700	0.339500
C	-6.132500	-1.257400	-1.792200
C	-2.277900	0.565300	2.170400
C	-2.392800	0.470400	3.616200
C	-3.393200	-0.058200	4.442800
H	-4.282500	-0.512500	4.007800
C	-3.205800	0.021800	5.824600
C	-0.428800	1.486200	3.016000
C	-1.235500	1.058300	4.150200
C	-1.034500	1.160000	5.533100
H	-0.132100	1.624500	5.927900
C	-2.023600	0.643300	6.374700
C	1.499300	2.459500	2.112400
C	2.796800	3.097400	2.257700
C	3.548500	3.441900	3.388200
H	3.174200	3.217400	4.386500
C	4.777800	4.073900	3.184700
C	2.233900	2.878400	0.047300
C	3.256700	3.371500	0.959100
C	4.479300	4.016800	0.735300
H	4.815900	4.223800	-0.279400
C	5.243100	4.372300	1.851500
C	1.413400	2.499400	-2.112000
C	1.536300	2.579200	-3.558200
C	2.546300	3.090200	-4.384500
H	3.448800	3.517500	-3.949900
C	2.347300	3.031300	-5.765300
C	-0.443200	1.594800	-2.957700
C	0.363600	2.020500	-4.091300
C	0.140200	1.963600	-5.473300
H	-0.777100	1.529700	-5.867800
C	1.133900	2.472500	-6.315500
N	-1.621500	0.996400	-3.085400
N	-2.051100	0.749200	-0.707800
N	-3.207000	0.115700	1.333200
N	-1.082500	1.185300	1.827800
N	0.758000	2.067600	3.144600
N	1.175500	2.337900	0.766600
N	2.342900	2.948100	-1.274800
N	0.206900	1.901800	-1.768900
O	-6.454300	-1.448800	-4.104500
O	-4.057200	-0.458700	6.747300
O	-1.980400	0.651300	7.714200
O	5.625100	4.442700	4.161600
O	6.435200	4.982700	1.808300
O	3.228900	3.454100	-6.689900
O	1.080700	2.484100	-7.654600
C	-0.061600	1.949700	-8.320200
H	-0.983400	2.459100	-7.991200
H	0.102000	2.139600	-9.387400
H	-0.143300	0.865400	-8.150300
C	4.436400	4.071100	-6.264500
H	5.053700	3.372200	-5.674200
H	4.970300	4.350600	-7.180200
H	4.230000	4.973600	-5.665700
C	7.011500	5.320400	0.548800
H	6.335500	5.970400	-0.032100
H	7.933100	5.865400	0.780900
H	7.257400	4.414200	-0.026200
C	5.247900	4.248800	5.517700
H	5.106500	3.177000	5.741600
H	6.073600	4.644000	6.120900
H	4.320500	4.796900	5.752900
C	-0.858800	1.226900	8.380800
H	-0.719600	2.278500	8.081600
H	-1.091700	1.175700	9.450500
H	0.056100	0.648000	8.179300
C	-5.281300	-1.043600	6.322800
H	-5.100800	-1.938300	5.701500
H	-5.811100	-1.333400	7.237800
H	-5.889800	-0.320700	5.755300
C	-6.093300	-1.221600	-5.460200
H	-5.981100	-0.143300	-5.664200
H	-5.154000	-1.742300	-5.714400
H	-6.912700	-1.627100	-6.063000
O	-7.334900	-1.843600	-1.746900
C	-7.958400	-2.112800	-0.477900
H	-7.995900	-1.177000	0.108600
H	-7.348100	-2.849900	0.071100
C	-9.355000	-2.647200	-0.744300
H	-9.909500	-1.905100	-1.343500
H	-9.273200	-3.556200	-1.363300
C	-10.118000	-2.959900	0.548700
H	-10.173500	-2.047900	1.171200
H	-9.546900	-3.700200	1.137800
C	-11.530500	-3.489100	0.293700
H	-12.137000	-2.755300	-0.261000
H	-11.507400	-4.418500	-0.297300
H	-12.048900	-3.705900	1.239600

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Y	4.944900	1.551500	0.020400
C	7.418900	-0.626800	0.634400
C	8.106600	-1.740000	-0.014000
C	8.739300	-2.885300	0.490200
H	8.797700	-3.044800	1.566800
C	9.246300	-3.807700	-0.424700
C	7.283000	-0.255700	-1.554500
C	8.021000	-1.504500	-1.393900
C	8.562800	-2.403200	-2.323400
H	8.478500	-2.199400	-3.390500
C	9.157000	-3.567900	-1.838200
C	6.589700	1.541400	-2.901900
C	6.575400	2.233600	-4.187200
C	6.926700	1.830300	-5.483400
H	7.319800	0.828000	-5.653200
C	6.722600	2.733700	-6.527800
C	5.791100	3.579500	-2.506800
C	6.072800	3.518200	-3.937500
C	5.900500	4.450100	-4.970100
H	5.503200	5.440500	-4.749600
C	6.205800	4.049000	-6.270600
C	5.295300	4.832400	-0.580600
C	5.041100	6.114000	0.070400
C	4.735200	7.387500	-0.431500
H	4.679500	7.548000	-1.508200
C	4.476500	8.407700	0.484000
C	5.428500	4.460200	1.608300
C	5.127300	5.879600	1.449700
C	4.909700	6.904600	2.382000
H	4.976600	6.693300	3.448300
C	4.562400	8.165700	1.898000
C	6.124300	2.664700	2.956500
C	6.571700	2.141600	4.243800
C	6.547700	2.671800	5.542100
H	6.157400	3.675200	5.711900
C	7.000400	1.865800	6.586300
C	6.920300	0.625000	2.560600
C	7.075300	0.857500	3.994100
C	7.571100	0.051000	5.028800
H	7.951400	-0.945200	4.807600
C	7.513600	0.548800	6.330400
N	6.879200	0.200300	-0.320400
N	7.116900	0.332100	-2.735800
N	6.045600	2.354600	-1.935800
N	5.409100	4.699300	-1.897800
N	5.450100	3.855700	0.373300
N	5.694200	3.911400	2.790000
N	6.282800	1.701000	1.988700
N	7.401800	-0.455400	1.952900
O	9.829600	-4.989600	-0.087800
O	9.664700	-4.559500	-2.615500
O	6.956700	2.463000	-7.839800
O	6.029100	4.814400	-7.379200
O	4.107500	9.673200	0.148000
O	4.257700	9.236800	2.674900
O	6.980000	2.219000	7.899800
O	7.893300	-0.137100	7.438600
C	9.568500	-4.423000	-4.022100
H	8.516300	-4.396700	-4.353100
H	10.090000	-3.516400	-4.375500
H	10.059100	-5.309100	-4.445000
C	9.998400	-5.278300	1.284200
H	10.624300	-4.517200	1.783300
H	9.028600	-5.341200	1.810000
H	10.501600	-6.251800	1.333700
C	8.361600	-1.464100	7.276300
H	8.635500	-1.811700	8.280600
H	7.576700	-2.121300	6.865000
H	9.252600	-1.500200	6.625400
C	6.534500	3.518500	8.229800
H	7.159200	4.294200	7.752100
H	5.482300	3.676400	7.931800
H	6.618800	3.603200	9.320700
C	7.511600	1.207700	-8.169100
H	8.492400	1.057300	-7.684300
H	6.841400	0.377400	-7.878900
H	7.640200	1.204600	-9.259200
C	5.473900	6.108100	-7.216500
H	6.100700	6.735800	-6.558100
H	5.448700	6.552800	-8.219700
H	4.448000	6.058400	-6.813500
C	4.048200	10.003200	-1.223700
H	5.028200	9.869000	-1.715500
H	3.295600	9.393700	-1.757400
H	3.757800	11.061200	-1.272000
C	4.267600	9.065700	4.081600
H	3.508400	8.333700	4.404600
H	5.262600	8.751100	4.441900
H	4.025700	10.048900	4.505600
Cd	1.751400	0.305600	0.005300
C	4.393100	-1.778700	-0.668700
C	4.739900	-2.612300	-1.807500
C	5.279800	-3.903400	-1.895100
H	5.495200	-4.466000	-0.987300
C	5.547200	-4.411300	-3.164200
C	3.943700	-0.578600	-2.491800
C	4.465500	-1.854800	-2.955500
C	4.732800	-2.351200	-4.239000
H	4.515600	-1.743200	-5.116400
C	5.279600	-3.629500	-4.341200

C	3.099400	1.563900	-2.888900	H	1.515800	6.281800	7.552300	H	-2.242200	3.740000	-6.533000
C	2.702500	2.632300	-3.792000	H	0.995900	4.706700	6.872000	C	-2.129100	5.670600	5.335000
C	2.707200	2.727400	-5.190400	C	1.319800	-3.021600	0.487800	H	-2.969200	5.471200	4.645600
H	3.039700	1.882800	-5.792800	C	1.676300	-3.931100	1.567400	H	-2.467400	6.346200	6.131500
C	2.303800	3.932600	-5.760500	C	2.211200	-5.226800	1.566600	H	-1.301100	6.146500	4.784800
C	2.440700	3.263800	-1.607500	H	2.431600	-5.725400	0.623500	C	-0.418800	1.399800	8.140100
C	2.296800	3.706100	-2.985200	C	2.430100	-5.840500	2.798400	H	-0.493000	1.761900	9.173300
C	1.889800	4.925700	-3.545900	C	0.877400	-1.949400	2.389700	H	-1.093200	0.538400	8.009100
H	1.582400	5.746800	-2.899900	C	1.382800	-3.262100	2.764300	H	0.622100	1.092400	7.935900
C	1.899400	5.038500	-4.934800	C	1.584700	-3.870800	4.010500	O	-2.353700	6.562200	-2.962800
C	2.277600	3.627000	0.696000	H	1.349400	-3.330900	4.925600	C	-2.686500	7.321100	-1.801400
C	1.959700	4.471900	1.834900	C	2.104600	-5.164000	4.024900	H	-1.792200	7.428600	-1.158400
C	1.481500	5.786500	1.921900	C	0.062700	0.172300	2.941700	H	-3.465400	6.794200	-1.224200
H	1.266000	6.349100	1.014200	C	-0.327700	1.177300	3.918400	C	-3.189500	8.681200	-2.258800
C	1.324000	6.337300	3.191500	C	-0.308100	1.184900	5.319400	H	-2.406800	9.166700	-2.867400
C	2.745900	2.433700	2.518400	H	0.051400	0.312700	5.864100	H	-4.056700	8.526700	-2.922600
C	2.262000	3.725400	2.983100	C	-0.770700	2.326700	5.970600	C	-3.584700	9.585400	-1.086800
C	2.111200	4.267200	4.267100	C	-0.637400	1.940800	1.782000	H	-4.362500	9.080000	-0.487300
H	2.356600	3.669600	5.143800	C	-0.783700	2.285200	3.187700	H	-2.716400	9.717800	-0.415700
C	1.646600	5.577000	4.368900	C	-1.264800	3.435900	3.828900	C	-4.095000	10.956900	-1.532600
C	3.571500	0.284000	2.915400	H	-1.613000	4.282500	3.240300	H	-4.984700	10.859300	-2.176100
C	3.997300	-0.773200	3.818600	C	-1.262000	3.450900	5.222400	H	-4.372600	11.581200	-0.668800
C	4.053100	-0.844700	5.217200	N	-0.129500	0.660400	1.661900	H	-3.327300	11.501000	-2.107300
H	3.721500	0.000300	5.819700	N	0.521100	-1.027700	3.276000	Y	-4.453300	-2.114600	-0.022000
C	4.568400	-2.006200	5.787900	N	0.845700	-1.832800	1.012400	C	-5.013300	-4.829300	-1.910400
C	4.248900	-1.408700	1.634000	N	1.440200	-3.334400	-0.796200	C	-4.705300	-6.256100	-1.923200
C	4.430700	-1.835600	3.012800	N	-0.948200	2.770300	0.793000	C	-4.528800	-7.177100	-2.965700
C	4.954400	-3.010200	3.573100	O	-1.702000	4.486400	5.986800	H	-4.650800	-6.858000	-4.000400
H	5.288800	-3.820700	2.927300	O	-0.807100	2.489400	7.319700	C	-4.164700	-8.482300	-2.630400
C	5.025900	-3.091400	4.962400	O	2.349400	-5.889700	5.148500	C	-4.783000	-5.438800	0.216000
N	3.929500	-0.550200	-1.108300	O	2.948900	-7.086100	2.963300	C	-4.562500	-6.640300	-0.582700
N	3.565200	0.395100	-3.310300	C	1.116200	-2.509400	-1.784400	C	-4.236700	-7.957600	-0.229000
N	2.945300	1.976300	-1.575100	C	1.252500	-2.858400	-3.191000	H	-4.125100	-8.228100	0.820000
N	2.136800	4.024400	-0.562000	C	1.683000	-4.028000	-3.833000	C	-4.016600	-8.874800	-1.257200
N	2.764700	2.407100	1.134900	H	1.995000	-4.889000	-3.243200	C	-5.191200	-4.423000	2.296700
N	3.119700	1.458200	3.336800	C	1.706600	-4.033500	-5.225800	C	-5.408700	-4.520600	3.736800
N	3.748700	-0.118800	1.602500	C	0.442200	-0.730800	-2.944000	C	-5.197700	-5.555900	4.659100
N	4.548900	-2.170300	0.589400	C	0.843000	-1.732300	-3.921400	H	-4.821700	-6.520500	4.316600
O	6.070200	-5.640800	-3.412800	C	0.873700	-1.720300	-5.322200	C	-5.448900	-5.294000	6.005900
O	5.603100	-4.243700	-5.508200	H	0.551500	-0.833600	-5.866700	C	-5.965200	-2.442500	2.948300
O	2.254000	4.180200	-7.095900	C	1.311300	-2.871900	-5.973500	C	-5.899000	-3.272300	4.147500
O	1.546600	6.153800	-5.624300	C	-0.399600	1.380600	-2.393500	C	-6.194200	-3.007600	5.491500
O	0.873700	7.595200	3.440500	C	-0.914000	2.688900	-2.767600	H	-6.568400	-2.027700	5.784100
O	1.460300	6.243900	5.537000	C	-1.167700	3.278900	-4.013700	C	-5.948600	-4.013500	6.425600
O	4.689000	-2.226200	7.123600	H	-0.968200	2.723500	-4.929300	C	-6.718500	-0.502900	1.853500
O	5.516600	-4.152900	5.652500	C	-1.661100	4.581500	-4.027500	C	-7.458700	0.755200	1.864400
C	4.360600	-1.170000	8.011800	C	-0.815000	2.463400	-0.491500	C	-7.961600	1.549800	2.904800
H	3.309600	-0.855100	7.892100	C	-1.161200	3.376600	-1.569600	H	-7.843300	1.229200	3.939500
H	4.505300	-1.571900	9.022800	C	-1.644800	4.692300	-1.568600	C	-8.575100	2.756700	2.568900
H	5.026600	-0.303200	7.867300	H	-1.827700	5.204900	-0.626200	C	-6.945100	0.108100	-0.272800
C	5.933700	-5.295300	4.922100	C	-1.889600	5.295300	-2.801400	C	-7.602800	1.139900	0.523300
H	6.739500	-5.043900	4.209700	N	-0.354600	1.268300	-1.015600	C	-8.252700	2.330300	0.169500
H	6.318200	-6.003000	5.668000	N	-0.029900	0.463200	-3.279200	H	-8.345400	2.607600	-0.880200
H	5.090300	-5.757500	4.384500	N	0.621400	-1.224000	-1.664200	C	-8.719700	3.151400	1.195200
C	6.463900	-6.439400	-2.309700	O	-1.963600	5.284200	-5.152200	C	-6.540600	-0.909200	-2.353600
H	5.613500	-6.647700	-1.637200	O	1.405400	-3.012000	-7.322400	C	-6.755300	-0.980300	-3.795600
H	6.827000	-7.383800	-2.736200	O	2.088800	-5.091600	-5.990400	C	-7.293500	-0.072100	-4.718600
H	7.278900	-5.962800	-1.739900	C	2.135300	-5.273500	6.407100	H	-7.672100	0.890900	-4.376900
C	5.315300	-3.572100	-6.724200	H	1.086200	-4.946900	6.523100	C	-7.290900	-0.431600	-6.067400
H	5.835800	-2.600300	-6.779500	H	2.359700	-6.041300	7.159200	C	-5.763800	-2.888600	-3.005100
H	5.686400	-4.227400	-7.522800	H	2.810500	-4.414400	6.554100	C	-6.267100	-2.228800	-4.205500
H	4.230900	-3.421700	-6.852700	C	3.223000	-7.859900	1.807000	C	-6.295300	-2.619400	-5.552300
C	2.734900	3.184200	-7.982600	H	3.948500	-7.353900	1.147100	H	-5.904000	-3.593500	-5.844400
H	3.810100	2.996500	-7.831000	H	3.658700	-8.798700	2.171500	C	-6.787900	-1.709400	-6.486800
H	2.173700	2.239200	-7.871000	H	2.301300	-8.082900	1.246600	N	-4.979000	-4.363200	-0.618200
H	2.577300	3.580500	-8.994400	C	2.572800	-6.253600	-5.338400	N	-4.838200	-5.461200	1.545100
C	1.074400	7.274800	-4.894100	H	1.814300	-6.678200	-4.656400	N	-5.466300	-3.144100	1.875900
H	1.830800	7.633300	-4.174600	H	2.787100	-6.977600	-6.135500	N	-6.498000	-1.223400	2.948800
H	0.883700	8.058100	-5.639100	H	3.499800	-6.044400	-4.780200	N	-6.367200	-0.818400	0.563100
H	0.136600	7.042200	-4.363800	C	0.960300	-1.944700	-8.143100	N	-6.989500	0.091600	-1.602400
C	0.631800	8.453100	2.338100	H	1.515900	-1.013900	-7.931500	N	-5.879900	-2.037400	-1.931000
H	-0.129300	8.032200	1.658300	H	1.158000	-2.257500	-9.176300	N	-5.329800	-4.146200	-3.006100
H	0.256900	9.392000	2.765100	H	-0.120600	-1.767800	-8.019300	O	-3.900000	-9.466000	-3.532200
H	1.559000	8.655700	1.776800	C	-1.692600	4.690100	-6.410500	O	-3.631100	-10.164200	-1.074000
C	1.692900	5.551600	6.752200	H	-2.041800	5.409200	-7.163100	O	-5.233200	-6.177400	7.018000
H	2.733900	5.188500	6.815200	H	-0.614000	4.516300	-6.548700	O	-6.121700	-3.885400	7.766200

O	-9.053100	3.657100	3.469800
O	-7.720800	0.368100	-7.080500
O	-6.817700	-1.917200	-7.829100
C	-6.291200	-3.133600	-8.328700
H	-5.213500	-3.226600	-8.112400
H	-6.827400	-4.005900	-7.913600
H	-6.440900	-3.103000	-9.415400
C	-4.071600	-9.172500	-4.903000
H	-5.110900	-8.875400	-5.126500
H	-3.392000	-8.365800	-5.235100
H	-3.831200	-10.095500	-5.446100
C	-3.411800	-10.615000	0.250700
H	-2.585200	-10.065200	0.732500
H	-4.324700	-10.522200	0.864800
H	-3.140100	-11.675600	0.166300
C	-4.787900	-7.473400	6.682200
H	-5.507800	-7.992000	6.023500
H	-3.802500	-7.450900	6.181500
H	-4.701000	-8.023400	7.628600
C	-6.562500	-2.635600	8.266100
H	-7.543700	-2.355700	7.844200
H	-6.660200	-2.763800	9.352300
H	-5.830000	-1.836800	8.058700
C	-8.991600	3.321400	4.839500
H	-9.557600	2.398300	5.056500
H	-7.948600	3.186400	5.180100
H	-9.444200	4.160700	5.382200
C	-8.275600	1.622900	-6.744800
H	-9.161400	1.514000	-6.094400
H	-7.538100	2.271500	-6.236600
H	-8.575300	2.088300	-7.692600
O	-9.323400	4.353400	1.006200
C	-9.521000	4.809400	-0.329700
H	-8.542000	4.977600	-0.814800
H	-10.063900	4.040300	-0.910100
C	-10.327500	6.097600	-0.272300
H	-11.282800	5.893400	0.240700
H	-9.785600	6.827200	0.353200
C	-10.587400	6.691500	-1.660500
H	-9.621300	6.877100	-2.163600
H	-11.118700	5.948900	-2.282900
C	-11.397100	7.988600	-1.616200
H	-10.875400	8.763500	-1.030500
H	-11.566700	8.390200	-2.627700
H	-12.382700	7.827100	-1.149300
Cd	-1.260400	-0.869600	-0.007600
C	-1.789700	-4.179900	-0.737200
C	-1.325200	-5.420800	-0.138400
C	-0.886200	-6.626600	-0.702000
H	-0.839300	-6.736800	-1.784400
C	-0.549500	-7.664200	0.164900
C	-1.918100	-3.904500	1.469400
C	-1.413900	-5.251000	1.251100
C	-1.081200	-6.287000	2.135200
H	-1.161400	-6.132600	3.211100
C	-0.653300	-7.494700	1.589400
C	-2.592900	-2.164900	2.878500
C	-2.830000	-1.614300	4.201900
C	-2.660900	-2.153400	5.485900
H	-2.267700	-3.161900	5.605700
C	-3.035600	-1.368500	6.573400
C	-3.403600	-0.112300	2.573800
C	-3.348600	-0.325000	4.011400
C	-3.732300	0.474600	5.097200
H	-4.135600	1.471200	4.924600
C	-3.579800	-0.052000	6.379000
C	-3.898100	1.206400	0.708500
C	-4.391500	2.436100	0.109600
C	-4.890100	3.618600	0.672900
H	-4.938900	3.728100	1.755400
C	-5.338400	4.612100	-0.195400
C	-3.788200	0.923200	-1.498900
C	-4.330700	2.255400	-1.280000
C	-4.779700	3.245400	-2.165500
H	-4.726700	3.080900	-3.240600
C	-5.288800	4.422000	-1.619200
C	-3.094900	-0.808600	-2.907100
C	-2.886700	-1.370400	-4.230700
C	-3.116400	-0.855000	-5.515000
H	-3.510500	0.153200	-5.634800
C	-2.852500	-1.683200	-6.603000
C	-2.303600	-2.869300	-2.603400
C	-2.396000	-2.670600	-4.040300
C	-2.128800	-3.515700	-5.126600
H	-1.752500	-4.522900	-4.954200
C	-2.363200	-3.021100	-6.408800
N	-2.157100	-3.286200	0.255000
N	-2.122500	-3.389400	2.676300
N	-2.961800	-1.244400	1.911500
N	-3.837500	1.014000	2.019700
N	-3.554900	0.303300	-0.283700
N	-3.580200	0.410200	-2.705000
N	-2.750000	-1.739100	-1.941100
N	-1.865000	-3.993800	-2.049300
O	-0.111400	-8.889100	-0.226200
O	-0.307500	-8.592600	2.310800
O	-2.933900	-1.748800	7.874900
O	-3.915200	0.592800	7.526600
O	-5.771600	5.466400	-2.341300
O	-3.025600	-1.331700	-7.904300
O	-2.163900	-3.719000	-7.557000
C	-5.704500	5.393600	-3.756300
H	-6.263000	4.521600	-4.140400
H	-6.173800	6.314200	-4.126200
H	-4.660500	5.352300	-4.107200
C	-4.401200	1.921400	7.435000
H	-5.318800	1.972000	6.820900
H	-4.636500	2.226200	8.462800
H	-3.638200	2.600600	7.019600
C	-2.508000	-3.071200	8.158000
H	-3.218900	-3.813900	7.763500
H	-1.500500	-3.265900	7.748800
H	-2.474600	-3.147500	9.252800
C	-0.319600	-8.498300	3.726100
H	-1.323600	-8.235400	4.102500
H	-0.044000	-9.494600	4.095200
H	0.417400	-7.761700	4.085100
C	-0.078900	-9.181500	-1.612700
H	0.580000	-8.481700	-2.157700
H	0.325800	-10.198000	-1.696500
H	-1.090300	-9.156900	-2.051400
C	-1.622900	-5.026200	-7.465200
H	-2.268700	-5.686200	-6.858800
H	-1.582300	-5.406900	-8.493900
H	-0.605600	-5.010900	-7.042500
C	-3.604600	-0.068100	-8.188600
H	-2.999700	0.756100	-7.772000
H	-3.624000	0.013700	-9.283400
H	-4.635200	-0.003800	-7.801800
O	-5.851400	5.805500	0.204900
C	-6.078500	6.004400	1.599600
H	-5.120800	5.932500	2.149300
H	-6.750700	5.214700	1.977200
C	-6.708500	7.374200	1.793400
H	-6.000100	8.153000	1.461200
H	-7.589800	7.446300	1.134900
C	-7.127000	7.617800	3.247400
H	-7.842500	6.831900	3.547500
H	-6.247700	7.504500	3.907900
C	-7.754100	8.995200	3.469300
H	-8.048500	9.136300	4.521100
H	-7.050500	9.802400	3.206100
H	-8.656000	9.124900	2.848800

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[5]$^{+1}$ with butoxy

Y	4.528900	-1.851400	0.078800
C	5.062300	-5.171300	0.110700
C	4.991000	-6.331300	-0.776100
C	4.814400	-7.700800	-0.535000
H	4.704600	-8.066300	0.485600
C	4.776700	-8.561100	-1.635800
C	5.343100	-4.395400	-1.951600
C	5.163700	-5.839000	-2.076500
C	5.154500	-6.690000	-3.188700
H	5.293100	-6.280600	-4.188900
C	4.936700	-8.051200	-2.970300
C	6.034000	-2.352000	-2.886000
C	6.591900	-1.596500	-4.006500
C	6.785800	-1.909500	-5.359300
H	6.498000	-2.888500	-5.739600
C	7.344000	-0.929900	-6.185100
C	6.656000	-0.385600	-2.062200
C	6.979200	-0.355200	-3.485700
C	7.564300	0.627900	-4.293100
H	7.857900	1.584400	-3.860700
C	7.725800	0.348600	-5.651400
C	6.920800	0.510800	0.094900
C	7.521000	1.497900	0.990700
C	8.195200	2.705500	0.757300
H	8.351600	3.055300	-0.262100
C	8.639600	3.432800	1.864900
C	6.627900	-0.260200	2.157600
C	7.331800	1.012900	2.290300
C	7.794000	1.714700	3.411300
H	7.634400	1.312200	4.409800
C	8.428000	2.939900	3.198500
C	5.949700	-2.307200	3.091600
C	5.920600	-3.235600	4.221100
C	6.222900	-3.085400	5.581400
H	6.557800	-2.120800	5.963000
C	6.070400	-4.197600	6.414100
C	5.314800	-4.270700	2.267500
C	5.516000	-4.471500	3.700200
C	5.382100	-5.603100	4.514900
H	5.069000	-6.551800	4.082100
C	5.638000	-5.459600	5.879600
N	5.204500	-4.025200	-0.634200
N	5.673000	-3.628300	-2.985300
N	6.026200	-1.568900	-1.756400
N	7.021200	0.584300	-1.229300
N	6.337100	-0.489900	0.832700
N	6.409700	-1.063900	3.193100
N	5.515300	-2.946100	1.954900
N	5.061500	-5.276500	1.437100
O	4.590400	-9.900400	-1.563000
O	4.849600	-8.983200	-3.949000
O	7.570000	-1.076900	-7.511800
O	8.226400	1.217800	-6.561400
O	8.880200	3.753300	4.182600
O	6.299500	-4.200000	7.749000
O	5.500800	-6.448200	6.796200
C	5.064000	-8.572900	-5.288100
H	4.302600	-7.844000	-5.615700
H	6.067600	-8.130800	-5.415800
H	4.986400	-9.480800	-5.899200
C	4.484800	-10.494200	-0.284600
H	5.390400	-10.314400	0.320800
H	3.604300	-10.117700	0.266200
H	4.371300	-11.572200	-0.457200
C	5.144300	-7.741200	6.339400
H	5.128700	-8.382100	7.230100
H	4.145600	-7.743600	5.869200
H	5.885800	-8.131500	5.621200
C	6.786900	-3.015400	8.347900
H	7.751400	-2.707100	7.907500
H	6.065700	-2.184700	8.248800
H	6.929400	-3.247100	9.411300
C	7.282500	-2.325800	-8.108300
H	7.864500	-3.139800	-7.643000
H	6.206100	-2.569000	-8.038000
H	7.564600	-2.233500	-9.163900
C	8.688200	2.476900	-6.103200
H	9.495900	2.360500	-5.359900
H	9.081100	2.995200	-6.988200
H	7.870300	3.073600	-5.661500
C	8.770300	3.307800	5.524400
H	7.716200	3.172900	5.822200

H	9.315500	2.360700	5.677100	C	0.508400	-8.992800	2.317200	C	-0.271900	-0.855400	-6.571400
H	9.225200	4.093100	6.141200	H	1.393400	-9.090000	1.664800	C	0.562700	2.080000	-1.621000
O	9.284800	4.620600	1.799200	H	0.265500	-9.972000	2.748500	C	1.003500	3.458700	-1.481800
C	9.623400	5.149500	0.521800	H	-0.351100	-8.631900	1.730600	C	1.308200	4.448800	-2.426500
H	10.233300	4.414800	-0.036300	C	1.017700	-7.737900	-4.899100	H	1.225200	4.231300	-3.491200
H	8.702300	5.333000	-0.064300	H	0.127800	-7.543300	-4.274300	C	1.724300	5.691900	-1.953800
C	10.394200	6.442100	0.740100	H	0.777400	-8.504800	-5.645600	C	0.678300	2.488900	0.567600
H	11.274000	6.220900	1.367500	H	1.840500	-8.097400	-4.257900	C	1.096000	3.709800	-0.103500
H	9.761500	7.135000	1.321100	C	2.454800	-3.554900	-7.982000	C	1.528300	4.950800	0.386100
C	10.834000	7.100900	-0.571600	H	3.477600	-3.187600	-7.786400	H	1.595800	5.121100	1.459300
H	11.458600	6.392800	-1.145200	H	2.412800	-3.993500	-8.987000	C	1.849200	5.939500	-0.542400
H	9.945900	7.300900	-1.198600	H	1.740000	-2.718700	-7.920400	N	0.367900	1.519100	-0.370300
C	11.607600	8.403100	-0.357200	C	4.660600	3.317700	-6.631700	N	0.396500	1.483700	-2.795200
H	12.520000	8.230100	0.236400	H	5.325000	2.440100	-6.702600	N	-0.318900	-0.658500	-1.910600
H	11.911100	8.849900	-1.316700	H	3.611500	2.988500	-6.736000	O	2.042200	6.752400	-2.739500
H	10.996300	9.145600	0.181400	H	4.902600	4.024800	-7.434600	O	-0.117500	-0.576600	-7.890700
Cd	1.292600	-0.793900	0.025900	C	5.025600	5.021000	5.008200	O	-1.041100	-2.912700	-7.405200
C	2.187300	-3.697000	-1.601300	H	4.211100	5.382600	4.355500	C	-2.599400	-7.139900	4.147100
C	2.072000	-4.129300	-2.984000	H	5.261900	5.788800	5.755000	H	-3.235500	-6.299200	4.475900
C	1.699900	-5.355900	-3.550100	H	5.919800	4.818500	4.395300	H	-2.989200	-8.075300	4.567200
H	1.416400	-6.187700	-2.907100	C	3.621500	0.826300	8.091100	H	-1.565700	-6.987700	4.500100
C	1.730700	-5.466600	-4.938400	H	4.234700	-0.076600	7.922400	C	-2.728300	-8.177000	-1.136200
C	2.785600	-1.958500	-2.863300	H	3.816100	1.214200	9.098000	H	-1.769300	-8.038800	-1.664300
C	2.455300	-3.040100	-3.779400	H	2.552200	0.573000	7.999700	H	-2.998400	-9.240400	-1.146900
C	2.492000	-3.135600	-5.178300	O	5.315500	5.406000	-3.309600	H	-3.520100	-7.596900	-1.637700
H	2.791900	-2.277900	-5.778800	C	5.594400	6.270100	-2.206400	C	-1.468500	-4.255600	-7.239900
C	2.130500	-4.352600	-5.758000	H	6.334000	5.788200	-1.539700	H	-2.401300	-4.310300	-6.652100
C	3.485000	0.230300	-2.428400	H	4.669900	6.446700	-1.630200	H	-1.653900	-4.638100	-8.251900
C	3.923600	1.541800	-2.874400	C	6.139300	7.574500	-2.766400	H	-0.687100	-4.866400	-6.759700
C	4.136100	2.067500	-4.156200	H	7.028100	7.351300	-3.381400	C	0.300700	0.727300	-8.264400
H	3.949400	1.453000	-5.034900	H	5.385000	8.005500	-3.446200	H	1.280800	0.975900	-7.820800
C	4.609900	3.374600	-4.250300	C	6.493800	8.585700	-1.671300	H	0.391600	0.710000	-9.357200
C	3.858300	1.436000	-0.591000	H	5.595700	8.790800	-1.061900	H	-0.444900	1.483600	-7.974100
C	4.166500	2.300200	-1.720300	H	7.234700	8.138000	-0.984100	C	2.024700	6.584300	-4.147900
C	4.643400	3.615700	-1.799400	C	7.045900	9.900100	-2.225800	H	2.274400	7.566100	-4.569600
H	4.824900	4.188700	-0.891000	H	6.315500	10.389100	-2.890800	H	2.779200	5.848300	-4.470000
C	4.866500	4.153900	-3.067900	H	7.287400	10.605800	-1.415800	H	1.025500	6.278000	-4.502900
C	3.680800	1.036000	1.707200	H	7.965800	9.731300	-2.809400	C	0.892900	3.700400	7.239000
C	3.801100	1.467100	3.089700	C	-1.126200	-3.086400	-0.565900	H	0.189500	4.289900	6.625000
C	4.209600	2.682100	3.656100	C	-1.530600	-4.311800	0.105700	H	0.937900	4.128500	8.248800
H	4.491100	3.514700	3.014300	C	-1.899600	-5.572900	-0.383400	H	1.897600	3.727400	6.788800
C	4.257700	2.766400	5.046300	H	-1.914700	-5.760400	-1.455600	C	-0.654800	-1.354800	8.267100
C	3.099200	-0.706900	2.968500	C	-2.251900	-6.550600	0.545100	H	-0.604700	-1.384300	9.363000
C	3.443400	0.369100	3.885900	C	-1.043000	-2.666700	1.622100	H	-1.694300	-1.527800	7.946900
C	3.488100	0.438800	5.285500	C	-1.497100	-4.040900	1.482400	H	0.001600	-2.139900	7.851300
H	3.205500	-0.424400	5.886000	C	-1.864500	-5.009500	2.426500	O	2.279100	7.185600	-0.222700
C	3.897200	1.639700	5.866400	H	-1.834200	-4.775500	3.489600	C	2.327200	7.559900	1.155300
C	2.383400	-2.890700	2.533700	C	-2.249500	-6.263600	1.955200	H	3.039300	6.904400	1.691900
C	1.948800	-4.202900	2.980700	C	-0.443100	-0.823600	2.930300	H	1.329100	7.429800	1.606300
C	1.772400	-4.740900	4.262100	C	-0.247800	-0.180400	4.220500	C	2.759200	9.014700	1.238100
H	1.957200	-4.125600	5.142100	C	-0.387400	-0.649500	5.534300	H	3.754300	9.124000	0.773300
C	1.378600	-6.074700	4.358200	H	-0.698300	-1.677400	5.717400	H	2.059700	9.619500	0.637300
C	2.026500	-4.101400	0.696200	C	-0.130900	0.243600	6.573400	C	2.787200	9.533100	2.679900
C	1.731600	-4.970100	1.826000	C	0.226300	1.259900	2.505500	H	1.781300	9.418400	3.121400
C	1.336400	-6.313200	1.907300	C	0.154500	1.136700	3.953100	H	3.464000	8.902000	3.284800
H	1.171600	-6.890600	0.998200	C	0.401500	2.050600	4.986700	C	3.228000	10.994200	2.783500
C	1.161800	-6.865500	3.176400	H	0.709400	3.068500	4.754600	H	2.550500	11.654200	2.217700
N	2.635200	-2.385200	-1.554200	C	0.250400	1.603600	6.298300	H	3.233500	11.337000	3.829900
N	3.181800	-0.755300	-3.263200	N	-0.145000	0.066700	1.911600	H	4.243800	11.134300	2.378900
N	3.468100	0.186900	-1.043000	N	-0.859500	-2.075800	2.796200	Y	-4.992200	1.260900	-0.079200
N	3.960300	1.823400	0.676200	N	-0.831800	-2.110900	0.371400	C	-6.759900	0.668100	-2.877200
N	3.269500	-0.286700	1.661200	N	-1.073100	-2.962700	-1.885800	C	-7.400900	-0.434200	-3.591000
N	2.696200	-1.908100	3.368600	N	0.609200	2.370900	1.886800	C	-7.719700	-0.634100	-4.941500
N	2.436400	-2.859400	1.149300	O	0.439800	2.366300	7.404900	H	-7.481600	0.134300	-5.677400
N	1.917400	-4.487500	-0.570100	O	-0.209700	-0.059500	7.893600	C	-8.331200	-1.837600	-5.300000
O	1.398100	-6.585500	-5.631100	O	-2.642500	-7.299300	2.737900	C	-7.274600	-0.850700	-1.340900
O	2.106400	-4.600200	-7.087700	O	-2.619900	-7.818700	0.232900	C	-7.721200	-1.393000	-2.620700
O	4.861300	4.021800	-5.417800	C	-0.706600	-1.846600	-2.504400	C	-8.358400	-2.593900	-2.958500
O	4.629500	3.872600	5.739500	C	-0.648000	-1.718900	-3.952500	H	-8.597200	-3.320400	-2.183300
O	3.984100	1.866600	7.197300	C	-0.957900	-2.612000	-4.987300	C	-8.643200	-2.826600	-4.304900
O	1.164900	-6.733300	5.525400	H	-1.318700	-3.613300	-4.755600	C	-7.334200	-0.892900	1.008900
O	0.775500	-8.140100	3.419900	C	-0.776300	-2.175000	-6.298400	C	-7.838100	-1.473600	2.252100
C	1.381600	-6.034900	6.740000	C	-0.003800	0.225700	-2.928500	C	-8.508600	-2.671600	2.535900
H	0.726500	-5.148900	6.817100	C	-0.186500	-0.421000	-4.219000	H	-8.748800	-3.367300	1.733000
H	1.136000	-6.739800	7.543200	C	0.017000	0.027100	-5.531500	C	-8.841700	-2.937500	3.867100
H	2.434400	-5.718700	6.839900	H	0.379400	1.038000	-5.713700	C	-6.874200	0.573700	2.612600

C	-7.542000	-0.550400	3.262400	H	-4.808500	-3.692000	-3.664000	H	-6.309400	-5.196900	-4.728600
C	-7.891900	-0.787300	4.597900	C	-5.366400	-5.183900	-2.177100	C	-3.661100	-0.131100	-8.353600
H	-7.652200	-0.050100	5.362800	C	-4.328400	-2.054700	0.441700	H	-4.656400	-0.384200	-7.949700
C	-8.522600	-1.994000	4.905000	C	-4.721100	-3.266600	-0.263300	H	-3.713100	-0.090200	-9.448500
C	-6.150600	2.809500	2.671500	C	-5.181300	-4.513000	0.185100	H	-2.929100	-0.899000	-8.053700
C	-6.038200	4.085300	3.375600	H	-5.272300	-4.711100	1.252800	C	-2.028100	4.864100	-7.149200
C	-6.217000	4.447100	4.718500	C	-5.506100	-5.472300	-0.774000	H	-1.083900	4.896000	-6.576900
H	-6.500600	3.694700	5.453900	C	-3.957400	-0.847500	2.409500	H	-1.867000	5.301000	-8.142700
C	-6.010100	5.783500	5.070900	C	-3.949300	-0.742200	3.859200	H	-2.797200	5.446600	-6.613900
C	-5.623300	4.324700	1.134800	C	-4.286000	-1.658800	4.863400				
C	-5.700700	5.038700	2.406800	H	-4.608800	-2.665000	4.596600	471			
C	-5.515000	6.386900	2.736000	C	-4.211900	-1.229300	6.186200	**[5]**$^{+2}$ with butoxy			
H	-5.256200	7.106800	1.961100	C	-3.295600	1.225800	2.891800	Y	5.020600	1.061600	-0.087700
C	-5.647200	6.756600	4.075900	C	-3.541300	0.564800	4.165000	C	5.707100	4.221100	-0.998600
C	-5.576000	4.371200	-1.215300	C	-3.462600	1.012200	5.492000	C	5.652000	5.589000	-0.488000
C	-5.601900	5.125100	-2.467600	H	-3.142600	2.029800	5.707900	C	5.605000	6.828600	-1.136700
C	-5.426800	6.484900	-2.759600	C	-3.799700	0.112500	6.504300	H	5.573900	6.876100	-2.224900
H	-5.233600	7.195600	-1.957200	C	-2.657400	3.087700	1.629200	C	5.595000	7.981600	-0.345800
C	-5.498600	6.883000	-4.097500	C	-2.208100	4.466300	1.526400	C	5.798200	4.065100	1.213100
C	-6.023700	2.900400	-2.818700	C	-1.927900	5.431200	2.501800	C	5.714300	5.492100	0.906700
C	-5.878800	4.195700	-3.477600	H	-2.025300	5.182400	3.557400	C	5.739300	6.636100	1.715100
C	-5.981500	4.580300	-4.820500	C	-1.550700	6.700900	2.069700	H	5.817100	6.540800	2.798300
H	-6.200300	3.836100	-5.585000	C	-2.483300	3.538400	-0.547100	C	5.670000	7.885200	1.087400
C	-5.766900	5.923600	-5.133800	C	-2.105000	4.754700	0.158100	C	6.308900	2.347600	2.736000
N	-6.640100	0.352900	-1.546100	C	-1.727200	6.027300	-0.292500	C	6.773000	1.943400	4.061900
N	-7.549500	-1.442700	-0.182300	H	-1.651400	6.230800	-1.359300	C	6.910000	2.651100	5.261600
N	-6.704000	0.299100	1.275500	C	-1.451100	7.002400	0.666000	H	6.616100	3.698100	5.315100
N	-6.579300	1.696500	3.260300	C	-2.838400	2.324900	-2.514900	C	7.427600	1.969900	6.367500
N	-5.828000	2.981200	1.346800	C	-2.850900	2.222100	-3.964300	C	6.916900	0.220600	2.560700
N	-5.460100	4.953200	-0.025700	C	-2.549400	3.150600	-4.969400	C	7.160800	0.602600	3.951100
N	-5.764100	3.035000	-1.474800	H	-2.224300	4.154300	-4.702300	C	7.712300	-0.087200	5.039100
N	-6.429400	1.813600	-3.468200	C	-2.703900	2.746600	-6.294100	H	8.035000	-1.121800	4.926000
O	-8.675700	-2.181700	-6.563800	C	-3.516200	0.257300	-2.997800	C	7.837800	0.596300	6.253700
O	-9.206900	-3.960000	-4.787600	C	-3.284500	0.923900	-4.270900	C	7.297600	-1.254300	0.769200
O	-9.467900	-4.057600	4.297900	C	-3.445600	0.502700	-5.598600	C	7.953100	-2.452200	0.248200
O	-8.871300	-2.384000	6.154300	H	-3.781900	-0.509800	-5.816000	C	8.587500	-3.524600	0.886100
O	-6.121600	6.277400	6.326400	C	-3.155500	1.417500	-6.611400	H	8.623500	-3.570900	1.973500
O	-5.447300	8.008800	4.552600	N	-4.000700	-1.064200	-0.467800	C	9.158600	-4.516800	0.085000
O	-5.328500	8.152800	-4.535300	N	-4.313500	-1.951900	1.766400	C	7.217200	-1.095100	-1.442100
O	-5.781900	6.432400	-6.389100	N	-3.573200	0.360100	1.848200	C	7.907300	-2.350600	-1.147000
C	-6.105500	5.564100	-7.461800	N	-2.878900	2.483400	2.789400	C	8.503600	-3.317900	-1.967300
H	-5.363800	4.753200	-7.565200	N	-2.831300	2.553900	0.361400	H	8.482000	-3.206500	-3.050900
H	-7.108600	5.124100	-7.330600	N	-2.491700	3.433100	-1.871200	C	9.123200	-4.409500	-1.350000
H	-6.095800	6.184600	-8.366700	N	-3.258600	1.130200	-1.953900	C	6.695800	0.619300	-2.965300
C	-8.461100	-1.241700	-7.598100	N	-3.925900	-1.001600	-2.894900	C	6.832100	1.193700	-4.300700
H	-9.014600	-0.305100	-7.412700	O	-5.708600	-6.207300	-2.999800	C	7.280600	0.652400	-5.512000
H	-7.387700	-1.008400	-7.715800	O	-5.952300	-6.720000	-0.501900	H	7.580300	-0.392900	-5.565300
H	-8.834000	-1.709500	-8.517700	O	-4.503100	-2.000100	7.265600	C	7.324300	1.493500	-6.627800
C	-9.606600	-4.956700	-3.862300	O	-3.766900	0.388600	7.828300	C	6.098500	2.749400	-2.789600
H	-8.743700	-5.364500	-3.306900	O	-1.246500	7.737300	2.892700	C	6.460400	2.539800	-4.191600
H	-10.347000	-4.563700	-3.144100	O	-1.065800	8.270800	0.393500	C	6.529700	3.405400	-5.290200
H	-10.066600	-5.755300	-4.457900	O	-2.450800	3.530400	-7.373300	H	6.263200	4.455900	-5.178400
C	-9.874700	-5.011400	3.336500	O	-3.252100	1.162500	-7.936700	C	6.954800	2.878600	-6.515000
H	-10.575800	-4.573600	2.605000	C	-0.909800	8.658200	-0.963100	N	5.727300	3.332900	0.052600
H	-9.008600	-5.434800	2.794900	H	-1.848900	8.525100	-1.526900	N	6.006700	3.608200	2.445200
H	-10.379500	-5.810000	3.893100	H	-0.646300	9.723400	-0.942300	N	6.347700	1.270100	1.880400
C	-8.653100	-1.482500	7.224900	H	-0.097900	8.093100	-1.450100	N	7.297000	-0.953200	2.064400
H	-9.198000	-0.535400	7.068000	C	-1.345300	7.533900	4.291900	N	6.811500	-0.499600	-0.273000
H	-9.038600	-1.979400	8.122700	H	-0.671500	6.726600	4.629300	N	7.111700	-0.610000	-2.676300
H	-7.579100	-1.264900	7.358800	H	-1.041500	8.480000	4.758000	N	6.190700	1.564100	-2.101100
C	-6.535800	5.402300	7.357600	H	-2.379400	7.293300	4.592400	N	5.821200	3.952700	-2.294700
H	-7.529000	4.970700	7.146600	C	-3.344300	1.678300	8.245000	O	5.523000	9.241000	-0.824300
H	-5.811000	4.580500	7.505000	H	-3.985200	2.466200	7.813400	O	5.674500	9.072300	1.729500
H	-6.586900	6.008500	8.270300	H	-3.444100	1.687000	9.337300	O	7.591300	2.508900	7.594000
C	-5.153700	9.039700	3.626000	H	-2.291700	1.861600	7.975000	O	8.340200	0.065700	7.387900
H	-4.200100	8.853200	3.100400	C	-4.943300	-3.329000	7.040700	O	9.777500	-5.621700	0.553100
H	-5.960600	9.152800	2.882800	H	-5.891000	-3.348900	6.477800	O	9.730400	-5.422200	-2.002600
H	-5.069700	9.961300	4.215200	H	-4.183800	-3.918400	6.497700	O	7.706400	1.109900	-7.863900
C	-5.121300	9.171600	-3.576900	H	-5.100600	-3.767500	8.034500	O	7.064000	3.583200	-7.660700
H	-5.967600	9.239900	-2.870400	C	-6.095600	-7.111000	0.854400	C	5.837300	9.083600	3.136700
H	-4.190200	9.006800	-3.005700	H	-6.792000	-6.444100	1.391300	H	4.999900	8.570900	3.642400
H	-5.041300	10.109000	-4.140600	H	-6.511900	-8.126300	0.831000	H	6.786500	8.606600	3.434700
Cd	-1.756600	0.202100	-0.024900	H	-5.122400	-7.129300	1.371400	H	5.849500	10.139200	3.432700
C	-4.138300	-1.609600	-1.733800	C	-5.626100	-5.998900	-4.400400	C	5.555300	9.436800	-2.228600
C	-4.593000	-2.986000	-1.631600	H	-4.595900	-5.748300	-4.709300	H	6.484100	9.032100	-2.666500
C	-4.908000	-3.940700	-2.607800	H	-5.925900	-6.945800	-4.865500	H	4.686900	8.968300	-2.722800

H	5.522200	10.522500	-2.383500	O	5.069100	-4.872600	5.382300	C	0.927800	-2.710800	1.617200
C	6.807700	4.976200	-7.629400	O	5.537400	-6.231300	3.264100	C	1.314000	-4.105100	1.474400
H	6.992000	5.341800	-8.646900	O	4.803400	-4.655900	-5.778000	C	1.579800	-5.107900	2.418800
H	5.760100	5.186500	-7.349400	O	4.311200	-2.595400	-7.215700	H	1.506300	-4.890600	3.483600
H	7.481300	5.491800	-6.925300	O	1.754700	6.081500	-5.497000	C	1.947700	-6.365400	1.944400
C	8.193300	-0.210600	-8.046000	O	1.509300	7.503700	-3.383100	C	1.023600	-3.121800	-0.572300
H	9.079300	-0.398000	-7.416200	C	1.931600	5.390900	-6.721300	C	1.395500	-4.357700	0.096300
H	7.417800	-0.962500	-7.815100	H	1.244700	4.529000	-6.801700	C	1.780000	-5.613000	-0.396600
H	8.472700	-0.286100	-9.103200	H	1.704300	6.114200	-7.514600	H	1.840700	-5.784700	-1.469900
C	7.316600	3.889400	7.770500	H	2.969500	5.034600	-6.834500	C	2.063800	-6.614900	0.530500
H	7.949700	4.509400	7.113600	C	1.281000	8.364900	-2.272600	N	0.752600	-2.140600	0.367000
H	6.254200	4.118400	7.574300	H	2.172900	8.427500	-1.626900	N	0.788100	-2.109600	2.792500
H	7.550000	4.111100	8.819000	H	1.073400	9.352000	-2.702300	N	0.154900	0.059500	1.910800
C	8.853500	-1.254100	7.352300	H	0.410900	8.032400	-1.686200	O	2.459300	-7.871900	0.217200
H	9.674000	-1.345400	6.621100	C	1.675300	7.039600	4.951200	O	2.222700	-7.438500	2.723300
H	9.237200	-1.457900	8.359800	H	0.778600	6.884400	4.326100	O	0.370000	-0.033600	7.888700
H	8.065000	-1.987100	7.105700	H	1.464900	7.804000	5.709500	O	-0.470100	2.329900	7.410200
C	9.955600	-5.757500	1.953900	H	2.506900	7.376900	4.309200	C	-1.902600	6.635400	-4.132600
H	10.545800	-4.920500	2.363700	C	3.050500	2.803300	7.986600	H	-2.576600	5.822000	-4.455200
H	8.987000	-5.811900	2.481700	H	4.058200	2.401500	7.787300	H	-2.259900	7.587300	-4.543200
H	10.503100	-6.696000	2.098700	H	3.024400	3.239900	8.991600	H	-0.880200	6.443800	-4.495900
C	9.825800	-5.361000	-3.414100	H	2.301800	1.996800	7.920500	C	-0.856400	3.688400	7.255000
H	8.826900	-5.370000	-3.886600	C	4.897200	-4.181700	6.606100	H	-1.790100	3.774300	6.672400
H	10.371000	-4.457900	-3.740800	H	5.596400	-3.331200	6.686700	H	-1.025300	4.069000	8.269700
H	10.381700	-6.254800	-3.720100	H	3.864100	-3.808400	6.717400	H	-0.057000	4.276000	6.775300
Cd	1.753500	0.132600	-0.028500	H	5.112000	-4.908600	7.399300	C	0.747800	-1.348300	8.268600
C	2.782700	3.006300	1.601800	C	5.759800	-7.094300	2.153500	H	1.718200	-1.629400	7.822600
C	2.676100	3.436600	2.987000	H	6.528500	-6.684200	1.477500	H	0.841900	-1.329500	9.360800
C	2.328900	4.664700	3.566700	H	6.116700	-8.039100	2.579800	H	-0.023300	-2.082000	7.982500
H	2.054000	5.508100	2.934300	H	4.824900	-7.275600	1.599900	C	2.206700	-7.281900	4.134300
C	2.354200	4.757500	4.957800	C	5.152300	-5.829700	-5.066500	H	2.416700	-8.275600	4.547900
C	3.319100	1.242000	2.855800	H	4.330400	-6.163600	-4.409500	H	2.986700	-6.578100	4.465400
C	3.026200	2.332100	3.776100	H	5.350200	-6.597500	-5.823900	H	1.217300	-6.941900	4.487500
C	3.069700	2.410400	5.174000	H	6.059100	-5.673200	-4.456000	C	2.537000	-8.244000	-1.150600
H	3.353200	1.541800	5.764900	C	3.990300	-1.532700	-8.105700	H	3.241200	-7.597100	-1.701800
C	2.740900	3.631300	5.767700	H	4.642500	-0.659300	-7.936300	H	2.909500	-9.275200	-1.159300
C	3.930100	-0.974700	2.424200	H	4.163800	-1.927400	-9.113700	H	1.544700	-8.211900	-1.628700
C	4.307000	-2.307000	2.867300	H	2.932800	-1.239600	-8.007900	C	1.160500	-4.334900	-7.253300
C	4.480600	-2.860300	4.143100	C	-0.560500	2.520600	0.571200	H	0.431400	-4.893000	-6.640400
H	4.299700	-2.254200	5.030000	C	-0.917800	3.760600	-0.097600	H	1.181800	-4.756400	-8.265200
C	4.887000	-4.191700	4.225900	C	-1.234400	5.035300	0.394200	H	2.164500	-4.410100	-6.805900
C	4.252400	-2.186000	0.581300	H	-1.236000	5.223900	1.466600	C	-0.161500	0.782400	-8.271100
C	4.524500	-3.066600	1.708800	C	-1.551200	6.027900	-0.532000	H	-0.109400	0.804900	-9.367100
C	4.945400	-4.400800	1.772600	C	-0.499600	2.099500	-1.618000	H	-1.193500	1.002800	-7.952500
H	5.114300	-4.967100	0.857900	C	-0.900400	3.489700	-1.475100	H	0.530500	1.536500	-7.856600
C	5.135400	-4.964500	3.035500	C	-1.233900	4.473400	-2.417300	O	-1.857300	7.307700	-0.216000
C	4.083700	-1.785300	-1.717900	H	-1.218600	4.239400	-3.481400	C	-1.923400	7.682400	1.163000
C	4.173100	-2.221500	-3.102300	C	-1.567000	5.740700	-1.944200	H	-0.960500	7.448000	1.654600
C	4.505700	-3.453700	-3.681800	C	0.025200	0.236000	-2.929700	H	-2.719200	7.101700	1.660100
H	4.735700	-4.309000	-3.048900	C	0.193100	-0.412100	-4.221100	C	-2.216700	9.171800	1.237700
C	4.528600	-3.531900	-5.074300	C	0.071000	0.064400	-5.533800	H	-1.414500	9.723200	0.717900
C	3.569800	-0.015600	-2.971900	H	-0.197200	1.104100	-5.716400	H	-3.148900	9.373700	0.684600
C	3.863400	-1.104500	-3.892600	C	0.289300	-0.836600	-6.574300	C	-2.349600	9.668700	2.681500
C	3.894900	-1.162500	-5.291400	C	0.613800	-1.874200	-2.509000	H	-3.155000	9.104600	3.185100
H	3.657700	-0.279700	-5.883500	C	0.543300	-1.745600	-3.955600	H	-1.420500	9.439300	3.235700
C	4.237000	-2.378600	-5.885500	C	0.750000	-2.668000	-4.991400	C	-2.639500	11.167800	2.775100
C	2.937500	2.195000	-2.540100	H	1.016500	-3.698300	-4.761300	H	-2.731800	11.491800	3.823100
C	2.541900	3.522700	-2.983700	C	0.614900	-2.212800	-6.301400	H	-1.834500	11.759800	2.310100
C	2.355000	4.071300	-4.259200	N	0.290700	-0.665800	-1.912300	H	-3.580200	11.423000	2.261000
H	2.490400	3.452400	-5.144400	N	-0.342400	1.503500	-2.793000	Y	-4.574900	-1.667400	0.088100
C	1.996900	5.417800	-4.341600	N	-0.306600	1.533600	-0.367200	C	-6.070600	-1.847700	3.090200
C	2.636300	3.413300	-0.697700	N	-0.508500	2.392100	1.891200	C	-6.618400	-0.993400	4.140700
C	2.366100	4.294400	-1.825500	N	0.955100	-2.998000	-1.891800	C	-6.847100	-1.214700	5.503500
C	2.019800	5.649900	-1.890400	O	0.768400	-2.978100	-7.408700	H	-6.571200	-2.165300	5.957400
H	1.896500	6.229200	-0.976600	O	0.222000	-0.530900	-7.892000	C	-7.430400	-0.183100	6.245800
C	1.842600	6.216100	-3.153900	O	-1.924400	6.790600	-2.720800	C	-6.636700	0.059300	2.108100
N	3.183100	1.681200	1.547100	C	-0.185600	1.262900	2.508200	C	-6.980900	0.209600	3.522000
N	3.665700	0.026800	3.258500	C	-0.129700	1.130200	3.954900	C	-7.597000	1.241900	4.240600
N	3.914100	-0.922700	1.040300	C	-0.404200	2.033300	4.991900	H	-7.897800	2.158100	3.734700
N	4.334600	-2.581900	-0.682600	H	-0.728800	3.047200	4.763500	C	-7.814300	1.048900	5.609300
N	3.729200	-0.448200	-1.663800	C	-0.235100	1.588200	6.302700	C	-6.874800	0.771900	-0.119800
N	3.210400	1.197000	-3.374100	C	0.438000	-0.837000	2.929600	C	-7.477200	1.687600	-1.087200
N	2.997800	2.156600	-1.157200	C	0.283600	-0.185500	4.219000	C	-8.139000	2.910200	-0.931300
N	2.541800	3.804900	0.567300	C	0.474600	-0.642100	5.531400	H	-8.248500	3.351100	0.059100
O	2.020400	5.864900	5.663300	H	0.800800	-1.665400	5.712300	C	-8.641700	3.534000	-2.077600
O	2.734400	3.867300	7.095900	C	0.221400	0.249200	6.573100	C	-6.645600	-0.184100	-2.109100

C	-7.338000	1.083100	-2.342700
C	-7.863300	1.675500	-3.498500
H	-7.769100	1.175100	-4.460900
C	-8.509600	2.909400	-3.366600
C	-6.042900	-2.329900	-2.860200
C	-6.094800	-3.355700	-3.898700
C	-6.451600	-3.301100	-5.251000
H	-6.733600	-2.351300	-5.705200
C	-6.429900	-4.491700	-5.983600
C	-5.487100	-4.240700	-1.877300
C	-5.749000	-4.562400	-3.279800
C	-5.753400	-5.771400	-3.987700
H	-5.508600	-6.704800	-3.481100
C	-6.086700	-5.735100	-5.346100
C	-5.238300	-4.950100	0.351000
C	-5.236300	-6.035700	1.328900
C	-5.159800	-7.426000	1.183800
H	-5.055400	-7.867400	0.192800
C	-5.219600	-8.209000	2.339900
C	-5.479500	-3.996600	2.339800
C	-5.392100	-5.436200	2.583900
C	-5.488100	-6.205300	3.751500
H	-5.638200	-5.721800	4.715600
C	-5.392400	-7.595900	3.630000
N	-6.036100	-1.157900	1.899200
N	-6.966900	0.965800	1.191100
N	-6.328100	-0.306100	-0.778900
N	-6.462100	-1.087000	-3.070500
N	-5.610200	-2.886700	-1.678000
N	-5.260000	-5.175600	-0.959100
N	-5.318800	-3.739700	1.000500
N	-5.764500	-3.123800	3.302700
O	-7.685700	-0.238600	7.570200
O	-8.386300	1.951500	6.434100
O	-9.056600	3.605300	-4.384800
O	-6.721000	-4.592500	-7.297100
O	-6.125400	-6.811600	-6.159600
O	-5.131700	-9.555800	2.361900
O	-5.457000	-8.465900	4.659700
C	-5.715000	-7.964000	5.958700
H	-4.907300	-7.290800	6.298300
H	-6.676300	-7.422600	5.996400
H	-5.761900	-8.838100	6.617900
C	-7.442200	-1.454400	8.257600
H	-8.036400	-2.280500	7.831600
H	-6.372000	-1.726300	8.233100
H	-7.749900	-1.281400	9.296400
C	-8.879600	3.158400	5.882600
H	-8.066000	3.760400	5.439400
H	-9.646300	2.965700	5.113300
H	-9.329000	3.711900	6.716100
C	-9.056500	3.030100	-5.679400
H	-9.589200	2.064600	-5.689000
H	-9.578000	3.743200	-6.328900
H	-8.027900	2.878600	-6.052100
C	-7.176200	-3.436300	-7.982100
H	-8.101900	-3.042400	-7.526900
H	-6.410000	-2.642400	-7.989900
H	-7.381900	-3.756100	-9.009900
C	-5.890900	-8.092100	-5.603400
H	-4.867200	-8.172100	-5.193600
H	-6.618100	-8.324600	-4.806800
H	-6.009700	-8.807500	-6.426900
C	-5.070600	-10.251500	1.127100
H	-5.961100	-10.047300	0.509600
H	-4.163600	-9.985600	0.557200
H	-5.040300	-11.317800	1.383000
O	-9.277000	4.723400	-2.089100
C	-9.577300	5.364100	-0.847900
H	-10.182100	4.683700	-0.220600
H	-8.639300	5.580600	-0.303000
C	-10.335700	6.645000	-1.155700
H	-11.243100	6.386600	-1.726800
H	-9.714400	7.269400	-1.820400
C	-10.709800	7.429700	0.106500
H	-11.327300	6.792200	0.764400
H	-9.793200	7.662200	0.679000
C	-11.462400	8.726200	-0.198200
H	-12.399700	8.524100	-0.741100
H	-11.719600	9.264400	0.727000
H	-10.855100	9.402000	-0.822600
Cd	-1.307900	-0.738900	0.027100
C	-3.633000	1.160600	1.748100
C	-4.022100	2.557700	1.647000
C	-4.274700	3.536900	2.616600
H	-4.163800	3.300000	3.673800
C	-4.669400	4.801600	2.176800
C	-3.812600	1.609600	-0.428300
C	-4.149000	2.838400	0.277300
C	-4.556200	4.097300	-0.179700
H	-4.654800	4.288000	-1.247000
C	-4.825900	5.081200	0.773300
C	-3.491700	0.397700	-2.403000
C	-3.479500	0.295300	-3.853600
C	-3.755500	1.225800	-4.864600
H	-4.018000	2.250100	-4.606500
C	-3.682300	0.789600	-6.188400
C	-2.915600	-1.701300	-2.884100
C	-3.131400	-1.028700	-4.157300
C	-3.064900	-1.486900	-5.479800
H	-2.799700	-2.522700	-5.689100
C	-3.350400	-0.577200	-6.498900
C	-2.343100	-3.592500	-1.631200
C	-1.935200	-4.985100	-1.529600
C	-1.668100	-5.960200	-2.499400
H	-1.734600	-5.709600	-3.557600
C	-1.323100	-7.238100	-2.059500
C	-2.184800	-4.047600	0.545400
C	-1.849400	-5.276600	-0.160000
C	-1.516500	-6.557500	0.299300
H	-1.464700	-6.760500	1.367400
C	-1.260600	-7.544400	-0.653900
C	-2.483300	-2.829100	2.520700
C	-2.478100	-2.721800	3.970700
C	-2.188500	-3.648300	4.981700
H	-1.881200	-4.661100	4.722200
C	-2.310300	-3.226100	6.305800
C	-3.081800	-0.736500	3.002200
C	-2.867900	-1.409500	4.275700
C	-3.008100	-0.972700	5.598200
H	-3.320600	0.048800	5.808800
C	-2.736900	-1.887100	6.618600
N	-3.522400	0.606800	0.484000
N	-3.802400	1.514200	-1.751700
N	-3.158000	-0.822300	-1.839800
N	-2.545500	-2.972500	-2.789100
N	-2.497300	-3.050900	-0.365600
N	-2.182400	-3.948500	1.868900
N	-2.860700	-1.621500	1.958100
N	-3.439300	0.538200	2.906300
O	-4.922100	5.855700	2.989600
O	-3.893300	1.573900	-7.271200
O	-3.331100	-0.862700	-7.817400
O	-1.011200	-8.275100	-2.872100
O	-0.929600	-8.821800	-0.373200
O	-2.039800	-3.994400	7.388000
O	-2.826200	-1.620500	7.938400
C	-0.789400	-9.214400	0.987800
H	-1.724700	-9.047200	1.548800
H	-0.564600	-10.287400	0.965500
H	0.043700	-8.678700	1.470400
C	-1.094100	-8.084000	-4.273500
H	-0.392300	-7.302500	-4.616200
H	-0.822600	-9.043300	-4.729000
H	-2.117800	-7.807300	-4.579400
C	-2.961900	-2.173500	-8.232500
H	-3.635400	-2.933000	-7.801400
H	-3.061100	-2.176800	-9.325400
H	-1.917300	-2.396300	-7.961800
C	-4.275100	2.921600	-7.064000
H	-5.223000	2.986800	-6.502000
H	-3.496000	3.483900	-6.520100
H	-4.410700	3.357100	-8.061700
C	-4.843000	5.662200	4.389900
H	-3.825000	5.370300	4.701400
H	-5.102100	6.626100	4.845300
H	-5.557300	4.891000	4.728500
C	-3.188300	-0.308800	8.353700
H	-4.175400	-0.021900	7.952800
H	-3.237800	-0.346900	9.448500
H	-2.427000	0.427800	8.049100
C	-1.662900	-5.343600	7.180500
H	-0.722200	-5.416300	6.605500
H	-1.514900	-5.774500	8.178100
H	-2.452100	-5.903300	6.650200
O	-5.234200	6.334700	0.489800
C	-5.420200	6.714400	-0.880100
H	-6.102100	5.996100	-1.369900
H	-4.447500	6.687000	-1.400600
C	-6.010600	8.114600	-0.904000
H	-6.951200	8.112900	-0.326800
H	-5.322100	8.799400	-0.381300
C	-6.266900	8.616100	-2.329600
H	-5.316300	8.609200	-2.892800
H	-6.938100	7.909600	-2.850700
C	-6.874400	10.019400	-2.370000
H	-7.041200	10.352000	-3.406000
H	-7.845300	10.048300	-1.848400
H	-6.213200	10.754700	-1.883200

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[5]$^{+3}$ with butoxy

Y	5.044300	0.905600	-0.110100
C	6.478500	1.856000	2.783900
C	6.999600	1.312400	4.038100
C	7.256200	1.901000	5.280800
H	7.016800	2.950100	5.451800
C	7.839800	1.105100	6.274900
C	7.002200	-0.256700	2.370200
C	7.331500	-0.022500	3.777400
C	7.936200	-0.828800	4.747900
H	8.213900	-1.856700	4.514200
C	8.181900	-0.266700	6.006300
C	7.281800	-1.550900	0.427500
C	7.909800	-2.695000	-0.234900
C	8.580500	-3.816300	0.265600
H	8.664400	-3.972400	1.340300
C	9.144400	-4.708000	-0.656300
C	7.135700	-1.162000	-1.749700
C	7.817300	-2.448700	-1.609700
C	8.394100	-3.313500	-2.547600
H	8.336900	-3.087400	-3.611700
C	9.051600	-4.454600	-2.070600
C	6.631900	0.715900	-3.072100
C	6.778800	1.428200	-4.342200
C	7.230300	1.017300	-5.601300
H	7.507500	-0.022100	-5.773000
C	7.324500	1.983000	-6.610300
C	6.111200	2.829800	-2.659000
C	6.450700	2.763500	-4.081300
C	6.560000	3.749600	-5.068300
H	6.328400	4.788700	-4.835200
C	6.988300	3.357000	-6.341900
C	5.828000	4.123600	-0.715600
C	5.868100	5.434900	-0.068100
C	5.906100	6.734500	-0.585000
H	5.860200	6.900400	-1.660500
C	6.020600	7.796700	0.320800
C	5.976900	3.734500	1.461000
C	5.962700	5.189200	1.306200
C	6.101300	6.233600	2.227300
H	6.204000	6.019500	3.291100
C	6.119300	7.545600	1.734900
N	6.437100	0.870700	1.824700
N	7.330500	-1.384300	1.745900
N	6.775000	-0.684600	-0.512000
N	7.012800	-0.549100	-2.924200
N	6.170500	1.574100	-2.102200

N	5.892800	3.985000	-2.036400	C	2.513600	4.520300	3.638600	N	-0.259300	1.552100	-0.320700
N	5.832700	3.129200	0.235600	H	2.261600	5.383400	3.023500	N	-0.412400	2.366200	1.960000
N	6.210200	3.149900	2.632700	C	2.537900	4.583700	5.032600	N	0.179300	0.014000	1.919500
O	8.139200	1.524100	7.517500	C	3.406300	1.086600	2.854700	N	0.752500	-2.193800	2.746000
O	8.751100	-0.912900	7.040400	C	3.149400	2.164600	3.801000	N	-0.320600	1.577900	-2.745800
O	9.810400	-5.829400	-0.331100	C	3.191100	2.213000	5.199800	O	-1.745300	6.905700	-2.536400
O	9.647700	-5.378400	-2.843200	H	3.446200	1.323300	5.773600	O	-0.325000	2.174700	7.473900
O	7.732500	1.742400	-7.869000	C	2.889900	3.428700	5.818700	O	0.461400	-0.216700	7.889400
O	7.138200	4.183300	-7.392600	N	3.916800	-1.059300	0.986400	C	0.861000	-2.773400	1.557200
O	6.061600	9.097100	-0.019300	N	4.267400	-2.694500	-0.773800	C	1.201600	-4.174800	1.379000
O	6.240400	8.650300	2.491400	N	3.719800	-0.520400	-1.705400	C	1.441400	-5.206800	2.298000
C	9.224700	-2.236900	6.848400	N	3.234400	1.173400	-3.375400	H	1.381400	-5.014100	3.368000
H	8.399800	-2.926200	6.597900	N	3.075800	2.093500	-1.135100	C	1.765700	-6.464700	1.791500
H	9.987900	-2.273900	6.052200	N	2.685900	3.717600	0.626100	C	0.922800	-3.137400	-0.643400
H	9.675300	-2.535800	7.801600	N	3.272800	1.554600	1.556700	C	1.263200	-4.397600	-0.006700
C	7.948500	2.891200	7.849100	N	3.718200	-0.149500	3.227900	C	1.606900	-5.651900	-0.531000
H	8.543400	3.545900	7.191100	O	4.942100	-5.133900	5.242800	H	1.656800	-5.801700	-1.609000
H	6.883400	3.175300	7.783200	O	5.326600	-6.472400	3.101000	C	1.867800	-6.684000	0.369600
H	8.292200	3.000400	8.884200	O	4.576700	-4.693700	-5.904000	C	0.530600	-1.834100	-2.547200
C	6.454800	8.508600	3.887400	O	4.115700	-2.602800	-7.297100	C	0.448500	-1.671000	-3.988900
H	6.559800	9.527100	4.280700	O	1.868000	6.122000	-5.387800	C	0.612300	-2.576600	-5.046800
H	5.597500	8.012300	4.376500	O	1.665300	7.505900	-3.249600	H	0.843700	-3.621100	-4.844000
H	7.374400	7.936500	4.092700	O	2.234800	5.681600	5.758600	C	0.479400	-2.087900	-6.346100
C	6.087000	9.448600	-1.395600	O	2.876900	3.637000	7.148400	C	0.005600	0.303400	-2.915000
H	6.961700	9.006900	-1.902000	C	1.925400	6.886400	5.076500	C	0.141200	-0.319900	-4.220500
H	5.164400	9.126400	-1.908600	H	1.022400	6.773200	4.450400	C	0.024100	0.190200	-5.522500
H	6.158800	10.541900	-1.424900	H	1.741100	7.636200	5.854300	H	-0.207900	1.242300	-5.679000
C	10.058200	-6.112900	1.037600	H	2.767100	7.211400	4.440900	C	0.203100	-0.693800	-6.585000
H	10.641400	-5.304500	1.511000	C	3.191200	2.557900	8.023700	N	0.252500	-0.629900	-1.919300
H	9.116300	-6.259200	1.593800	H	4.191000	2.147800	7.804300	N	0.842900	-2.981900	-1.959400
H	10.640600	-7.041200	1.052900	H	3.184200	2.984500	9.033900	N	0.691100	-2.167900	0.320900
C	9.709100	-5.168400	-4.245200	H	2.432000	1.762100	7.959200	O	0.136500	-0.357100	-7.893500
H	10.239500	-4.231600	-4.485000	C	4.811900	-4.463300	6.485400	O	0.592400	-2.831400	-7.469700
H	10.267100	-6.019800	-4.653400	H	3.794200	-4.053000	6.616200	O	2.226300	-7.941100	0.027400
H	8.699300	-5.142500	-4.691800	H	5.005000	-5.216200	7.258800	O	2.011300	-7.562300	2.541000
C	8.196000	0.443900	-8.206900	H	5.545800	-3.643900	6.575600	C	-0.684700	3.545000	7.359700
H	9.057900	0.155300	-7.582900	C	5.538300	-7.321900	1.978200	H	-1.624300	3.663600	6.791800
H	7.396400	-0.308800	-8.097900	H	6.324600	-6.917800	1.318800	H	-0.833800	3.902100	8.385600
H	8.505600	0.499100	-9.256900	H	5.866700	-8.283300	2.391800	H	0.119500	4.127600	6.884000
C	6.938200	5.576500	-7.207000	H	4.605900	-7.469100	1.410600	C	0.816500	-1.547500	8.241600
H	5.897700	5.796700	-6.913300	C	4.903400	-5.893800	-5.221300	H	1.775600	-1.838300	7.778800
H	7.626000	5.978800	-6.444400	H	5.825300	-5.775900	-4.627200	H	0.923600	-1.549700	9.332400
H	7.151400	6.043100	-8.175200	H	4.082300	-6.214400	-4.556300	H	0.026300	-2.258300	7.952000
Cd	1.751600	0.078900	-0.035000	H	5.061600	-6.650300	-5.998900	C	2.000800	-7.446500	3.957300
C	3.944200	-1.139400	2.370300	C	3.845700	-1.513800	-8.173700	H	1.022400	-7.087800	4.320600
C	4.277200	-2.493700	2.783300	H	4.541900	-0.677000	-7.992500	H	2.182000	-8.458100	4.341100
C	4.432500	-3.075500	4.047900	H	3.998100	-1.903400	-9.186900	H	2.802700	-6.775900	4.305400
H	4.281800	-2.479300	4.947000	H	2.804000	-1.169900	-8.068200	C	2.295200	-8.287000	-1.350000
C	4.781700	-4.425700	4.103600	C	2.016800	5.455900	-6.630300	H	3.018000	-7.646600	-1.885700
C	4.210600	-2.324100	0.500800	H	1.309900	4.612600	-6.721800	H	2.638300	-9.327900	-1.379500
C	4.457800	-3.237400	1.607600	H	1.797700	6.202100	-7.403400	H	1.304500	-8.217500	-1.825800
C	4.820500	-4.589800	1.644400	H	3.046000	5.080200	-6.761600	C	0.928400	-4.207900	-7.354600
H	4.957800	-5.147200	0.719200	C	1.498000	8.366800	-2.128000	H	0.923100	-4.604000	-8.377600
C	4.988400	-5.185500	2.896500	H	2.409200	8.389100	-1.506200	H	1.932600	-4.335000	-6.920300
C	4.032500	-1.868600	-1.788500	H	1.315700	9.364400	-2.544800	H	0.182100	-4.750600	-6.747500
C	4.088100	-2.281200	-3.182300	H	0.632000	8.061900	-1.521000	C	-0.194100	0.979200	-8.245800
C	4.364800	-3.514800	-3.784800	C	0.445000	-0.913400	2.915400	H	0.532300	1.694700	-7.821000
H	4.578000	-4.388200	-3.169700	C	0.325000	-0.286600	4.220600	H	-0.147000	1.020300	-9.340400
C	4.356100	-3.574700	-5.179000	C	0.518800	-0.778500	5.519700	H	-1.213000	1.235200	-7.914500
C	3.561000	-0.058400	-3.003100	H	0.818700	-1.813800	5.676200	C	-1.759500	6.783100	-3.952700
C	3.803300	-1.140700	-3.948500	C	0.303700	0.096900	6.583800	H	-2.466400	5.999500	-4.277000
C	3.803700	-1.178300	-5.349000	C	-0.118600	1.213700	2.548500	H	-2.094900	7.755700	-4.332700
H	3.582500	-0.280500	-5.923800	C	-0.052200	1.045800	3.990400	H	-0.751900	6.568500	-4.341400
C	4.085700	-2.399200	-5.966900	C	-0.290500	1.933700	5.050800	O	-1.619300	7.366800	-0.024800
C	3.002400	2.161000	-2.517600	H	-0.589000	2.960700	4.848800	C	-1.643200	7.722600	1.362600
C	2.637600	3.507800	-2.930000	C	-0.120800	1.454300	6.348500	H	-2.448800	7.161700	1.866400
C	2.445100	4.080400	-4.193900	C	-0.472300	2.526000	0.643700	H	-0.678900	7.444700	1.828000
H	2.555600	3.474000	-5.092700	C	-0.795900	3.791100	0.005600	C	-1.880700	9.219800	1.466900
C	2.111500	5.434100	-4.249800	C	-1.064600	5.064400	0.528400	H	-1.072500	9.750500	0.935200
C	2.757000	3.352200	-0.648300	H	-1.045500	5.230900	1.605100	H	-2.818400	9.464000	0.941100
C	2.494600	4.261400	-1.756000	C	-1.361700	6.086500	-0.370800	C	-1.958900	9.698300	2.921200
C	2.173500	5.623900	-1.793400	C	-0.449000	2.153000	-1.555900	H	-2.770700	9.155100	3.437500
H	2.070400	6.190800	-0.869200	C	-0.804500	3.550200	-1.377700	H	-1.024400	9.427800	3.447100
C	1.985500	6.215200	-3.045400	C	-1.120600	4.563400	-2.294800	C	-2.192900	11.205000	3.044100
C	2.913600	2.891000	1.641400	H	-1.128700	4.353100	-3.362800	H	-2.246400	11.515100	4.098800
C	2.826700	3.295300	3.035700	C	-1.408400	5.831100	-1.788700	H	-1.379800	11.775600	2.567100

H	-3.137100	11.501100	2.559500
Y	-4.613500	-1.522100	0.109500
C	-5.393500	-4.765600	0.555800
C	-5.465700	-5.795300	1.593000
C	-5.493400	-7.193400	1.526700
H	-5.407900	-7.699700	0.565800
C	-5.647400	-7.902700	2.724500
C	-5.621300	-3.690500	2.480300
C	-5.610800	-5.117000	2.807800
C	-5.790300	-5.804400	4.013600
H	-5.931400	-5.255500	4.944200
C	-5.798400	-7.204900	3.974500
C	-6.159700	-1.487300	3.098800
C	-6.724000	-0.567500	4.087400
C	-7.030500	-0.720700	5.444300
H	-6.803600	-1.655300	5.956500
C	-7.645800	0.352000	6.102200
C	-6.654800	0.373400	2.000800
C	-7.037200	0.607100	3.394100
C	-7.673400	1.682200	4.025200
H	-7.935700	2.575700	3.459700
C	-7.970000	1.559000	5.388700
C	-6.854000	0.961300	-0.267100
C	-7.449200	1.823000	-1.289400
C	-8.131100	3.042200	-1.206600
H	-8.254400	3.538700	-0.245000
C	-8.654600	3.581600	-2.388400
C	-6.628400	-0.114400	-2.191100
C	-7.307200	1.143600	-2.504700
C	-7.842900	1.651200	-3.692700
H	-7.747900	1.091200	-4.622700
C	-8.509700	2.881500	-3.638300
C	-6.086400	-2.317100	-2.810400
C	-6.190100	-3.405700	-3.783100
C	-6.591700	-3.430100	-5.123700
H	-6.856400	-2.505300	-5.635100
C	-6.653900	-4.672600	-5.765700
C	-5.594800	-4.178300	-1.711600
C	-5.880400	-4.580700	-3.089000
C	-5.958400	-5.835600	-3.704700
H	-5.742700	-6.740900	-3.137500
C	-6.336700	-5.882500	-5.052800
N	-5.426800	-3.516600	1.130200
N	-5.893800	-2.757800	3.387900
N	-6.076600	-0.867300	1.874400
N	-6.952700	1.233100	1.030900
N	-6.317400	-0.161200	-0.853400
N	-6.466500	-1.075300	-3.096900
N	-5.667400	-2.810600	-1.596600
N	-5.407400	-5.066300	-0.738900
O	-5.685400	-9.243000	2.823900
O	-5.954300	-8.003500	5.044700
O	-7.994100	0.359500	7.400400
O	-8.571800	2.503100	6.133600
O	-9.071400	3.499900	-4.692300
O	-7.013800	-4.857700	-7.048500
O	-6.452300	-7.006800	-5.780500
C	-6.268400	-8.262200	-5.143600
H	-5.239500	-8.367800	-4.756500
H	-6.986300	-8.398400	-4.318500
H	-6.447500	-9.019600	-5.914900
C	-5.661400	-10.023800	1.638300
H	-6.513700	-9.776800	0.983400
H	-4.718100	-9.880500	1.082600
H	-5.739500	-11.068000	1.963600
C	-6.219800	-7.417000	6.309300
H	-5.378100	-6.783500	6.641500
H	-7.142900	-6.814400	6.283100
H	-6.346600	-8.252400	7.008100
C	-7.823700	-0.823700	8.166800
H	-8.397500	-1.661600	7.735900
H	-6.759100	-1.108100	8.236900
H	-8.207100	-0.592400	9.167100
C	-9.030900	3.689300	5.502600
H	-9.763300	3.460900	4.711000
H	-9.514400	4.281000	6.289800
H	-8.193700	4.264700	5.072100
C	-9.081100	2.844400	-5.951000
H	-8.055700	2.681200	-6.325700
H	-9.608200	1.877100	-5.891300
H	-9.618000	3.512100	-6.634800
C	-7.456200	-3.743900	-7.807900
H	-8.339600	-3.273500	-7.344100
H	-6.657500	-2.991000	-7.920700
H	-7.727700	-4.139500	-8.793900
O	-9.320000	4.745100	-2.472800
C	-9.605700	5.483300	-1.280400
H	-10.199600	4.852400	-0.594300
H	-8.658400	5.740800	-0.770600
C	-10.368800	6.736200	-1.676500
H	-11.284500	6.435100	-2.212000
H	-9.756900	7.306400	-2.396300
C	-10.724700	7.615500	-0.472400
H	-11.333000	7.030700	0.240800
H	-9.799700	7.889800	0.067800
C	-11.481100	8.886000	-0.864600
H	-12.425800	8.644100	-1.377300
H	-11.725700	9.492000	0.020800
H	-10.882400	9.511800	-1.546400
Cd	-1.320300	-0.694000	0.035400
C	-2.562300	-2.815000	2.489600
C	-2.530300	-2.742200	3.942500
C	-2.247000	-3.702400	4.922900
H	-1.977600	-4.717000	4.632500
C	-2.323300	-3.308700	6.259000
C	-3.088300	-0.716600	3.030400
C	-2.872800	-1.426300	4.285400
C	-2.968300	-1.016400	5.621400
H	-3.239000	0.009600	5.863600
C	-2.696500	-1.962600	6.613000
C	-3.593500	1.226600	1.826900
C	-3.933300	2.639000	1.764500
C	-4.132300	3.599900	2.763700
H	-4.019600	3.330900	3.812700
C	-4.474500	4.892900	2.363600
C	-3.782100	1.736200	-0.335200
C	-4.064900	2.958700	0.404800
C	-4.420200	4.246500	-0.014300
H	-4.520500	4.472400	-1.075500
C	-4.631300	5.216900	0.968000
C	-3.521600	0.561000	-2.342800
C	-3.521400	0.497200	-3.795200
C	-3.768400	1.465800	-4.776200
H	-3.998000	2.490800	-4.488000
C	-3.706400	1.068600	-6.113300
C	-3.016200	-1.542500	-2.882300
C	-3.216100	-0.829400	-4.137600
C	-3.163300	-1.249400	-5.471600
H	-2.926500	-2.284000	-5.714900
C	-3.413200	-0.298100	-6.464900
C	-2.490400	-3.480500	-1.680000
C	-2.117800	-4.884800	-1.617400
C	-1.880300	-5.836700	-2.617600
H	-1.954400	-5.557200	-3.667600
C	-1.553600	-7.133200	-2.217300
C	-2.322300	-3.995300	0.483300
C	-2.024000	-5.214300	-0.256900
C	-1.710100	-6.512400	0.163700
H	-1.644700	-6.746900	1.225100
C	-1.478400	-7.477600	-0.819800
N	-2.908500	-1.580900	1.961300
N	-3.406200	0.571100	2.968800
N	-3.514400	0.700400	0.546900
N	-3.788600	1.670600	-1.661400
N	-3.221200	-0.684200	-1.812900
N	-2.684100	-2.826600	-2.820600
N	-2.614000	-2.965700	-0.398900
N	-2.301100	-3.926900	1.809400
O	-2.054400	-4.108000	7.314600
O	-2.735500	-1.726300	7.937000
O	-4.672900	5.932600	3.203900
O	-3.892200	1.888300	-7.170100
O	-3.392200	-0.539700	-7.789200
O	-1.271400	-8.151900	-3.058900
O	-1.157400	-8.763000	-0.581300
C	-3.095900	-1.852700	-8.251000
H	-3.803700	-2.588300	-7.834000
H	-3.208000	-1.815300	-9.341400
H	-2.062500	-2.137300	-8.000300
C	-4.237200	3.242900	-6.928200
H	-3.438900	3.767700	-6.374200
H	-4.361200	3.705300	-7.915300
H	-5.180400	3.319800	-6.363300
C	-4.593200	5.703800	4.600900
H	-5.334200	4.954500	4.925400
H	-3.583600	5.365100	4.895500
H	-4.810400	6.666600	5.078300
C	-3.075400	-0.424000	8.400800
H	-4.063900	-0.112900	8.022300
H	-3.109300	-0.497700	9.494500
H	-2.310500	0.312700	8.109700
C	-1.727800	-5.467300	7.073500
H	-0.800700	-5.558400	6.480100
H	-1.577100	-5.922400	8.060100
H	-2.546500	-5.987800	6.548400
C	-1.038000	-9.210200	0.765300
H	-1.971300	-9.035700	1.325700
H	-0.845500	-10.288600	0.702800
H	-0.193900	-8.718000	1.272500
C	-1.369700	-7.927700	-4.456000
H	-0.655300	-7.155100	-4.789600
H	-1.125700	-8.883200	-4.934000
H	-2.390600	-7.622000	-4.740700
O	-4.981900	6.492300	0.725800
C	-5.200600	6.920400	-0.626700
H	-5.901800	6.223300	-1.120000
H	-4.241600	6.899100	-1.172100
C	-5.778400	8.325300	-0.588200
H	-6.708900	8.309000	0.004800
H	-5.075000	8.983900	-0.051800
C	-6.053500	8.883400	-1.989300
H	-5.112600	8.890200	-2.568500
H	-6.739600	8.203400	-2.526600
C	-6.649400	10.292100	-1.965200
H	-5.973500	11.002600	-1.462600
H	-6.829800	10.665100	-2.984800
H	-7.610900	10.309200	-1.426700

471

[5]$^{+4}$ with butoxy

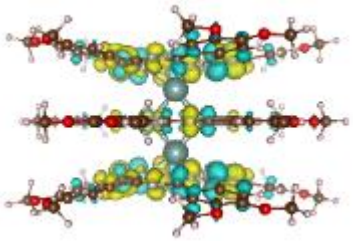
Y	-4.621100	-1.484400	0.103900
C	-6.841400	1.017000	-0.266300
C	-7.438100	1.883300	-1.284400
C	-8.126900	3.097700	-1.193400
H	-8.250100	3.590500	-0.229500
C	-8.662900	3.636300	-2.371300
C	-6.623300	-0.053000	-2.192900
C	-7.300800	1.207200	-2.501700
C	-7.847100	1.713300	-3.686000
H	-7.759800	1.153700	-4.617300
C	-8.523200	2.939600	-3.624500
C	-6.097700	-2.258100	-2.820600
C	-6.218600	-3.342600	-3.795300
C	-6.638300	-3.359400	-5.130200
H	-6.899400	-2.431700	-5.637700
C	-6.730400	-4.602100	-5.773000
C	-5.621600	-4.125900	-1.728800
C	-5.919200	-4.522200	-3.105600
C	-6.026000	-5.775400	-3.718400
H	-5.820800	-6.685000	-3.153900
C	-6.422900	-5.817200	-5.062500
C	-5.426900	-4.723500	0.536900
C	-5.516900	-5.756900	1.568800
C	-5.573600	-7.152700	1.494300
H	-5.494600	-7.656700	0.530800
C	-5.754900	-7.867300	2.686500
C	-5.648100	-3.654200	2.463500
C	-5.658200	-5.081600	2.786400

C	-5.862800	-5.771200	3.986400	C	-3.038200	-1.512900	-2.886100	H	-3.133400	-0.503900	9.497400
H	-6.005400	-5.225200	4.918700	C	-3.229400	-0.794900	-4.140200	H	-2.335300	0.315900	8.117300
C	-5.901800	-7.172100	3.940200	C	-3.174700	-1.213000	-5.474900	O	-4.933500	6.528300	0.739100
C	-6.170900	-1.449100	3.090500	H	-2.944300	-2.247700	-5.719700	C	-5.168800	6.964300	-0.610800
C	-6.738100	-0.531700	4.080900	C	-3.416100	-0.257100	-6.467100	H	-5.873100	6.266300	-1.097900
C	-7.064500	-0.697000	5.430200	C	-2.528000	-3.459000	-1.687800	H	-4.214800	6.946700	-1.164900
H	-6.849300	-1.635300	5.939300	C	-2.167000	-4.867100	-1.630400	C	-5.750300	8.367000	-0.558700
C	-7.691500	0.370300	6.088600	C	-1.935700	-5.818800	-2.631900	H	-6.671900	8.345000	0.047600
C	-6.650000	0.418000	1.998700	H	-2.007300	-5.537900	-3.682500	H	-5.041700	9.026500	-0.030600
C	-7.041700	0.647900	3.390800	C	-1.615600	-7.118100	-2.233900	C	-6.048500	8.928500	-1.954100
C	-7.687800	1.717400	4.019800	C	-2.366900	-3.980500	0.473500	H	-5.116700	8.940700	-2.547900
H	-7.946300	2.613500	3.455800	C	-2.075400	-5.199800	-0.270700	H	-6.740500	8.247700	-2.482700
C	-8.005000	1.584600	5.378900	C	-1.769100	-6.499700	0.149900	C	-6.649200	10.335000	-1.915600
N	-6.310300	-0.107100	-0.856000	H	-1.706000	-6.737000	1.210500	H	-5.968100	11.046400	-1.421700
N	-6.466200	-1.011500	-3.102300	C	-1.541800	-7.465900	-0.836200	H	-6.846700	10.710000	-2.931000
N	-5.680500	-2.757200	-1.607900	C	-2.601300	-2.803000	2.484400	H	-7.602200	10.346600	-1.362300
N	-5.441100	-5.018700	-0.759500	C	-2.568400	-2.734900	3.936900	C	-0.427200	2.151100	-1.568500
N	-5.448900	-3.475100	1.115100	C	-2.292300	-3.699300	4.914900	C	-0.772000	3.551700	-1.396500
N	-5.913700	-2.722100	3.375100	H	-2.031300	-4.715900	4.625900	C	-1.076900	4.563600	-2.319000
N	-6.078400	-0.825800	1.867700	C	-2.363800	-3.306300	6.254400	H	-1.082700	4.349900	-3.385800
N	-6.938800	1.285100	1.032400	C	-3.112400	-0.703300	3.029000	C	-1.357100	5.835600	-1.819000
O	-9.097000	3.554100	-4.668200	C	-2.900800	-1.416700	4.282300	C	-0.454800	2.533000	0.630200
O	-7.111100	-4.782600	-7.044700	C	-2.990300	-1.007000	5.617800	C	-0.767500	3.797300	-0.013400
O	-6.569300	-6.935600	-5.786900	H	-3.252500	0.021000	5.862700	C	-1.027800	5.075700	0.504200
O	-5.825100	-9.202300	2.779900	C	-2.724300	-1.956800	6.609600	H	-1.010700	5.246200	1.579900
O	-6.087100	-7.971100	4.999500	C	-3.602100	1.248000	1.830600	C	-1.312900	6.096800	-0.400700
O	-8.061500	0.367900	7.376700	C	-3.928600	2.664400	1.770900	C	-0.115700	1.225000	2.541300
O	-8.619600	2.517200	6.119400	C	-4.120800	3.625200	2.772600	C	-0.053400	1.063200	3.983500
C	-9.126300	2.903200	-5.932600	H	-4.014600	3.353300	3.821700	C	-0.286800	1.956000	5.040500
H	-8.105700	2.747000	-6.323100	C	-4.449100	4.923700	2.374500	H	-0.577900	2.985500	4.834900
H	-9.650400	1.935600	-5.866400	C	-3.782700	1.764300	-0.330800	C	-0.125100	1.481600	6.341700
H	-9.676800	3.573900	-6.602600	C	-4.055000	2.988900	0.412100	C	0.431300	-0.905300	2.919200
C	-9.083600	3.708900	5.497400	C	-4.395900	4.279700	-0.007000	C	0.313500	-0.271900	4.220800
H	-9.580000	4.285900	6.286500	H	-4.489600	4.509600	-1.067000	C	0.499500	-0.760200	5.522800
H	-8.244600	4.295200	5.084300	C	-4.597600	5.251900	0.978400	H	0.790900	-1.796700	5.685100
H	-9.805600	3.481600	4.695700	N	-3.234100	-0.655100	-1.814400	C	0.289100	0.120300	6.583900
C	-7.913300	-0.819900	8.144200	N	-2.715500	-2.799200	-2.828200	N	0.174800	0.020100	1.918100
H	-8.484800	-1.651000	7.697600	N	-2.646700	-2.944100	-0.406300	N	-0.399100	2.377200	1.947200
H	-6.852500	-1.106700	8.234900	N	-2.347100	-3.914900	1.799300	N	-0.246100	1.552000	-0.329300
H	-8.317900	-0.587700	9.135700	N	-2.934000	-1.565600	1.957400	N	-0.300200	1.569900	-2.755000
C	-7.558000	-3.667000	-7.805800	N	-3.419900	0.587500	2.970200	N	0.730600	-2.188500	2.755200
H	-8.427800	-3.186800	-7.328600	N	-3.522500	0.724100	0.548900	O	0.440400	-0.186800	7.888900
H	-6.750900	-2.924900	-7.936200	N	-3.788300	1.703100	-1.657400	O	-0.325600	2.206400	7.462000
H	-7.849000	-4.067900	-8.782500	O	-3.878200	1.931700	-7.167300	O	-1.682700	6.908900	-2.569600
C	-6.408200	-8.201100	-5.158800	O	-3.391200	-0.494000	-7.788300	C	0.017400	0.291900	-2.920000
H	-7.121600	-8.322400	-4.327400	O	-1.341200	-8.135400	-3.073500	C	0.151500	-0.337700	-4.222100
H	-6.615600	-8.948300	-5.932600	O	-1.229700	-8.750100	-0.599500	C	0.039200	0.168600	-5.525500
H	-5.377300	-8.331300	-4.785300	O	-2.100400	-4.105700	7.307000	H	-0.185400	1.220900	-5.688200
C	-5.817300	-9.986800	1.593400	O	-2.758200	-1.721500	7.931600	C	0.213900	-0.721600	-6.585500
H	-6.660700	-9.717300	0.937000	O	-4.637500	5.962000	3.212600	C	0.527500	-1.847500	-2.541400
H	-4.867600	-9.869300	1.044100	C	-4.573700	5.736400	4.612100	C	0.449700	-1.690100	-3.984100
H	-5.925000	-11.027400	1.922000	H	-3.571200	5.387600	4.915900	C	0.609700	-2.601000	-5.038400
C	-6.360500	-7.394700	6.270600	H	-4.785100	6.702900	5.084900	H	0.833300	-3.647000	-4.831500
H	-5.512100	-6.782400	6.621800	H	-5.328000	4.996500	4.930500	C	0.482000	-2.117600	-6.339400
H	-7.272600	-6.776300	6.235100	C	-4.223600	3.288800	-6.932800	C	0.903400	-3.146400	-0.631000
H	-6.513900	-8.236200	6.955200	H	-3.427900	3.813700	-6.376200	C	1.231600	-4.406900	0.012300
O	-9.336000	4.790600	-2.449300	H	-4.342500	3.746400	-7.922300	C	1.566500	-5.667300	-0.506900
C	-9.627400	5.531800	-1.255900	H	-5.171200	3.365700	-6.373700	H	1.617100	-5.822000	-1.583200
H	-10.212700	4.894400	-0.568900	C	-3.116500	-1.810400	-8.261100	C	1.817000	-6.697400	0.399600
H	-8.679800	5.798800	-0.752000	H	-3.836900	-2.536500	-7.846800	C	0.839000	-2.773500	1.568300
C	-10.404400	6.775100	-1.653700	H	-3.228800	-1.763600	-9.349900	C	1.168400	-4.177900	1.396600
H	-11.318800	6.463100	-2.184600	H	-2.086700	-2.112700	-8.012100	C	1.398700	-5.207900	2.320800
H	-9.800800	7.349700	-2.377000	C	-1.443000	-7.919600	-4.472800	H	1.338200	-5.010700	3.389900
C	-10.765000	7.653600	-0.450000	H	-2.464500	-7.611000	-4.753100	C	1.714000	-6.471600	1.821200
H	-11.364400	7.064100	0.266700	H	-0.724800	-7.153600	-4.813000	N	0.676600	-2.170600	0.329500
H	-9.840600	7.939500	0.085700	H	-1.206100	-8.880000	-4.946300	N	0.829600	-2.995800	-1.947000
C	-11.536900	8.914400	-0.843400	C	-1.124200	-9.211100	0.744900	N	0.255800	-0.638100	-1.917200
H	-12.481100	8.660500	-1.350700	H	-2.060800	-9.032200	1.297900	O	1.947500	-7.567500	2.573500
H	-11.784200	9.519900	0.041400	H	-0.940000	-10.288800	0.673700	O	2.165400	-7.957500	0.063900
H	-10.948100	9.544800	-1.529500	H	-0.279200	-8.729500	1.261200	O	0.591100	-2.864200	-7.458900
Cd	-1.319200	-0.682700	0.032600	C	-1.793000	-5.472700	7.072800	O	0.154500	-0.391300	-7.892900
C	-3.529000	0.592800	-2.342300	H	-0.868300	-5.578300	6.479100	C	-1.704500	6.784600	-3.987000
C	-3.527100	0.532900	-3.795700	H	-1.648700	-5.923500	8.060900	H	-2.419500	6.006800	-4.305900
C	-3.764400	1.506400	-4.774900	H	-2.620300	-5.981600	6.550800	H	-2.030400	7.759600	-4.366800
H	-3.989300	2.531300	-4.485700	C	-3.099800	-0.421600	8.404100	H	-0.699500	6.558200	-4.379300
C	-3.700900	1.111800	-6.113800	H	-4.089200	-0.111800	8.028500	C	-0.157500	0.947900	-8.256800

H	0.577300	1.655800	-7.834900	C	9.155000	-4.759600	-0.562200	C	3.197700	2.243700	5.183300
H	-0.106700	0.978800	-9.351500	C	7.134500	-1.235500	-1.708000	H	3.441800	1.359200	5.768000
H	-1.174400	1.219800	-7.931700	C	7.815600	-2.521700	-1.550900	C	2.899400	3.468600	5.789700
C	0.907900	-4.246900	-7.343000	C	8.406100	-3.389500	-2.475900	C	3.944400	-1.141000	2.393200
H	0.151600	-4.777700	-6.738200	H	8.359600	-3.173800	-3.541800	C	4.263500	-2.493800	2.823800
H	0.899400	-4.641700	-8.365100	C	9.070500	-4.521300	-1.981000	C	4.408800	-3.064200	4.094500
H	1.908900	-4.387000	-6.906300	N	6.188000	1.502400	-2.097400	H	4.261200	-2.458300	4.987800
C	2.244400	-8.313000	-1.312100	N	5.929900	3.914900	-2.061800	C	4.743500	-4.418500	4.166000
H	2.579800	-9.356800	-1.331500	N	5.850600	3.086100	0.218900	C	4.209100	-2.348000	0.537000
H	1.258100	-8.237800	-1.796400	N	6.218900	3.132600	2.617900	C	4.443200	-3.251400	1.656600
H	2.977800	-7.681900	-1.842600	N	6.431700	0.842600	1.837300	C	4.791100	-4.606600	1.707200
C	1.927000	-7.452900	3.990800	N	7.310000	-1.418600	1.789600	H	4.927300	-5.176200	0.788700
H	0.948000	-7.087700	4.345100	N	6.769100	-0.741100	-0.479000	C	4.947200	-5.192900	2.966800
H	2.099600	-8.466300	4.374100	N	7.021000	-0.636300	-2.890200	C	4.045900	-1.915700	-1.758500
H	2.729900	-6.787600	4.345600	O	7.850300	1.607600	-7.835500	C	4.102100	-2.344200	-3.147700
C	0.793500	-1.516900	8.252500	O	7.272800	4.053000	-7.391000	C	4.371500	-3.586700	-3.735200
H	1.753700	-1.811500	7.794300	O	6.201300	9.042100	-0.107900	H	4.577700	-4.456100	-3.112000
H	0.897300	-1.510100	9.344100	O	6.364700	8.624100	2.404700	C	4.364000	-3.662400	-5.130100
H	0.003000	-2.227600	7.966300	O	8.182200	1.568400	7.504200	C	3.590900	-0.115400	-2.993100
C	-0.683200	3.577900	7.346900	O	8.776100	-0.873300	7.059100	C	3.827900	-1.210200	-3.927000
H	-0.830100	3.935700	8.373100	O	9.828200	-5.866900	-0.223400	C	3.828400	-1.261700	-5.325200
H	0.123200	4.158300	6.871400	O	9.681300	-5.444500	-2.735800	H	3.615000	-0.369700	-5.910500
H	-1.622900	3.696800	6.778800	C	9.765000	-5.252800	-4.142500	C	4.102100	-2.492600	-5.931200
O	-1.559700	7.378700	-0.063400	H	8.763100	-5.242400	-4.603800	N	3.109600	2.058300	-1.150700
C	-1.576600	7.750200	1.322200	H	10.293100	-4.315000	-4.382600	N	2.726800	3.707400	0.591400
H	-0.613900	7.465000	1.786400	H	10.336900	-6.105000	-4.527800	N	3.290800	1.548700	1.547500
H	-2.387100	7.202100	1.832200	C	8.318500	0.304500	-8.162600	N	3.720500	-0.139400	3.239300
C	-1.797000	9.250700	1.412000	H	9.165200	0.017500	-7.518200	N	3.919500	-1.075600	1.008800
H	-0.985900	9.766600	0.870400	H	7.511800	-0.443400	-8.071000	N	4.268700	-2.732300	-0.732100
H	-2.734700	9.500200	0.888700	H	8.650900	0.359100	-9.205100	N	3.738500	-0.565300	-1.688800
C	-1.861400	9.745300	2.861900	C	7.095100	5.454000	-7.228000	N	3.274800	1.113800	-3.380600
H	-2.675600	9.216000	3.389000	H	6.051400	5.695200	-6.960600	O	1.947700	6.053100	-5.447400
H	-0.926300	9.470500	3.384700	H	7.775200	5.851600	-6.456600	O	1.741700	7.456300	-3.326500
C	-2.079200	11.255600	2.969600	H	7.338000	5.902300	-8.197400	O	2.262500	5.723300	5.704000
H	-2.122500	11.576900	4.021200	C	6.247200	9.386300	-1.486200	O	2.878700	3.688500	7.114000
H	-1.263300	11.812600	2.481600	H	7.114400	8.918300	-1.980800	O	4.891200	-5.116300	5.309600
H	-3.023400	11.556200	2.488300	H	5.320000	9.085900	-2.004000	O	5.268200	-6.477400	3.185900
Y	5.050500	0.865800	-0.103500	H	6.349700	10.476800	-1.519900	O	4.576400	-4.786500	-5.841700
C	6.650300	0.630400	-3.054900	C	6.583500	8.506200	3.804000	O	4.130600	-2.710300	-7.256700
C	6.817800	1.327700	-4.329900	H	7.491700	7.917000	4.014000	C	5.491600	-7.344200	2.076200
C	7.291200	0.901600	-5.575900	H	6.714500	9.529400	4.174800	H	6.287300	-6.951400	1.422400
H	7.565800	-0.140900	-5.734400	H	5.716600	8.040500	4.305200	H	5.809600	-8.300300	2.506600
C	7.417300	1.858900	-6.593300	C	8.012800	2.943800	7.824800	H	4.565100	-7.493700	1.500100
C	6.144200	2.751100	-2.669100	H	8.606400	3.582900	7.150100	C	4.772400	-4.436800	6.550700
C	6.498600	2.668900	-4.087100	H	6.950200	3.237700	7.771900	H	3.760800	-4.014100	6.679600
C	6.638400	3.646500	-5.077800	H	8.374000	3.059100	8.853100	H	4.958000	-5.189300	7.325900
H	6.418100	4.690200	-4.857400	C	9.255700	-2.200600	6.890300	H	5.518700	-3.627400	6.633300
C	7.090300	3.239400	-6.342100	H	8.430400	-2.896400	6.662200	C	3.192700	2.624200	8.008000
C	5.861500	4.069900	-0.742700	H	10.010800	-2.247500	6.088500	H	4.193900	2.212500	7.795700
C	5.918100	5.388600	-0.111700	H	9.715500	-2.477300	7.844700	H	3.184000	3.066300	9.011100
C	5.987500	6.680000	-0.645900	C	10.082100	-6.138100	1.148900	H	2.434900	1.826900	7.953400
H	5.951600	6.833200	-1.723300	H	10.656500	-5.320000	1.613700	C	1.974400	6.931300	5.016000
C	6.125700	7.751900	0.246700	H	9.141000	-6.293100	1.705100	H	2.825500	7.243100	4.387100
C	5.997800	3.705400	1.437800	H	10.674200	-7.059900	1.168200	H	1.075300	6.826800	4.385100
C	6.004200	5.159400	1.265900	Cd	1.749700	0.064000	-0.032400	H	1.794300	7.684900	5.790200
C	6.166500	6.209500	2.174700	C	3.046900	2.114600	-2.534200	C	1.585700	8.338900	-2.218800
H	6.266500	6.008000	3.240700	C	2.692000	3.459200	-2.963700	H	2.498500	8.361000	-1.600500
C	6.216500	7.515800	1.666200	C	2.509800	4.019800	-4.234400	H	1.413000	9.330400	-2.652100
C	6.479100	1.839500	2.785400	H	2.621600	3.405600	-5.126600	H	0.717800	8.051800	-1.605000
C	6.999100	1.308600	4.045700	C	2.182400	5.376300	-4.305500	C	2.105400	5.383300	-6.688900
C	7.272300	1.916800	5.275600	C	2.800600	3.326100	-0.678400	H	1.396000	4.542100	-6.782900
H	7.042800	2.970600	5.433400	C	2.549200	4.225800	-1.797200	H	1.894100	6.129100	-7.464200
C	7.864200	1.134200	6.276900	C	2.235000	5.588500	-1.849100	H	3.135100	5.006000	-6.808900
C	6.988200	-0.281100	2.398900	H	2.130400	6.165700	-0.931400	C	3.884400	-1.628700	-8.151300
C	7.322300	-0.030400	3.802500	C	2.054300	6.168800	-3.108300	H	4.592700	-0.802200	-7.974700
C	7.934300	-0.825800	4.777300	C	2.945400	2.889300	1.617400	H	4.038600	-2.036200	-9.156600
H	8.209900	-1.856000	4.555900	C	2.854500	3.309500	3.007500	H	2.848200	-1.268100	-8.057600
C	8.198500	-0.244200	6.026100	C	2.547200	4.543000	3.596000	C	4.903300	-5.985400	-5.155000
C	7.267800	-1.600700	0.472500	H	2.305100	5.403400	2.973200	H	4.082100	-6.299500	-4.486300
C	7.898800	-2.752300	-0.172600	C	2.561800	4.620300	4.990500	H	5.057900	-6.745100	-5.928400
C	8.575100	-3.861600	0.345800	C	3.419800	1.093600	2.851500	H	5.826800	-5.865200	-4.564500
H	8.656100	-4.004900	1.422600	C	3.164400	2.183900	3.785700				

4.7. Optical tansitions from DFT calculations

To evaluate the electron transfer by the optical transition, we used TD-Analy (ver. 1.13) which calculates differences in electron densities between ground and excited states.[24]. For visualization, VESTA 3.4.0 was used.[25]

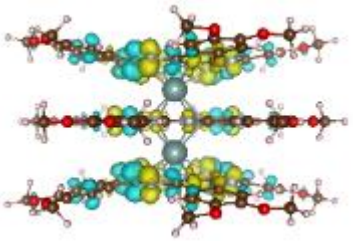


Singlet-A

15376 cm^{-1} (650.37 nm) f = 0.6068

Wavefunction

597 -> 600	0.14672
597 -> 601	-0.27254
597 -> 604	-0.10170
598 -> 602	0.50995
599 -> 604	-0.16285
599 -> 605	0.23163

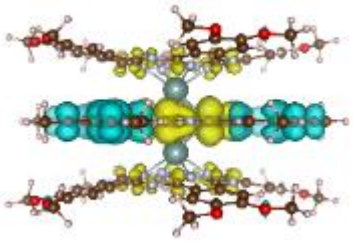


Singlet-A

15377 cm^{-1} (650.34 nm) f = 0.6068

Wavefunction

597 -> 600	0.27228
597 -> 601	0.14674
597 -> 605	0.10159
598 -> 603	0.51021
599 -> 604	0.23138
599 -> 605	0.16285

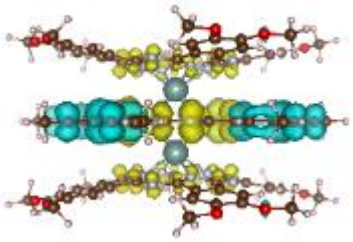


Singlet-A

18898 cm^{-1} (529.15 nm) f = 0.1716

Wavefunction

587 -> 600	-0.34500
587 -> 601	-0.20164
588 -> 600	0.43197
592 -> 600	-0.14518
597 -> 604	0.28164
597 -> 605	-0.12250

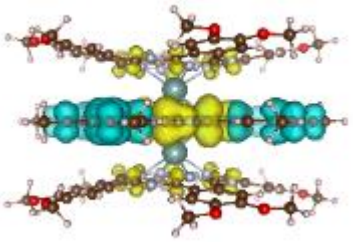


Singlet-A

18899 cm^{-1} (529.13 nm) f = 0.1718

Wavefunction

587 -> 600	-0.20304
587 -> 601	0.34393
588 -> 601	0.43183
592 -> 601	-0.14567

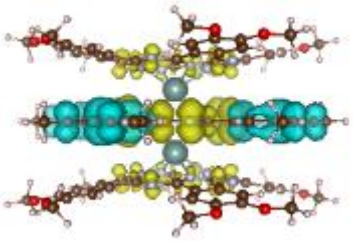


Singlet-A

19152 cm^{-1} (522.15 nm) f = 0.1717

Wavefunction

587 -> 600	0.50778
587 -> 601	0.25659
588 -> 600	0.33478
597 -> 604	0.17065



Singlet-A

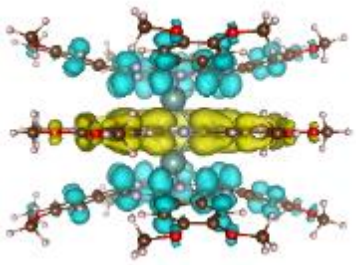
19152 cm^{-1} (522.13 nm) f = 0.1715

Wavefunction

587 -> 600	-0.25562
587 -> 601	0.50861
588 -> 601	-0.33465
597 -> 605	0.17091

597 -> 604	-0.12282
597 -> 605	-0.28184

Fig. S278. Light-induced electron transfer direction (isosurface value 0.0002), transition wavelength and wavefunction in **[3]^{0}**. The electron moves from the blue to the yellow regions. MO 599 is HOMO.

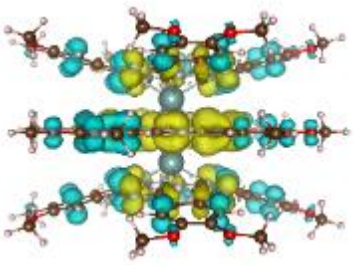


Singlet-AU

5604 cm^{-1} (1784.38 nm) f = 0.3751

Wavefunction

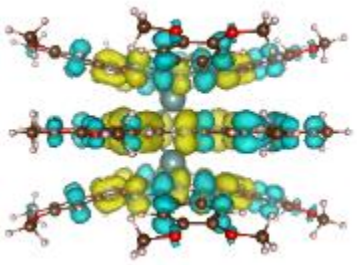
598 -> 599	0.74332
598 <- 599	-0.23190



Singlet-AU

14429 cm1 (693.04 nm) f = 0.3130

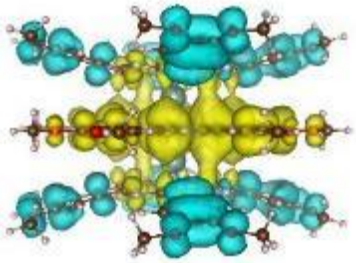
583 -> 599	-0.15529
586 -> 599	0.10793
588 -> 601	0.16844
597 -> 600	0.44236
598 -> 602	0.42807
598 -> 603	-0.15700



Singlet-AU

14431 cm1 (692.93 nm) f = 0.3126

584 -> 599	0.15545
585 -> 599	0.10817
588 -> 600	-0.16864
597 -> 601	0.44171
598 -> 602	0.15634
598 -> 603	0.42883

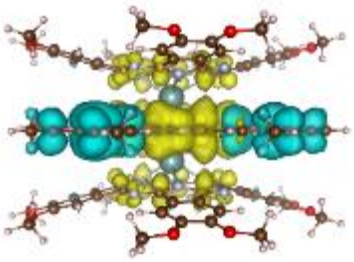


Singlet-AU

15318 cm^{-1} (652.82 nm) f = 0.0250

Wavefunction

594 -> 600	0.68918

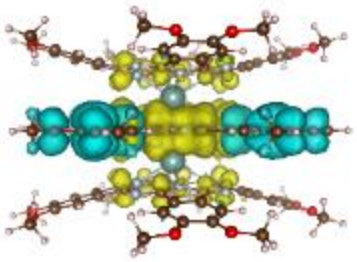


Singlet-AU

16089 cm^{-1} (621.54 nm) f = 0.0599

Wavefunction

584 -> 599	0.16317
587 -> 601	-0.11020
588 -> 600	0.52949
588 -> 601	0.37016
597 -> 601	0.13098



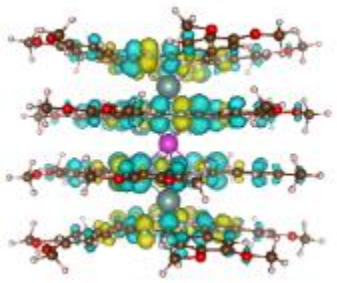
Singlet-AU

16091 cm^{-1} (621.46 nm) f = 0.0603

Wavefunction

583 -> 599	0.16273
587 -> 600	-0.11090
588 -> 600	-0.36987
588 -> 601	0.52963
597 -> 600	-0.13079

Fig. S279. Light-induced electron transfer direction (isosurface value 0.0002), transition wavelength and wavefunction in **[3]**$^{2+}$. The electron moves from the blue to the yellow regions. MO 598 is HOMO.

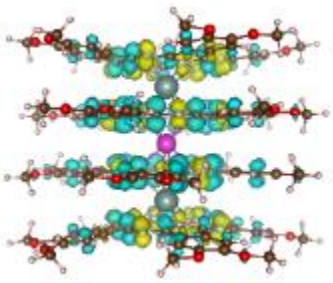


Singlet-B

15424 cm^{-1} (648.32 nm) f = 0.1939

Wavefunction

802 -> 808	0.41077
802 -> 809	0.14431
803 -> 809	-0.16181
803 -> 810	-0.11216
803 -> 811	-0.10150
803 -> 812	0.10204
803 -> 813	0.17177
804 -> 811	0.10342
804 -> 813	0.23162
805 -> 812	0.24861

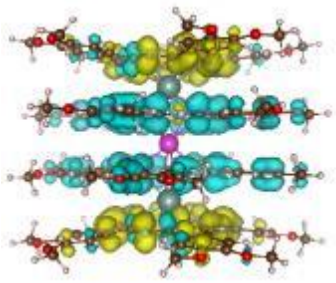


Singlet-B

15424 cm^{-1} (648.32 nm) f = 0.1939

Wavefunction

802 -> 808	-0.14431
802 -> 809	0.41077
803 -> 808	0.16181
803 -> 810	0.10151
803 -> 811	-0.11217
803 -> 812	0.17177
803 -> 813	-0.10203
804 -> 810	-0.10342
804 -> 812	0.23162
805 -> 813	-0.24861

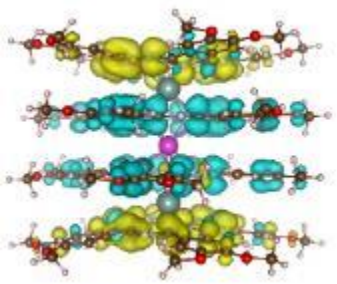


Singlet-B

16129 cm^{-1} (620.01 nm) f = 0.1023

Wavefunction

803 -> 810	0.59280
803 -> 811	0.24604
804 -> 810	0.13058
804 -> 813	0.12773

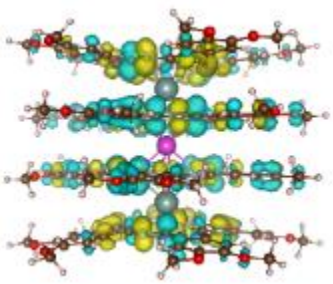


Singlet-B

16129 cm^{-1} (620.01 nm) f = 0.1023

Wavefunction

803 -> 810	-0.24604
803 -> 811	0.59280
804 -> 811	0.13058
804 -> 812	0.12774

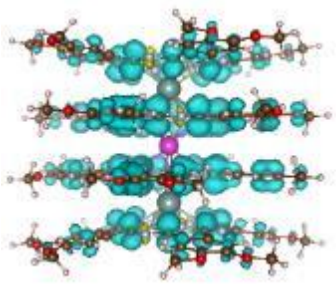


Singlet-B

16789 cm^{-1} (595.63 nm) f = 0.3432

Wavefunction

792 -> 806	0.13515
802 -> 809	-0.15640
802 -> 810	0.10602
803 -> 812	0.58592
804 -> 811	-0.10522
805 -> 813	0.15613



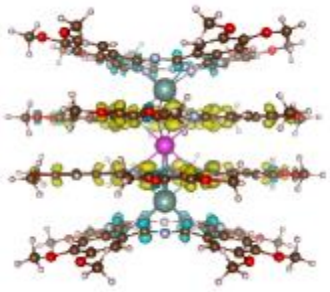
Singlet-B

16789 cm^{-1} (595.63 nm) f = 0.3432

Wavefunction

792 -> 807	-0.13514
802 -> 808	-0.15639
802 -> 811	-0.10602
803 -> 813	0.58593
804 -> 810	-0.10522
805 -> 812	-0.15613

Fig. S280. Light-induced electron transfer direction (isosurface value 0.0002), transition wavelength and wavefunction in **[4]^{0}**. The electron moves from the blue to the yellow regions. MO 805 is HOMO.

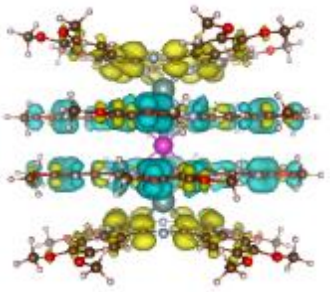


Singlet-A

1433 cm^{-1} (6978.14 nm) f = 0.0450

Wavefunction

803 -> 805	-0.15738
804 -> 805	0.93831
804 <- 805	-0.63616

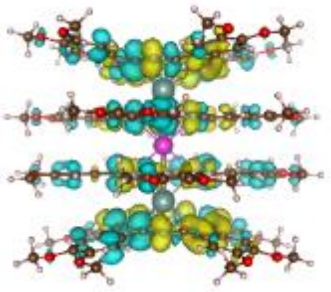


Singlet-A

5818 cm^{-1} (1718.78 nm) f = 0.2371

Wavefunction

803 -> 805	0.69160
804 -> 805	0.20679
804 <- 805	-0.13647

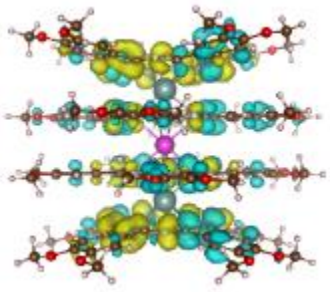


Singlet-B

12773 cm^{-1} (782.93 nm) f = 0.1163

Wavefunction

802 -> 808	0.16114
802 -> 809	0.16102
803 -> 807	0.33612
804 -> 810	0.55575

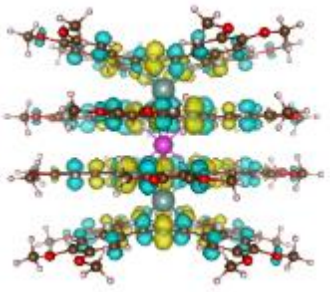


Singlet-B

12773 cm^{-1} (782.92 nm) f = 0.1162

Wavefunction

802 -> 808	-0.16106
802 -> 809	0.16113
803 -> 806	-0.33583
804 -> 811	0.55593

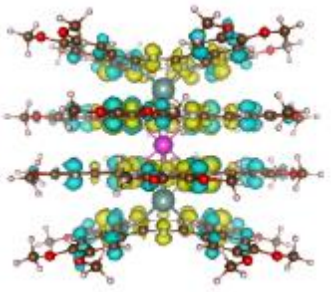


Singlet-B

15009 cm^{-1} (666.27 nm) f = 0.2027

Wavefunction

784 -> 805	0.17000
802 -> 808	0.54414
802 -> 809	0.11491
803 -> 809	-0.23903
804 -> 810	-0.12240
804 -> 813	0.11433



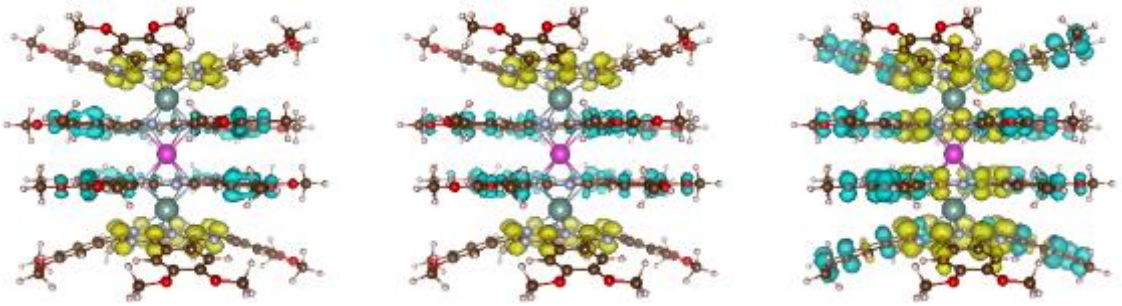
Singlet-B

15009 cm^{-1} (666.26 nm) f = 0.2027

Wavefunction

785 -> 805	-0.17009
802 -> 808	-0.11488
802 -> 809	0.54426
803 -> 808	0.23882
804 -> 811	-0.12240
804 -> 812	-0.11421

Fig. S281. Light-induced electron transfer direction (isosurface value 0.0002), transition wavelength and wavefunction in **[4]**$^{2+}$. The electron moves from blue to yellow region. MO 804 is HOMO.



Singlet-A

6248 cm^{-1} (1600.44 nm) f= 0.0632

Wavelength	
802 -> 805	0.34993
803 -> 804	0.61392

Singlet-A

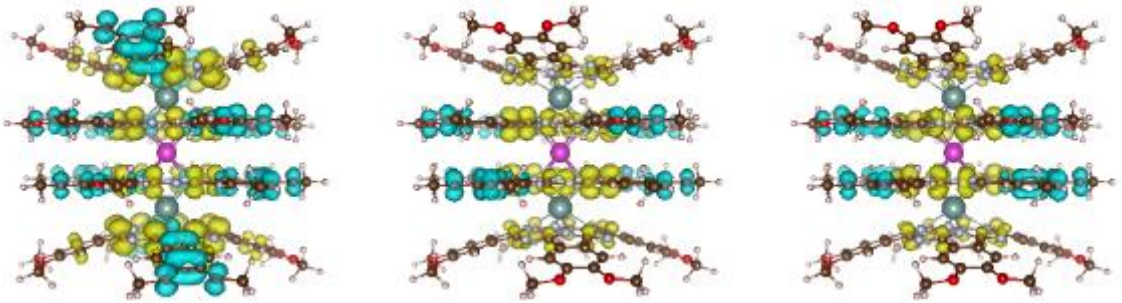
7814 cm^{-1} (1279.81 nm) f= 0.4634

Wavelength	
802 -> 805	0.61556
803 -> 804	-0.35668

Singlet-A

9278 cm^{-1} (1077.77 nm) f= 0.0131

Wavelengh	
791 -> 804	0.57350
795 -> 805	-0.30853
798 -> 804	0.15143
799 -> 804	0.18864



Singlet-A

9278 cm^{-1} (1077.77 nm) f= 0.0131

Wavelength	
790 -> 804	0.57349
794 -> 805	-0.30859
798 -> 804	0.17965
799 -> 804	-0.15127

Singlet-A

12119 cm^{-1} (825.17 nm) f= 0.0364

Wavelength	
786 -> 805	-0.37602
787 -> 804	0.10647
787 -> 805	0.27636
803 -> 806	0.47493
803 -> 807	0.12443

Singlet-A

12119 cm^{-1} (825.17 nm) f= 0.0364

Wavelength	
786 -> 804	0.10664
786 -> 805	0.27644
787 -> 805	0.37568
803 -> 806	-0.12425
803 -> 807	0.47518

Fig. S282. Light-induced electron transfer direction (isosurface value 0.0002), transition wavelength and wavefunction in **[4]**$^{4+}$. The electron moves from blue to yellow region. MO 803 is HOMO.

4.8. Natural orbital analysis for **[4]**$^{2+}$ and **[5]**$^{2+}$

Computational details

Natural orbital (NO) analyses for **[4]**$^{2+}$ and **[5]**$^{2+}$ were performed using the DFT optimized structures of singlet states listed in section 3.7 (shown in Fig. S261 and S272, respectively). The calculations were done with Gaussian 09 (revision C01) using Becke's three parameter hybrid (B3LYP[16-17]) functional, Stuttgart RSC 1997 ECP[23, 26] for Y and Cd and 6-31G*[20-22] for other atoms. In order to get the *J* values between the pair of the spins, single-point calculations for anti-ferromagnetic (AFM) coupling state (S = 0) and ferromagnetic (FM) state (S = 1) were continued until the total energies being converged within 10^{-7} Hartree.

Table S30. Total energies, $<S^2>$ values and *J* values calculated by Yamaguchi equation for **[4]**$^{2+}$ and **[5]**$^{2+}$.

	AFM state		FM state		J / cm^{-1}
	Total Energy / hartree	$<S^2>$	Total Energy / hartree	$<S^2>$	
[4]$^{2+}$	-10577.59477181	1.02530594	-10577.59461524	2.03178845	-34
[5]$^{2+}$	-13328.68984292	1.02596929	-13328.68982980	2.02754717	-3

Table S31. Occupation numbers of natural orbitals (NOs) and calculated *y* values of each orbital.

	[4]$^{2+}$		
	Occupation number	Overlap*	*y* values
LUNO-5	0.00067		
LUNO-4	0.00234		
LUNO-3	0.00234		
LUNO-2	0.00237		
LUNO-1	0.00237		
LUNO-0	0.92210		
HONO+0	1.07790	0.07790	0.8451
HONO+1	1.99763	0.99763	0.0000
HONO+2	1.99763	0.99763	0.0000
HONO+3	1.99766	0.99766	0.0000
HONO+4	1.99766	0.99766	0.0000
HONO+5	1.99933	0.99933	0.0000

* overlap is calculated by (occupation number) – 1

Table S32. Occupation numbers of natural orbitals (NOs) and calculated *y* values of each orbital.

	[5]$^{2+}$		
	Occupation number	Overlap*	*y* values
LUNO-5	0.00053		
LUNO-4	0.00187		
LUNO-3	0.00187		
LUNO-2	0.00187		
LUNO-1	0.00187		
LUNO-0	0.96109		
HONO+0	1.03891	0.00369	0.9223
HONO+1	1.99813	0.99660	0.0000
HONO+2	1.99813	0.99660	0.0000
HONO+3	1.99813	0.99660	0.0000
HONO+4	1.99813	0.99905	0.0000
HONO+5	1.99947	0.99905	0.0000

* overlap is calculated by (occupation number) – 1

Table S33. Orbital energies of $[4]^{2+}$.

Orbital Energy / eV	$[4]^{2+}$			
	AFM		FM	
	Alpha	Beta	Alpha	Beta
LUMO+10	-4.130	-4.130	-3.968	-4.133
LUMO+9	-4.157	-4.157	-4.126	-5.177
LUMO+8	-5.210	-5.211	-4.163	-5.177
LUMO+7	-5.210	-5.211	-5.386	-5.261
LUMO+6	-5.454	-5.453	-5.386	-5.261
LUMO+5	-5.454	-5.453	-5.515	-5.705
LUMO+4	-5.770	-5.770	-5.515	-5.705
LUMO+3	-5.770	-5.770	-5.832	-5.994
LUMO+2	-6.053	-6.053	-5.832	-5.994
LUMO+1	-6.053	-6.053	-6.080	-6.693
LUMO+0	-6.719	-6.719	-6.080	-6.747
HOMO-0	-7.570	-7.569	-7.541	-7.815
HOMO-1	-7.852	-7.852	-7.590	-7.898
HOMO-2	-8.103	-8.103	-8.033	-8.463
HOMO-3	-8.464	-8.464	-8.151	-8.466
HOMO-4	-8.470	-8.470	-8.468	-8.466
HOMO-5	-8.470	-8.470	-8.471	-8.483
HOMO-6	-8.482	-8.481	-8.471	-8.496
HOMO-7	-8.500	-8.500	-8.488	-8.521
HOMO-8	-8.523	-8.523	-8.509	-8.521
HOMO-9	-8.523	-8.523	-8.532	-8.524
HOMO-10	-8.527	-8.526	-8.532	-8.567

Table S34. Orbital energies of $[5]^{2+}$.

Orbital Energy / eV	$[5]^{2+}$			
	AFM		FM	
	Alpha	Beta	Alpha	Beta
LUMO+10	-4.871	-4.871	-3.906	-4.852
LUMO+9	-4.871	-4.871	-5.034	-4.898
LUMO+8	-5.078	-5.078	-5.034	-4.898
LUMO+7	-5.078	-5.078	-5.129	-5.220
LUMO+6	-5.268	-5.268	-5.129	-5.220
LUMO+5	-5.268	-5.268	-5.306	-5.528
LUMO+4	-5.569	-5.569	-5.306	-5.528
LUMO+3	-5.569	-5.569	-5.633	-5.659
LUMO+2	-5.710	-5.711	-5.633	-5.659
LUMO+1	-5.710	-5.711	-5.734	-6.362
LUMO+0	-6.374	-6.373	-5.734	-6.384
HOMO-0	-7.203	-7.203	-7.196	-7.339
HOMO-1	-7.357	-7.357	-7.209	-7.539
HOMO-2	-7.581	-7.581	-7.381	-7.626
HOMO-3	-7.829	-7.829	-7.794	-8.160
HOMO-4	-8.162	-8.162	-7.856	-8.160
HOMO-5	-8.162	-8.162	-8.164	-8.170
HOMO-6	-8.172	-8.172	-8.164	-8.178
HOMO-7	-8.180	-8.180	-8.175	-8.189
HOMO-8	-8.191	-8.191	-8.181	-8.208
HOMO-9	-8.211	-8.211	-8.193	-8.211
HOMO-10	-8.214	-8.214	-8.219	-8.211

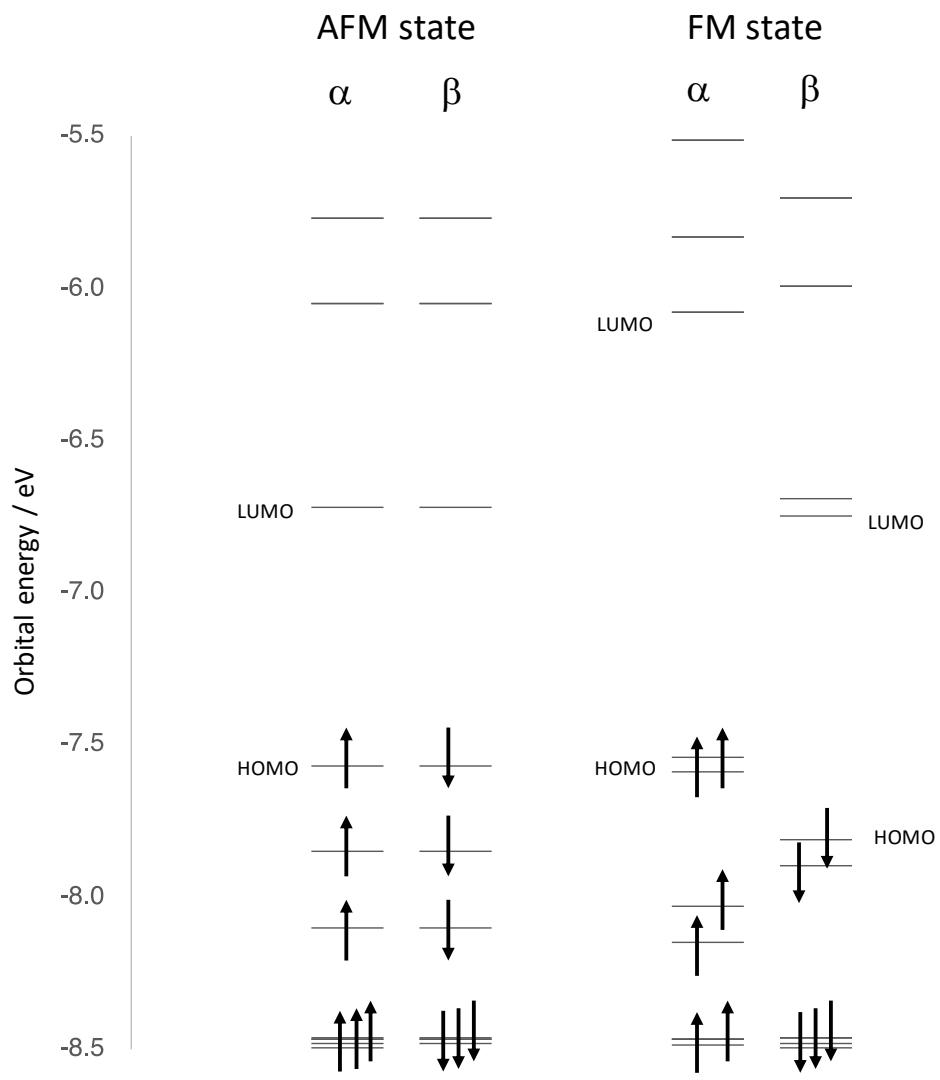


Fig. S283. Orbital energy diagram of **[4]**$^{4+}$.

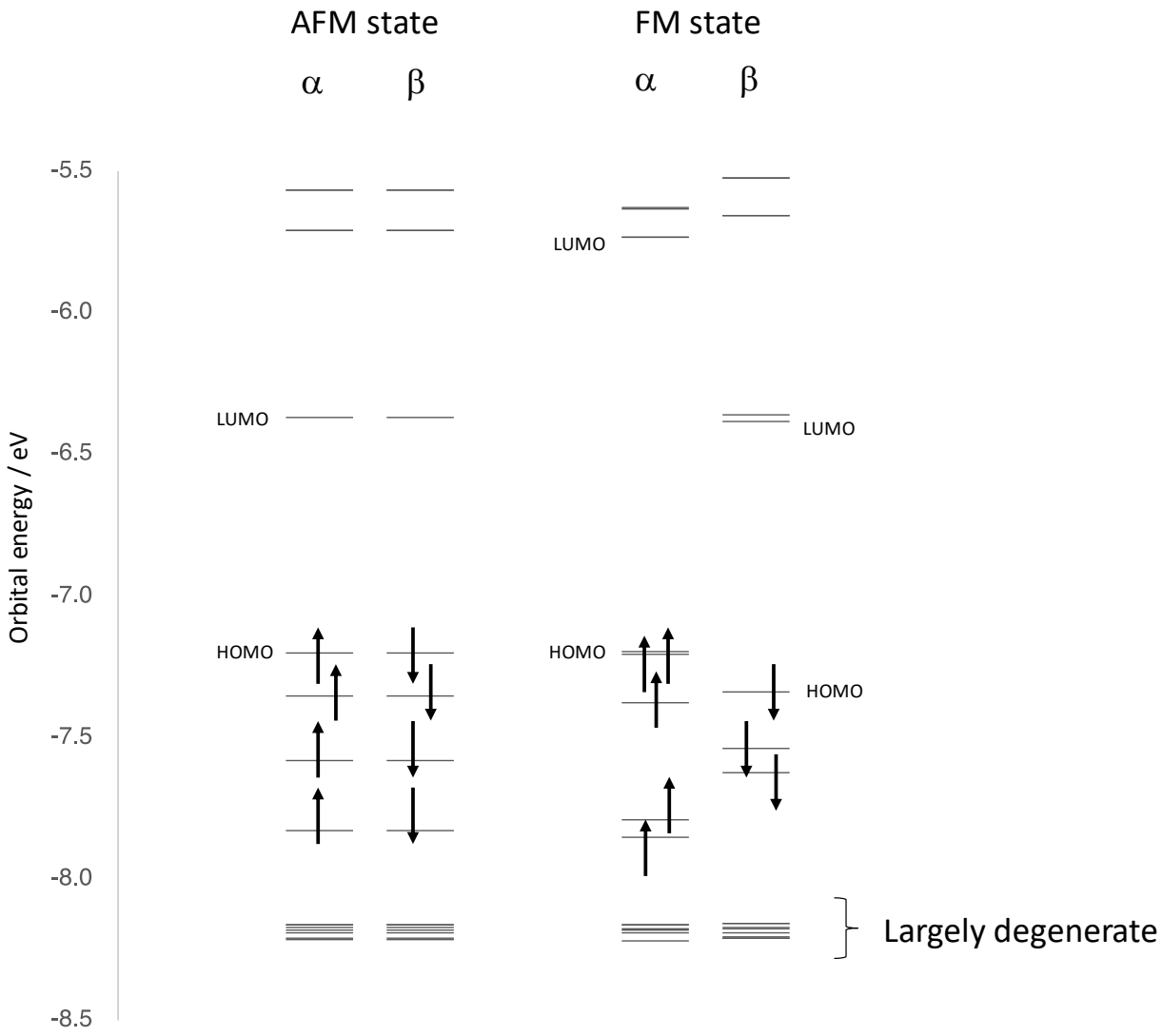


Fig. S284. Orbital energy diagram of **[4]**$^{4+}$.

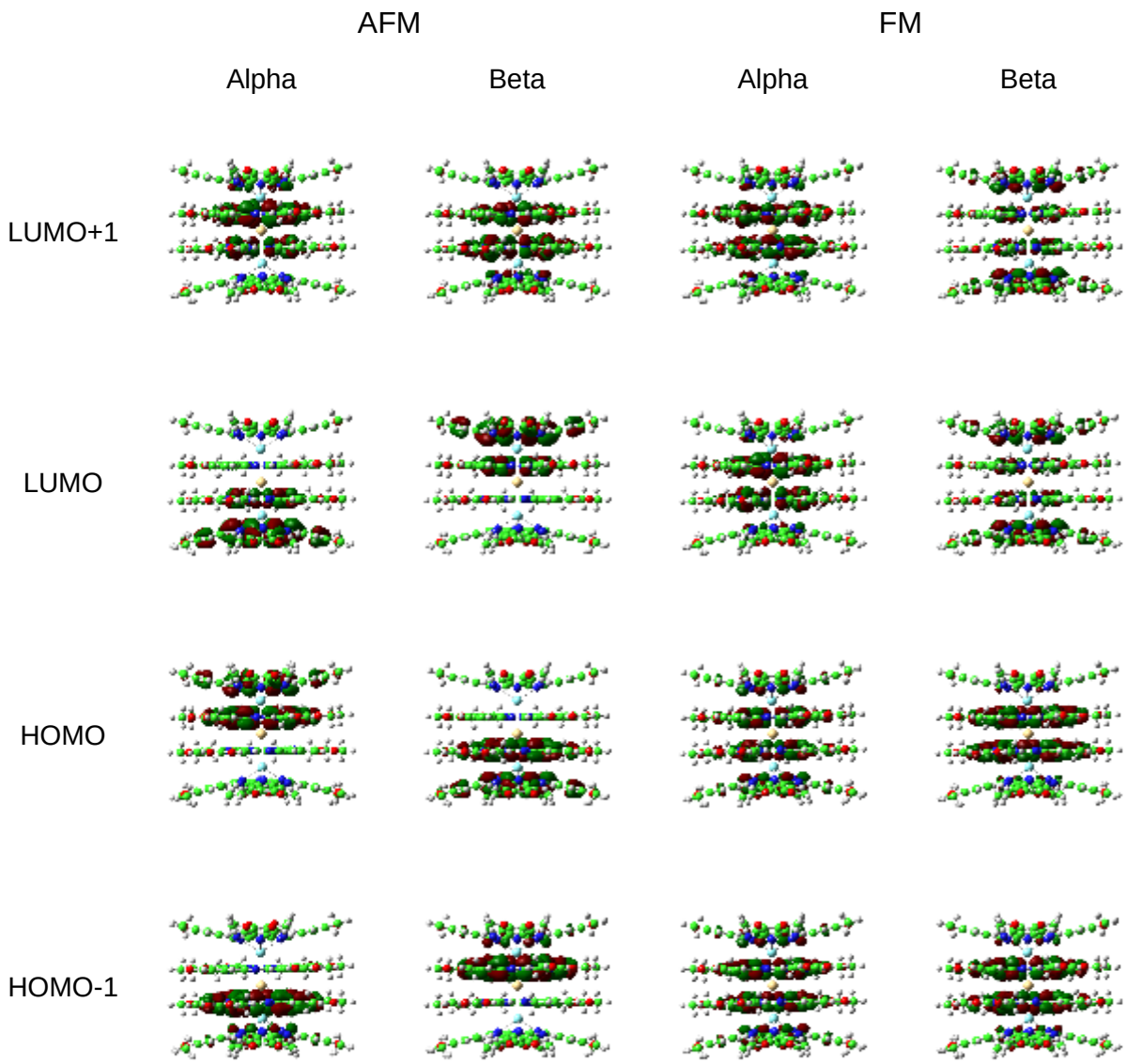


Fig. S285. Molecular orbitals of **[4]**$^{2+}$ in AFM and FM states.

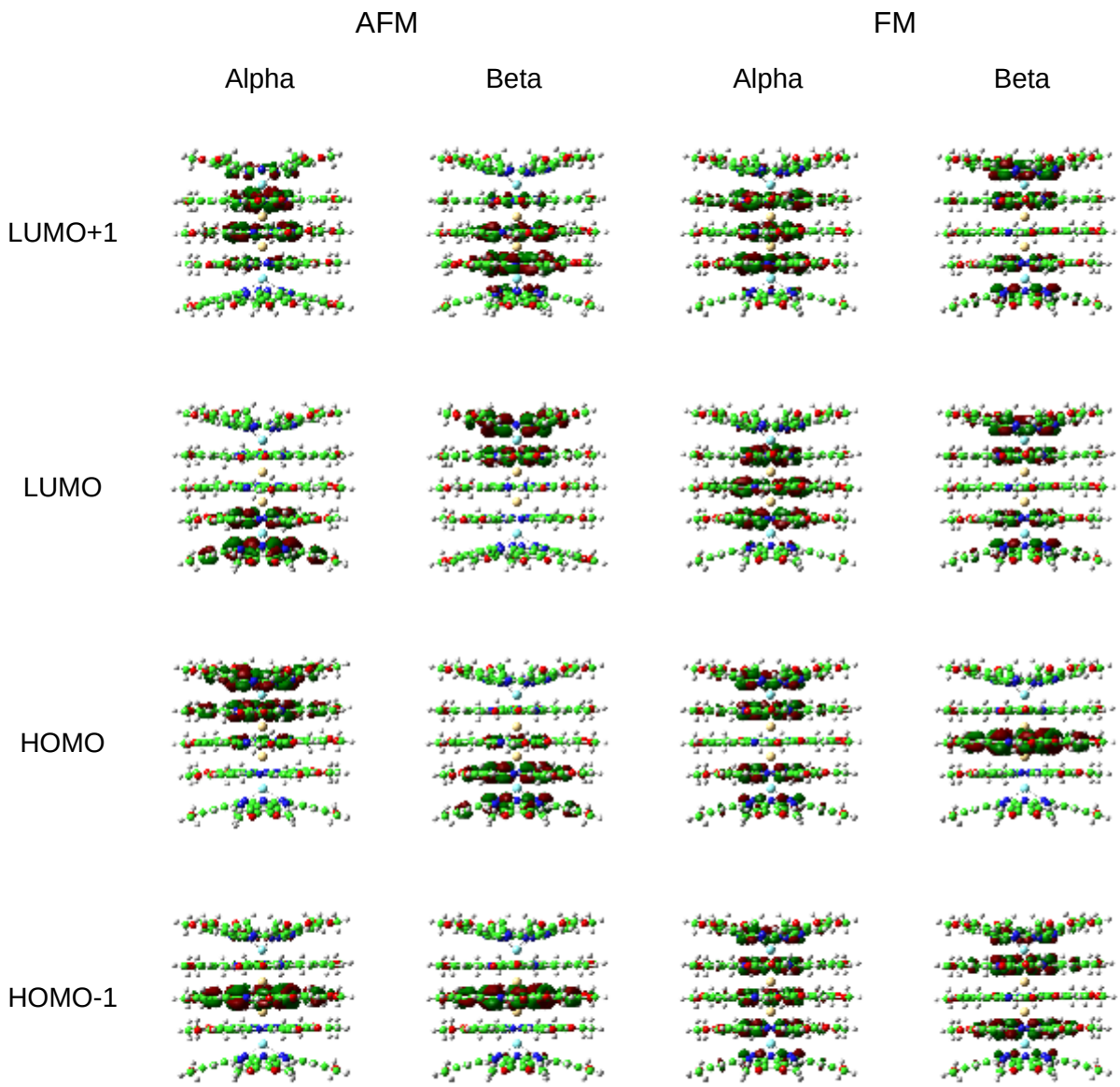
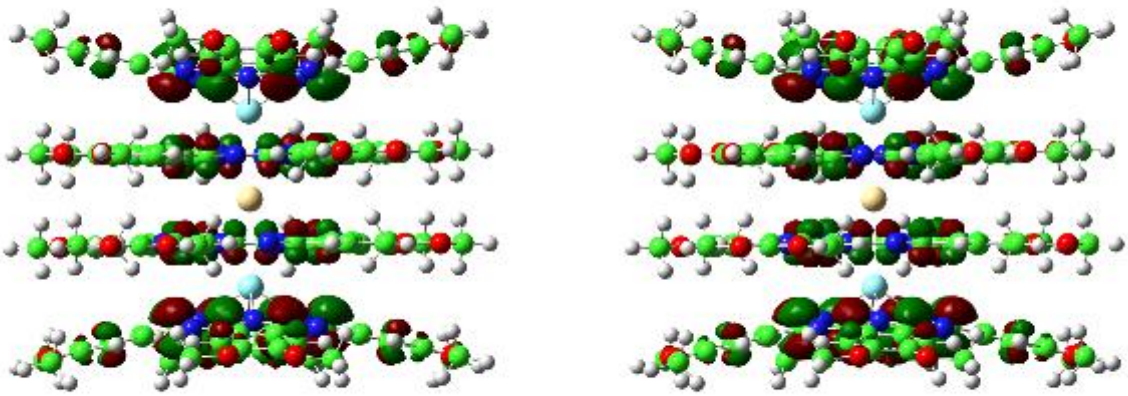
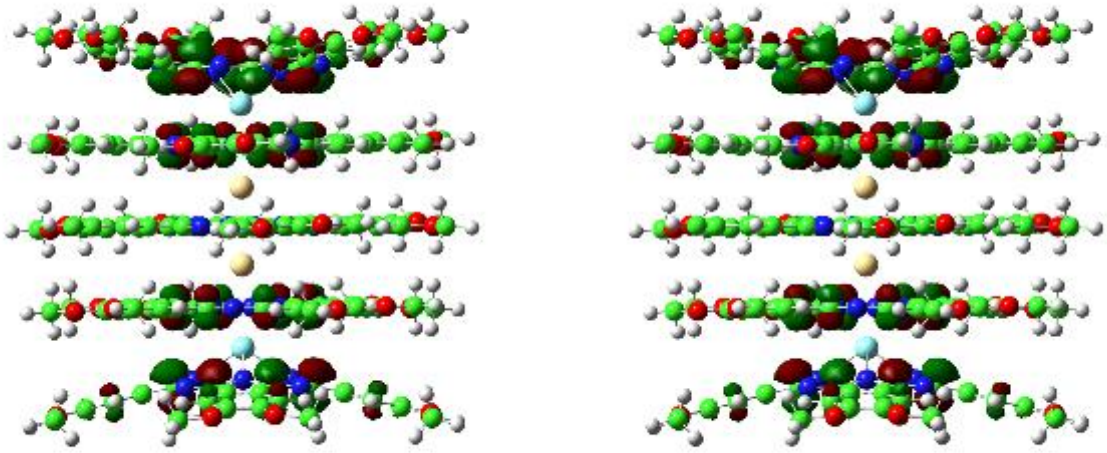


Fig. S286. Molecular orbitals of **[5]**$^{2+}$ in AFM and FM states.



HOMO LUMO

Fig. S287. Natural orbitals of **[4]**$^{2+}$.



HOMO LUMO

Fig. S288. Natural orbitals of **[5]**$^{2+}$.

5. *Ab Initio* Ligand Field Calculations

5.1. General Information

Choice of molecular fragments: in the case of the triple-deckers, a diamagnetic Lu(III) ion was used instead of the Tb(III) ion in the calculations. The calculations were based on the XRD data for those complexes for which crystals of good quality could have been obtained. The structures used in the calculations contained two ligands each. Due to previous reports[27] on the importance of avoiding the simplification or reduction o the size of the molecular fragments used in the calculations, we did not completely replace the alkoxy groups with aromatic H atoms. Instead, the –OBu chains were turned into –OMe groups (this practically halved the number of atoms in the calculation). If the molecule in question had 2 different Tb(III) ions, these are herein described as simply numbered (1 and 2), or, if the coordination environment changed from square antiprismatic (SAP) to (almost) square prismatic (SP), then the distinction is made with labels "SAP" and "SP".

Details about the *ab initio* (CASSCF[28]) calculations: these were done with the software Molcas 8.2[29], utilizing the RASSCF and RASSI modules, as well as the SINGLE_ANISO and POLY_ANISO modules for magnetic properties. Choice of the basis sets (all ANO-RCC[30-32]): due to the still significant size of the fragments used in the calculations, we chose to do calculations with a VDZP basis on the Tb(III) ion, VDZP basis on N atoms, VDZ basis on C and H atoms and VDZP on Cd(II) or Lu(III) ions. Number of roots taken into account for Tb(III) (8 electrons in 7 orbitals active space): multiplicity 7: 7 out of 7, multiplicity 5: 140 out of 140, multiplicity 3:588 out of 588. We tested of our choice of basis sets and the number of roots in the case of the neutral triple-decker (**[3]^0**) against the i) TVZP basis set on the Tb(III) ion and ii) consideration of singlet states. The comparison is given in a corresponding table below. We did not observe a significant improvement with the VTZP basis on the Tb(III) ion or with the inclusion of the singlet state (roots 121 out of 490) with regards to how well we could fit the experimental data with the theoretical model. For some of the compounds, especially for those which showed possible inter- and intramolecular dipole-dipole interactions to be of relevance, we used the corresponding "aniso" files in the POLY_ANISO module to improve the agreement in the fit of experimental DC data with the theoretical model.

Choice of the number of paired electrons: from a strict consideration of total charge (metal ions and ligands), some fragments which were used in the calculations would have contained an unpaired electron on the ligands. For this reason, in such cases two calculations on the same molecular fragment were always made: one with the addition of another electron to the total fragment, and one with the removal of one electron from the total fragment, in order to round the number of electron pairs and make sure that the only unpaired electrons were in the 4f shell. In all such instances, results from both calculations were tabulated below and some slight differences in the E-levels, g-factors, ligand field parameters and weights of M_J components can be observed. Both sets of calculated LF parameters obtained in this approach were deemed equally valid for fitting of the DC SQUID data, so we fitted the experimental data with the one of the two theoretical models which gave a better quality of the fit. The numbers of electron pairs are indicated in captions of figures with easy axes.

The plots of the easy axes for all calculated species (ground state) show that structural distortions induced by the successive oxidations, do not influence significantly the direction of the magnetic easy axes, i.e. all axes point approximately perpendicular to the plane of the ligands. On the other hand, the structural changes have a significant influence on the ligand field experienced by the lanthanide ion, as is shown in the tabulated data below. In every figure that contains the plot of the calculated easy axes, the molecular fragment is shown from two perspectives, differing by ca. 90 degrees from one another with respect to the rotation around the axis perpendicular to two ligands. [33]

Formalism for crystal field parameters tabulated below: Hamiltonian Hcf = SUM_{n,m} alpha(n) * [B(n,m) * O(n,m) + C(n,m) * W(n,m)]; where: O(n,m) = 0.5 * ((-1)**m * Y(n,+m) + Y(n,-m)); W(n,m) = -0.5 *

((-1)**m * Y(n,+m) - Y(n,-m)) * I; (I = imaginary unit; n - the rank of the ITO, = 2, 4, 6; m - the component of the ITO, = 0, 1, ... n; alpha(n) - Stevens coefficients. Reference is given here. [34]

5.2. Triple-Deckers **[3]**

Table S35. Energy spectrum and composition of wave functions of **[3]^0** predicted by computational methods described above, with varying settings (2nd column: TZVP on the Tb(III) ion, other atoms with same basis sets as above, 3rd column: including 121 roots of the singlet state). Both show differences which are not significant in the context of this work. (a) 453 electron pairs. (b) 454 electron pairs.

	[3]^0	**[3]^0** (VTZP)	**[3]^0** (singlet)	**[3]$^{2+}$**	**[3]$^{2+}$ (a)**	**[3]$^{2+}$ (b)**
Nr.	*E* (cm^{-1})	*E* (cm^{-1})	*E* (cm^{-1})	*E* (cm^{-1})	*E* (cm^{-1})	*E* (cm^{-1})
1	0	0	0	0	0.000	0
2	0.025	0.027	0.025	0.359	0.359	0.16
3	231.972	239.620	232.282	113.685	113.685	141.461
4	233.303	240.937	233.607	115.420	115.420	144.014
5	295.298	308.422	295.924	143.877	143.877	171.322
6	311.848	326.375	312.519	154.424	154.424	181.254
7	321.419	336.579	322.127	186.426	186.426	201.113
8	329.705	345.183	330.419	193.130	193.130	206.772
9	358.602	372.712	359.178	225.626	225.626	249.917
10	420.276	438.394	421.042	252.428	252.428	274.951
11	437.064	456.114	437.890	256.184	256.184	279.472
12	448.799	468.634	449.654	284.695	284.695	306.392
13	452.367	472.456	453.248	289.210	289.210	309.147

Table S36. Main values of the *g*-tensor of the lowest Kramers doublets for the indicated complex (fragment). (a) 453 electron pairs. (b) 454 electron pairs.

	$[3]^0$			$[3]^{2+}$ (a)			$[3]^{2+}$ (b)		
Nr.	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z
1	0.00E+00	2.17E-07	17.923	0.00E+00	1.57E-07	17.850	1.00E-08	3.47E-07	17.891
2	0.00E+00	1.42E-07	14.158	0.00E+00	0.00E+00	16.371	0.00E+00	8.70E-08	16.408
3	2.90E-08	1.69E-07	14.064	0.00E+00	3.00E-08	14.368	0.00E+00	3.00E-08	13.530
4	7.00E-08	2.09E-07	15.274	0.00E+00	9.70E-08	11.352	0.00E+00	1.03E-07	10.417
5	0.00E+00	1.35E-07	8.003	2.30E-07	3.76E-07	9.479	2.24E-07	4.28E-07	10.134
6	5.45E-07	8.10E-07	4.062	1.32E-07	7.07E-07	6.968	0.00E+00	0.00E+00	8.028

Table S37. *Ab initio* crystal-field parameters B_k^q (in cm^{-1}) for the molecular fragments of triple-decker series made from XRD data. (a) 453 electron pairs. (b) 454 electron pairs.

			$[3]^0$		$[3]^{2+}$ (a)		$[3]^{2+}$ (b)	
		1/alpha(n)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)
n	m							
2	0		3.22E+02	0.00E+00	1.23E+02	0.00E+00	1.49E+02	0.00E+00
2	1	-99	-1.76E+01	-1.76E+01	-3.00E+01	-3.00E+01	5.50E+01	5.50E+01
2	2		-1.82E+01	-2.05E+01	-4.38E+01	-1.33E+01	4.53E+01	-7.12E+00
4	0		-1.14E+02	0.00E+00	-1.22E+02	0.00E+00	-1.25E+02	0.00E+00
4	1		-9.15E+00	-2.03E+00	-1.55E+01	2.68E+01	2.82E+01	7.96E+00
4	2	8167.5	-1.75E+00	-1.75E+00	1.85E+00	1.85E+00	-1.38E+00	-1.38E+00
4	3		3.06E+00	6.49E+00	8.29E+00	-3.52E+00	7.93E+00	3.71E+00
4	4		1.03E+02	-7.79E+01	2.78E+01	-1.03E+02	-6.33E+01	-7.98E+01
6	0		-1.06E+01	0.00E+00	-4.54E+00	0.00E+00	-3.72E+00	0.00E+00
6	1		-4.12E-01	-3.78E-01	4.41E-01	-7.09E-01	-1.22E+00	-4.57E-01
6	2		8.49E-01	1.35E+00	1.56E+00	-4.48E-03	-1.71E+00	7.08E-01
6	3	-891891	6.08E+00	6.08E+00	9.90E+00	9.90E+00	7.49E+00	7.49E+00
6	4		3.27E+01	-5.34E+01	3.56E+00	-1.79E+00	-6.11E+00	-1.18E+01
6	5		-7.85E-01	-2.78E+00	2.54E+00	1.38E+00	-1.38E+00	-9.79E-01
6	6		-2.03E+00	-7.17E-01	-1.52E+00	2.17E+00	-1.83E+00	-1.84E+00

Table S38. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[3]^{0}**.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.70	0.40	1.20	0.10	0.40	0.10	0.30	0.10	1.00
-5	0.00	0.00	68.80	69.70	0.80	15.00	4.60	10.60	0.80	1.50	4.90	4.70	0.80
-4	0.30	0.30	1.80	2.00	44.90	2.80	22.30	10.00	69.60	48.90	4.40	5.20	9.30
-3	0.30	0.30	6.90	2.30	2.90	43.50	6.60	45.60	5.30	4.30	52.70	53.90	13.60
-2	1.40	1.00	1.70	1.10	29.00	11.80	62.40	9.90	5.80	10.90	12.90	9.20	67.90
-1	0.10	0.00	14.60	11.30	2.10	52.30	14.60	50.60	9.70	7.30	44.70	44.20	6.60
0	0.10	0.00	1.10	1.40	65.20	0.90	25.60	9.50	0.90	69.50	5.10	2.00	11.70
1	0.10	0.00	14.60	11.30	2.10	52.30	14.60	50.60	9.70	7.30	44.70	44.20	6.60
2	1.40	1.00	1.70	1.10	29.00	11.80	62.40	9.90	5.80	10.90	12.90	9.20	67.90
3	0.30	0.30	6.90	2.30	2.90	43.50	6.60	45.60	5.30	4.30	52.70	53.90	13.60
4	0.30	0.30	1.80	2.00	44.90	2.80	22.30	10.00	69.60	48.90	4.40	5.20	9.30
5	0.00	0.00	68.80	69.70	0.80	15.00	4.60	10.60	0.80	1.50	4.90	4.70	0.80
6	70.70	70.70	0.00	0.00	0.70	0.40	1.20	0.10	0.40	0.10	0.30	0.10	1.00

Table S39. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[3]$^{2+}$**. Number of electron pairs 453.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.40	70.60	1.20	4.10	0.40	4.80	0.40	0.80	3.20	1.40	1.20	1.30	1.60
-5	0.10	0.10	24.20	9.70	28.90	12.40	60.20	63.80	3.20	16.40	14.60	10.70	4.80
-4	1.70	1.50	6.20	22.70	13.20	7.60	12.70	9.00	42.10	34.80	40.10	37.10	54.80
-3	0.60	0.50	27.30	6.90	17.80	19.10	27.90	15.20	30.50	38.10	37.30	51.40	33.20
-2	6.10	4.00	11.90	31.60	10.10	59.50	8.30	10.20	40.50	39.60	36.00	14.80	16.40
-1	0.20	0.20	58.10	21.20	54.90	11.90	18.20	22.00	25.40	19.80	21.70	24.80	8.80
0	1.40	0.60	14.50	75.80	33.30	37.90	8.10	7.40	0.70	14.70	7.00	7.30	32.40
1	0.20	0.20	58.10	21.20	54.90	11.90	18.20	22.00	25.40	19.80	21.70	24.80	8.80
2	6.10	4.00	11.90	31.60	10.10	59.50	8.30	10.20	40.50	39.60	36.00	14.80	16.40
3	0.60	0.50	27.30	6.90	17.80	19.10	27.90	15.20	30.50	38.10	37.30	51.40	33.20
4	1.70	1.50	6.20	22.70	13.20	7.60	12.70	9.00	42.10	34.80	40.10	37.10	54.80
5	0.10	0.10	24.20	9.70	28.90	12.40	60.20	63.80	3.20	16.40	14.60	10.70	4.80
6	70.40	70.60	1.20	4.10	0.40	4.80	0.40	0.80	3.20	1.40	1.20	1.30	1.60

Table S40. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[3]$^{2+}$**. Number of electron pairs 454.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.60	70.60	0.70	2.90	0.30	3.00	0.20	0.50	2.30	0.70	1.00	1.20	1.40
-5	0.00	0.00	27.40	11.10	37.40	13.40	58.90	60.40	2.50	15.20	10.20	8.40	4.70
-4	1.40	1.30	5.90	23.30	11.60	10.90	10.80	9.10	45.90	36.10	40.40	35.00	52.00
-3	0.30	0.20	27.90	5.60	17.90	14.70	27.00	18.40	29.50	40.50	31.70	52.10	36.80
-2	4.00	2.80	10.80	34.00	2.20	59.30	7.60	8.00	37.60	33.00	44.10	18.50	16.50
-1	0.20	0.10	57.20	19.10	52.00	3.20	24.50	28.60	24.50	23.90	17.60	24.30	12.70
0	0.80	0.40	9.50	74.50	29.40	43.60	7.30	10.50	0.00	18.20	4.50	11.00	31.10
1	0.20	0.10	57.20	19.10	52.00	3.20	24.50	28.60	24.50	23.90	17.60	24.30	12.70
2	4.00	2.80	10.80	34.00	2.20	59.30	7.60	8.00	37.60	33.00	44.10	18.50	16.50
3	0.30	0.20	27.90	5.60	17.90	14.70	27.00	18.40	29.50	40.50	31.70	52.10	36.80
4	1.40	1.30	5.90	23.30	11.60	10.90	10.80	9.10	45.90	36.10	40.40	35.00	52.00
5	0.00	0.00	27.40	11.10	37.40	13.40	58.90	60.40	2.50	15.20	10.20	8.40	4.70
6	70.60	70.60	0.70	2.90	0.30	3.00	0.20	0.50	2.30	0.70	1.00	1.20	1.40

Fig. S289. $[3]^{0}$: plot of the fragment of the triple-decker (overall oxidation state 0) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 455.

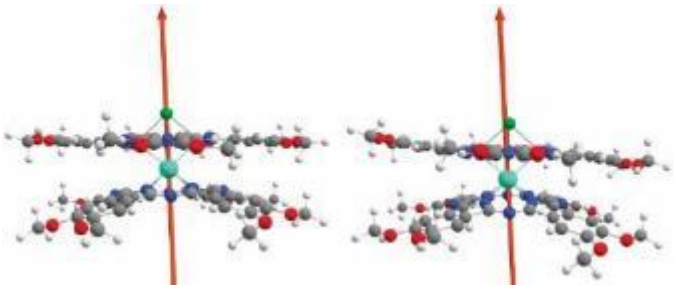


Fig. S290. $[3]^{2+}$ (a): plot of the fragment of the triple-decker (overall oxidation state +2) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 453.

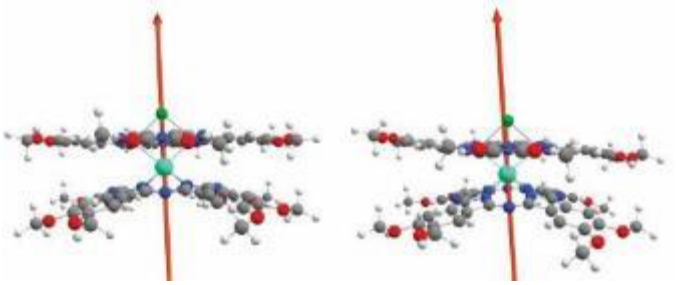


Fig. S291. $[3]^{2+}$ (b): plot of the fragment of the triple-decker (overall oxidation state +2) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 454.

5.3. Quadruple-Deckers **[4]**

Table S41. Energy spectrum of quadruple-decker series as predicted by computational methods described above. (a) 444 electron pairs ; (b) 443 electron pairs.

	$[4]^0$ Tb1 (a)	$[4]^0$ Tb2 (a)	$[4]^{2+}$ Tb1 (a)	$[4]^{2+}$ Tb1 (b)	$[4]^{2+}$ Tb2 (a)	$[4]^{2+}$ Tb2 (b)
Nr.	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})
1	0.000	0.000	0.000	0.000	0.000	0.000
2	0.008	0.009	0.009	0.014	0.012	0.018
3	259.257	262.617	243.106	239.671	240.125	235.856
4	259.736	263.550	243.106	239.671	240.125	235.856
5	363.097	359.922	334.790	317.783	312.967	292.681
6	386.206	379.693	356.084	337.503	329.808	309.156
7	388.334	409.969	356.088	337.506	329.813	309.162
8	396.688	413.687	358.666	339.923	331.251	310.263
9	414.391	424.559	370.382	362.715	360.527	351.624
10	508.686	515.931	404.749	394.065	390.562	379.409
11	533.265	540.296	424.327	411.333	408.047	391.421
12	555.408	554.931	424.329	411.338	408.057	393.131
13	564.228	564.777	426.801	411.747	408.782	393.141

Table S42. Energy spectrum of the quadruple-decker series as predicted by computational methods described above. (a) 444 electron pairs ; (b) 443 electron pairs.

	$[4]^{4+}$ Tb1 (a)	$[4]^{4+}$ Tb1 (b)	$[4]^{4+}$ Tb2 (a)	$[4]^{4+}$ Tb2 (b)
Nr.	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})
1	0.000	0.000	0.000	0.000
2	0.008	0.017	0.013	0.010
3	246.567	235.093	242.325	252.557
4	246.583	235.135	242.325	252.557
5	319.482	276.183	299.865	320.127
6	335.527	293.086	309.718	332.770
7	335.637	293.293	319.449	341.848
8	339.339	296.875	319.452	341.850
9	367.153	345.713	373.721	391.447
10	389.608	363.324	473.102	499.586
11	402.194	364.718	501.186	529.846
12	404.896	371.318	501.189	529.849
13	405.295	371.710	516.193	546.335

Table S43. Main values of the *g*-tensor of the lowest Kramers doublets for the indicated complex (fragment). (a) 444 electron pairs ; (b) 443 electron pairs.

Nr.	$[4]^0$ Tb1 (a)			$[4]^0$ Tb2 (a)		
	g_x	g_y	g_z	g_x	g_y	g_z
1	0.00E+00	1.50E-08	17.928	0.00E+00	3.10E-08	17.928
2	6.00E-09	2.60E-08	14.490	0.00E+00	0.00E+00	14.473
3	2.38E-07	1.78E-06	10.109	0.00E+00	1.69E-07	14.831
4	2.13E-07	1.77E-06	10.107	0.00E+00	5.70E-08	6.530
5	3.00E-08	3.30E-08	5.871	0.00E+00	6.00E-08	5.606
6	4.20E-08	8.10E-08	2.849	1.20E-08	3.40E-08	2.678

Table S44. Main values of the *g*-tensor of the lowest Kramers doublets for the indicated complex (fragment). (a) 444 electron pairs ; (b) 443 electron pairs.

Nr.	$[4]^{2+}$ Tb1 (a)			$[4]^{2+}$ Tb1 (b)			$[4]^{2+}$ Tb2 (a)			$[4]^{2+}$ Tb2 (b)		
	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z
1	2.00E-09	2.00E-09	17.925	2.00E-09	2.00E-09	17.925	2.00E-09	3.00E-09	17.924	1.00E-09	2.00E-09	17.923
2	1.00E-09	4.00E-09	14.503	1.00E-09	4.00E-09	14.503	7.00E-09	1.00E-08	14.406	3.00E-09	9.00E-09	14.191
3	2.52E-05	3.65E-04	10.764	2.52E-05	3.65E-04	10.764	1.15E-05	6.37E-04	11.113	1.49E-05	3.43E-04	11.142
4	2.53E-05	4.33E-04	12.760	2.53E-05	4.33E-04	12.760	1.15E-05	7.25E-04	12.656	1.48E-05	3.85E-04	12.497
5	2.10E-08	2.90E-08	8.460	2.10E-08	2.90E-08	8.460	1.80E-08	4.60E-08	9.283	1.50E-08	3.10E-08	9.776
6	3.40E-08	1.00E-07	5.195	3.40E-08	1.00E-07	5.195	8.40E-08	1.61E-07	5.496	6.04E-05	9.21E-05	12.407

Table S45. Main values of the *g*-tensor of the lowest Kramers doublets for the indicated complex (fragment). (a) 444 electron pairs; (b) 443 electron pairs.

Nr.	$[4]^{4+}$ Tb1 (a)			$[4]^{4+}$ Tb1 (b)			$[4]^{4+}$ Tb2 (a)			$[4]^{4+}$ Tb2 (b)		
	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z
1	0.00E+00	1.00E-09	17.924	2.00E-09	4.00E-09	17.921	0.00E+00	1.00E-09	17.926	1.00E-09	1.00E-09	17.927
2	4.00E-09	1.20E-08	14.425	6.00E-09	7.00E-09	13.866	1.10E-08	2.50E-08	13.901	1.00E-09	2.00E-09	14.077
3	2.02E-06	3.13E-05	11.552	4.09E-06	2.11E-05	11.441	5.00E-09	1.34E-07	0.016	7.00E-09	2.00E-08	0.009
4	1.99E-06	3.40E-05	12.488	4.09E-06	2.23E-05	12.107	1.02E-07	2.19E-07	1.861	1.80E-08	2.30E-08	2.202
5	1.00E-08	3.70E-08	9.753	3.60E-08	4.10E-08	2.065	2.00E-09	1.50E-08	7.833	5.00E-09	8.00E-09	7.568
6	1.00E-05	1.48E-05	11.949	5.66E-06	6.91E-06	6.994	2.00E-08	2.40E-08	3.200	4.20E-08	5.80E-08	3.034

Table S46. *Ab initio* crystal-field parameters B_k^q (in cm^{-1}) for the molecular fragments of quintuple-decker series made from XRD data. Part 1. (a) 444 electron pairs: (b) 443 electron pairs.

			$[4]^0$ Tb1 (a)		$[4]^0$ Tb2 (a)		$[4]^{2+}$ Tb1 (a)		$[4]^{2+}$ Tb1 (b)		$[4]^{2+}$ Tb2 (a)		$[4]^{2+}$ Tb2 (b)	
n	m	1/alpha(n)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)
2	0		4.19E+02	0.00E+00	4.24E+02	0.00E+00	3.29E+02	0.00E+00	3.09E+02	0.00E+00	3.03E+02	0.00E+00	2.81E+02	0.00E+00
2	1	-99	1.80E+01	1.80E+01	-1.50E+00	-1.50E+00	-6.13E-02	-6.13E-02	3.03E-02	3.03E-02	-7.82E-02	-7.82E-02	1.14E-01	1.14E-01
2	2		2.39E+01	1.52E+01	-5.32E+00	5.88E+01	6.10E-03	-1.32E-03	1.50E-03	-6.61E-03	-1.53E-02	6.32E-03	-1.21E-02	1.36E-02
4	0		-1.09E+02	0.00E+00	-1.12E+02	0.00E+00	-1.19E+02	0.00E+00	-1.21E+02	0.00E+00	-1.22E+02	0.00E+00	-1.25E+02	0.00E+00
4	1		9.20E+00	-1.08E+01	-3.00E-01	2.57E+00	-3.10E-02	-4.63E-02	1.23E-02	-2.43E-02	-3.98E-02	4.21E-02	5.72E-02	-3.60E-02
4	2	8167.5	-1.71E+00	-1.71E+00	3.38E+00	3.38E+00	-2.11E-03	-2.11E-03	3.81E-03	3.81E-03	-3.65E-04	-3.65E-04	-7.09E-04	-7.09E-04
4	3		-7.47E+00	9.61E-01	-2.40E+00	-5.56E+00	9.31E-03	-2.90E-02	-7.27E-05	3.36E-02	4.47E-04	-2.27E-03	-6.91E-03	2.43E-03
4	4		1.66E+01	1.52E+02	1.47E+02	1.45E+01	-3.69E+01	6.21E+01	5.83E+01	-5.02E+01	-4.62E+00	-7.85E+01	-7.65E+01	-3.31E+01
6	0		-1.38E+01	0.00E+00	-1.50E+01	0.00E+00	-9.92E+00	0.00E+00	-9.25E+00	0.00E+00	-7.32E+00	0.00E+00	-6.40E+00	0.00E+00
6	1		5.55E-01	-9.85E-01	1.16E+00	-4.64E-01	2.40E-03	2.33E-03	-7.63E-03	-3.18E-03	1.08E-03	-2.31E-03	-4.11E-03	1.83E-03
6	2		-6.34E-01	-5.96E-01	1.42E+00	-3.98E+00	-1.19E-03	-1.07E-03	2.26E-03	6.51E-03	6.08E-04	1.31E-04	6.61E-04	-1.87E-04
6	3	-891891	-4.76E+00	-4.76E+00	-3.03E-01	-3.03E-01	-1.19E-03	-1.19E-03	5.60E-03	5.60E-03	-3.42E-03	-3.42E-03	4.83E-03	4.83E-03
6	4		-1.03E+01	9.96E+01	9.63E+01	-1.24E+01	-1.66E+00	1.95E+01	7.52E+00	-1.76E+01	1.68E+01	-2.82E+01	-1.70E+01	-2.76E+01
6	5		-1.42E+00	-7.26E+00	3.53E+00	-3.97E-01	-2.82E-03	8.89E-03	7.59E-03	-9.33E-04	-1.37E-03	-1.04E-02	1.46E-02	5.91E-03
6	6		-1.59E+00	2.11E+00	-2.72E+00	6.47E+00	-4.62E-04	-6.66E-04	-3.01E-03	-2.98E-03	7.15E-04	1.02E-03	1.04E-03	-7.22E-04

Table S47. *Ab initio* crystal-field parameters B_k^q (in cm^{-1}) for the molecular fragments of quadruple-decker series made from XRD data. Part 2. (a) 444 electron pairs; (b) 443 electron pairs.

			$[4]^{4+}$ Tb1 (a)		**$[4]^{4+}$ Tb1 (b)**		**$[4]^{4+}$ Tb2 (a)**		**$[4]^{4+}$ Tb2 (b)**	
		1/alpha(n)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)
n	m									
2	0		3.01E+02	0.00E+00	2.56E+02	0.00E+00	3.53E+02	0.00E+00	3.80E+02	0.00E+00
2	1	-99	2.17E+00	2.17E+00	-4.82E-01	-4.82E-01	2.14E-02	2.14E-02	2.19E-02	2.19E-02
2	2		-7.56E-01	-1.73E-01	-7.42E-01	2.78E-01	3.23E-03	3.86E-03	4.48E-04	4.15E-03
4	0		-1.28E+02	0.00E+00	-1.31E+02	0.00E+00	-1.12E+02	0.00E+00	-1.13E+02	0.00E+00
4	1		1.07E+00	-7.00E-01	-2.38E-01	-4.48E-02	1.04E-02	3.76E-02	1.06E-02	1.09E-02
4	2	8167.5	-3.76E-03	-3.76E-03	-6.37E-02	-6.37E-02	8.04E-04	8.04E-04	9.16E-04	9.16E-04
4	3		3.56E-02	2.01E-01	3.21E-02	9.75E-02	-1.05E-02	-2.12E-02	9.48E-03	-3.34E-02
4	4		6.35E+01	2.12E+01	2.42E+01	-6.88E+01	-1.38E+02	-1.28E+02	-7.32E+01	-1.80E+02
6	0		-5.75E+00	0.00E+00	-3.94E+00	0.00E+00	-7.03E+00	0.00E+00	-7.92E+00	0.00E+00
6	1		-9.81E-02	6.58E-02	3.19E-02	-2.58E-03	4.13E-04	-1.02E-04	-2.67E-04	3.03E-03
6	2		9.02E-03	-1.68E-02	2.20E-03	-1.43E-02	-7.50E-04	-9.44E-04	-4.19E-04	-9.42E-04
6	3	-891891	-2.09E-02	-2.09E-02	4.32E-03	4.32E-03	-1.57E-02	-1.57E-02	-2.91E-03	-2.91E-03
6	4		1.47E+01	7.69E+00	6.87E+00	-1.15E+01	-7.04E+01	-9.28E+01	-2.76E+01	-1.17E+02
6	5		-1.15E-01	4.77E-02	2.41E-02	-3.55E-02	-1.22E-02	1.83E-02	-8.60E-04	6.31E-03
6	6		-2.37E-02	4.75E-03	1.14E-02	1.66E-02	8.10E-04	-3.76E-04	8.75E-04	2.80E-04

Table S48. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **$[4]^0$** Tb1 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.10	0.00	0.40	0.50	0.50	0.20	0.50	0.20	0.10	0.20	0.60
-5	0.00	0.00	70.10	70.30	2.50	4.90	4.40	8.00	0.40	0.70	2.50	4.20	0.30
-4	0.50	0.50	2.70	2.90	57.20	19.10	23.40	6.60	64.10	39.40	3.50	2.00	9.00
-3	0.10	0.10	3.90	0.60	10.20	46.60	14.30	47.50	16.40	1.60	50.60	48.60	6.50
-2	0.70	0.60	1.20	1.50	5.30	26.00	63.00	9.50	15.40	15.70	4.10	5.50	68.60
-1	0.20	0.20	7.70	6.40	6.10	41.50	16.20	50.00	19.50	2.70	49.00	50.80	2.20
0	0.00	0.10	1.10	2.30	55.80	8.30	3.00	9.00	1.70	79.80	3.00	2.00	18.10
1	0.20	0.20	7.70	6.40	6.10	41.50	16.20	50.00	19.50	2.70	49.00	50.80	2.20
2	0.70	0.60	1.20	1.50	5.30	26.00	63.00	9.50	15.40	15.70	4.10	5.50	68.60
3	0.10	0.10	3.90	0.60	10.20	46.60	14.30	47.50	16.40	1.60	50.60	48.60	6.50
4	0.50	0.50	2.70	2.90	57.20	19.10	23.40	6.60	64.10	39.40	3.50	2.00	9.00
5	0.00	0.00	70.10	70.30	2.50	4.90	4.40	8.00	0.40	0.70	2.50	4.20	0.30
6	70.70	70.70	0.10	0.00	0.40	0.50	0.50	0.20	0.50	0.20	0.10	0.20	0.60

Table S49. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **$[4]^0$** Tb2(a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.60	0.10	0.50	0.30	0.30	0.30	0.10	0.10	0.60
-5	0.00	0.00	70.00	70.50	0.40	9.80	1.60	1.40	2.70	0.30	4.80	1.70	0.50
-4	0.40	0.40	0.70	0.70	48.60	2.20	33.80	67.00	21.10	38.80	0.90	0.80	6.40
-3	0.20	0.10	5.30	0.80	1.50	46.90	2.00	15.80	51.70	0.50	45.60	52.60	1.30
-2	0.80	0.60	0.90	0.50	35.00	3.30	60.50	7.50	3.00	8.70	1.20	1.40	70.40
-1	0.10	0.10	8.50	5.60	0.20	51.90	3.60	14.20	43.20	1.30	53.80	47.10	1.50
0	0.10	0.00	0.60	0.00	53.10	1.30	18.60	1.40	0.00	82.60	0.20	2.20	0.80
1	0.10	0.10	8.50	5.60	0.20	51.90	3.60	14.20	43.20	1.30	53.80	47.10	1.50
2	0.80	0.60	0.90	0.50	35.00	3.30	60.50	7.50	3.00	8.70	1.20	1.40	70.40
3	0.20	0.10	5.30	0.80	1.50	46.90	2.00	15.80	51.70	0.50	45.60	52.60	1.30
4	0.40	0.40	0.70	0.70	48.60	2.20	33.80	67.00	21.10	38.80	0.90	0.80	6.40
5	0.00	0.00	70.00	70.50	0.40	9.80	1.60	1.40	2.70	0.30	4.80	1.70	0.50
6	70.70	70.70	0.00	0.00	0.60	0.10	0.50	0.30	0.30	0.30	0.10	0.10	0.60

Table S50. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **$[4]^{2+}$** Tb1 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00	0.00	1.00
-5	0.00	0.00	70.30	70.10	0.00	7.60	7.60	0.00	0.00	0.00	3.30	3.30	0.00
-4	0.00	0.00	0.00	0.00	49.00	0.10	0.10	0.00	70.70	50.90	0.00	0.10	0.00
-3	0.00	0.00	1.50	1.50	0.00	39.30	39.30	0.10	0.10	0.00	58.80	58.70	0.40
-2	1.10	1.00	0.00	0.00	0.00	0.00	0.10	70.70	0.00	0.00	0.40	0.20	70.70
-1	0.00	0.00	8.20	8.10	0.00	58.30	58.30	0.10	0.10	0.10	39.20	39.20	0.20
0	0.00	0.00	0.00	0.00	72.10	0.00	0.00	0.00	0.00	69.30	0.00	0.00	0.00
1	0.00	0.00	8.10	8.20	0.00	58.30	58.30	0.10	0.10	0.10	39.20	39.20	0.20
2	1.10	1.00	0.00	0.00	0.00	0.00	0.10	70.70	0.00	0.00	0.40	0.20	70.70
3	0.00	0.00	1.50	1.50	0.00	39.30	39.30	0.10	0.10	0.00	58.70	58.80	0.40
4	0.00	0.00	0.00	0.00	49.00	0.10	0.10	0.00	70.70	50.90	0.00	0.10	0.00
5	0.00	0.00	70.10	70.30	0.00	7.60	7.60	0.00	0.00	0.00	3.30	3.30	0.00
6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.10	0.00	0.00	0.00	0.00	1.00

Table S51. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **[4]**$^{2+}$ Tb1 (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.30	0.00	0.00	0.00	0.00	1.10
-5	0.00	0.00	70.10	69.80	0.00	9.70	9.80	0.00	0.00	0.00	3.60	3.60	0.10
-4	0.00	0.00	0.00	0.00	44.70	0.00	0.00	0.00	70.70	54.80	0.00	0.00	0.00
-3	0.00	0.00	2.10	2.10	0.00	37.60	37.60	0.10	0.00	0.00	59.80	59.80	1.30
-2	1.30	1.10	0.00	0.00	0.00	0.00	0.10	70.70	0.00	0.00	0.30	1.50	70.70
-1	0.00	0.00	10.20	10.20	0.00	59.10	59.10	0.10	0.00	0.00	37.50	37.50	0.80
0	0.00	0.00	0.00	0.00	77.50	0.00	0.00	0.00	0.00	63.20	0.00	0.00	0.00
1	0.00	0.00	10.20	10.20	0.00	59.10	59.10	0.10	0.00	0.00	37.50	37.50	0.80
2	1.30	1.10	0.00	0.00	0.00	0.00	0.10	70.70	0.00	0.00	0.30	1.50	70.70
3	0.00	0.00	2.10	2.10	0.00	37.60	37.60	0.10	0.00	0.00	59.80	59.80	1.30
4	0.00	0.00	0.00	0.00	44.70	0.00	0.00	0.00	70.70	54.80	0.00	0.00	0.00
5	0.00	0.00	69.80	70.10	0.00	9.70	9.80	0.00	0.00	0.00	3.60	3.60	0.10
6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.30	0.00	0.00	0.00	0.00	1.10

Table S52. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **[4]**$^{2+}$ Tb2 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.20	0.00	0.00	0.00	0.00	1.00
-5	0.00	0.00	69.90	70.00	0.00	9.80	9.80	0.00	0.00	0.00	3.40	3.50	0.10
-4	0.00	0.00	0.00	0.00	43.40	0.00	0.00	0.00	70.70	55.80	0.10	0.10	0.00
-3	0.00	0.00	2.30	2.30	0.00	37.70	37.70	0.10	0.00	0.10	59.80	59.80	1.60
-2	1.20	1.00	0.00	0.00	0.00	0.00	0.10	70.70	0.00	0.00	1.70	0.80	70.70
-1	0.00	0.00	10.10	10.10	0.00	59.00	59.00	0.10	0.10	0.10	37.60	37.60	1.00
0	0.00	0.00	0.00	0.00	79.00	0.00	0.10	0.00	0.00	61.30	0.10	0.00	0.00
1	0.00	0.00	10.10	10.10	0.00	59.00	59.00	0.10	0.10	0.10	37.60	37.60	1.00
2	1.20	1.00	0.00	0.00	0.00	0.00	0.10	70.70	0.00	0.00	1.70	0.80	70.70
3	0.00	0.00	2.30	2.30	0.00	37.70	37.70	0.10	0.00	0.10	59.80	59.80	1.60
4	0.00	0.00	0.00	0.00	43.40	0.00	0.00	0.00	70.70	55.80	0.10	0.10	0.00
5	0.00	0.00	70.00	69.90	0.00	9.80	9.80	0.00	0.00	0.00	3.40	3.50	0.10
6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.20	0.00	0.00	0.00	0.00	1.00

Table S53. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[4]**$^{2+}$ Tb2 (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.40	0.00	0.00	1.20	0.00	0.00
-5	0.00	0.00	69.30	69.30	0.00	13.40	13.40	0.00	0.00	0.00	0.10	3.90	3.90
-4	0.00	0.00	0.00	0.00	39.30	0.00	0.00	0.00	70.70	58.80	0.00	0.10	0.10
-3	0.00	0.00	3.50	3.50	0.00	36.10	36.10	0.10	0.00	0.10	0.80	60.70	60.70
-2	1.40	1.20	0.00	0.00	0.00	0.10	0.20	70.70	0.00	0.00	70.70	1.00	0.00
-1	0.00	0.00	13.50	13.50	0.00	59.30	59.30	0.10	0.10	0.10	0.50	36.00	36.00
0	0.00	0.00	0.00	0.00	83.10	0.10	0.00	0.00	0.00	55.60	0.00	0.10	0.00
1	0.00	0.00	13.50	13.50	0.00	59.30	59.30	0.10	0.10	0.10	0.50	36.00	36.00
2	1.40	1.20	0.00	0.00	0.00	0.10	0.20	70.70	0.00	0.00	70.70	1.00	0.00
3	0.00	0.00	3.50	3.50	0.00	36.10	36.10	0.10	0.00	0.10	0.80	60.70	60.70
4	0.00	0.00	0.00	0.00	39.30	0.00	0.00	0.00	70.70	58.80	0.00	0.10	0.10
5	0.00	0.00	69.30	69.30	0.00	13.40	13.40	0.00	0.00	0.00	0.10	3.90	3.90
6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.40	0.00	0.00	1.20	0.00	0.00

Table S54. Weights of M_J components (in %) in the wavefunctions of the J = 6 ground state for **[4]**$^{4+}$ Tb1 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.90	0.10	0.10
-5	0.00	0.00	70.00	70.00	0.30	9.40	9.40	0.10	0.10	0.40	0.60	2.90	3.00
-4	0.00	0.00	0.30	0.30	39.40	1.00	0.40	0.40	70.70	58.60	1.10	2.30	1.70
-3	0.00	0.00	1.90	1.80	0.60	33.80	33.70	1.70	0.80	1.90	10.40	61.60	61.70
-2	1.00	0.90	0.10	0.10	0.20	1.10	1.30	70.70	0.40	1.60	69.60	10.00	7.40
-1	0.00	0.00	9.70	9.70	0.10	61.40	61.40	0.70	1.60	1.80	6.80	33.00	33.50
0	0.00	0.00	0.20	0.20	83.00	0.10	0.90	0.20	0.00	55.80	1.30	1.40	0.60
1	0.00	0.00	9.70	9.70	0.10	61.40	61.40	0.70	1.60	1.80	6.80	33.00	33.50
2	1.00	0.90	0.10	0.10	0.20	1.10	1.30	70.70	0.40	1.60	69.60	10.00	7.40
3	0.00	0.00	1.90	1.80	0.60	33.80	33.70	1.70	0.80	1.90	10.40	61.60	61.70
4	0.00	0.00	0.30	0.30	39.40	1.00	0.40	0.40	70.70	58.60	1.10	2.30	1.70
5	0.00	0.00	70.00	70.00	0.30	9.40	9.40	0.10	0.10	0.40	0.60	2.90	3.00
6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.90	0.10	0.10

Table S55. Weights of M_J components (in %) in the wavefunctions of the J = 6 ground state for **[4]**$^{4+}$ Tb1 (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.50	0.00	1.30	0.30	0.00	0.00
-5	0.00	0.00	68.30	68.40	0.10	17.70	17.70	0.10	0.00	0.00	0.10	3.70	3.80
-4	0.00	0.00	0.10	0.10	32.00	0.00	0.10	0.30	70.70	12.50	61.80	1.10	0.70
-3	0.00	0.00	4.40	4.30	0.10	30.40	30.40	0.20	0.30	0.60	1.20	63.70	63.60
-2	1.50	1.30	0.10	0.00	0.40	0.10	0.20	70.70	0.20	69.30	13.90	0.80	0.40
-1	0.00	0.00	17.60	17.50	0.00	61.30	61.30	0.10	0.30	0.50	0.70	30.30	30.70
0	0.00	0.00	0.10	0.00	89.10	0.10	0.00	0.40	0.00	8.80	44.50	0.60	0.30
1	0.00	0.00	17.60	17.50	0.00	61.30	61.30	0.10	0.30	0.50	0.70	30.30	30.70
2	1.50	1.30	0.10	0.00	0.40	0.10	0.20	70.70	0.20	69.30	13.90	0.80	0.40
3	0.00	0.00	4.40	4.30	0.10	30.40	30.40	0.20	0.30	0.60	1.20	63.70	63.60
4	0.00	0.00	0.10	0.10	32.00	0.00	0.10	0.30	70.70	12.50	61.80	1.10	0.70
5	0.00	0.00	68.30	68.40	0.10	17.70	17.70	0.10	0.00	0.00	0.10	3.70	3.80
6	70.70	70.70	0.00	0.00	0.00	0.00	0.00	1.50	0.00	1.30	0.30	0.00	0.00

Table S56. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **[4]**$^{4+}$ Tb2 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.60
-5	0.00	0.00	68.90	68.70	0.00	0.00	15.50	15.50	0.00	0.00	4.80	4.80	0.00
-4	0.00	0.00	0.00	0.00	52.40	0.00	0.00	0.00	70.70	47.50	0.00	0.00	0.00
-3	0.00	0.00	7.20	7.20	0.00	0.00	47.90	47.90	0.00	0.00	51.50	51.50	0.00
-2	0.90	0.60	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	0.00	0.00	70.70
-1	0.00	0.00	14.50	14.50	0.00	0.00	49.60	49.60	0.00	0.00	48.20	48.30	0.00
0	0.00	0.00	0.00	0.00	67.20	0.00	0.10	0.00	0.00	74.10	0.00	0.00	0.00
1	0.00	0.00	14.50	14.50	0.00	0.00	49.60	49.60	0.00	0.00	48.30	48.20	0.00
2	0.90	0.60	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	0.00	0.00	70.70
3	0.00	0.00	7.20	7.20	0.00	0.00	47.90	47.90	0.00	0.00	51.50	51.50	0.00
4	0.00	0.00	0.00	0.00	52.40	0.00	0.00	0.00	70.70	47.50	0.00	0.00	0.00
5	0.00	0.00	68.70	68.90	0.00	0.00	15.50	15.50	0.00	0.00	4.80	4.80	0.00
6	70.70	70.70	0.00	0.00	0.00	0.90	0.00	0.00	0.00	0.00	0.00	0.00	0.60

Table S57. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state for **[4]**$^{4+}$ Tb2 (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	0.50
-5	0.00	0.00	69.40	69.10	0.00	0.00	13.30	13.30	0.00	0.00	4.60	4.60	0.00
-4	0.00	0.00	0.00	0.00	53.70	0.00	0.00	0.00	70.70	46.00	0.00	0.00	0.00
-3	0.00	0.00	6.00	6.00	0.00	0.00	48.80	48.80	0.00	0.00	50.80	50.80	0.00
-2	0.80	0.50	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	0.00	0.00	70.70
-1	0.00	0.00	12.80	12.70	0.00	0.00	49.40	49.40	0.00	0.00	49.00	49.00	0.00
0	0.00	0.00	0.00	0.00	65.00	0.00	0.00	0.00	0.00	76.00	0.00	0.00	0.00
1	0.00	0.00	12.70	12.80	0.00	0.00	49.40	49.40	0.00	0.00	49.00	49.00	0.00
2	0.80	0.50	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	0.00	0.00	70.70
3	0.00	0.00	6.00	6.00	0.00	0.00	48.80	48.80	0.00	0.00	50.80	50.80	0.00
4	0.00	0.00	0.00	0.00	53.70	0.00	0.00	0.00	70.70	46.00	0.00	0.00	0.00
5	0.00	0.00	69.10	69.40	0.00	0.00	13.30	13.30	0.00	0.00	4.60	4.60	0.00
6	70.70	70.70	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	0.50

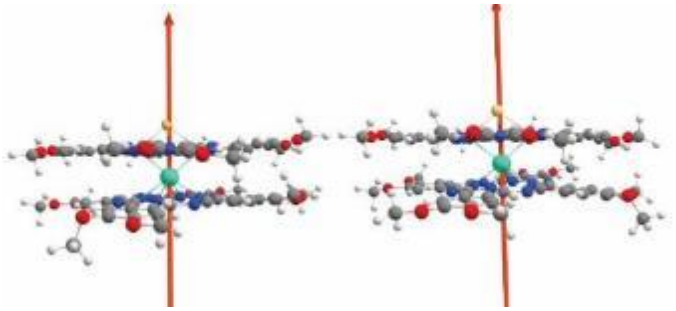


Fig. S292. [4]^{0} Tb1: plot of the fragment of the quadruple-decker (overall neutral oxidation state) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 444.

Fig. S293. $[4]^{0}$ Tb2: plot of the fragment of the quadruple-decker (overall neutral oxidation state) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 444.

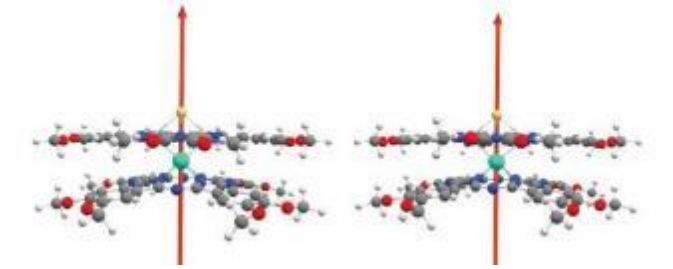


Fig. S294. $[4]^{2+}$ Tb1 (a): plot of the fragment of the quadruple-decker (overall oxidation state +2) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 2. Nr. of electron pairs in calculation: 444.

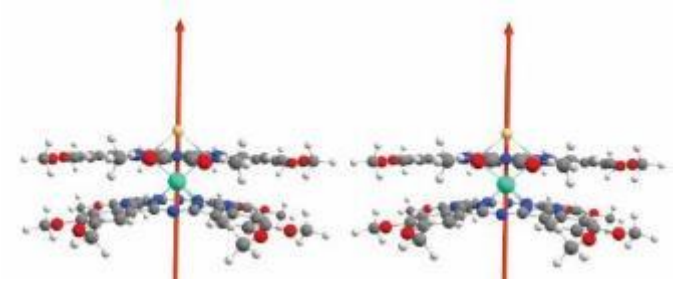


Fig. S295. $[4]^{+2}$ Tb1 (b): plot of the fragment of the quadruple-decker (overall oxidation state +2) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 2. Nr. of electron pairs in calculation: 443.

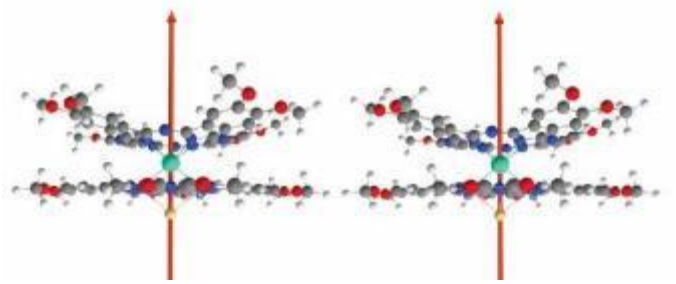


Fig. S296. $[4]^{2+}$ Tb2 (a): plot of the fragment of the quadruple-decker (overall oxidation state +2) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr.1. Nr. of electron pairs in calculation: 444.

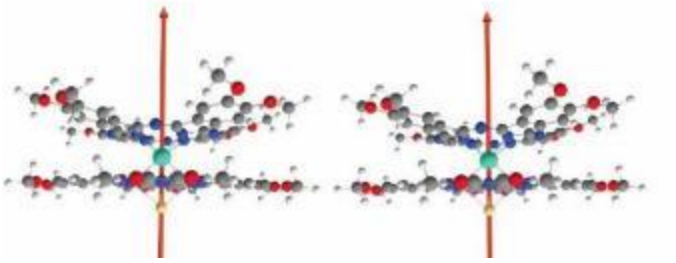


Fig. S297. $[4]^{2+}$ Tb2 (b): plot of the fragment of the quadruple-decker (overall oxidation state +2) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 1. Nr. of electron pairs in calculation: 443.

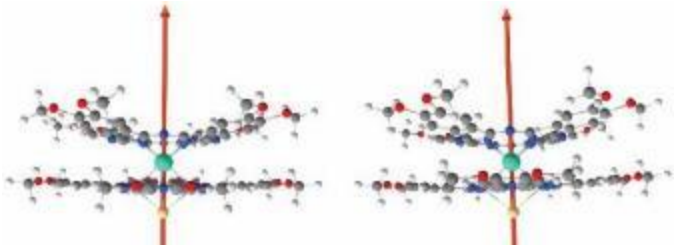


Fig. S298. $[4]^{4+}$ Tb1 (a): plot of the fragment of the quadruple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 1 (SAP coordination). Nr. of electron pairs in calculation: 444.

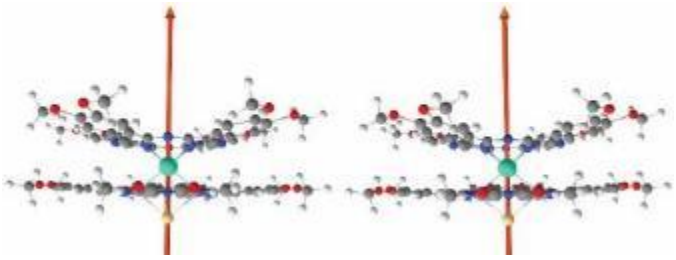


Fig. S299. $[4]^{4+}$ Tb1 (b): plot of the fragment of the quadruple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 1 (SAP coordination). Nr. of electron pairs in calculation:443.

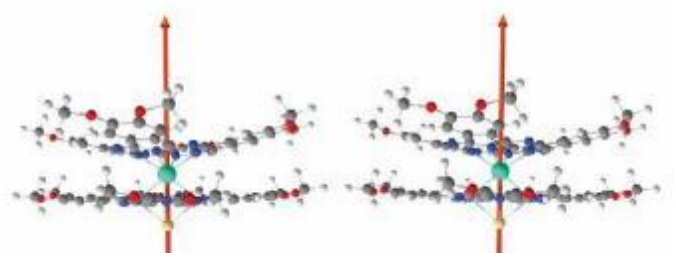


Fig. S300. $[4]^{4+}$ Tb2 (a): plot of the fragment of the quadruple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 2 (SP coordination). Nr. of electron pairs in calculation:444.

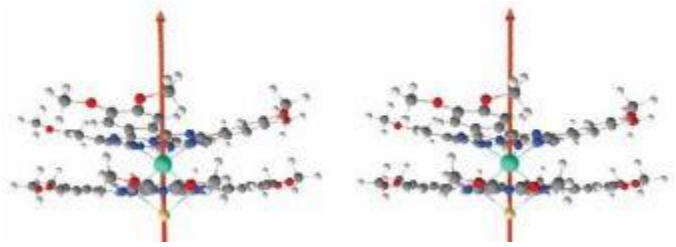


Fig. S301. $[4]^{4+}$ Tb2 (b): plot of the fragment of the quadruple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Crystallographically district Tb(III) ion Nr. 2 (SP coordination). Nr. of electron pairs in calculation: 443.

5.4. Quintuple-Deckers **[5]**

Table S58. Energy spectrum of quintuple-decker series predicted by as computational methods described above. (a) 444 electron pairs; (b) 443 electron pairs.

	$[5]^0$ (a)	**$[5]^0$ (b)**	**$[5]^{4+}$ Tb1 (a)**	**$[5]^{4+}$ Tb1 (b)**	**$[5]^{4+}$ Tb2 (a)**	**$[5]^{4+}$ Tb2 (b)**
Nr.	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})	E (cm^{-1})
1	0.000	0.000	0.000	0.000	0.000	0.000
2	0.007	0.005	0.005	0.011	0.002	0.003
3	263.694	272.621	269.608	258.596	232.742	239.011
4	265.434	274.193	270.700	260.843	239.524	245.986
5	356.560	375.245	369.584	329.783	277.427	288.201
6	377.491	398.670	384.978	343.182	279.213	290.865
7	412.302	428.942	412.435	389.029	283.108	294.073
8	425.879	445.355	444.526	414.350	308.765	321.889
9	440.374	458.638	465.749	418.997	368.517	380.496
10	529.773	554.161	468.787	424.270	439.098	453.510
11	548.688	572.981	469.432	434.240	453.752	468.958
12	584.887	612.938	516.522	475.482	561.572	583.962
13	590.479	618.695	518.813	479.431	562.240	584.677

Table S59. Main values of the *g*-tensor of the lowest Kramers doublets for the indicated complex (fragment). (a) 444 electron pairs; (b) 443 electron pairs.

	$[5]^0$ (a)			**$[5]^0$ (b)**		
Nr.	g_x	g_y	g_z	g_x	g_y	g_z
1	1.20E-08	3.40E-08	17.926	0.00E+00	8.00E-09	17.927
2	0.00E+00	2.00E-08	14.426	0.00E+00	1.20E-08	14.444
3	1.80E-08	1.05E-07	14.845	0.00E+00	0.00E+00	14.694
4	9.20E-08	1.94E-07	7.434	3.00E-08	1.12E-07	6.331
5	8.90E-08	1.06E-07	5.555	4.50E-08	7.10E-08	5.504
6	5.90E-08	1.31E-07	2.358	2.86E-07	6.15E-07	2.186

Table S60. Main values of the *g*-tensor of the lowest Kramers doublets for the indicated complex (fragment). (a) 444 electron pairs; (b) 443 electron pairs.

	$[5]^{4+}$ Tb1 (a)			**$[5]^{4+}$ Tb1 (b)**			**$[5]^{4+}$ Tb2 (a)**			**$[5]^{4+}$ Tb2 (b)**		
Nr.	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z	g_x	g_y	g_z
1	1.00E-09	1.00E-09	17.922	0.00E+00	0.00E+00	17.921	3.00E-09	3.00E-09	17.927	1.00E-09	2.00E-09	17.926
2	2.00E-09	4.00E-09	14.477	2.00E-09	4.00E-09	14.297	2.00E-09	1.60E-08	13.291	7.00E-09	1.60E-08	13.458
3	0.00E+00	1.69E-07	15.740	0.00E+00	1.69E-07	15.928	1.25E-07	1.75E-07	1.457	1.10E-08	2.40E-08	1.640
4	3.00E-09	8.00E-09	8.260	2.60E-08	8.40E-08	6.710	5.10E-08	1.78E-07	1.145	1.10E-08	1.20E-08	1.386
5	1.28E-07	4.63E-07	3.837	0.00E+00	2.70E-08	13.702	7.00E-09	2.00E-08	6.105	1.10E-08	1.60E-08	5.908
6	1.36E-07	4.46E-07	3.284	0.00E+00	1.22E-07	5.417	3.30E-08	1.59E-07	3.366	1.40E-08	2.20E-08	3.318

Table S61. *Ab initio* crystal-field parameters B_k^q (in cm^{-1}) for the molecular fragments of quintuple-decker series made from XRD data. (a) 444 electron pairs; (b) 443 electron pairs.

			[5]^0 (a)		**[5]^0 (b)**		**[5]$^{4+}$ Tb1 (a)**		**[5]$^{4+}$ Tb1 (b)**		**[5]$^{4+}$ Tb2 (a)**		**[5]$^{4+}$ Tb2 (b)**	
		1/alpha(n)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)	B(n,m)	C(n,m)
n	m													
2	0		4.39E+02	0.00E+00	4.63E+02	0.00E+00	3.99E+02	0.00E+00	3.51E+02	0.00E+00	3.44E+02	0.00E+00	3.60E+02	0.00E+00
2	1	-99	-8.94E+00	-8.94E+00	-2.00E+01	-2.00E+01	-3.48E-03	-3.48E-03	-2.15E-03	-2.15E-03	2.14E-04	2.14E-04	2.77E-03	2.77E-03
2	2		3.56E+01	-8.59E+01	-1.61E+01	9.30E+01	-2.19E+01	-1.16E+02	5.29E+01	-9.75E+01	-1.15E+02	5.92E+01	-1.04E+02	9.13E+01
4	0		-1.09E+02	0.00E+00	-1.09E+02	0.00E+00	-1.23E+02	0.00E+00	-1.28E+02	0.00E+00	-1.09E+02	0.00E+00	-1.10E+02	0.00E+00
4	1		-4.72E+00	-1.53E+01	-1.06E+01	7.09E+00	-1.50E-03	1.46E-03	-7.93E-04	1.24E-03	3.68E-04	3.19E-04	1.06E-03	6.48E-04
4	2	8167.5	5.48E+00	5.48E+00	-3.87E+00	-3.87E+00	-2.81E+00	-2.81E+00	3.45E+00	3.45E+00	-2.05E+01	-2.05E+01	-1.83E+01	-1.83E+01
4	3		-6.48E+00	8.57E+00	-8.93E+00	-2.43E+00	1.73E-04	1.16E-03	-8.05E-04	6.08E-04	1.06E-03	-1.91E-03	-4.67E-04	1.12E-03
4	4		-4.56E+00	1.57E+02	4.53E+01	1.57E+02	1.08E+01	-6.67E+01	7.45E+01	-6.25E+00	1.22E+02	-1.79E+02	3.84E+01	-2.20E+02
6	0		-1.39E+01	0.00E+00	-1.43E+01	0.00E+00	-1.15E+01	0.00E+00	-1.02E+01	0.00E+00	-1.92E+00	0.00E+00	-2.69E+00	0.00E+00
6	1		-1.03E+00	-1.10E+00	-1.43E+00	9.56E-01	7.87E-04	-6.24E-04	8.94E-04	-3.51E-04	7.36E-04	2.95E-04	-8.83E-04	-3.73E-04
6	2		-3.01E+00	5.86E+00	2.43E+00	-5.87E+00	-7.94E-01	4.97E+00	-3.93E+00	3.21E+00	-3.24E+00	1.61E+00	-3.22E+00	2.04E+00
6	3	-891891	-3.33E+00	-3.33E+00	-4.38E+00	-4.38E+00	-1.12E-04	-1.12E-04	-9.12E-05	-9.12E-05	2.59E-03	2.59E-03	-2.74E-03	-2.74E-03
6	4		1.84E+01	1.03E+02	4.82E+01	9.68E+01	6.67E+00	-1.89E+01	1.62E+01	3.00E+00	7.87E+01	-1.10E+02	2.73E+01	-1.36E+02
6	5		-4.54E+00	2.63E+00	4.20E+00	-7.74E-02	-4.71E-04	-2.40E-04	9.34E-05	-5.89E-04	1.51E-03	9.82E-04	-2.78E-03	7.02E-04
6	6		9.24E+00	2.50E+00	-9.19E+00	2.04E+00	-3.35E+00	8.87E-02	1.45E+00	-3.14E+00	-7.68E-01	8.46E+00	5.05E+00	7.84E+00

Table S62. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[5]^0** (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.10	0.00	0.50	0.20	0.60	1.00	0.40	0.30	0.20	0.20	0.70
-5	0.00	0.00	69.60	70.40	2.30	11.60	2.00	3.60	3.00	0.20	4.00	4.00	1.10
-4	0.90	0.90	2.70	2.60	47.00	7.40	60.30	45.10	24.90	35.20	1.40	3.90	13.40
-3	0.20	0.20	7.50	2.80	7.10	46.30	18.80	12.60	51.30	2.70	45.50	49.70	6.50
-2	0.70	0.50	0.90	1.80	37.80	13.10	26.80	50.50	9.50	21.60	3.40	5.80	67.30
-1	0.10	0.10	9.50	4.90	7.80	49.70	14.50	11.60	40.50	1.40	53.80	49.60	3.20
0	0.00	0.10	2.30	0.90	49.90	7.10	12.20	14.80	2.70	81.10	0.10	3.90	22.00
1	0.10	0.10	9.50	4.90	7.80	49.70	14.50	11.60	40.50	1.40	53.80	49.60	3.20
2	0.70	0.50	0.90	1.80	37.80	13.10	26.80	50.50	9.50	21.60	3.40	5.80	67.30
3	0.20	0.20	7.50	2.80	7.10	46.30	18.80	12.60	51.30	2.70	45.50	49.70	6.50
4	0.90	0.90	2.70	2.60	47.00	7.40	60.30	45.10	24.90	35.20	1.40	3.90	13.40
5	0.00	0.00	69.60	70.40	2.30	11.60	2.00	3.60	3.00	0.20	4.00	4.00	1.10
6	70.70	70.70	0.10	0.00	0.50	0.20	0.60	1.00	0.40	0.30	0.20	0.20	0.70

Table S63. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[5]^0** (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.50	0.10	0.60	1.00	0.30	0.30	0.20	0.20	0.60
-5	0.00	0.00	69.80	70.50	1.00	10.50	1.30	2.50	3.40	0.20	3.60	4.10	0.90
-4	0.90	0.90	1.80	1.70	49.00	3.80	62.60	45.40	16.70	33.60	0.90	3.10	13.50
-3	0.20	0.20	6.90	2.60	4.90	47.60	13.10	8.20	54.30	1.80	45.60	48.50	5.20
-2	0.60	0.40	0.60	1.20	36.50	9.70	27.60	52.10	6.70	23.60	2.50	5.00	66.80
-1	0.10	0.10	8.70	4.70	5.60	50.00	9.50	8.50	41.30	2.40	53.80	50.90	3.20
0	0.00	0.10	1.50	0.00	49.20	5.40	10.40	12.70	4.60	81.30	0.90	3.60	25.10
1	0.10	0.10	8.70	4.70	5.60	50.00	9.50	8.50	41.30	2.40	53.80	50.90	3.20
2	0.60	0.40	0.60	1.20	36.50	9.70	27.60	52.10	6.70	23.60	2.50	5.00	66.80
3	0.20	0.20	6.90	2.60	4.90	47.60	13.10	8.20	54.30	1.80	45.60	48.50	5.20
4	0.90	0.90	1.80	1.70	49.00	3.80	62.60	45.40	16.70	33.60	0.90	3.10	13.50
5	0.00	0.00	69.80	70.50	1.00	10.50	1.30	2.50	3.40	0.20	3.60	4.10	0.90
6	70.70	70.70	0.00	0.00	0.50	0.10	0.60	1.00	0.30	0.30	0.20	0.20	0.60

Table S64. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[5]**$^{4+}$ Tb1 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	1.10	0.00	1.20	0.70	0.00	0.00	0.50	0.70	0.00
-5	0.00	0.00	69.80	70.40	0.00	10.60	0.00	0.00	4.40	4.10	0.00	0.00	4.30
-4	1.20	1.20	0.00	0.00	41.30	0.00	67.70	56.80	0.00	0.00	5.00	21.30	0.00
-3	0.00	0.00	7.30	5.30	0.00	38.50	0.00	0.00	65.80	39.80	0.00	0.00	50.30
-2	0.80	0.70	0.00	0.00	41.10	0.00	20.10	36.90	0.00	0.00	55.00	59.30	0.00
-1	0.00	0.00	8.30	4.10	0.00	58.30	0.00	0.00	25.60	58.30	0.00	0.00	49.50
0	0.20	0.10	0.00	0.00	56.60	0.00	4.90	28.60	0.00	0.10	62.40	45.40	0.00
1	0.00	0.00	8.30	4.10	0.00	58.30	0.00	0.00	25.60	58.30	0.00	0.00	49.50
2	0.80	0.70	0.00	0.00	41.10	0.00	20.10	36.90	0.00	0.00	55.00	59.30	0.00
3	0.00	0.00	7.30	5.30	0.00	38.50	0.00	0.00	65.80	39.80	0.00	0.00	50.30
4	1.20	1.20	0.00	0.00	41.30	0.00	67.70	56.80	0.00	0.00	5.00	21.30	0.00
5	0.00	0.00	69.80	70.40	0.00	10.60	0.00	0.00	4.40	4.10	0.00	0.00	4.30
6	70.70	70.70	0.00	0.00	1.10	0.00	1.20	0.70	0.00	0.00	0.50	0.70	0.00

Table S65. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[5]**$^{4+}$ Tb1 (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	1.30	0.00	1.00	0.90	0.00	0.60	0.00	0.90	0.00
-5	0.00	0.00	68.80	70.30	0.00	15.70	0.00	0.00	3.40	0.00	6.30	0.00	5.20
-4	1.10	1.10	0.00	0.00	34.40	0.00	65.80	52.30	0.00	32.40	0.00	26.50	0.00
-3	0.00	0.00	9.20	5.30	0.00	35.50	0.00	0.00	35.00	0.00	66.80	0.00	54.30
-2	1.20	1.00	0.00	0.00	42.60	0.00	24.80	47.20	0.00	43.50	0.00	58.80	0.00
-1	0.00	0.00	13.30	6.00	0.00	59.10	0.00	0.00	61.30	0.00	22.40	0.00	45.00
0	0.20	0.10	0.00	0.00	63.30	0.00	10.40	8.90	0.00	64.20	0.00	41.10	0.00
1	0.00	0.00	13.30	6.00	0.00	59.10	0.00	0.00	61.30	0.00	22.40	0.00	45.00
2	1.20	1.00	0.00	0.00	42.60	0.00	24.80	47.20	0.00	43.50	0.00	58.80	0.00
3	0.00	0.00	9.20	5.30	0.00	35.50	0.00	0.00	35.00	0.00	66.80	0.00	54.30
4	1.10	1.10	0.00	0.00	34.40	0.00	65.80	52.30	0.00	32.40	0.00	26.50	0.00
5	0.00	0.00	68.80	70.30	0.00	15.70	0.00	0.00	3.40	0.00	6.30	0.00	5.20
6	70.70	70.70	0.00	0.00	1.30	0.00	1.00	0.90	0.00	0.60	0.00	0.90	0.00

Table S66. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[5]**$^{4+}$ Tb2 (a).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.70	0.30	0.00	0.00	0.80	0.50	0.00	0.00	0.20
-5	0.00	0.00	65.50	69.10	0.00	0.00	13.40	26.60	0.00	0.00	2.20	6.50	0.00
-4	0.90	0.80	0.00	0.00	46.00	27.30	0.00	0.00	68.80	42.90	0.00	0.00	23.80
-3	0.00	0.00	14.10	5.70	0.00	0.00	52.50	39.30	0.00	0.00	57.10	47.00	0.00
-2	0.20	0.10	0.00	0.00	31.60	61.40	0.00	0.00	16.30	39.40	0.00	0.00	58.40
-1	0.00	0.00	22.70	13.70	0.00	0.00	45.50	52.40	0.00	0.00	41.60	52.40	0.00
0	0.20	0.00	0.00	0.00	61.50	31.00	0.00	0.00	0.10	56.70	0.00	0.00	45.20
1	0.00	0.00	22.70	13.70	0.00	0.00	45.50	52.40	0.00	0.00	41.60	52.40	0.00
2	0.20	0.10	0.00	0.00	31.60	61.40	0.00	0.00	16.30	39.40	0.00	0.00	58.40
3	0.00	0.00	14.10	5.70	0.00	0.00	52.50	39.30	0.00	0.00	57.10	47.00	0.00
4	0.90	0.80	0.00	0.00	46.00	27.30	0.00	0.00	68.80	42.90	0.00	0.00	23.80
5	0.00	0.00	65.50	69.10	0.00	0.00	13.40	26.60	0.00	0.00	2.20	6.50	0.00
6	70.70	70.70	0.00	0.00	0.70	0.30	0.00	0.00	0.80	0.50	0.00	0.00	0.20

Table S67. Weights of M_J components (in %) in the wavefunctions of the J=6 ground state for **[5]**$^{4+}$ Tb2 (b).

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.70	0.00	0.00	0.70	0.60	0.00	0.00	0.90	0.50	0.00	0.00	0.30
-5	0.00	0.00	65.90	69.50	0.00	0.00	11.30	25.50	0.00	0.00	1.90	6.60	0.00
-4	1.00	1.00	0.00	0.00	47.00	27.30	0.00	0.00	68.50	42.30	0.00	0.00	23.70
-3	0.00	0.00	13.70	4.00	0.00	0.00	52.90	39.50	0.00	0.00	57.00	46.80	0.00
-2	0.10	0.10	0.00	0.00	30.00	61.80	0.00	0.00	17.60	39.60	0.00	0.00	58.30
-1	0.00	0.00	21.70	12.30	0.00	0.00	45.60	52.80	0.00	0.00	41.80	52.60	0.00
0	0.30	0.00	0.00	0.00	61.50	29.30	0.00	0.00	0.30	57.30	0.00	0.00	45.60
1	0.00	0.00	21.70	12.30	0.00	0.00	45.60	52.80	0.00	0.00	41.80	52.60	0.00
2	0.10	0.10	0.00	0.00	30.00	61.80	0.00	0.00	17.60	39.60	0.00	0.00	58.30
3	0.00	0.00	13.70	4.00	0.00	0.00	52.90	39.50	0.00	0.00	57.00	46.80	0.00
4	1.00	1.00	0.00	0.00	47.00	27.30	0.00	0.00	68.50	42.30	0.00	0.00	23.70
5	0.00	0.00	65.90	69.50	0.00	0.00	11.30	25.50	0.00	0.00	1.90	6.60	0.00
4	1.00	1.00	0.00	0.00	47.00	27.30	0.00	0.00	68.50	42.30	0.00	0.00	23.70

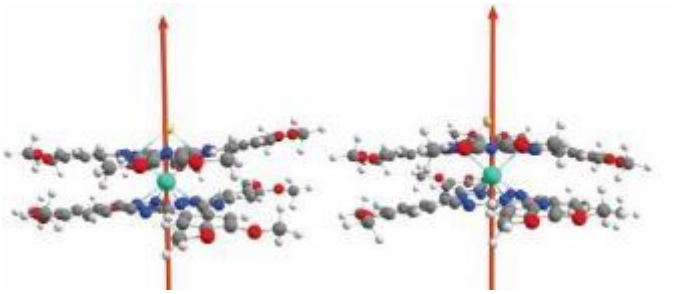


Fig. S302. [5]^{0} (a): plot of the fragment of the quintuple-decker (overall oxidation state 0) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 444.

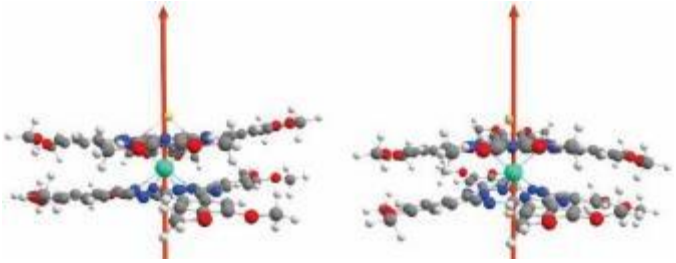


Fig. S303. [5]^{0} (b): plot of the fragment of the quintuple-decker (overall oxidation state 0) used in the ab initio calculation, together with the calculated easy axis direction. Nr. of electron pairs in calculation: 443.

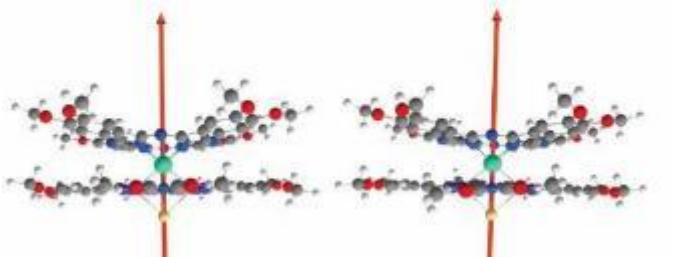


Fig. S304. $[5]^{4+}$ Tb1 (a): lot of the fragment of the quintuple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Square-antiprismatic coordinated Tb(III) ion. Nr. of electron pairs in calculation: 444.

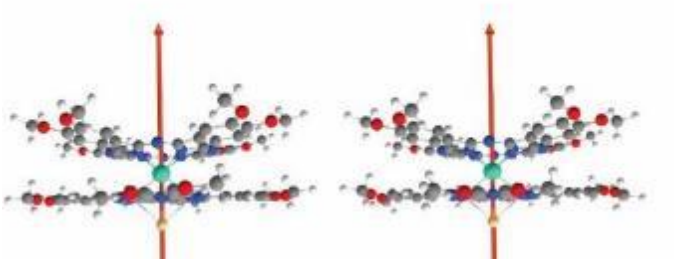


Fig. S305. $[5]^{4+}$ Tb1 (b): plot of the fragment of the quintuple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Square-antiprismatic coordinated Tb(III) ion. Nr. of electron pairs in calculation: 443.

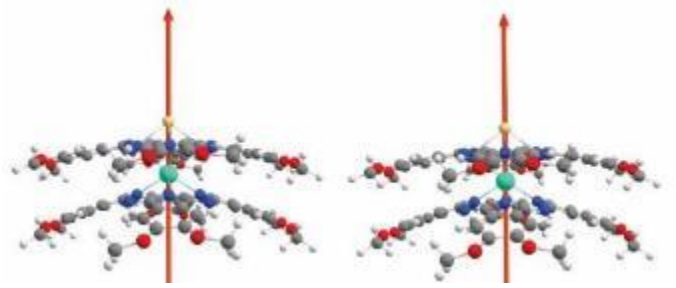


Fig. S306. $[5]^{4+}$ Tb2 (a): plot of the fragment of the quintuple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Square-prismatic coordinated Tb(III) ion. Nr. of electron pairs in calculation: 444.

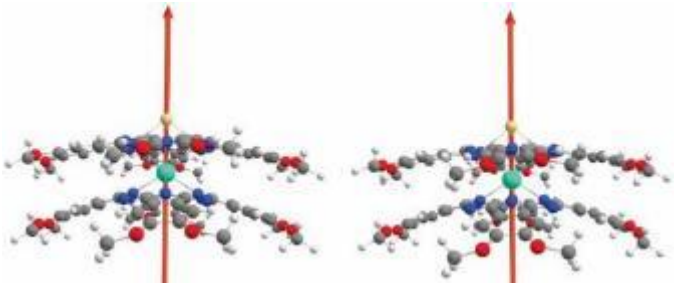


Fig. S307. [5]$^{4+}$ Tb2 (b): plot of the fragment of the quintuple-decker (overall oxidation state +4) used in the ab initio calculation, together with the calculated easy axis direction. Square-prismatic coordinated Tb(III) ion. Nr. of electron pairs in calculation: 443.

5.5. XYZ coordinates for the input files

[3]^{0}

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Tb	0.000000	0.000000	0.000000
Cd	0.000000	0.000000	3.224100
O	7.747678	-1.248584	1.254800
O	7.751023	1.253118	1.254200
O	1.248584	7.747778	1.254800
O	-1.253118	7.751123	1.254200
O	-1.248684	-7.747678	1.254800
O	1.253118	-7.751023	1.254200
O	-7.747778	1.248684	1.254800
O	-7.751123	-1.253118	1.254200
O	-6.808302	-4.021533	-2.684400
O	-5.033348	-5.876730	-2.703800
O	6.808201	4.021633	-2.684400
O	5.033348	5.876830	-2.703800
O	4.021533	-6.808202	-2.684400
O	5.876730	-5.033348	-2.703800
O	-4.021633	6.808301	-2.684400
O	-5.876830	5.033348	-2.703800
N	1.930500	0.000000	1.599400
N	2.396593	-2.401311	1.600000
N	1.385864	-1.388939	-1.295600
N	-0.005199	-3.379804	-1.501100
N	-0.000000	1.930600	1.599400
N	2.401311	2.396693	1.600000
N	0.000000	-1.930500	1.599400
N	-2.401311	-2.396593	1.600000
N	-1.930600	-0.000000	1.599400
N	-2.396693	2.401311	1.600000
N	1.388939	1.385864	-1.295600
N	3.379804	-0.005199	-1.501100
N	-1.389039	-1.385864	-1.295600
N	-3.379804	0.005199	-1.501100
N	-1.385864	1.389039	-1.295600
N	0.005199	3.379804	-1.501100
C	1.112617	-2.762209	1.593400
C	2.770591	-1.110478	1.595100
C	4.152363	0.704081	1.562500
C	4.150138	-0.702820	1.568000
C	6.514347	-0.717151	1.374500
C	6.517957	0.714952	1.376100
C	5.337207	1.438918	1.478100
C	5.334994	-1.435784	1.480500
C	-1.159804	-2.728021	-1.462500
C	1.159807	-2.746380	-1.467400
C	7.891734	2.683306	1.372000
C	7.891371	-2.685295	1.364800
C	2.762209	1.112717	1.593400
C	1.110478	2.770691	1.595100
C	-0.704081	4.152363	1.562500
C	0.702820	4.150238	1.568000
C	0.717151	6.514347	1.374500
C	-0.714952	6.518057	1.376100
C	-1.438918	5.337207	1.478100
C	1.435784	5.335094	1.480500
C	-2.683306	7.891734	1.372000
C	2.685295	7.891471	1.364800
C	-2.762309	-1.112617	1.593400
C	-1.110478	-2.770591	1.595100
C	0.703981	-4.152363	1.562500
C	-0.702920	-4.150138	1.568000
C	-0.717251	-6.514347	1.374500
C	0.714952	-6.517957	1.376100
C	1.438818	-5.337207	1.478100
C	-1.435884	-5.334994	1.480500
C	2.683206	-7.891734	1.372000
C	-2.685295	-7.891371	1.364800
C	-1.112717	2.762309	1.593400
C	-2.770691	1.110478	1.595100
C	-4.152363	-0.703981	1.562500
C	-4.150238	0.702920	1.568000
C	-6.514347	0.717251	1.374500
C	-6.518057	-0.714952	1.376100
C	-5.337207	-1.438818	1.478100
C	-5.335094	1.435884	1.480500
C	-7.891734	-2.683206	1.372000
C	-7.891471	2.685295	1.364800
C	2.728021	-1.159804	-1.462500
C	2.746380	1.159907	-1.467400
C	-2.728121	1.159804	-1.462500
C	-2.746480	-1.159807	-1.467400
C	1.159804	2.728121	-1.462500
C	-1.159907	2.746480	-1.467400
C	-4.594844	-4.596557	-2.296300
C	4.594744	4.596557	-2.296300
C	4.596557	-4.594744	-2.296300
C	-4.596557	4.594844	-2.296300
C	-4.022867	-6.810502	-2.689000
C	-4.985658	-2.321200	-1.949700
C	-3.143190	-4.521355	-1.996500
C	-5.411959	-3.606265	-2.256300
C	2.154434	-3.593961	-1.679100
C	-7.644408	-2.884952	-2.586200
C	-2.727178	-3.253896	-1.719800
C	4.022767	6.810502	-2.689000
C	4.985558	2.321299	-1.949700
C	3.143090	4.521355	-1.996500
C	5.411959	3.606365	-2.256300
C	-2.154534	3.594061	-1.679100
C	7.644408	2.884952	-2.586200
C	2.727078	3.253996	-1.719800
C	6.810502	-4.022767	-2.689000
C	2.321199	-4.985558	-1.949700
C	4.521355	-3.143090	-1.996500
C	3.606265	-5.411959	-2.256300
C	3.593961	2.154534	-1.679100
C	2.884952	-7.644408	-2.586200
C	3.253896	-2.727078	-1.719800
C	-2.321300	4.985658	-1.949700
C	-4.521355	3.143190	-1.996500
C	-3.606365	5.411959	-2.256300
C	-3.594062	-2.154434	-1.679100
C	-2.884952	7.644408	-2.586200
C	-6.810502	4.022867	-2.689000
C	-3.253996	2.727178	-1.719800
H	5.335429	2.368717	1.489600
H	5.332572	-2.365786	1.492700
H	-2.368717	5.335529	1.489600
H	2.365786	5.332572	1.492700
H	2.368717	-5.335429	1.489600
H	-2.365786	-5.332572	1.492700
H	-5.335529	-2.368717	1.489600
H	-5.332572	2.365786	1.492700
H	-5.577104	-1.604167	-1.923400
H	-2.578031	-5.260004	-1.997500
H	5.577104	1.604167	-1.923400
H	2.578031	5.260104	-1.997500
H	1.604167	-5.577104	-1.923400
H	5.260004	-2.578031	-1.997500
H	-1.604167	5.577104	-1.923400
H	-5.260104	2.578031	-1.997500
H	4.341732	7.672500	-2.141200
H	3.156528	6.391163	-2.221600
H	3.784491	7.094054	-3.692900
H	8.638646	3.146970	-2.882400
H	7.273088	2.112621	-3.227000
H	7.653825	2.535458	-1.574900
H	6.843328	-3.581747	-1.714700
H	6.541539	-3.278134	-3.408800
H	7.772651	-4.422769	-2.932100
H	3.146870	-8.638646	-2.882400
H	2.112621	-7.273088	-3.227000
H	2.535358	-7.653825	-1.574900
H	-3.102062	-6.335429	-2.421900
H	-3.928994	-7.249744	-3.660200
H	-4.251794	-7.572444	-1.973500
H	-8.638646	-3.146870	-2.882400
H	-7.273188	-2.112621	-3.227000
H	-7.653925	-2.535358	-1.574900
H	-8.920767	-2.951346	1.252900
H	-7.550739	-2.996894	2.336500
H	-7.308236	-3.162643	0.614000
H	-8.921536	2.950655	1.248700
H	-7.312266	3.161255	0.601300
H	-7.546670	3.005710	2.325800
H	-7.440570	4.131976	-1.831100
H	-6.311914	3.077077	-2.647400
H	-7.405234	4.073798	-3.577100
H	-3.146970	8.638646	-2.882400
H	-2.112621	7.273188	-3.227000
H	-2.535458	7.653925	-1.574900
H	-2.951446	8.920767	1.252900
H	-2.996994	7.550739	2.336500
H	-3.162643	7.308236	0.614000
H	-2.950655	-8.921436	1.248700
H	-3.161255	-7.312266	0.601300
H	-3.005710	-7.546670	2.325800
H	2.951346	-8.920667	1.252900
H	2.996894	-7.550739	2.336500
H	3.162643	-7.308136	0.614000
H	8.921436	-2.950655	1.248700
H	7.312266	-3.161155	0.601300
H	7.546670	-3.005610	2.325800
H	2.950655	8.921536	1.248700
H	3.161155	7.312266	0.601300
H	3.005610	7.546670	2.325800
H	8.920667	2.951446	1.252900
H	7.550739	2.996994	2.336500
H	7.308136	3.162643	0.614000

[3]$^{2+}$

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Tb	4.290600	12.884400	20.674500
Lu	7.192800	11.326600	19.685700
O	5.419700	16.345800	28.044700
O	-1.304000	11.922000	14.800900
O	4.408000	20.654600	18.032500
O	4.581900	14.061500	28.774800
O	-0.292200	7.615100	24.945900
O	5.438900	21.007900	20.345600
O	-0.116300	14.021300	13.938000
O	-1.359800	7.274400	22.637700
O	6.571900	16.801900	13.924700
O	2.055800	5.580600	17.844500
O	4.911500	7.409100	26.435600
O	9.427500	18.630400	22.515800
O	6.248300	9.293600	27.499000
O	9.327500	17.377400	24.723500
O	5.235100	14.917400	12.861200
O	2.155900	6.833600	15.636800
N	6.825700	13.489400	20.977200
N	5.703200	13.098900	18.526200
N	7.023000	15.060000	19.119900
N	4.411000	11.585200	17.111500
N	3.036500	15.353400	18.224700
N	4.891700	16.016800	22.577900
N	4.657700	10.721600	19.383000
N	5.780200	11.112100	21.834100
N	4.460400	9.151000	21.240400
N	7.072400	12.625800	23.248700
N	4.049100	15.205000	20.443700
N	4.058200	13.747000	22.844700
N	2.457800	11.772100	21.650000
N	2.431100	13.231600	19.276000
N	3.081100	11.840100	24.007900
N	1.092400	11.241900	19.704300
C	6.323000	14.320600	18.263800

C	7.232800	14.682500	20.377900
C	5.336600	13.690600	16.301900
C	4.231000	10.664200	18.060400
C	3.568600	8.697100	19.008500
C	3.559900	9.406500	17.809800
C	5.096500	12.705700	17.343200
C	4.988300	13.697900	14.952300
C	6.103200	14.706000	16.883500
C	5.447800	14.768000	14.195900
C	3.050400	7.397200	19.104100
C	2.574100	6.823100	17.936500
C	6.208200	15.828900	14.791200
C	3.071000	8.841600	16.622800
C	2.601600	7.541700	16.689400
C	6.544200	15.802300	16.144500
C	5.160400	9.890400	22.096400
C	4.250600	9.528500	19.982400
C	6.146800	10.520400	24.058300
C	7.252400	13.546800	22.299800
C	7.914800	15.513900	21.351800
C	7.923500	14.804500	22.550500
C	6.386900	11.505300	23.017000
C	6.495100	10.513100	25.408000
C	5.380200	9.505000	23.476700
C	6.035600	9.443000	26.164300
C	8.433000	16.813800	21.256100
C	8.909300	17.387900	22.423700
C	5.275200	8.382100	25.569000
C	8.412400	15.369400	23.737500
C	8.881800	16.669300	23.670900
C	4.939200	8.408700	24.215700
C	5.168500	15.843700	25.674400
C	1.494000	10.214600	23.086100
C	0.910800	10.046800	21.840100
C	2.437900	11.319400	22.962100
C	1.503200	11.047500	20.966700
C	4.176200	17.228100	19.312400
C	4.597200	16.152900	21.285600
C	1.163200	14.315700	15.980200
C	-0.408600	12.457300	15.668200
C	3.789500	12.973700	23.946500
C	-0.084100	11.914500	16.900800
C	1.491800	12.273500	18.960800
C	2.410400	14.168500	18.262600
C	4.715100	17.427300	20.579700
C	4.045100	18.275200	18.397800
C	3.733000	15.840800	19.259900
C	1.489100	13.751600	17.212000
C	4.259700	13.649000	25.155300
C	-0.452500	8.286200	22.702600
C	4.759800	14.888800	24.747300
C	4.607300	14.231200	27.435300
C	1.122500	9.443700	24.188700
C	0.234000	13.648000	15.194800
C	-0.084800	9.084900	21.622200
C	5.163200	18.681700	20.992600
C	4.606000	14.926300	23.289900
C	0.899300	12.572300	17.656800
C	4.476300	19.535900	18.798600
C	5.084800	15.512000	27.019200
C	4.168900	13.289400	26.506200
C	0.142500	8.465900	23.983300
C	5.047600	19.736100	20.092100
C	9.752700	19.287100	21.287800
C	7.169900	17.992700	14.443600
C	4.582300	13.838900	12.186200
C	2.235500	7.445500	14.346800
C	1.730600	4.923900	19.072400
C	4.313500	6.218300	25.916700
C	6.901100	10.372100	28.174000
C	9.247900	16.765500	26.013500
C	6.054400	21.254200	21.612700
C	3.681500	20.558500	16.804500
C	0.689400	15.037500	13.335300
C	-1.850200	10.643900	15.137200
C	-1.784200	6.835700	21.344500
C	0.393400	7.614400	26.200800
C	3.968000	12.876000	29.287200
C	5.687700	17.713300	27.723600
H	6.632300	17.784300	27.226000
H	4.917300	18.086400	27.081500
H	5.713800	18.292300	28.623000
H	4.473400	13.020700	14.578100
H	-1.074000	9.907700	15.116800
H	-2.277000	10.685200	16.117500
H	-2.608400	10.382500	14.428800
H	0.745400	15.882700	13.989000
H	1.673600	14.655600	13.160800
H	0.251900	15.334400	12.405100
H	-2.166200	7.669100	20.792800
H	-0.952700	6.412300	20.820900
H	-2.551200	6.097500	21.452200
H	1.374700	7.208300	26.070900
H	0.467900	8.617000	26.567100
H	-0.149500	7.017400	26.903500
H	3.012900	12.740300	28.824300
H	4.590300	12.031800	29.075200
H	3.841300	12.968800	30.345600
H	4.220700	19.939100	16.118700
H	2.719300	20.129600	16.992000
H	3.560900	21.535100	16.384200
H	5.445600	20.843300	22.390800
H	7.020400	20.794600	21.635300
H	6.157700	22.309000	21.760000
H	8.238700	16.465700	26.204400
H	9.886200	15.907100	26.041100
H	9.559400	17.465700	26.760200
H	7.830700	10.585700	27.689100
H	6.276600	11.240400	28.146200
H	7.084600	10.097100	29.191600
H	5.059000	5.630900	25.422600
H	3.888800	5.653200	26.720000
H	3.545300	6.479600	25.219300
H	0.897700	5.415400	19.530200
H	1.477800	3.903100	18.874900
H	2.573100	4.961600	19.731100
H	1.572600	8.284600	14.308600
H	3.238000	7.774600	14.169400
H	1.955300	6.735200	13.597200
H	5.124700	12.932200	12.354800
H	3.586100	13.733700	12.562200
H	4.547500	14.043900	11.136600
H	-0.501000	11.144300	17.213600
H	7.609400	18.549400	13.642400
H	6.421200	18.588100	14.923000
H	7.926600	17.731600	15.153600
H	10.016800	20.304800	21.486700
H	10.578300	18.788400	20.824500
H	8.906500	19.259500	20.633600
H	3.834100	12.461400	26.770900
H	5.527300	18.809500	21.838900
H	-0.483400	8.984700	20.789600
H	1.508900	9.575500	25.023300
H	3.683600	18.134000	17.552700
H	1.553100	15.110100	15.696100
H	5.486200	16.671700	25.402700
H	3.027300	6.941300	19.913700
H	8.456000	17.269700	20.446500
H	3.062400	9.321200	15.825200
H	7.040700	16.485300	16.535600
H	7.010000	11.190300	25.782100
H	8.421000	14.889800	24.535000
H	4.442700	7.725700	23.824600

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Tb	3.104400	10.016900	3.360800
Cd	3.522600	9.698600	6.630000
O	10.460400	6.703000	4.843700
O	11.114600	9.187300	4.759000
O	6.624600	17.016900	5.455000
O	4.163700	17.728800	5.421600
O	-3.849500	13.180600	5.462700
O	-4.553000	10.729600	5.308600
O	-0.067400	2.810500	4.561200
O	2.354700	2.171600	4.045000
O	8.934600	15.254400	1.962100
O	6.986600	16.914600	2.080300
O	-2.305200	15.985900	2.280600
O	-3.863500	13.969600	2.113700
O	-3.019800	5.032100	1.671900
O	-1.019300	3.306700	1.325200
O	8.233700	4.240900	1.397100
O	9.822600	6.248700	1.276400
N	4.951000	6.946300	4.697300
N	5.117600	9.417800	4.805200
N	6.199000	11.604000	4.956700
N	3.821300	11.776900	5.082600
N	1.619200	12.852800	5.375400
N	1.457800	10.427100	5.257200
N	0.367700	8.237900	5.162200
N	2.779200	8.068900	4.977300
N	6.285500	10.464400	1.641100
N	4.226600	11.667500	1.998100
N	2.649900	13.508400	2.159900
N	1.510800	11.349700	2.242100
N	-0.352000	9.751300	2.044300
N	1.759600	8.538400	2.003200
N	3.288700	6.754000	1.620600
N	4.476900	8.835100	1.795200
C	-4.801800	12.901400	1.960900
C	-1.474000	17.143800	2.396000
C	5.931500	17.875800	2.168400
C	10.004100	14.305600	1.934000
C	10.723700	7.357200	1.341800
C	7.360000	3.129700	1.613500
C	0.026200	2.335600	1.231500
C	-3.507500	4.392800	0.489400
C	5.606000	8.103100	4.771800
C	7.083000	8.165500	4.720500
C	8.031100	7.155400	4.702500
C	9.361000	7.575300	4.797500
C	6.229700	10.282600	4.792400
C	7.435500	9.496600	4.712700
C	8.744900	9.906300	4.687100
C	9.772500	8.903500	4.720500
C	5.059100	12.250800	5.054300
C	5.040800	13.683600	5.213600
C	6.069900	14.653300	5.262400
C	5.773100	15.936300	5.385600
C	2.952600	12.860000	5.246900
C	3.720100	14.091200	5.295700
C	3.349300	15.437500	5.365100
C	4.400900	16.359000	5.401000
C	0.979800	11.704800	5.377900
C	-0.507800	11.684300	5.460100
C	-1.474300	12.653400	5.516600
C	-2.807000	12.289200	5.437000
C	0.331100	9.551700	5.252100
C	-0.841600	10.329600	5.390800
C	-2.232800	9.940300	5.334300
C	-3.153600	10.931100	5.347100
C	1.473600	7.520900	5.036300
C	1.529300	6.107400	4.882300
C	0.459200	5.160900	4.887400
C	0.794200	3.873000	4.628000
C	3.616700	6.940600	4.743600
C	2.825400	5.751300	4.707600
C	3.167800	4.415400	4.404600
C	2.196400	3.481500	4.355800
C	8.020900	16.720100	5.370300

C	2.806700	18.138900	5.234100
C	-3.521000	14.571700	5.507300
C	-4.933400	9.354500	5.211500
C	-1.453500	3.136100	4.693700
C	3.661300	1.779600	3.616000
C	10.098100	5.319700	4.846300
C	11.473000	10.570300	4.696500
C	5.588200	11.542600	1.777200
C	6.156200	12.904900	1.777200
C	7.470200	13.331400	1.787500
C	7.684800	14.696700	1.892800
C	3.849600	12.953200	2.005800
C	5.118500	13.754200	1.946700
C	5.290700	15.139000	1.990400
C	6.587300	15.574300	1.987800
C	1.550700	12.703500	2.188200
C	0.212000	13.256000	2.224100
C	-0.275000	14.605600	2.278000
C	-1.687800	14.723400	2.237000
C	0.111500	11.022300	2.159900
C	-0.703500	12.176300	2.134200
C	-2.054800	12.361600	2.129100
C	8.436300	6.609600	1.317500
C	7.603700	5.443500	1.389400
C	5.822100	9.206700	1.607700
C	6.650400	8.062500	1.443400
C	8.016100	7.824800	1.309800
C	-0.650900	4.606600	1.376600
C	4.441200	7.514600	1.646300
C	5.747200	6.933800	1.469000
C	6.228900	5.647400	1.433100
C	-1.689500	5.523100	1.541000
C	2.056400	7.221600	1.754100
C	0.838200	6.489500	1.569200
C	0.661300	5.091400	1.443400
C	-2.538900	13.647300	2.136800
C	0.339800	8.663400	1.941600
C	-0.180600	7.388700	1.692500
C	-1.528700	6.876300	1.710500
H	11.064400	11.004800	3.808100
H	11.083800	11.078700	5.553800
H	12.538900	10.662100	4.680800
H	8.193800	12.718400	1.725900
H	9.482200	5.113900	5.696700
H	9.558400	5.090600	3.951200
H	10.982600	4.719400	4.892900
H	3.945300	2.359100	2.762500
H	4.361300	1.944800	4.408200
H	3.655000	0.741600	3.356300
H	-1.623700	3.590300	5.647400
H	-1.735400	3.817800	3.918600
H	-2.038700	2.243800	4.614000
H	-4.527800	8.934700	4.314800
H	-4.556300	8.819600	6.058100
H	-6.000600	9.280400	5.189200
H	-2.954900	14.776300	6.391900
H	-2.941600	14.829100	4.645500
H	-4.420900	15.150400	5.518000
H	2.436600	17.737300	4.314000
H	2.209900	17.778900	6.046000
H	2.758100	19.207300	5.202100
H	-0.438000	5.420100	5.062000
H	8.298300	16.076000	6.178400
H	8.226300	16.233500	4.439700
H	8.582900	17.628700	5.429300
H	4.556100	15.739700	2.021200
H	4.072900	4.178900	4.237600
H	-2.489200	9.025800	5.290600
H	-1.230200	13.566500	5.606500
H	2.438100	15.709800	5.388200
H	6.977400	14.382100	5.205900
H	0.303000	15.359700	2.334500
H	7.792900	6.237100	4.633100
H	8.966000	10.828700	4.648500
H	-3.539500	3.334400	0.643500
H	-4.491600	4.751200	0.270200
H	-2.856400	4.614400	-0.330300
H	-4.591000	12.367900	1.057700
H	-4.723300	12.235700	2.795000
H	-5.793300	13.301300	1.915800
H	-0.894400	17.078800	3.293000
H	-0.819300	17.198500	1.551500
H	-2.086500	18.020500	2.429900
H	10.547600	8.009300	0.512000
H	10.565900	7.891600	2.255200
H	11.731700	6.999900	1.307100
H	0.628700	2.542000	0.371800
H	0.633400	2.379200	2.111500
H	-0.401300	1.358800	1.141300
H	6.851600	3.252300	2.547000
H	6.643100	3.080000	0.820800
H	7.931600	2.225400	1.634700
H	9.924200	13.653000	2.778200
H	9.948000	13.731400	1.032900
H	10.940400	14.822300	1.970000
H	5.296400	17.787900	1.311800
H	5.360400	17.698200	3.055700
H	6.348400	18.860700	2.203700
H	-2.644800	11.618700	2.118800
H	-2.275500	7.452100	1.836300
H	1.404500	4.501800	1.404800
H	5.631600	4.907600	1.438200
H	8.626400	8.546800	1.217400

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Tb	3.961100	9.353200	9.900400
Cd	3.522600	9.698600	6.630000
O	-3.228500	6.307400	11.729200
O	-1.943000	4.148400	11.236100
O	7.063000	1.993800	10.298700
O	9.213900	3.359000	10.188300
O	11.397300	12.194200	11.593100
O	9.994700	14.462900	11.623900
O	1.323200	16.531600	12.463700
O	-0.911100	15.253800	12.571600
O	11.600200	9.327600	8.187600
O	11.290800	11.852100	8.174800
O	3.746100	17.303400	8.965800
O	1.262800	16.882300	8.904100
O	-4.068200	9.544400	8.608800
O	-3.698300	7.056300	8.218400
O	3.701700	1.676200	7.278400
O	6.177800	2.096300	6.965100
N	0.816200	10.017800	11.731800
N	2.389500	8.204100	11.318300
N	3.306100	5.978500	11.159100
N	5.061000	7.575300	11.025500
N	7.354500	8.444700	11.071800
N	5.779400	10.288100	11.184800
N	4.897400	12.522600	11.564900
N	3.076600	10.928700	11.462100
N	6.484900	7.496800	7.840900
N	5.676700	9.782500	8.069500
N	5.792800	12.199700	8.277500
N	3.488000	11.384300	8.377700
N	1.049400	11.435600	8.585700
N	1.877200	9.177700	8.380200
N	1.773000	6.733300	8.159300
N	4.067100	7.570100	8.082300
C	1.190800	8.758400	11.559200
C	0.190300	7.673700	11.585700
C	-1.216400	7.643300	11.732100
C	-1.810900	6.455200	11.608500
C	2.281100	6.854200	11.277200
C	0.912100	6.523500	11.390200
C	0.235300	5.262200	11.313200
C	-1.141000	5.277900	11.400500
C	4.598400	6.279400	11.058900
C	-1.258800	2.930300	10.931100
C	5.669600	5.301200	10.920200
C	5.656700	3.941300	10.763600
C	6.917700	3.359200	10.565800
C	6.492600	7.474700	10.999800
C	6.848300	6.083800	10.835500
C	8.098900	5.462200	10.594100
C	8.076100	4.083900	10.411700
C	7.049700	9.733800	11.225800
C	8.019400	10.807500	11.392800
C	9.415600	10.805100	11.423600
C	10.025800	12.039100	11.554600
C	5.889500	11.659100	11.387600
C	7.285700	11.961300	11.523800
C	7.936600	13.215800	11.590500
C	9.306400	13.234500	11.639300
C	3.595400	12.211400	11.616200
C	2.555900	13.172200	11.906400
C	2.613100	14.520100	12.127300
C	1.447000	15.148800	12.312200
C	1.697100	11.049200	11.683000
C	1.370500	12.413100	11.942400
C	0.158300	13.096700	12.217200
C	0.188500	14.471700	12.361000
C	6.635100	8.777800	7.946200
C	7.957400	9.421800	7.979600
C	9.236200	8.838000	7.984700
C	10.321600	9.692400	8.097700
C	6.327000	11.067600	8.084900
C	7.767000	10.779600	8.010400
C	8.835700	11.704100	8.079700
C	10.117100	11.137200	8.084900
C	4.471300	12.404000	8.380200
C	3.826900	13.655200	8.516300
C	4.341400	14.970100	8.644700
C	3.408400	15.989300	8.816800
C	2.264500	11.992900	8.488100
C	2.445700	13.407000	8.598500
C	1.584000	14.470100	8.747500
C	2.002800	15.756800	8.824500
C	0.895800	10.145100	8.513800
C	-0.420300	9.468200	8.531700
C	-1.710800	10.072800	8.665300
C	-2.746700	9.162700	8.554900
C	1.241200	7.893500	8.290300
C	-0.202000	8.135100	8.346800
C	-1.261900	7.222300	8.262100
C	-2.560300	7.783800	8.362200
C	3.106700	6.550700	8.013000
C	3.749100	5.283300	7.815200
C	3.165900	4.021900	7.738200
C	4.017400	2.994800	7.414600
C	5.240700	6.929900	7.828000
C	5.073600	5.532900	7.668800
C	5.945000	4.538100	7.373500
C	5.454200	3.250200	7.275900
C	2.343100	1.359500	7.592600
C	7.580300	2.283700	6.758100
C	11.836300	7.917900	8.232400
C	11.195100	13.274900	8.281600
C	5.136900	17.605500	9.104900
C	-0.149600	16.670000	8.973800
C	-4.368700	10.933600	8.766400
C	-3.558800	5.648900	8.007300
C	-4.003200	7.492300	11.931100
C	-2.161700	14.573800	12.707200
C	2.536500	17.288400	12.453300
C	10.715200	14.792700	12.814300
C	12.235900	11.048000	11.426100
C	10.398500	4.099200	9.882100
C	5.866000	1.211600	10.308900
H	6.039600	0.287200	9.798700

H	5.578700	1.012300	11.320200	O	10.569500	1.048000	3.628900	C	8.703700	15.083800	3.704400
H	5.083900	1.749900	9.815500	O	8.048000	0.881600	3.326100	C	7.757800	5.732900	4.573100
H	-0.842600	2.991700	9.947300	O	6.622800	16.144200	3.628900	C	9.686100	4.524300	4.360200
H	-0.473800	2.774700	11.641400	O	9.144200	16.310600	3.326100	C	5.945400	7.224900	4.611300
H	-1.948000	2.113100	10.976500	O	1.048000	6.622800	3.628900	C	8.294900	4.405300	4.302900
H	-1.714700	8.433000	11.909000	O	3.362800	2.694000	7.930500	C	10.516800	3.421300	4.150900
H	0.714100	4.451200	11.202700	O	16.310600	8.048000	3.326100	C	9.913700	2.203400	3.841800
H	-2.435200	14.139400	11.768300	O	0.881600	9.144200	3.326100	C	7.681200	3.200900	3.962800
H	-2.070600	13.803000	13.443700	O	11.651500	15.833700	7.853400	C	8.488500	2.108500	3.704400
H	-2.915200	15.270100	13.010900	O	13.829400	14.498200	7.930500	C	11.459300	7.757800	4.573100
H	10.257400	4.635500	8.967000	O	15.833700	5.540700	7.853400	C	12.667900	9.686100	4.360200
H	10.601400	4.790700	10.673100	N	9.645500	10.211200	7.726800	C	9.967400	5.945400	4.611300
H	11.223000	3.425400	9.777200	N	7.885100	11.901500	7.748600	C	12.786900	8.294900	4.302900
H	11.766200	14.757200	12.616400	N	5.989400	10.748600	4.555000	C	13.771000	10.516800	4.150900
H	10.445400	15.777800	13.133200	N	10.563600	8.792800	4.780400	C	14.988900	9.913700	3.841800
H	10.473300	14.089800	13.583900	N	10.211200	7.546700	7.726800	C	13.991400	7.681200	3.962800
H	11.730600	10.179700	11.794200	N	5.290700	7.885100	7.748600	C	15.083800	8.488500	3.704400
H	12.459000	10.917500	10.387800	N	6.981100	9.645500	7.726800	C	13.848800	2.090000	7.986800
H	13.145700	11.189200	11.971400	N	8.792800	6.628600	4.780400	C	6.719900	0.550800	7.898700
H	2.313300	18.317600	12.264100	N	6.443700	5.989400	4.555000	C	2.090000	3.343400	7.986800
H	3.021800	17.197300	13.402600	N	11.202800	6.443700	4.555000	C	0.550800	10.472300	7.898700
H	3.182300	16.916500	11.685500	N	8.399400	10.563600	4.780400	C	3.343300	15.102200	7.986800
H	-5.034900	7.280400	11.742400	N	10.748600	11.202800	4.555000	C	0.761600	10.525300	2.975500
H	-3.886600	7.827000	12.940700	N	11.901500	9.307200	7.748600	C	5.198300	16.161100	3.753600
H	-3.667700	8.256200	11.261100	N	7.546700	6.981100	7.726800	C	10.525300	16.430700	2.975500
H	-4.527700	5.197100	7.962600	N	9.307200	5.290700	7.748600	C	16.161100	11.994000	3.753600
H	-3.041800	5.475800	7.086600	N	6.628600	8.399400	4.780400	C	16.430700	6.666900	2.975500
H	-3.002500	5.220500	8.814700	C	5.732900	9.434400	4.573100	C	16.641400	6.719900	7.898700
H	-4.012500	11.269800	9.717700	C	4.524300	7.506100	4.360200	C	15.102200	13.848900	7.986800
H	-3.890900	11.492300	7.988900	C	4.727900	10.256900	7.752200	C	10.472300	16.641400	7.898700
H	-5.427400	11.078100	8.710600	C	7.224900	11.246800	4.611300	C	1.031200	5.198300	3.753600
H	-0.633900	17.581700	9.255100	C	9.149700	11.513600	7.739400	C	6.666900	0.761600	2.975500
H	-0.510600	16.354800	8.017100	C	6.875200	11.036700	7.747600	C	11.994000	1.031200	3.753600
H	-0.361300	15.914500	9.701400	C	5.477800	11.434600	7.773600	H	12.414600	1.802500	3.142900
H	5.515700	17.141700	9.991700	C	4.405300	8.897300	4.302900	H	12.264500	1.197900	4.775300
H	5.669100	17.235300	8.253600	C	3.421300	6.675400	4.150900	H	12.368600	0.080600	3.436000
H	5.266600	18.665400	9.173400	C	3.342900	10.255200	7.756200	H	3.497100	5.750700	4.216000
H	12.100400	13.662900	8.699600	C	2.702600	11.480300	7.804000	H	6.063900	0.900200	3.848500
H	11.041700	13.696000	7.309900	C	2.203400	7.278500	3.841800	H	6.417600	1.505700	2.248100
H	10.371500	13.530400	8.915100	C	3.468000	12.709200	7.853400	H	6.485600	-0.210800	2.567600
H	11.469900	7.524100	9.157300	C	4.859600	12.685500	7.822700	H	1.802900	4.777700	3.143300
H	11.328900	7.445200	7.417500	C	3.200900	9.511100	3.962800	H	1.197300	4.927800	4.775400
H	12.886800	7.729600	8.155800	C	2.108500	8.703700	3.704400	H	0.080800	4.823700	3.435400
H	8.058400	1.330500	6.670700	C	10.256900	12.464400	7.752200	H	9.921300	16.519400	6.989700
H	7.736500	2.844800	5.860500	C	11.513600	8.042500	7.739400	H	9.865400	16.340300	8.726900
H	7.995300	2.816100	7.588300	C	11.036700	10.317100	7.747600	H	10.748000	17.668900	8.013500
H	2.154100	1.581100	8.622200	C	11.434600	11.714500	7.773600	H	15.103800	13.135700	8.784500
H	1.689600	1.941500	6.976700	C	10.255200	13.849400	7.756200	H	15.288300	13.347700	7.059900
H	2.168900	0.319000	7.413800	C	11.480300	14.489600	7.804000	H	15.867000	14.577400	8.158200
H	4.857800	3.430400	10.789200	C	12.709200	13.724200	7.853400	H	16.520000	7.270500	6.989300
H	6.868700	4.720000	7.239900	C	12.685500	12.332700	7.822700	H	16.339700	7.327200	8.726400
H	2.239300	3.883700	7.897400	C	6.935400	4.727900	7.752200	H	17.668800	6.444300	8.014300
H	-1.119200	6.290800	8.146500	C	5.678600	9.149700	7.739400	H	16.298400	6.064200	3.849700
H	-1.842200	11.001000	8.814300	C	6.155500	6.875200	7.747600	H	15.682600	6.416000	2.252800
H	0.650600	14.293900	8.798800	C	5.757700	5.477800	7.773600	H	17.400900	6.487000	2.561700
H	5.275300	15.147600	8.613900	C	6.937100	3.342900	7.756200	H	15.390300	12.414700	3.142300
H	9.351900	7.898400	7.910200	C	5.712000	2.702600	7.804000	H	15.993700	12.264500	4.775200
H	8.695200	12.642800	8.120800	C	4.483100	3.468000	7.853400	H	17.112000	12.368500	3.436700
H	-0.657400	12.616900	12.304500	C	4.506800	4.859600	7.822700	H	11.128100	16.297800	3.849500
H	9.918500	10.002000	11.356800	C	12.464400	6.935400	7.752200	H	10.776000	15.683000	2.252300
H	3.442700	14.986100	12.145300	C	8.042500	5.678600	7.739400	H	10.705400	17.401100	2.562300
H	7.438500	14.023100	11.603400	C	10.317100	6.155500	7.747600	H	4.777700	15.389400	3.143300
H	8.908400	5.959800	10.558100	C	11.714500	5.757700	7.773600	H	4.927800	15.995000	4.775400
				C	13.849400	6.937100	7.756200	H	4.823700	17.111500	3.435400
				C	14.489600	5.712000	7.804000	H	0.900200	11.128300	3.848500
[4]$^{2+}$ Tb1				C	13.724200	4.483100	7.853400	H	1.505700	10.774600	2.248100
178				C	12.332700	4.506800	7.822700	H	-0.210800	10.706600	2.567500
Tb	8.596100	8.596100	6.097600	C	9.434400	11.459300	4.573100	H	4.059400	15.102500	8.781900
Cd	8.596100	8.596100	9.362000	C	7.506100	12.667900	4.360200	H	3.841100	15.290100	7.058500
O	14.498200	3.362800	7.930500	C	11.246800	9.967400	4.611300	H	2.615300	15.866500	8.162300
O	16.144200	10.569500	3.628900	C	8.897300	12.786900	4.302900	H	7.268300	0.668900	6.987600
O	1.358500	11.651500	7.853400	C	6.675400	13.771000	4.150900	H	7.329300	0.855400	8.723800
O	2.694000	13.829400	7.930500	C	7.278500	14.988900	3.841800	H	6.444400	-0.476100	8.018700
O	5.540700	1.358500	7.853400	C	9.511100	13.991400	3.962800	H	0.668900	9.923900	6.987600

H	0.855300	9.862900	8.723800
H	-0.476200	10.747800	8.018700
H	13.132700	2.089800	8.781900
H	13.351100	1.902100	7.058500
H	14.576800	1.325700	8.162300
H	2.861300	9.460100	7.727600
H	2.089800	4.059500	8.781900
H	1.902100	3.841100	7.058500
H	1.325700	2.615400	8.162300
H	13.695200	11.441500	4.216000
H	14.058100	6.755200	3.911200
H	11.441500	3.497100	4.216000
H	6.755200	3.134100	3.911200
H	9.460100	14.331000	7.727600
H	5.357300	13.471100	7.834900
H	3.134100	10.437100	3.911200
H	13.471100	11.834900	7.834900
H	7.732100	2.861300	7.727600
H	3.721200	5.357300	7.834900
H	14.331000	7.732100	7.727600
H	5.750700	13.695200	4.216000
H	11.834900	3.721200	7.834900
H	10.437100	14.058100	3.911200

[4]$^{2+}$ Tb2

178

Tb	8.596100	8.596100	12.639400
Cd	8.596100	8.596100	9.362000
O	8.487100	16.475300	11.183800
O	12.602300	1.847800	14.889800
O	14.542200	3.483100	14.904300
O	15.344400	12.602300	14.889800
O	13.709100	14.542200	14.904300
O	1.111000	10.982400	11.309700
O	0.716900	8.487100	11.183800
O	6.209800	1.111000	11.309700
O	4.590000	15.344400	14.889800
O	2.650000	13.709100	14.904300
O	1.847800	4.590000	14.889800
O	10.982400	16.081300	11.309700
O	8.705100	0.716900	11.183800
O	16.081300	6.209800	11.309700
O	16.475300	8.705100	11.183800
O	3.483100	2.650000	14.904300
N	10.113500	9.856000	13.961800
N	8.900100	11.960600	14.165800
N	10.631000	5.888000	10.991300
N	7.336300	10.113500	13.961800
N	5.231600	8.900100	14.165800
N	8.326900	6.685700	10.984700
N	11.304200	10.631000	10.991300
N	7.078700	7.336300	13.961800
N	8.292200	5.231600	14.165800
N	6.561300	11.304200	10.991300
N	9.856000	7.078700	13.961800
N	6.685700	8.865400	10.984700
N	5.888000	6.561300	10.991300
N	8.865400	10.506500	10.984700
N	11.960600	8.292200	14.165800
N	10.506500	8.326900	10.984700
C	7.672900	11.437700	14.130200
C	10.015900	11.222800	14.126900
C	13.610400	10.934600	14.497300
C	12.240900	10.726600	14.325300
C	11.341400	11.795300	14.331900
C	11.772900	13.121800	14.514200
C	13.131100	13.335000	14.695400
C	14.053300	12.234000	14.692800
C	11.437700	9.519300	14.130200
C	11.222800	7.176400	14.126900
C	10.934600	3.581800	14.497300
C	10.726600	4.951400	14.325300
C	11.795300	5.850900	14.331900
C	10.094500	0.379000	11.169300
C	13.121800	5.419300	14.514200
C	13.335000	4.061200	14.695400
C	12.234000	3.139000	14.692800
C	5.754600	7.672900	14.130200
C	5.969500	10.015900	14.126900
C	6.257600	13.610400	14.497300
C	6.465700	12.240900	14.325300
C	5.397000	11.341400	14.331900
C	4.070400	11.772900	14.514200
C	3.857300	13.131100	14.695400
C	4.958200	14.053300	14.692800
C	9.519300	5.754600	14.130200
C	7.176400	5.969500	14.126900
C	3.581800	6.257600	14.497300
C	4.951400	6.465700	14.325300
C	5.850900	5.397000	14.331900
C	5.419300	4.070400	14.514200
C	4.061200	3.857300	14.695400
C	3.139000	4.958200	14.692800
C	4.346700	1.534400	15.137800
C	0.856100	5.615500	14.988100
C	11.576700	0.856100	14.988100
C	15.657800	4.346700	15.137800
C	16.336100	11.576700	14.988100
C	5.615500	16.336100	14.988100
C	1.534300	12.845600	15.137800
C	12.845600	15.657900	15.137800
C	7.886100	11.492700	10.983700
C	6.020400	10.092900	10.996300
C	4.585900	9.875200	11.027900
C	4.376800	8.498100	11.003500
C	3.524100	10.782600	11.121800
C	2.248700	10.255500	11.191300
C	3.091200	7.950700	11.044000
C	2.032800	8.834100	11.134700
C	11.492700	9.306200	10.983700
C	10.092900	11.171900	10.996300
C	9.875200	12.606400	11.027900
C	8.498100	12.815400	11.003500
C	10.782600	13.668200	11.121800
C	10.255500	14.943500	11.191300
C	7.950700	14.101100	11.044000
C	8.834100	15.159400	11.134700
C	5.699600	7.886100	10.983700
C	7.099400	6.020400	10.996300
C	7.317000	4.585900	11.027900
C	8.694100	4.376800	11.003500
C	6.409600	3.524100	11.121800
C	6.936700	2.248700	11.191300
C	9.241500	3.091200	11.044000
C	8.358200	2.032800	11.134700
C	9.306200	5.699600	10.983700
C	11.171900	7.099400	10.996300
C	12.606400	7.317000	11.027900
C	12.815400	8.694100	11.003500
C	13.668200	6.409600	11.121800
C	14.943500	6.936700	11.191300
C	14.101100	9.241500	11.044000
C	15.159400	8.358200	11.134700
C	0.378900	7.097700	11.169300
C	1.235200	12.406800	11.285800
C	7.097700	16.813300	11.169300
C	12.406800	15.957000	11.285800
C	16.813200	10.094500	11.169300
C	15.957000	4.785400	11.285800
C	4.785400	1.235200	11.285800
H	4.464800	1.825900	12.118300
H	4.483900	1.709100	10.375000
H	4.341600	0.263400	11.346100
H	14.208400	10.222600	14.481500
H	15.366200	4.464900	12.118300
H	15.483200	4.484000	10.375000
H	16.928800	4.341600	11.346200
H	10.542500	0.749900	10.271200
H	10.577400	0.818900	12.016800
H	10.203300	-0.684700	11.209300
H	12.727300	15.366200	12.118300
H	12.708200	15.483200	10.375000
H	12.850600	16.928800	11.346200
H	6.649700	16.442400	10.271200
H	6.614800	16.373300	12.016700
H	6.988900	17.877000	11.209300
H	1.826000	12.727300	12.118300
H	1.709000	12.708300	10.375000
H	0.263400	12.850600	11.346200
H	0.749700	6.649800	10.271100
H	0.819000	6.614700	12.016700
H	-0.684800	6.988900	11.209400
H	16.442400	10.542500	10.271200
H	16.373300	10.577400	12.016700
H	17.876900	10.203300	11.209300
H	14.238100	10.160700	11.011600
H	13.521400	5.491400	11.136500
H	11.169500	13.829500	14.513300
H	10.222600	2.983800	14.481500
H	13.829500	6.022800	14.513300
H	6.969600	14.208400	14.481500
H	10.160700	2.954200	11.011600
H	5.491400	3.670900	11.136500
H	3.670900	11.700900	11.136500
H	3.362700	11.169500	14.513300
H	7.031500	14.238100	11.011600
H	2.983800	6.969600	14.481500
H	6.022800	3.362700	14.513300
H	4.945900	1.359200	14.268700
H	4.982100	1.743800	15.972800
H	3.758300	0.665400	15.346400
H	1.097100	6.268000	15.801100
H	0.830600	6.175600	14.076700
H	-0.101600	5.170300	15.159900
H	11.700900	13.521400	11.136500
H	10.924300	1.097100	15.801200
H	11.016600	0.830800	14.076800
H	12.021900	-0.101600	15.159700
H	15.833000	4.945900	14.268800
H	15.448400	4.982100	15.972800
H	16.526800	3.758300	15.346400
H	16.095100	10.924300	15.801200
H	16.361400	11.016500	14.076800
H	17.293800	12.021900	15.159700
H	6.268000	16.095200	15.801100
H	6.175600	16.361500	14.076700
H	5.170300	17.293800	15.159800
H	2.954200	7.031500	11.011600
H	1.359100	12.246300	14.268800
H	1.743700	12.210200	15.972900
H	0.665400	13.434000	15.346300
H	12.246300	15.833100	14.268800
H	12.210200	15.448500	15.972900
H	13.434000	16.526800	15.346300

[4]$^{4+}$ Tb1

178

Tb	0.000000	0.000000	0.000000
Cd	0.000000	0.000000	3.224100
O	7.747678	-1.248584	1.254800
O	7.751023	1.253118	1.254200
O	1.248584	7.747778	1.254800
O	-1.253118	7.751123	1.254200
O	-1.248684	-7.747678	1.254800
O	1.253118	-7.751023	1.254200
O	-7.747778	1.248684	1.254800
O	-7.751123	-1.253118	1.254200
O	-6.808302	-4.021533	-2.684400
O	-5.033348	-5.876730	-2.703800
O	6.808201	4.021633	-2.684400
O	5.033348	5.876830	-2.703800
O	4.021533	-6.808202	-2.684400
O	5.876730	-5.033348	-2.703800
O	-4.021633	6.808301	-2.684400
O	-5.876830	5.033348	-2.703800
N	1.930500	0.000000	1.599400
N	2.396593	-2.401311	1.600000
N	1.385864	-1.388939	-1.295600
N	-0.005199	-3.379804	-1.501100
N	-0.000000	1.930600	1.599400
N	2.401311	2.396693	1.600000
N	0.000000	-1.930500	1.599400
N	-2.401311	-2.396593	1.600000
N	-1.930600	-0.000000	1.599400

N	-2.396693	2.401311	1.600000	C	2.321199	-4.985558	-1.949700	H	8.920667	2.951446	1.252900
N	1.388939	1.385864	-1.295600	C	4.521355	-3.143090	-1.996500	H	7.550739	2.996994	2.336500
N	3.379804	-0.005199	-1.501100	C	3.606265	-5.411959	-2.256300	H	7.308136	3.162643	0.614000
N	-1.389039	-1.385864	-1.295600	C	3.593961	2.154534	-1.679100				
N	-3.379804	0.005199	-1.501100	C	2.884952	-7.644408	-2.586200				
N	-1.385864	1.389039	-1.295600	C	3.253896	-2.727078	-1.719800	**[4]**$^{4+}$ Tb2			
N	0.005199	3.379804	-1.501100	C	-2.321300	4.985658	-1.949700	178			
C	1.112617	-2.762209	1.593400	C	-4.521355	3.143190	-1.996500	Tb	0.000000	0.000000	0.000000
C	2.770591	-1.110478	1.595100	C	-3.606365	5.411959	-2.256300	Cd	0.000000	0.000000	3.266400
C	4.152363	0.704081	1.562500	C	-3.594062	-2.154434	-1.679100	O	1.245707	-7.656456	-2.594900
C	4.150138	-0.702820	1.568000	C	-2.884952	7.644408	-2.586200	O	-1.274590	-7.652917	-2.590800
C	6.514347	-0.717151	1.374500	C	-6.810502	4.022867	-2.689000	O	7.794115	-1.009855	1.295600
C	6.517957	0.714952	1.376100	C	-3.253996	2.727178	-1.719800	O	7.046301	-3.463354	1.454300
C	5.337207	1.438918	1.478100	H	5.335429	2.368717	1.489600	O	-7.656456	-1.245707	-2.594900
C	5.334994	-1.435784	1.480500	H	5.332572	-2.365786	1.492700	O	-7.652917	1.274590	-2.590800
C	-1.159804	-2.728021	-1.462500	H	-2.368717	5.335529	1.489600	O	7.656456	1.245807	-2.594900
C	1.159807	-2.746380	-1.467400	H	2.365786	5.332572	1.492700	O	7.652917	-1.274490	-2.590800
C	7.891734	2.683306	1.372000	H	2.368717	-5.335429	1.489600	O	-1.245807	7.656456	-2.594900
C	7.891371	-2.685295	1.364800	H	-2.365786	-5.332572	1.492700	O	1.274490	7.652917	-2.590800
C	2.762209	1.112717	1.593400	H	-5.335529	-2.368717	1.489600	O	-1.009955	-7.794115	1.295600
C	1.110478	2.770691	1.595100	H	-5.332572	2.365786	1.492700	O	-3.463354	-7.046301	1.454300
C	-0.704081	4.152363	1.562500	H	-5.577104	-1.604167	-1.923400	O	1.009855	7.794115	1.295600
C	0.702820	4.150238	1.568000	H	-2.578031	-5.260004	-1.997500	O	3.463354	7.046301	1.454300
C	0.717151	6.514347	1.374500	H	5.577104	1.604167	-1.923400	O	-7.794115	1.009955	1.295600
C	-0.714952	6.518057	1.376100	H	2.578031	5.260104	-1.997500	O	-7.046301	3.463354	1.454300
C	-1.438918	5.337207	1.478100	H	1.604167	-5.577104	-1.923400	N	1.968003	0.000000	-1.306500
C	1.435784	5.335094	1.480500	H	5.260004	-2.578031	-1.997500	N	2.379105	-2.392977	-1.547100
C	-2.683306	7.891734	1.372000	H	-1.604167	5.577104	-1.923400	N	1.838784	-0.542358	1.716600
C	2.685295	7.891471	1.364800	H	-5.260104	2.578031	-1.997500	N	1.628093	-2.983666	1.680100
C	-2.762309	-1.112617	1.593400	H	4.341732	7.672500	-2.141200	N	-0.000100	-1.968003	-1.306500
C	-1.110478	-2.770591	1.595100	H	3.156528	6.391163	-2.221600	N	-2.392977	-2.379105	-1.547100
C	0.703981	-4.152363	1.562500	H	3.784491	7.094054	-3.692900	N	0.000000	1.968103	-1.306500
C	-0.702920	-4.150138	1.568000	H	8.638646	3.146970	-2.882400	N	2.392977	2.379105	-1.547100
C	-0.717251	-6.514347	1.374500	H	7.273088	2.112621	-3.227000	N	-1.968103	0.000100	-1.306500
C	0.714952	-6.517957	1.376100	H	7.653825	2.535458	-1.574900	N	-2.379105	2.392977	-1.547100
C	1.438818	-5.337207	1.478100	H	6.843328	-3.581747	-1.714700	N	-0.542358	-1.838784	1.716600
C	-1.435884	-5.334994	1.480500	H	6.541539	-3.278134	-3.408800	N	-2.983766	-1.628093	1.680100
C	2.683206	-7.891734	1.372000	H	7.772651	-4.422769	-2.932100	N	0.542358	1.838884	1.716600
C	-2.685295	-7.891371	1.364800	H	3.146870	-8.638646	-2.882400	N	2.983666	1.628193	1.680100
C	-1.112717	2.762309	1.593400	H	2.112621	-7.273088	-3.227000	N	-1.838884	0.542358	1.716600
C	-2.770691	1.110478	1.595100	H	2.535358	-7.653825	-1.574900	N	-1.628193	2.983766	1.680100
C	-4.152363	-0.703981	1.562500	H	-3.102062	-6.335429	-2.421900	C	-0.711388	-4.141470	-1.758800
C	-4.150238	0.702920	1.568000	H	-3.928994	-7.249744	-3.660200	C	0.695502	-4.148615	-1.757800
C	-6.514347	0.717251	1.374500	H	-4.251794	-7.572444	-1.973500	C	1.103304	-2.764979	-1.512300
C	-6.518057	-0.714952	1.376100	H	-8.638646	-3.146870	-2.882400	C	2.765707	-1.116102	-1.510200
C	-5.337207	-1.438818	1.478100	H	-7.273188	-2.112621	-3.227000	C	1.423445	-5.296286	-2.021500
C	-5.335094	1.435884	1.480500	H	-7.653925	-2.535358	-1.574900	C	-1.438748	-5.289704	-2.029100
C	-7.891734	-2.683206	1.372000	H	-8.920767	-2.951346	1.252900	C	-0.729134	-6.453441	-2.292200
C	-7.891471	2.685295	1.364800	H	-7.550739	-2.996894	2.336500	C	0.704547	-6.464636	-2.298200
C	2.728021	-1.159804	-1.462500	H	-7.308236	-3.162643	0.614000	C	5.520089	-0.011278	1.505100
C	2.746380	1.159907	-1.467400	H	-8.921536	2.950655	1.248700	C	2.328017	-1.854880	1.702300
C	-2.728121	1.159804	-1.462500	H	-7.312266	3.161255	0.601300	C	-2.697169	-7.746443	-2.802900
C	-2.746480	-1.159807	-1.467400	H	-7.546670	3.005710	2.325800	C	2.663112	-7.761721	-2.796300
C	1.159804	2.728121	-1.462500	H	-7.440570	4.131976	-1.831100	C	8.283700	-0.007674	1.056700
C	-1.159907	2.746480	-1.467400	H	-6.311914	3.077077	-2.647400	C	4.177160	-0.504054	1.623300
C	-4.594844	-4.596557	-2.296300	H	-7.405234	4.073798	-3.577100	C	6.441875	-1.189413	1.417800
C	4.594744	4.596557	-2.296300	H	-3.146970	8.638646	-2.882400	C	6.029862	-2.579141	1.497800
C	4.596557	-4.594744	-2.296300	H	-2.112621	7.273188	-3.227000	C	4.688957	-2.899621	1.617300
C	-4.596557	4.594844	-2.296300	H	-2.535458	7.653925	-1.574900	C	3.781520	-1.854513	1.656100
C	-4.022867	-6.810502	-2.689000	H	-2.951446	8.920767	1.252900	C	0.279364	-2.944930	1.688700
C	-4.985658	-2.321200	-1.949700	H	-2.996994	7.550739	2.336500	C	6.704807	-4.523714	1.315200
C	-3.143190	-4.521355	-1.996500	H	-3.162643	7.308236	0.614000	C	-4.141470	0.711388	-1.758800
C	-5.411959	-3.606265	-2.256300	H	-2.950655	-8.921436	1.248700	C	-4.148715	-0.695501	-1.757800
C	2.154434	-3.593961	-1.679100	H	-3.161255	-7.312266	0.601300	C	-2.765079	-1.103303	-1.512300
C	-7.644408	-2.884952	-2.586200	H	-3.005710	-7.546670	2.325800	C	-1.116202	-2.765706	-1.510200
C	-2.727178	-3.253896	-1.719800	H	2.951346	-8.920667	1.252900	C	-5.296386	-1.423445	-2.021500
C	4.022767	6.810502	-2.689000	H	2.996894	-7.550739	2.336500	C	-5.289704	1.438748	-2.029100
C	4.985558	2.321299	-1.949700	H	3.162643	-7.308136	0.614000	C	-6.453541	0.729134	-2.292200
C	3.143090	4.521355	-1.996500	H	8.921436	-2.950655	1.248700	C	-6.464736	-0.704547	-2.298200
C	5.411959	3.606365	-2.256300	H	7.312266	-3.161155	0.601300	C	-7.746543	2.697169	-2.802900
C	-2.154534	3.594061	-1.679100	H	7.546670	-3.005610	2.325800	C	-7.761721	-2.663112	-2.796300
C	7.644408	2.884952	-2.586200	H	2.950655	8.921536	1.248700	C	4.141470	-0.711388	-1.758800
C	2.727078	3.253996	-1.719800	H	3.161155	7.312266	0.601300	C	4.148615	0.695502	-1.757800
C	6.810502	-4.022767	-2.689000	H	3.005610	7.546670	2.325800	C	2.764979	1.103404	-1.512300

C	1.116102	2.765807	-1.510200
C	5.296286	1.423445	-2.021500
C	5.289704	-1.438748	-2.029100
C	6.453441	-0.729134	-2.292200
C	6.464636	0.704547	-2.298200
C	7.746443	-2.697169	-2.802900
C	7.761721	2.663112	-2.796300
C	0.711388	4.141470	-1.758800
C	-0.695501	4.148715	-1.757800
C	-1.103403	2.765079	-1.512300
C	-2.765806	1.116202	-1.510200
C	-1.423445	5.296386	-2.021500
C	1.438748	5.289704	-2.029100
C	0.729134	6.453541	-2.292200
C	-0.704547	6.464736	-2.298200
C	2.697169	7.746543	-2.802900
C	-2.663112	7.761721	-2.796300
C	-0.011278	-5.520089	1.505100
C	-1.854880	-2.328017	1.702300
C	-0.007674	-8.283700	1.056700
C	-0.504154	-4.177160	1.623300
C	-1.189513	-6.441875	1.417800
C	-2.579141	-6.029862	1.497800
C	-2.899721	-4.688957	1.617300
C	-1.854613	-3.781520	1.656100
C	-2.944930	-0.279364	1.688700
C	-4.523814	-6.704807	1.315200
C	0.011278	5.520189	1.505100
C	1.854880	2.328117	1.702300
C	0.007674	8.283700	1.056700
C	0.504054	4.177160	1.623300
C	1.189414	6.441975	1.417800
C	2.579141	6.029862	1.497800
C	2.899621	4.689057	1.617300
C	1.854513	3.781620	1.656100
C	2.944931	0.279464	1.688700
C	4.523714	6.704907	1.315200
C	-5.520189	0.011278	1.505100
C	-2.328117	1.854880	1.702300
C	-8.283700	0.007674	1.056700
C	-4.177160	0.504154	1.623300
C	-6.441975	1.189514	1.417800
C	-6.029862	2.579141	1.497800
C	-4.689057	2.899721	1.617300
C	-3.781620	1.854613	1.656100
C	-0.279464	2.944931	1.688700
C	-6.704907	4.523814	1.315200
H	2.353557	-5.290934	-2.015200
H	-2.368632	-5.280756	-2.034000
H	5.773871	0.883246	1.486100
H	4.407493	-3.784293	1.669700
H	-5.290934	-2.353557	-2.015200
H	-5.280856	2.368633	-2.034000
H	5.290934	2.353557	-2.015200
H	5.280756	-2.368532	-2.034000
H	-2.353557	5.290934	-2.015200
H	2.368533	5.280856	-2.034000
H	0.883146	-5.773871	1.486100
H	-3.784393	-4.407493	1.669700
H	-0.883246	5.773971	1.486100
H	3.784293	4.407593	1.669700
H	-5.773971	-0.883146	1.486100
H	-4.407593	3.784393	1.669700
H	2.916805	-8.776299	-3.022400
H	3.173387	-7.456179	-1.906900
H	2.955598	-7.131169	-3.609800
H	-2.958373	-8.759353	-3.027800
H	-2.978183	-7.115713	-3.620300
H	-3.211082	-7.433676	-1.918000
H	-5.172014	-7.555690	1.289200
H	-4.606899	-6.164950	0.395100
H	-4.803217	-6.068280	2.128600
H	-8.776399	-2.916805	-3.022400
H	-7.456179	-3.173387	-1.906900
H	-7.131169	-2.955598	-3.609800
H	-8.759453	2.958374	-3.027800
H	-7.115813	2.978184	-3.620300
H	-7.433676	3.211082	-1.918000
H	-7.555790	5.172015	1.289200
H	-6.165050	4.606899	0.395100
H	-6.068380	4.803218	2.128600
H	-2.916905	8.776400	-3.022400
H	-3.173487	7.456180	-1.906900
H	-2.955598	7.131169	-3.609800
H	0.130371	9.345871	1.015400
H	-0.701093	8.035932	1.819100
H	-0.346494	7.928665	0.111500
H	2.958374	8.759454	-3.027800
H	2.978084	7.115814	-3.620300
H	3.210982	7.433676	-1.918000
H	5.172015	7.555790	1.289200
H	4.606799	6.165050	0.395100
H	4.803118	6.068380	2.128600
H	8.776300	2.916905	-3.022400
H	7.456180	3.173487	-1.906900
H	7.131169	2.955598	-3.609800
H	8.759354	-2.958373	-3.027800
H	7.115714	-2.978083	-3.620300
H	7.433676	-3.210982	-1.918000
H	-0.130471	-9.345771	1.015400
H	0.700993	-8.035932	1.819100
H	0.346494	-7.928565	0.111500
H	7.555690	-5.172014	1.289200
H	6.164950	-4.606799	0.395100
H	6.068280	-4.803117	2.128600
H	9.345771	-0.130371	1.015400
H	8.035932	0.701093	1.819100
H	7.928565	0.346494	0.111500
H	-9.345871	0.130471	1.015400
H	-8.035932	-0.700993	1.819100
H	-7.928665	-0.346494	0.111500

[5]^0

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Tb	22.975020	4.397370	13.604280
Cd	22.869730	4.349810	10.236010
O	24.000920	12.261640	15.313800
O	21.476290	12.177530	15.410870
O	15.254950	5.566870	13.729370
O	15.234160	3.096950	13.999800
O	21.728320	-3.211660	16.326160
O	24.261440	-3.123720	16.454450
O	30.660350	3.341650	15.715970
O	30.670750	5.888040	15.580760
O	21.162020	11.960360	11.988930
O	18.848630	10.957100	12.082540
O	15.531330	2.676380	10.511980
O	16.386940	0.302050	10.768540
O	24.896200	-3.184890	13.091440
O	27.212430	-2.121990	13.271730
O	30.658580	6.178610	12.089470
O	29.695590	8.537650	12.099880
N	22.879110	6.419490	14.852680
N	20.528830	6.805650	14.876950
N	20.958560	4.427500	14.870020
N	20.558780	2.034050	15.060700
N	22.929480	2.489030	15.015630
N	25.254090	2.144930	15.480210
N	24.889690	4.519260	15.036440
N	25.252760	6.882120	15.095380
N	22.303290	6.125090	11.794780
N	19.934240	5.612750	11.669970
N	21.262700	3.571060	11.864120
N	21.759520	1.231140	11.919590
N	23.759620	2.588440	12.006270
N	26.130380	3.112250	12.193490
N	24.803310	5.131000	12.020130
N	24.290480	7.497690	11.857180
C	23.937890	7.275930	15.008700
C	23.521870	8.640880	15.136980
C	24.233030	9.829960	15.199380
C	23.494640	10.992270	15.286060
C	25.303680	12.403110	15.400470
C	21.778100	7.210930	14.935890
C	22.145300	8.610300	15.130050
C	21.416820	9.780260	15.244460
C	22.071250	10.969330	15.327660
C	20.050370	12.204290	15.438610
C	20.154700	5.524810	14.797210
C	18.721310	5.142470	14.651600
C	17.588530	5.765690	14.329170
C	16.450560	5.035420	14.110740
C	15.204710	6.973880	13.507480
C	20.118480	3.318710	14.883890
C	18.732600	3.739290	14.700140
C	17.581350	2.978430	14.561460
C	16.440160	3.639880	14.245960
C	15.205190	1.663180	14.159280
C	21.832250	1.712880	15.192450
C	22.270110	0.359400	15.587690
C	21.571940	-0.802910	15.781840
C	22.256080	-1.926990	16.093870
C	20.342890	-3.337830	16.197890
C	24.019470	1.728180	15.362340
C	23.617140	0.393810	15.684770
C	24.373240	-0.757030	15.986400
C	23.653390	-1.926990	16.194420
C	25.714790	-3.161950	16.523790
C	25.669080	3.421940	15.299930
C	27.065680	3.846340	15.462880
C	28.251640	3.158130	15.625830
C	29.397490	3.907520	15.622360
C	30.792180	2.007290	15.476750
C	25.633130	5.624220	15.123110
C	27.032030	5.249530	15.345000
C	28.251660	5.998920	15.407410
C	29.434850	5.283940	15.601560
C	30.688630	7.268280	15.546090
C	22.976640	7.321810	11.822510
C	22.074650	8.438240	11.815580
C	22.250590	9.818490	11.864120
C	21.153730	10.613760	11.936930
C	22.447860	12.578990	11.929990
C	20.964090	6.453900	11.767040
C	20.775790	7.887670	11.836380
C	19.689420	8.698240	11.933460
C	19.827080	10.051720	11.964660
C	17.559910	10.487590	12.158820
C	20.042390	4.305150	11.645700
C	18.981780	3.379890	11.413410
C	17.648150	3.681930	11.104840
C	16.826900	2.638150	10.903760
C	15.047430	3.961040	10.407970
C	20.917040	2.259630	11.787840
C	19.449430	2.099050	11.527820
C	18.590010	1.009380	11.323260
C	17.304920	1.280840	11.028570
C	16.776510	-1.043790	10.959230
C	23.069310	1.368780	12.051340
C	23.942440	0.279110	12.304430
C	23.837480	-1.047610	12.498580
C	24.902000	-1.812290	12.838350
C	23.618110	-3.815750	12.987430
C	25.095910	2.286390	12.196950
C	25.258680	0.837320	12.411910
C	26.393190	0.095590	12.723940
C	26.201880	-1.265540	12.942360
C	28.524880	-1.582890	13.358400
C	25.986970	4.423670	12.051340
C	27.105050	5.348940	11.982000
C	28.431570	5.100420	12.013200

C	29.296780	6.239790	12.037470
C	31.300330	4.871010	12.176150
C	25.140230	6.423310	11.916120
C	26.610870	6.568600	11.954260
C	27.394800	7.734740	11.957730
C	28.738150	7.547390	12.047870
C	29.188270	9.864370	12.092940
H	25.183910	9.841430	15.188980
H	20.467210	9.753490	15.261790
H	17.569750	6.713890	14.252890
H	17.590790	2.034050	14.679330
H	20.626950	-0.822030	15.698630
H	25.319840	-0.730270	16.045340
H	28.269490	2.213750	15.736770
H	28.253980	6.943290	15.320730
H	23.120880	10.193180	11.843320
H	18.821780	8.315890	11.982000
H	17.341350	4.576610	11.042440
H	18.902920	0.114700	11.392610
H	22.988550	-1.464360	12.391100
H	27.252630	0.493220	12.782880
H	28.771820	4.213390	12.020130
H	27.007520	8.602650	11.898790
H	31.701960	7.611630	15.532840
H	30.192890	7.653280	16.412640
H	30.184890	7.609510	14.665910
H	31.818250	1.724750	15.587410
H	30.467780	1.789770	14.480580
H	30.194050	1.459070	16.174320
H	26.035720	-4.161030	16.732920
H	26.052070	-2.508860	17.301350
H	26.124990	-2.844070	15.588060
H	20.057090	-4.349820	16.395590
H	20.051190	-3.072670	15.203150
H	19.859310	-2.687630	16.896660
H	14.220670	1.300730	13.948930
H	15.471000	1.410680	15.164510
H	15.902430	1.214890	13.482670
H	15.958440	-1.689610	10.717180
H	17.057990	-1.192300	11.980800
H	17.607880	-1.267870	10.324000
H	14.024140	3.932600	10.096580
H	15.624530	4.502330	9.687650
H	15.117530	4.446660	11.358850
H	14.214130	7.253740	13.215370
H	15.893150	7.237460	12.731930
H	15.469140	7.486730	14.408580
H	16.884560	11.312530	12.249680
H	17.462250	9.850910	13.013220
H	17.329120	9.933610	11.272960
H	19.713900	13.217810	15.505430
H	19.699780	11.655390	16.287550
H	19.667820	11.759750	14.543660
H	22.334850	13.641880	11.978760
H	22.929770	12.313280	11.012350
H	23.042340	12.245290	12.754700
H	25.549380	13.444450	15.411850
H	25.769990	11.935800	14.558410
H	25.653080	11.944340	16.301770
H	30.002170	10.557670	12.135500
H	28.552890	10.007710	12.941850
H	28.627590	10.027150	11.196260
H	32.362460	4.996420	12.208300
H	31.035950	4.286490	11.319800
H	30.973150	4.371280	13.063910
H	29.212530	-2.358980	13.622450
H	28.547310	-0.817130	14.105400
H	28.802720	-1.166760	12.412600
H	23.717670	-4.860100	13.197960
H	23.236180	-3.686530	11.996310
H	22.943560	-3.372970	13.690150

[5]$^{4+}$ Tb1

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Tb	0.000000	0.000000	15.749620
Cd	0.000000	0.000000	19.093860
O	0.849840	7.778400	17.392110
O	-1.690080	7.681920	17.342160
O	-4.407650	-6.411770	13.432340
O	-6.239370	-4.617740	13.305190
O	6.433820	-4.379540	13.418710
O	4.654920	-6.215410	13.407360
O	7.809410	-0.863090	17.351240
O	7.660570	1.677190	17.151430
O	4.407650	6.411770	13.432340
O	6.239370	4.617740	13.305190
O	-6.433820	4.379540	13.418710
O	-4.654920	6.215410	13.407360
O	-0.849840	-7.778400	17.392110
O	1.690080	-7.681920	17.342160
O	-7.809410	0.863090	17.351240
O	-7.660570	-1.677190	17.151430
N	3.368150	0.058800	14.254260
N	-1.344380	-1.404320	14.442710
N	0.067220	-3.380770	14.265610
N	2.242240	2.487140	17.364860
N	1.416400	-1.338740	14.472230
N	1.896540	0.079150	17.351240
N	2.520710	-2.251210	17.364860
N	-0.117630	1.917280	17.344430
N	-3.368150	-0.058800	14.254260
N	1.344380	1.404320	14.442710
N	-0.067220	3.380770	14.265610
N	-1.416400	1.338740	14.472230
N	-2.242240	-2.487140	17.364860
N	-1.896540	-0.079150	17.351240
N	-2.520710	2.251210	17.364860
N	0.117630	-1.917280	17.344430
C	2.763180	-1.123150	14.320110
C	-2.371870	-3.462550	14.104410
C	-1.714090	5.257710	17.303560
C	1.130720	5.385860	17.389840
C	2.808800	-0.987470	17.360320
C	4.169980	-0.474890	17.348970
C	-1.089910	-2.785270	14.265610
C	3.485790	-2.381990	14.136200
C	2.693560	1.292760	17.255880
C	2.520710	-3.335540	14.099870
C	2.698360	1.232450	14.263340
C	-1.041900	6.467550	17.348970
C	1.238750	-2.709890	14.329190
C	5.238280	1.707340	17.205930
C	-0.905060	4.092720	17.387570
C	-2.664760	-4.816740	13.879630
C	0.357700	6.524090	17.378490
C	4.076360	0.930940	17.280850
C	-3.358550	-2.487520	14.045380
C	6.453030	1.070390	17.210470
C	-4.983810	-4.213710	13.641220
C	4.184380	-4.993880	13.661660
C	-4.674120	-2.800350	13.834220
C	4.818160	-2.619430	13.886440
C	-7.233250	-3.697360	12.937370
C	-3.985130	-5.144640	13.657120
C	0.969880	2.785270	17.364860
C	2.299850	7.929910	17.253610
C	5.401530	-1.130690	17.371670
C	-3.507390	-7.379640	13.237070
C	2.866410	-4.688600	13.879630
C	7.499720	-3.441070	13.336980
C	0.468130	4.179790	17.355780
C	7.636560	3.143320	16.972060
C	5.202270	-3.968730	13.659390
C	3.711450	-7.251500	13.078140
C	-3.113680	7.700010	17.301290
C	6.522650	-0.380670	17.339890
C	7.984660	-2.212380	17.569210

C	-1.272360	2.675970	17.333070
C	-2.763180	1.123150	14.320110
C	2.371870	3.462550	14.104410
C	1.089910	2.785270	14.265610
C	-3.485790	2.381990	14.136200
C	-2.520710	3.335540	14.099870
C	-2.698360	-1.232450	14.263340
C	-1.238750	2.709890	14.329190
C	2.664760	4.816740	13.879630
C	3.358550	2.487520	14.045380
C	4.983810	4.213710	13.641220
C	-4.184380	4.993880	13.661660
C	4.674120	2.800350	13.834220
C	-4.818160	2.619430	13.886440
C	7.233250	3.697360	12.937370
C	3.985130	5.144640	13.657120
C	3.507390	7.379640	13.237070
C	-2.866410	4.688600	13.879630
C	-7.499720	3.441070	13.336980
C	-5.202270	3.968730	13.659390
C	-3.711450	7.251500	13.078140
C	1.714090	-5.257710	17.303560
C	-1.130720	-5.385860	17.389840
C	-2.808800	0.987470	17.360320
C	-4.169980	0.474890	17.348970
C	-2.693560	-1.292760	17.255880
C	1.041900	-6.467550	17.348970
C	-5.238280	-1.707340	17.205930
C	0.905060	-4.092720	17.387570
C	-0.357700	-6.524090	17.378490
C	-4.076360	-0.930940	17.280850
C	-6.453030	-1.070390	17.210470
C	-0.969880	-2.785270	17.364860
C	-2.299850	-7.929910	17.253610
C	-5.401530	1.130690	17.371670
C	-0.468130	-4.179790	17.355780
C	-7.636560	-3.143320	16.972060
C	3.113680	-7.700010	17.301290
C	-6.522650	0.380670	17.339890
C	-7.984660	2.212380	17.569210
C	1.272360	-2.675970	17.333070
H	-2.639880	5.210560	17.224950
H	2.058870	5.429840	17.419810
H	5.189360	2.634020	17.155090
H	-1.999430	-5.466060	13.884190
H	-5.336690	-2.146090	13.814400
H	5.440060	-1.928050	13.866940
H	-6.913050	-3.146300	12.205350
H	-7.434910	-3.116830	13.686930
H	2.742510	7.593760	18.048440
H	2.612540	7.418880	16.492030
H	5.450240	-2.057630	17.411430
H	-2.954010	-7.487850	14.027280
H	-2.934130	-7.160360	12.487060
H	2.217290	-5.353290	13.880260
H	7.566220	-2.939800	14.165370
H	7.337080	-2.814890	12.613890
H	7.109230	3.365540	16.187580
H	7.215220	3.557120	17.742240
H	3.104490	-6.944060	12.386970
H	3.191200	-7.491540	13.861080
H	-3.455870	7.142540	18.017200
H	-3.409350	7.319150	16.460700
H	7.709860	-2.721050	16.789720
H	7.457710	-2.504520	18.329740
H	1.999430	5.466060	13.884190
H	5.336690	2.146090	13.814400
H	-5.440060	1.928050	13.866940
H	6.913050	3.146300	12.205350
H	7.434910	3.116830	13.686930
H	2.954010	7.487850	14.027280
H	2.934130	7.160360	12.487060
H	-2.217290	5.353290	13.880260
H	-7.566220	2.939800	14.165370

H	-7.337080	2.814890	12.613890
H	-3.104490	6.944060	12.386970
H	-3.191200	7.491540	13.861080
H	2.639880	-5.210560	17.224950
H	-2.058870	-5.429840	17.419810
H	-5.189360	-2.634020	17.155090
H	-2.742510	-7.593760	18.048440
H	-2.612540	-7.418880	16.492030
H	-5.450240	2.057630	17.411430
H	-7.109230	-3.365540	16.187580
H	-7.215220	-3.557120	17.742240
H	3.455870	-7.142540	18.017200
H	3.409350	-7.319150	16.460700
H	-7.709860	2.721050	16.789720
H	-7.457710	2.504520	18.329740
H	-8.108700	-4.236360	12.640780
H	2.523830	8.967330	17.117620
H	-4.035500	-8.288130	13.035440
H	8.407790	-3.978510	13.159570
H	8.640650	3.495720	16.860160
H	4.257890	-8.102900	12.729680
H	-3.463980	8.705770	17.404360
H	9.023570	-2.380160	17.762660
H	8.108700	4.236360	12.640780
H	4.035500	8.288130	13.035440
H	-8.407790	3.978510	13.159570
H	-4.257890	8.102900	12.729680
H	-2.523830	-8.967330	17.117620
H	-8.640650	-3.495720	16.860160
H	3.463980	-8.705770	17.404360
H	-9.023570	2.380160	17.762660

[5]$^{4+}$ Tb2

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Tb	0.000000	0.000000	25.453780
Cd	0.000000	0.000000	22.173350
O	6.244170	4.361450	28.481280
O	4.760550	6.137010	24.707690
O	-4.321220	6.204480	28.656110
O	6.486640	4.303030	24.551020
O	6.119330	-4.731560	24.816670
O	4.323620	-6.495820	24.600980
O	-6.143340	4.384440	28.783260
O	4.405250	6.153220	28.665190
O	-4.760550	-6.137010	24.707690
O	-6.486640	-4.303030	24.551020
O	-6.119330	4.731560	24.816670
O	-4.323620	6.495820	24.600980
O	-6.244170	-4.361450	28.481280
O	4.321220	-6.204480	28.656110
O	6.143340	-4.384440	28.783260
O	-4.405250	-6.153220	28.665190
N	1.322780	-1.428820	23.688230
N	-0.132040	-3.355510	23.826730
N	-1.402000	-1.297660	23.758620
N	1.392390	-1.409590	26.746610
N	0.019210	3.335540	27.071290
N	3.344150	-0.128150	23.858520
N	1.409200	1.390370	26.739800
N	3.346550	0.010180	27.103080
N	-1.322780	1.428820	23.688230
N	0.132040	3.355510	23.826730
N	1.402000	1.297660	23.758620
N	-3.344150	0.128150	23.858520
N	-1.392390	1.409590	26.746610
N	-0.019210	-3.335540	27.071290
N	-1.409200	-1.390370	26.739800
N	-3.346550	-0.010180	27.103080
C	3.502590	2.296060	23.922090
C	-1.255560	-2.702350	23.797220
C	2.602340	-4.851040	24.108270
C	4.719740	2.683510	27.645730
C	3.418570	2.404600	27.293800
C	5.223880	3.893350	24.308080
C	4.849370	2.551590	24.056050
C	3.905910	-5.189870	24.380740
C	4.914190	-4.213710	24.473830
C	3.372960	-7.488940	24.859810
C	-2.657550	4.707440	27.784230
C	3.322540	-2.581740	23.947070
C	-3.922710	5.001420	28.179300
C	-1.137920	2.743810	27.030420
C	2.931230	4.616990	24.171850
C	2.551920	3.338550	23.953880
C	2.727170	4.639600	27.786500
C	7.530930	3.297850	24.639570
C	2.655150	-1.247530	23.788130
C	4.258810	4.888350	24.383010
C	4.635710	-2.898340	24.253590
C	2.292650	-3.493830	23.917550
C	1.065900	-2.780750	23.781320
C	2.746380	1.134460	26.969120
C	-3.370560	2.438520	27.470900
C	-3.286530	7.191190	28.914950
C	-4.923800	3.987570	28.231520
C	3.387360	7.070590	29.103400
C	5.024620	3.946110	28.095290
C	3.826680	7.158780	25.064160
C	-4.647720	2.702350	27.856890
C	2.779990	1.044010	23.758620
C	7.259660	3.324230	28.715140
C	-2.391080	3.418460	27.375540
C	-7.041190	3.365690	29.160160
C	4.004330	4.929810	28.192920
C	2.729570	-1.183460	27.037230
C	1.181140	2.698580	27.019070
C	2.458300	3.373230	27.350560
C	7.142020	-3.765200	25.202660
C	-3.502590	-2.296060	23.922090
C	1.255560	2.702350	23.797220
C	-2.602340	4.851040	24.108270
C	-5.223880	-3.893350	24.308080
C	-4.849370	-2.551590	24.056050
C	-3.905910	5.189870	24.380740
C	-4.914190	4.213710	24.473830
C	-3.372960	7.488940	24.859810
C	-3.322540	2.581740	23.947070
C	-2.931230	-4.616990	24.171850
C	-2.551920	-3.338550	23.953880
C	-7.530930	-3.297850	24.639570
C	-2.655150	1.247530	23.788130
C	-4.258810	-4.888350	24.383010
C	-4.635710	2.898340	24.253590
C	-2.292650	3.493830	23.917550
C	-1.065900	2.780750	23.781320
C	-3.826680	-7.158780	25.064160
C	-2.779990	-1.044010	23.758620
C	-7.142020	3.765200	25.202660
C	-4.719740	-2.683510	27.645730
C	-3.418570	-2.404600	27.293800
C	2.657550	-4.707440	27.784230
C	3.922710	-5.001420	28.179300
C	1.137920	-2.743810	27.030420
C	-2.727170	-4.639600	27.786500
C	-2.746380	-1.134460	26.969120
C	3.370560	-2.438520	27.470900
C	3.286530	-7.191190	28.914950
C	4.923800	-3.987570	28.231520
C	-3.387360	-7.070590	29.103400
C	-5.024620	-3.946110	28.095290
C	4.647720	-2.702350	27.856890
C	-7.259660	-3.324230	28.715140
C	2.391080	-3.418460	27.375540
C	7.041190	-3.365690	29.160160
C	-4.004330	-4.929810	28.192920
C	-2.729570	1.183460	27.037230
C	-1.181140	-2.698580	27.019070
C	-2.458300	-3.373230	27.350560
H	1.941450	-5.503110	24.049900
H	5.381030	2.033850	27.579430
H	5.482990	1.875060	23.983280
H	2.888950	-7.721710	24.050880
H	2.739030	-7.195450	25.531110
H	-1.991220	5.356610	27.789340
H	2.301650	5.302490	24.178070
H	2.060600	5.287830	27.807870
H	7.660620	2.861060	23.783070
H	7.308890	2.627420	25.303700
H	5.295520	-2.244120	24.304720
H	-2.906260	7.506510	28.078490
H	-2.575910	6.802270	29.447240
H	2.731950	6.606930	29.646480
H	2.935120	7.457550	28.338190
H	3.186260	6.814300	25.706710
H	3.343070	7.457850	24.279360
H	-5.302480	2.039540	27.865200
H	7.532610	2.923970	27.873140
H	6.903060	2.624640	29.285330
H	-6.584920	2.702540	29.698110
H	-7.399860	2.930150	28.371360
H	6.781180	-3.118820	25.830160
H	7.473510	-3.290760	24.424400
H	-1.941450	5.503110	24.049900
H	-5.482990	-1.875060	23.983280
H	-2.888950	7.721710	24.050880
H	-2.739030	7.195450	25.531110
H	-2.301650	-5.302490	24.178070
H	-7.660620	-2.861060	23.783070
H	-7.308890	-2.627420	25.303700
H	-5.295520	2.244120	24.304720
H	-3.186260	-6.814300	25.706710
H	-3.343070	-7.457850	24.279360
H	-6.781180	3.118820	25.830160
H	-7.473510	3.290760	24.424400
H	-5.381030	-2.033850	27.579430
H	1.991220	-5.356610	27.789340
H	-2.060600	-5.287830	27.807870
H	2.906260	-7.506510	28.078490
H	2.575910	-6.802270	29.447240
H	-2.731950	-6.606930	29.646480
H	-2.935120	-7.457550	28.338190
H	5.302480	-2.039540	27.865200
H	-7.532610	-2.923970	27.873140
H	-6.903060	-2.624640	29.285330
H	6.584920	-2.702540	29.698110
H	7.399860	-2.930150	28.371360
H	3.898740	-8.347930	25.221180
H	8.433440	3.796010	24.926310
H	-3.732020	8.007460	29.444240
H	3.855790	7.842270	29.677830
H	4.369690	7.976250	25.490520
H	8.100170	3.786590	29.189120
H	-7.835300	3.807780	29.724820
H	7.942820	-4.305160	25.663180
H	-3.898740	8.347930	25.221180
H	-8.433440	-3.796010	24.926310
H	-4.369690	-7.976250	25.490520
H	-7.942820	4.305160	25.663180
H	3.732020	-8.007460	29.444240
H	-3.855790	-7.842270	29.677830
H	-8.100170	-3.786590	29.189120
H	7.835300	-3.807780	29.724820

6. Point-Charge Calculations

Table S68. Weights of M_J components (in %) in the wavefunctions of the J = 6 ground state and crystal field splitting energy for **[3]^0** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	1.03	0.00	0.00	0.00	0.00	0.00	0.00	0.80
-5	0.00	0.00	0.00	98.56	0.00	0.00	15.70	0.00	0.00	0.00	6.23	0.00	0.00
-4	0.00	0.00	0.00	0.00	50.31	0.00	0.00	0.00	70.71	49.68	0.00	0.00	0.00
-3	0.00	0.00	5.03	0.00	0.00	0.00	0.00	62.46	0.00	0.00	0.00	77.93	0.00
-2	1.03	0.80	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	0.00	0.00	70.71
-1	0.00	0.00	0.00	16.12	0.00	0.00	76.50	0.00	0.00	0.00	62.35	0.00	0.00
0	0.00	0.00	0.00	0.00	70.28	0.00	0.00	0.00	0.00	71.15	0.00	0.00	0.00
1	0.00	0.00	16.12	0.00	0.00	0.00	0.00	76.50	0.00	0.00	0.00	62.35	0.00
2	1.03	0.80	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	0.00	0.00	70.70
3	0.00	0.00	0.00	5.03	0.00	0.00	62.46	0.00	0.00	0.00	77.93	0.00	0.00
4	0.00	0.00	0.00	0.00	50.30	0.00	0.00	0.00	70.71	49.68	0.00	0.00	0.00
5	0.00	0.00	98.56	0.00	0.00	0.00	0.00	15.70	0.00	0.00	0.00	6.23	0.00
6	70.70	70.71	0.00	0.00	0.00	1.03	0.00	0.00	0.00	0.00	0.00	0.00	0.80
E / cm^{-1}	0.00	0.02	278.85	278.85	353.67	374.88	376.41	376.41	404.01	455.62	476.10	483.30	483.30

Table S69. Weights of M_J components (in %) in the wavefunctions of the J = 6 ground state and crystal field splitting energy for **[3]$^+$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.69	70.70	0.00	0.00	0.00	1.73	75.88	0.00	0.00	1.22	0.00	0.00	0.00
-5	0.00	0.00	64.59	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.34	0.00
-4	0.00	0.00	0.00	0.00	30.58	0.00	0.00	0.00	70.71	0.00	63.75	0.00	0.00
-3	0.00	0.00	0.00	31.29	0.00	0.00	0.00	36.28	0.00	0.00	0.00	0.00	87.78
-2	1.73	1.22	0.00	0.00	0.00	70.69	0.00	0.00	0.00	70.70	0.00	0.00	0.00
-1	0.00	0.00	69.63	0.00	0.00	0.00	54.09	0.00	0.00	0.00	0.00	47.18	0.00
0	0.00	0.00	0.00	0.00	90.16	0.00	0.00	0.00	0.00	0.00	43.25	0.00	0.00
1	0.00	0.00	0.00	69.63	0.00	0.00	0.00	54.09	0.00	0.00	0.00	0.00	47.18
2	1.73	1.22	0.00	0.00	0.00	70.69	0.00	0.00	0.00	70.70	0.00	0.00	0.00
3	0.00	0.00	31.29	0.00	0.00	0.00	36.28	0.00	0.00	0.00	0.00	87.78	0.00
4	0.00	0.00	0.00	0.00	30.58	0.00	0.00	0.00	70.71	0.00	63.75	0.00	0.00
5	0.00	0.00	0.00	64.59	0.00	0.00	0.00	75.88	0.00	0.00	0.00	0.00	8.34
6	70.69	70.70	0.00	0.00	0.00	1.73	0.00	0.00	0.00	1.22	0.00	0.00	0.00
E / cm^{-1}	0.00	0.04	216.60	216.60	219.13	235.64	249.68	249.68	317.44	334.39	340.06	340.97	340.97

Table S70. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[3]$^{2+}$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.68	70.70	0.00	0.00	0.00	2.17	0.00	0.00	0.00	1.42	0.00	0.00	0.00
-5	0.00	0.00	0.00	0.00	37.20	0.00	0.00	92.25	0.00	0.00	10.28	0.00	0.00
-4	0.00	0.00	27.15	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	65.29
-3	0.00	0.00	0.00	38.25	0.00	0.00	25.33	0.00	0.00	0.00	0.00	88.86	0.00
-2	2.16	1.42	0.00	0.00	0.00	70.67	0.00	0.00	0.00	70.69	0.00	0.00	0.00
-1	0.00	0.00	0.00	0.00	84.58	0.00	0.00	29.13	0.00	0.00	44.71	0.00	0.00
0	0.00	0.00	92.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	38.40
1	0.00	0.00	0.00	84.57	0.00	0.00	29.13	0.00	0.00	0.00	0.00	44.71	0.00
2	2.17	1.42	0.00	0.00	0.00	70.68	0.00	0.00	0.00	70.69	0.00	0.00	0.00
3	0.00	0.00	0.00	0.00	38.26	0.00	0.00	25.33	0.00	0.00	88.86	0.00	0.00
4	0.00	0.00	27.15	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	65.29
5	0.00	0.00	0.00	37.20	0.00	0.00	92.25	0.00	0.00	0.00	0.00	10.28	0.00
6	70.68	70.70	0.00	0.00	0.00	2.16	0.00	0.00	0.00	1.42	0.00	0.00	0.00
E / cm^{-1}	0.00	0.06	179.80	184.23	184.23	197.92	234.54	234.54	299.19	301.92	312.90	312.90	319.83

Table S71. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[3]$^{3+}$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.69	70.70	0.00	0.00	0.00	1.83	0.00	0.00	0.00	1.27	0.00	0.00	0.00
-5	0.00	0.00	0.00	50.10	0.00	0.00	0.00	86.10	0.00	0.00	8.73	0.00	0.00
-4	0.00	0.00	28.17	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	64.86
-3	0.00	0.00	0.00	0.00	35.11	0.00	29.44	0.00	0.00	0.00	0.00	88.88	0.00
-2	1.83	1.27	0.00	0.00	0.00	70.69	0.00	0.00	0.00	70.70	0.00	0.00	0.00
-1	0.00	0.00	0.00	79.10	0.00	0.00	0.00	41.47	0.00	0.00	44.98	0.00	0.00
0	0.00	0.00	91.72	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	39.84
1	0.00	0.00	0.00	0.00	79.10	0.00	41.47	0.00	0.00	0.00	0.00	44.98	0.00
2	1.83	1.27	0.00	0.00	0.00	70.69	0.00	0.00	0.00	70.70	0.00	0.00	0.00
3	0.00	0.00	0.00	35.11	0.00	0.00	0.00	29.44	0.00	0.00	88.88	0.00	0.00
4	0.00	0.00	28.17	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	50.10	0.00	86.10	0.00	0.00	0.00	0.00	8.73	0.00
6	70.69	70.70	0.00	0.00	0.00	1.83	0.00	0.00	0.00	1.27	0.00	0.00	0.00
E / cm^{-1}	0.00	0.05	203.42	205.42	205.42	221.51	243.25	243.25	311.41	319.78	328.99	328.99	331.79

Table S72. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[4]^0** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.67	0.00	0.00	0.00	0.55
-5	0.00	0.00	99.68	0.00	0.00	0.00	6.34	0.00	0.00	0.00	0.00	4.80	0.00
-4	0.00	0.00	0.00	0.00	63.20	70.71	0.00	0.00	0.00	31.73	0.00	0.00	0.00
-3	0.00	0.00	0.00	1.57	0.00	0.00	0.00	74.91	0.00	0.00	66.22	0.00	0.00
-2	0.67	0.55	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
-1	0.00	0.00	7.79	0.00	0.00	0.00	65.94	0.00	0.00	0.00	0.00	74.78	0.00
0	0.00	0.00	0.00	0.00	44.87	0.00	0.00	0.00	0.00	89.37	0.00	0.00	0.00
1	0.00	0.00	0.00	7.79	0.00	0.00	0.00	65.94	0.00	0.00	74.78	0.00	0.00
2	0.66	0.55	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
3	0.00	0.00	1.57	0.00	0.00	0.00	74.91	0.00	0.00	0.00	0.00	66.22	0.00
4	0.00	0.00	0.00	0.00	63.19	70.71	0.00	0.00	0.00	31.73	0.00	0.00	0.00
5	0.00	0.00	0.00	99.68	0.00	0.00	0.00	6.34	0.00	0.00	4.80	0.00	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.55
E / cm^{-1}	0.00	0.00	328.02	328.02	467.92	491.69	515.07	515.07	518.80	586.00	607.26	607.26	619.93

Table S73. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[4]$^+$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.74	0.00	0.00	0.00	70.71
-5	0.00	0.00	0.00	99.54	0.00	0.00	0.00	8.36	0.00	0.00	0.00	4.78	0.00
-4	0.00	0.00	0.00	0.00	57.79	70.71	0.00	0.00	0.00	40.75	0.00	0.00	0.00
-3	0.00	0.00	2.00	0.00	0.00	0.00	66.52	0.00	0.00	0.00	74.64	0.00	0.00
-2	0.74	0.62	0.00	0.00	0.00	0.00	0.00	0.00	70.70	0.00	0.00	0.00	70.71
-1	0.00	0.00	0.00	9.42	0.00	0.00	0.00	74.20	0.00	0.00	0.00	66.37	0.00
0	0.00	0.00	0.00	0.00	57.63	0.00	0.00	0.00	0.00	81.73	0.00	0.00	0.00
1	0.00	0.00	9.42	0.00	0.00	0.00	74.20	0.00	0.00	0.00	66.37	0.00	0.00
2	0.74	0.62	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	69.95
3	0.00	0.00	0.00	2.00	0.00	0.00	0.00	66.52	0.00	0.00	0.00	74.64	0.00
4	0.00	0.00	0.00	0.00	57.79	70.71	0.00	0.00	0.00	40.75	0.00	0.00	0.00
5	0.00	0.00	99.54	0.00	0.00	0.00	8.36	0.00	0.00	0.00	4.78	0.00	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.74	0.00	0.00	0.00	0.62
E / cm^{-1}	0.00	0.01	308.80	308.80	423.42	453.28	454.73	454.73	456.46	513.33	536.40	536.40	546.06

Table S74. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[4]$^{2+}$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.76	0.00	0.00	0.00	0.00	0.63
-5	0.00	0.00	0.00	99.45	0.00	9.31	0.00	0.00	0.00	0.00	0.00	4.78	0.00
-4	0.00	0.00	0.00	0.00	55.17	0.00	0.00	0.00	70.71	44.23	0.00	0.00	0.00
-3	0.00	0.00	2.26	0.00	0.00	0.00	63.64	0.00	0.00	0.00	77.11	0.00	0.00
-2	0.76	0.63	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	0.00	70.71
-1	0.00	0.00	0.00	10.22	0.00	76.57	0.00	0.00	0.00	0.00	0.00	63.50	0.00
0	0.00	0.00	0.00	0.00	62.55	0.00	0.00	0.00	0.00	78.02	0.00	0.00	0.00
1	0.00	0.00	10.22	0.00	0.00	0.00	76.57	0.00	0.00	0.00	63.50	0.00	0.00
2	0.76	0.64	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	0.00	70.71
3	0.00	0.00	0.00	2.26	0.00	63.64	0.00	0.00	0.00	0.00	0.00	77.11	0.00
4	0.00	0.00	0.00	0.00	55.17	0.00	0.00	0.00	70.71	44.23	0.00	0.00	0.00
5	0.00	0.00	99.45	0.00	0.00	0.00	9.30	0.00	0.00	0.00	4.78	0.00	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.76	0.00	0.00	0.00	0.00	0.64
E / cm^{-1}	0.00	0.01	305.96	305.96	412.68	440.22	440.22	441.74	446.27	498.54	521.87	521.87	530.33

Table S75. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[4]$^{3+}$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.65
-5	0.00	0.00	0.00	99.35	0.00	0.00	10.42	0.00	0.00	0.00	4.57	0.00	0.00
-4	0.00	0.00	0.00	0.00	50.81	0.00	0.00	0.00	70.71	49.18	0.00	0.00	0.00
-3	0.00	0.00	2.45	0.00	0.00	58.84	0.00	0.00	0.00	0.00	0.00	80.81	0.00
-2	0.78	0.65	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	0.00	70.71
-1	0.00	0.00	0.00	11.12	0.00	0.00	80.18	0.00	0.00	0.00	58.72	0.00	0.00
0	0.00	0.00	0.00	0.00	69.54	0.00	0.00	0.00	0.00	71.86	0.00	0.00	0.00
1	0.00	0.00	11.12	0.00	0.00	80.18	0.00	0.00	0.00	0.00	0.00	58.72	0.00
2	0.78	0.65	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	0.00	70.71
3	0.00	0.00	0.00	2.45	0.00	0.00	58.85	0.00	0.00	0.00	80.82	0.00	0.00
4	0.00	0.00	0.00	0.00	50.81	0.00	0.00	0.00	70.71	49.18	0.00	0.00	0.00
5	0.00	0.00	99.35	0.00	0.00	10.42	0.00	0.00	0.00	0.00	0.00	4.57	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.78	0.00	0.00	0.00	0.00	0.65
E / cm^{-1}	0.00	0.01	298.75	298.75	394.08	416.81	416.81	418.84	431.70	471.87	494.54	494.54	500.56

Table S76. Weights of M_J components (in %) in the wavefunctions of the J = 6 ground state and crystal field splitting energy for **[4]**$^{4+}$ by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.70	0.00	0.00	0.00	0.00	0.00	0.82	0.00	0.00	0.00	0.00	0.68
-5	0.00	0.00	99.18	0.00	0.00	11.93	0.00	0.00	0.00	0.00	0.00	4.64	0.00
-4	0.00	0.00	0.00	0.00	47.41	0.00	0.00	0.00	70.71	52.46	0.00	0.00	0.00
-3	0.00	0.00	0.00	2.90	0.00	0.00	56.21	0.00	0.00	0.00	82.65	0.00	0.00
-2	0.82	0.68	0.00	0.00	0.00	0.00	0.00	70.70	0.00	0.00	0.00	0.00	70.71
-1	0.00	0.00	12.47	0.00	0.00	81.84	0.00	0.00	0.00	0.00	0.00	56.09	0.00
0	0.00	0.00	0.00	0.00	74.20	0.00	0.00	0.00	0.00	67.04	0.00	0.00	0.00
1	0.00	0.00	0.00	12.47	0.00	0.00	81.84	0.00	0.00	0.00	56.10	0.00	0.00
2	0.82	0.68	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	0.00	70.70
3	0.00	0.00	2.90	0.00	0.00	56.21	0.00	0.00	0.00	0.00	0.00	82.65	0.00
4	0.00	0.00	0.00	0.00	47.41	0.00	0.00	0.00	70.71	52.47	0.00	0.00	0.00
5	0.00	0.00	0.00	99.18	0.00	0.00	11.93	0.00	0.00	0.00	4.64	0.00	0.00
6	70.70	70.71	0.00	0.00	0.00	0.00	0.00	0.82	0.00	0.00	0.00	0.00	0.68
E / cm^{-1}	0.00	0.01	294.70	294.70	380.23	400.68	400.68	402.83	423.29	458.45	480.08	480.08	484.51

Table S77. Weights of M_J components (in %) in the wavefunctions of the J = 6 ground state and crystal field splitting energy for **[5]**^{0} by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.59	0.00	0.00	0.00	0.50
-5	0.00	0.00	99.78	0.00	0.00	0.00	0.00	4.99	0.00	0.00	0.00	4.47	0.00
-4	0.00	0.00	0.00	0.00	65.37	70.71	0.00	0.00	0.00	26.96	0.00	0.00	0.00
-3	0.00	0.00	0.00	1.19	0.00	0.00	78.78	0.00	0.00	0.00	61.58	0.00	0.00
-2	0.59	0.50	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
-1	0.00	0.00	6.59	0.00	0.00	0.00	0.00	61.39	0.00	0.00	0.00	78.66	0.00
0	0.00	0.00	0.00	0.00	38.12	0.00	0.00	0.00	0.00	92.45	0.00	0.00	0.00
1	0.00	0.00	0.00	6.59	0.00	0.00	61.39	0.00	0.00	0.00	78.66	0.00	0.00
2	0.59	0.50	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
3	0.00	0.00	1.19	0.00	0.00	0.00	0.00	78.78	0.00	0.00	0.00	61.58	0.00
4	0.00	0.00	0.00	0.00	65.37	70.71	0.00	0.00	0.00	26.96	0.00	0.00	0.00
5	0.00	0.00	0.00	99.78	0.00	0.00	4.99	0.00	0.00	0.00	4.47	0.00	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.59	0.00	0.00	0.00	0.50
E / cm^{-1}	0.00	0.00	342.56	342.56	499.41	518.43	557.17	557.17	563.60	630.29	649.17	649.17	662.22

Table S78. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[5]**$^{+}$ by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.70	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.52
-5	0.00	0.00	0.00	99.73	0.00	0.00	0.00	5.84	0.00	0.00	4.35	0.00	0.00
-4	0.00	0.00	0.00	0.00	63.04	70.71	0.00	0.00	0.00	32.04	0.00	0.00	0.00
-3	0.00	0.00	1.28	0.00	0.00	0.00	72.90	0.00	0.00	0.00	0.00	68.44	0.00
-2	0.61	0.52	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
-1	0.00	0.00	0.00	7.17	0.00	0.00	0.00	68.20	0.00	0.00	72.78	0.00	0.00
0	0.00	0.00	0.00	0.00	45.31	0.00	0.00	0.00	0.00	89.15	0.00	0.00	0.00
1	0.00	0.00	7.17	0.00	0.00	0.00	68.20	0.00	0.00	0.00	0.00	72.78	0.00
2	0.61	0.53	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
3	0.00	0.00	0.00	1.28	0.00	0.00	0.00	72.90	0.00	0.00	68.44	0.00	0.00
4	0.00	0.00	0.00	0.00	63.04	70.71	0.00	0.00	0.00	32.04	0.00	0.00	0.00
5	0.00	0.00	99.73	0.00	0.00	0.00	5.84	0.00	0.00	0.00	0.00	4.35	0.00
6	70.71	70.70	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.53
E / cm^{-1}	0.00	0.00	330.19	330.19	470.80	491.72	514.86	514.86	518.68	572.70	594.20	594.20	606.03

Table S79. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[5]**$^{2+}$ by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.53
-5	0.00	0.00	0.00	99.73	0.00	0.00	0.00	6.12	0.00	0.00	4.16	0.00	0.00
-4	0.00	0.00	0.00	0.00	61.60	70.72	0.00	0.00	0.00	34.72	0.00	0.00	0.00
-3	0.00	0.00	1.26	0.00	0.00	0.00	69.49	0.00	0.00	0.00	0.00	71.90	0.00
-2	0.61	0.53	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
-1	0.00	0.00	0.00	7.29	0.00	0.00	0.00	71.65	0.00	0.00	69.38	0.00	0.00
0	0.00	0.00	0.00	0.00	49.09	0.00	0.00	0.00	0.00	87.12	0.00	0.00	0.00
1	0.00	0.00	7.29	0.00	0.00	0.00	71.65	0.00	0.00	0.00	0.00	69.38	0.00
2	0.61	0.53	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
3	0.00	0.00	0.00	1.26	0.00	0.00	0.00	69.49	0.00	0.00	71.90	0.00	0.00
4	0.00	0.00	0.00	0.00	61.61	70.71	0.00	0.00	0.00	34.72	0.00	0.00	0.00
5	0.00	0.00	99.73	0.00	0.00	0.00	6.12	0.00	0.00	0.00	0.00	4.16	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.53
E / cm^{-1}	0.00	0.00	324.95	324.95	458.98	480.35	497.38	497.38	500.73	547.67	570.09	570.09	580.80

Table S80. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[5]$^{3+}$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.53
-5	0.00	0.00	99.72	0.00	0.00	0.00	0.00	6.33	0.00	0.00	3.98	0.00	0.00
-4	0.00	0.00	0.00	0.00	60.16	70.71	0.00	0.00	0.00	37.15	0.00	0.00	0.00
-3	0.00	0.00	0.00	1.24	0.00	0.00	66.43	0.00	0.00	0.00	0.00	74.73	0.00
-2	0.61	0.53	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
-1	0.00	0.00	7.37	0.00	0.00	0.00	0.00	74.48	0.00	0.00	66.33	0.00	0.00
0	0.00	0.00	0.00	0.00	52.54	0.00	0.00	0.00	0.00	85.08	0.00	0.00	0.00
1	0.00	0.00	0.00	7.37	0.00	0.00	74.47	0.00	0.00	0.00	0.00	66.32	0.00
2	0.61	0.53	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
3	0.00	0.00	1.24	0.00	0.00	0.00	0.00	66.43	0.00	0.00	74.73	0.00	0.00
4	0.00	0.00	0.00	0.00	60.17	70.71	0.00	0.00	0.00	37.15	0.00	0.00	0.00
5	0.00	0.00	0.00	99.72	0.00	0.00	6.34	0.00	0.00	0.00	0.00	3.97	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.61	0.00	0.00	0.00	0.53
E / cm^{-1}	0.00	0.00	322.56	322.56	452.11	474.13	486.49	486.49	489.76	531.84	555.03	555.03	564.72

Table S81. Weights of M_J components (in %) in the wavefunctions of the $J = 6$ ground state and crystal field splitting energy for **[5]$^{4+}$** by using point charge calculations.

m_J	w.f. 1	w.f. 2	w.f. 3	w.f. 4	w.f. 5	w.f. 6	w.f. 7	w.f. 8	w.f. 9	w.f. 10	w.f. 11	w.f. 12	w.f. 13
-6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.00	0.54
-5	0.00	0.00	99.69	0.00	0.00	0.00	6.81	0.00	0.00	0.00	3.96	0.00	0.00
-4	0.00	0.00	0.00	0.00	58.48	70.71	0.00	0.00	0.00	39.75	0.00	0.00	0.00
-3	0.00	0.00	0.00	1.34	0.00	0.00	0.00	64.22	0.00	0.00	0.00	76.64	0.00
-2	0.62	0.54	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
-1	0.00	0.00	7.76	0.00	0.00	0.00	76.35	0.00	0.00	0.00	64.11	0.00	0.00
0	0.00	0.00	0.00	0.00	56.22	0.00	0.00	0.00	0.00	82.70	0.00	0.00	0.00
1	0.00	0.00	0.00	7.76	0.00	0.00	0.00	76.35	0.00	0.00	0.00	64.11	0.00
2	0.62	0.54	0.00	0.00	0.00	0.00	0.00	0.00	70.71	0.00	0.00	0.00	70.71
3	0.00	0.00	1.34	0.00	0.00	0.00	64.22	0.00	0.00	0.00	76.64	0.00	0.00
4	0.00	0.00	0.00	0.00	58.48	70.71	0.00	0.00	0.00	39.75	0.00	0.00	0.00
5	0.00	0.00	0.00	99.69	0.00	0.00	0.00	6.81	0.00	0.00	0.00	3.96	0.00
6	70.71	70.71	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.00	0.00	0.00	0.54
E / cm^{-1}	0.00	0.00	321.57	321.57	446.44	470.65	477.88	477.88	480.99	523.02	546.89	546.89	555.84

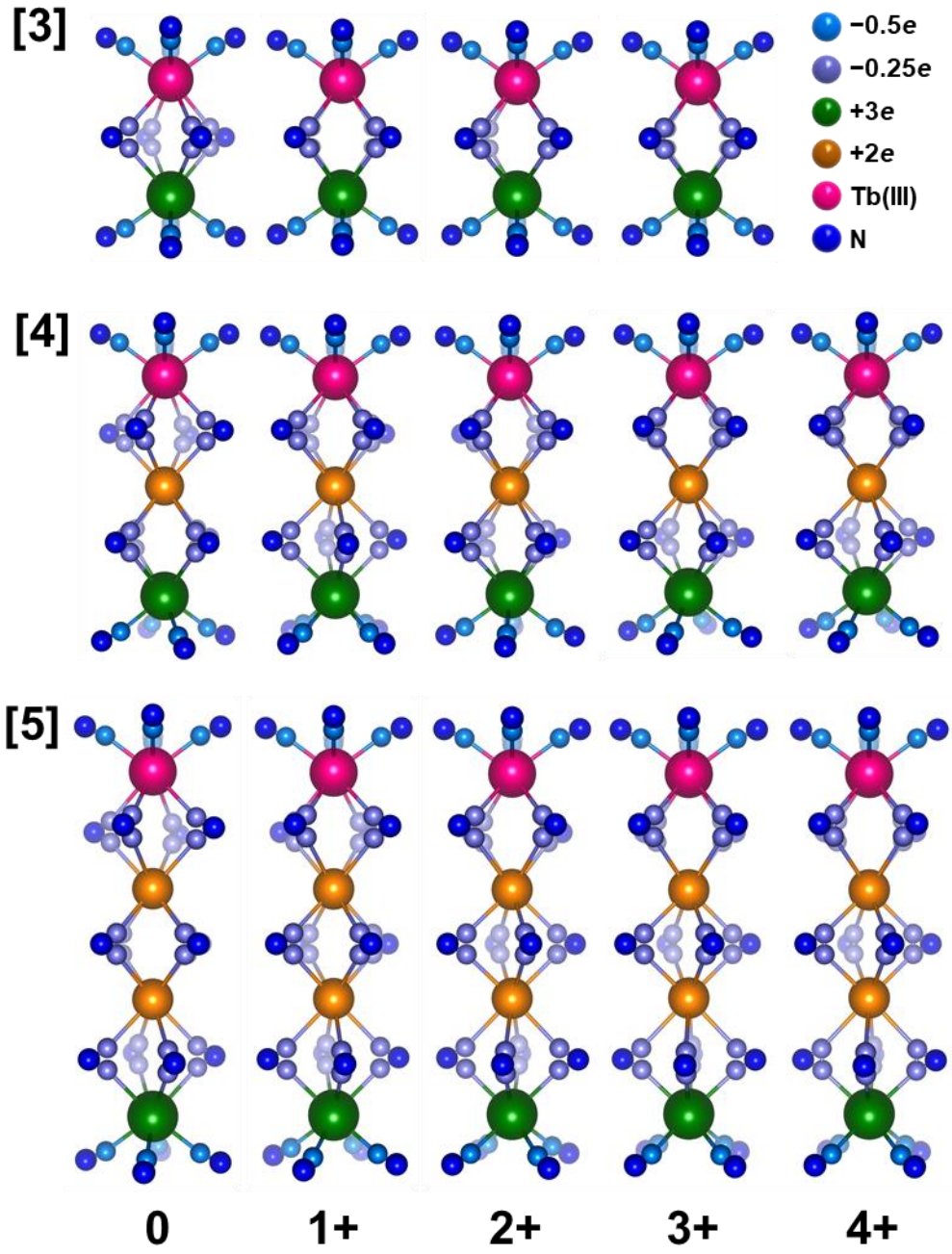

Fig. S308. Structural models for point charge calculations for (a) **[3]^0**, (b) **[4]^0** and (c) **[5]^0**. The coordinates of N atoms (deep blue) were averaged from DFT optimized structures. By applying the displacement parameter to the N atoms, negative charges of N atoms approach the metal ions. For Tb(III) ions and Cd(II) ions, +3*e* and +2*e* charges are assigned. Because of the −2*e* charge of the obPc ligand (which has four coordinating N atoms), a −0.5*e* charge is assigned to each of the N atoms of outer obPc ligands. For inner obPc, −0.25*e* charge is assigned to the ligand to metal bonds.

7. Additional XRD Data

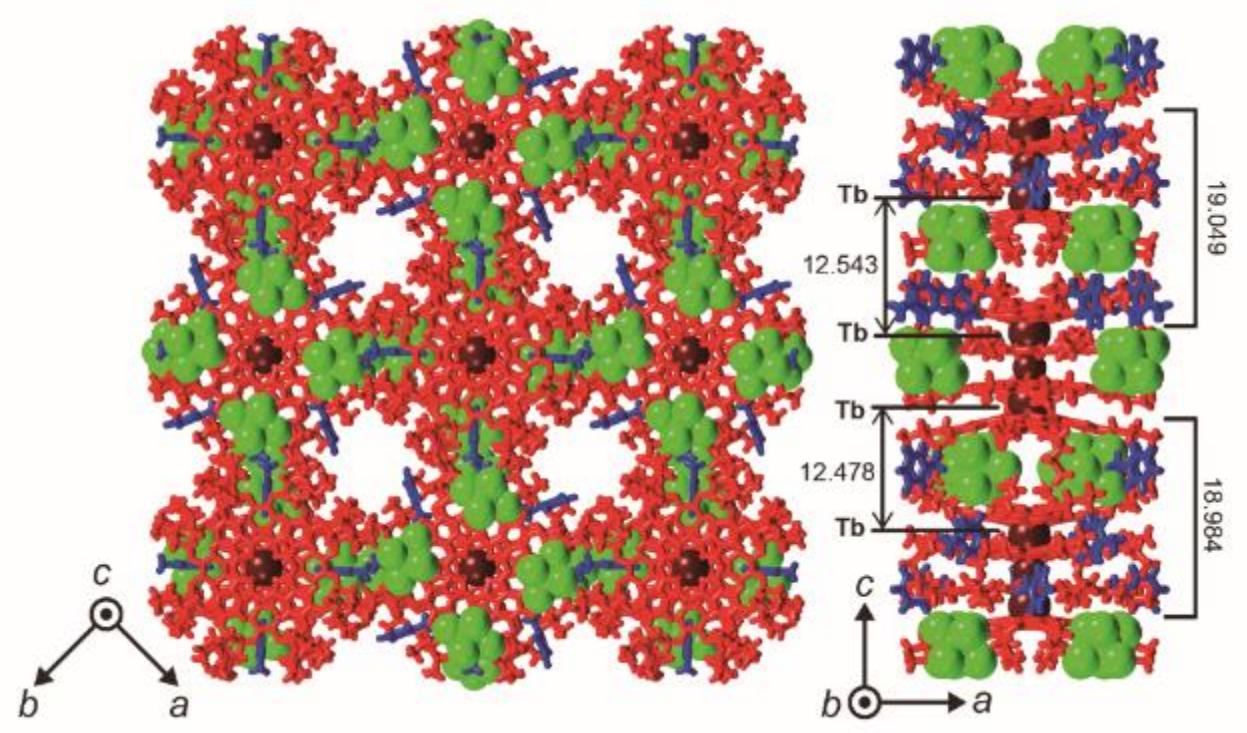

Fig. S309. Packing structures of **[4]**$^{4+}$ crystalized using toluene. Multiple-decker complexes, metal ions, $SbCl_6^-$ and toluene are shown in red, brown, green and blue respectively. Two crystallographically inequivalent **[4]**$^{4+}$ units were observed in this packing structure.

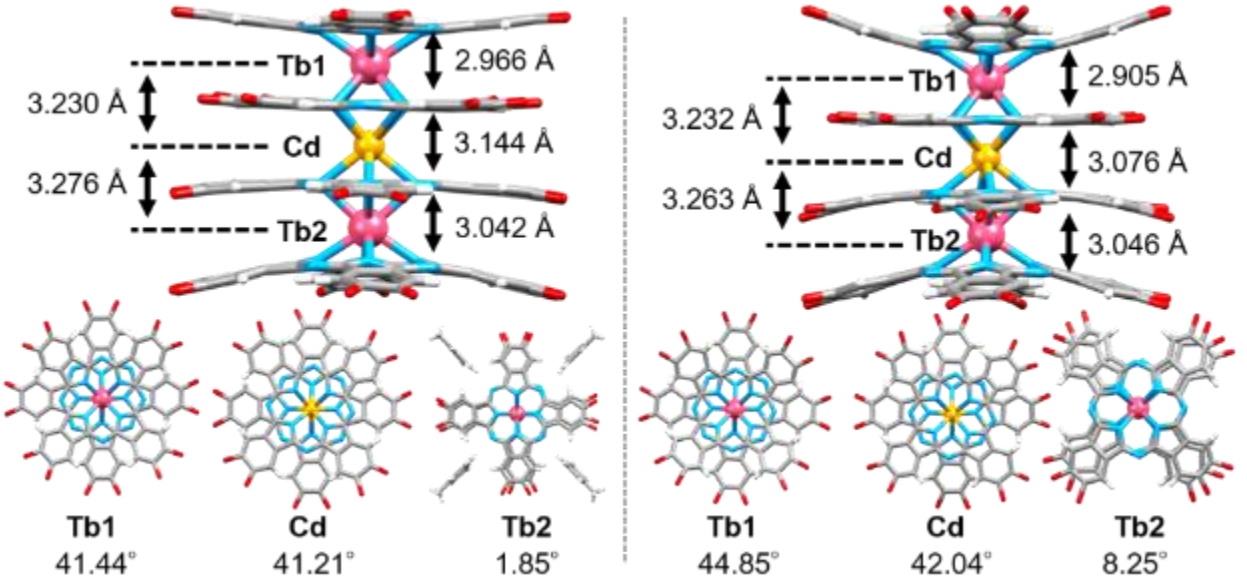

Fig. S310. Molecular structures of two crystallographically inequivalent **[4]**$^{4+}$ units crystalized using toluene. *n*-Butyl chains were omitted for clarity.

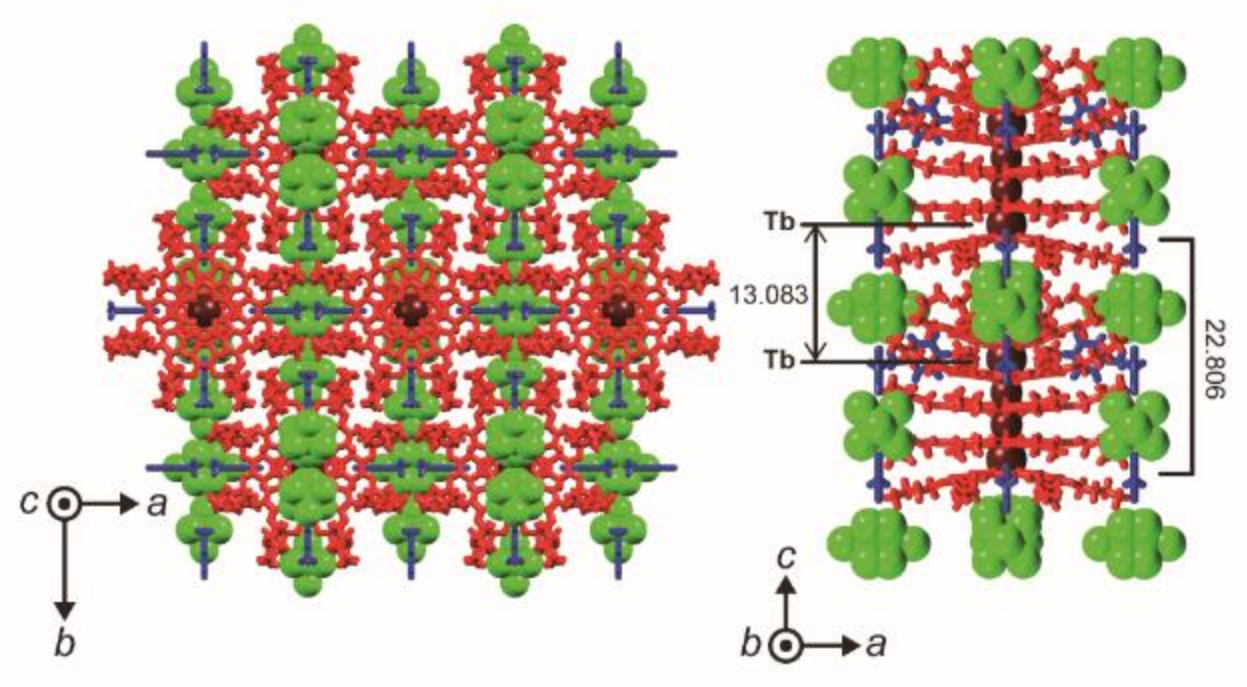

Fig. S311. Packing structures of **[5]**$^{4+}$ crystalized by slow diffusion using CH_2Cl_2 and toluene. Multiple-decker complexes, metal ions, $SbCl_6^-$ and toluene are shown in red, brown, green and blue respectively.

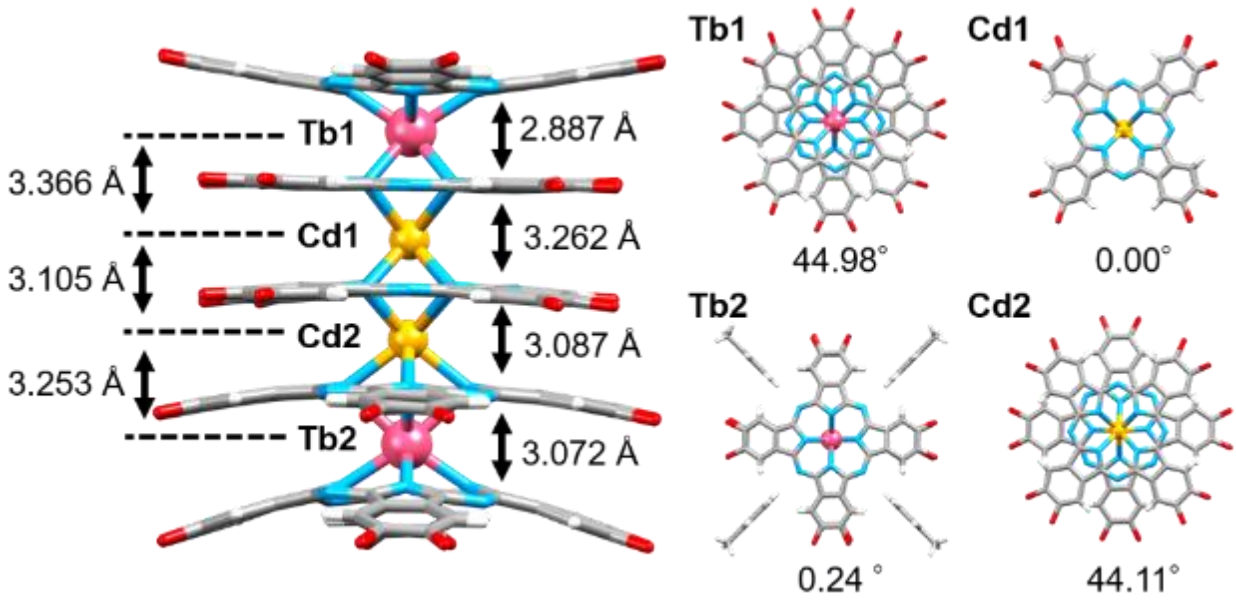

Fig. S312. Molecular structures of **[5]**$^{4+}$ units crystalized using CH_2Cl_2 and toluene. *n*-Butyl chains were omitted for clarity.

Table S82. Crystallographic data for multiple-decker complexes.

Name	**[3]$^{2+}$**	**[4]$^{2+}$**	**[4]$^{4+}$**	**[5]$^{4+}$**
T / K	100	100	100	120
Formula	$C_{130}H_{161}N_{13}O_{12}Cl_6SbTb$	$C_{86}H_{112}Cd_{0.25}Cl_3N_8O_8Sb_{0.5}Tb_{0.5}$	$C_{37.5}H_{48}Cd_{0.125}Cl_3N_4O_4Sb_{0.5}Tb_{0.25}$	$C_{190}H_{230}CdCl_{12}N_{20}O_{20}Sb_2Tb$
Z	4	16	16	4
Space group	$P2_1/c$	$P4/ncc$	$P4/nmm$	$Pnn2$
a / Å	13.49390(10)	34.38390(10)	30.45110(10)	24.0068(3)
b / Å	24.1820(2)	34.38390(10)	30.45110(10)	37.6897(3)
c / Å	40.3615(3)	32.9591(3)	19.4099(2)	22.7051(3)
α / Å	90	90	90	90
β / Å	92.8710(10)	90	90	90
γ / Å	90	90	90	90
V / Å	13153.81(18)	38966.0(4)	17998.2(2)	20543.8(4)
R_1	0.0492	0.0798	0.1116	0.1292
wR_2	0.1040	0.1498	0.1787	0.2257
GOF	1.021	1.031	1.017	1.035

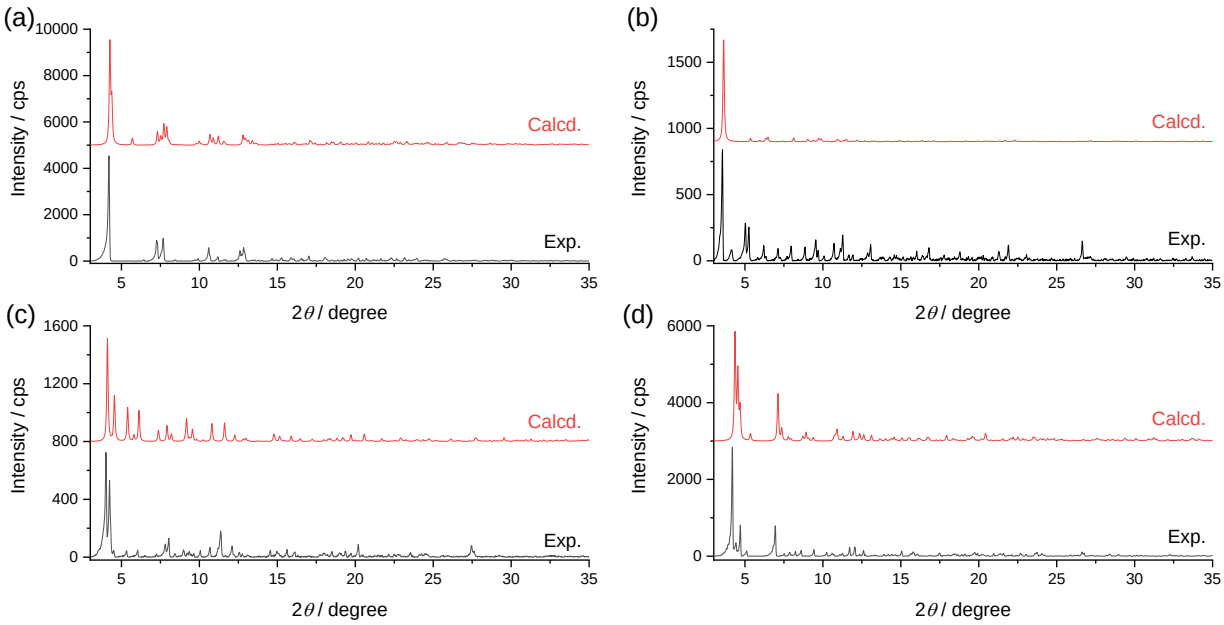

Fig. S313. Powder X-ray diffraction pattern for (a) **[3]**$^{2+}$, (b) **[4]**$^{2+}$, (c) **[4]**$^{4+}$ and (d) **[5]**$^{4+}$ at room temperature. Calculated patterns were obtained from cif files.

8. ESR Spectra

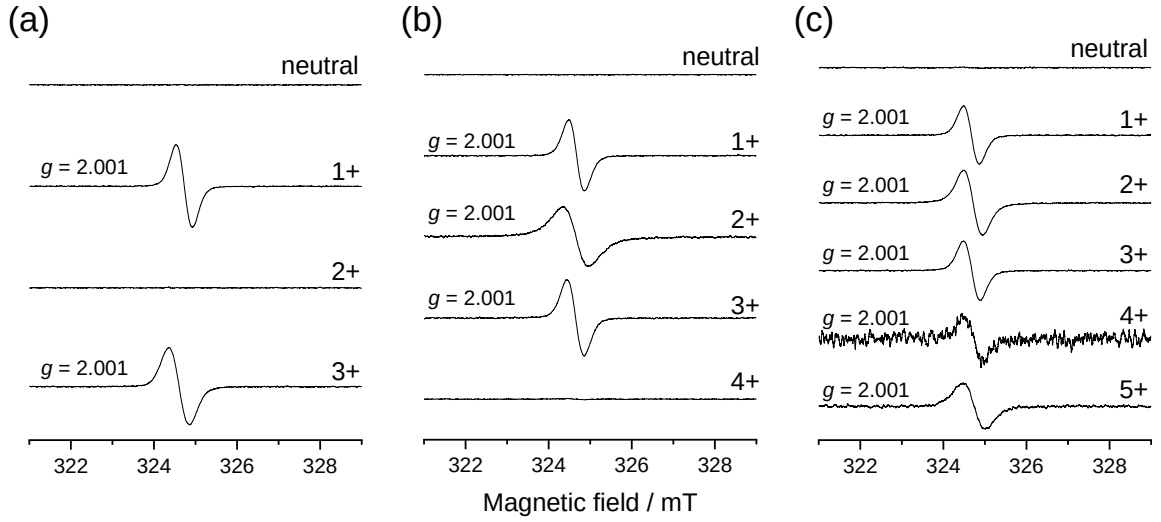

Fig. S314. ESR spectra of electrochemically synthesized Y(III) analogues of (a) **[3]**, (b) **[4]** and (c) **[5]** series, at room temperature and in CH_2Cl_2 containing 0.1 mM of TBA·PF_6.

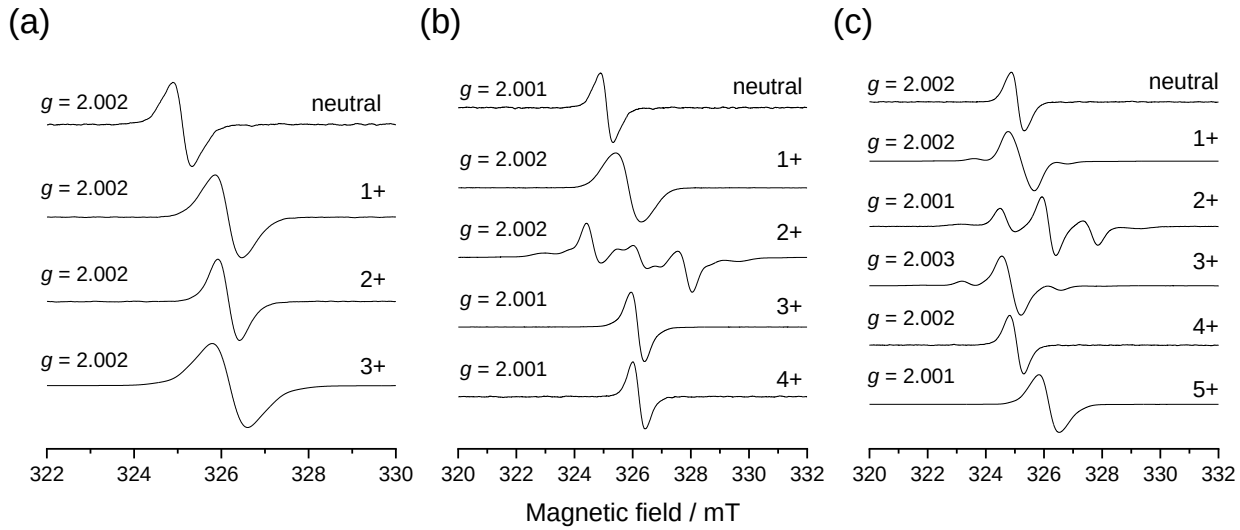

Fig. S315. ESR spectra of electrochemically synthesized Y(III) analogues of (a) **[3]**, (b) **[4]** and (c) **[5]** series at 80 K in CH_2Cl_2 containing 0.1 mM of TBA·PF_6. The signals in non-radical species stem from the impurities (contamination by radical species), detectable at low temperature. *g*-values were determined by using an Mn marker as a reference. $\mathbf{[4]}^{2+}$ and $\mathbf{[5]}^{2+}$ show multiple signals because of the zero-field splitting. Multiple signals in $\mathbf{[5]}^{+}$ and $\mathbf{[5]}^{3+}$ indicate the contamination by $\mathbf{[5]}^{2+}$.

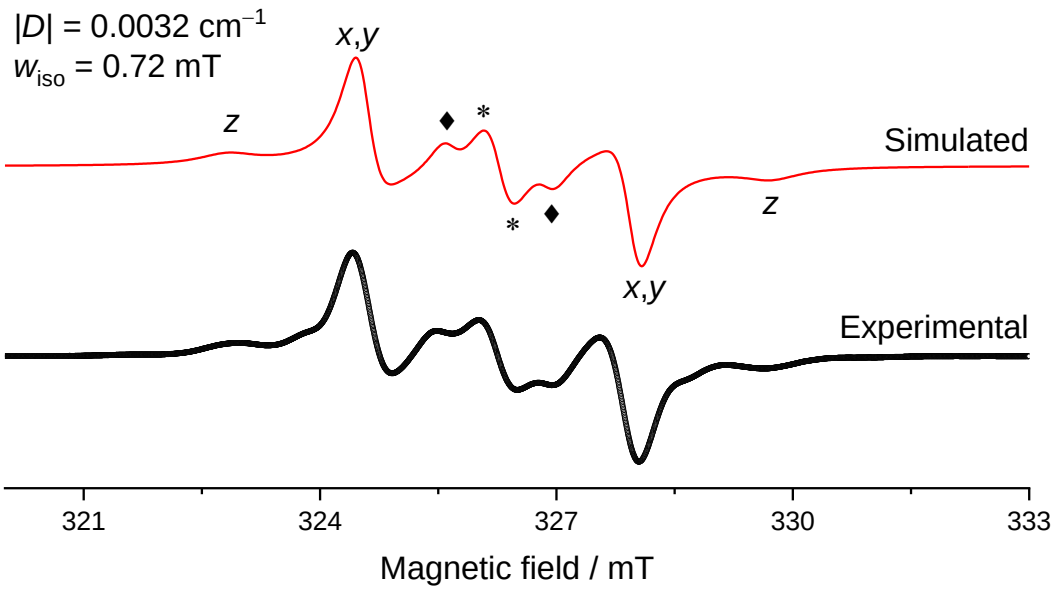

Fig. S316. Simulated and experimental ESR spectra for the Y(III) analogue of **[4]**$^{2+}$ at 80 K. From the simulations, a sign of the zero-field splitting parameter D could not be detmined. Isotropic linewidth for a Lorentzian function w_{iso} = 0.72 mT was applied for all the signals. The overall shape of signals was simulated by considering a monoradical species (*) and a triplet radical species with $|D|$ = 0.0012 cm^{-1} (♦).

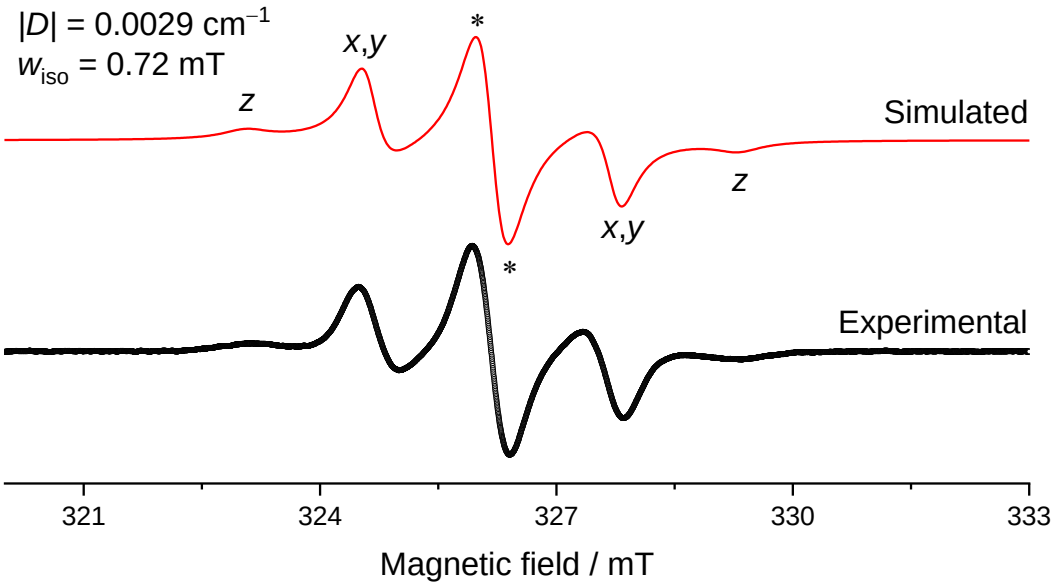

Fig. S317. Simulated and experimental ESR spectra for Y(III) analogue of **[5]**$^{2+}$ at 80 K. From the simulations, a sign of the zero-field splitting parameter D could not be detmined. Isotropic linewidth for a Lorentzian function w_{iso} = 0.72 mT was applied for all the signals. The overall shape of signals was simulated by considering the monoradical species (*).

9. UV-Vis-NIR Spectra

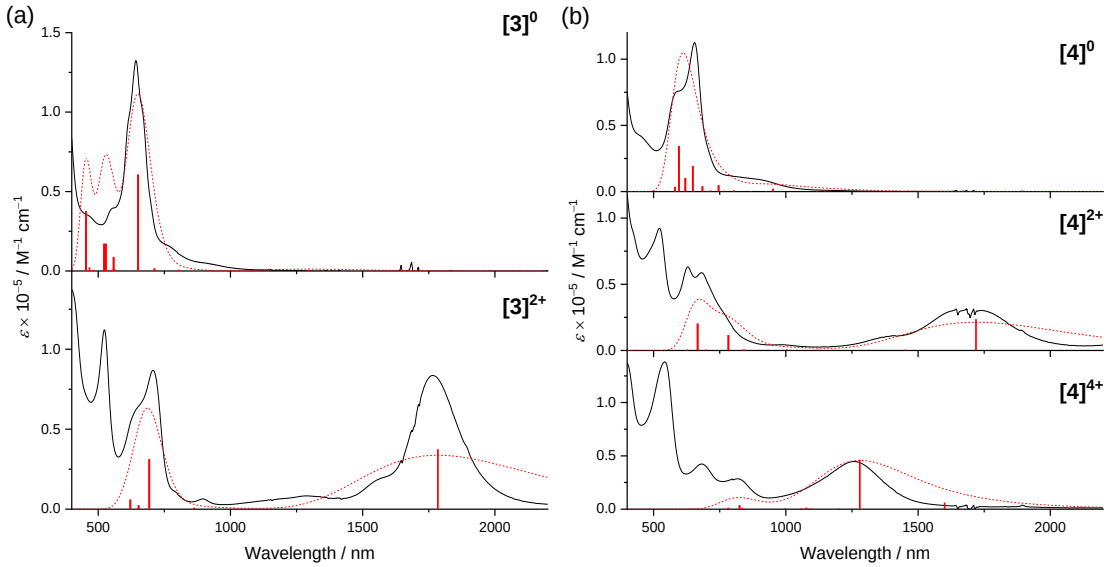

Fig. S318. Experimental UV-Vis-NIR spectra (black solid curves), oscillator strength (red rods) and theoretical spectra (red dotted curves) of (a) **[3]** and (b) **[4]** series in CH_2Cl_2. Polarizable continuum model was used to include the solvent effect. Half-width at half height of the theoretical spectra is 0.15 eV. B3LYP/Def2-SVP were used for $[\mathbf{3}]^{0}$, $[\mathbf{3}]^{2+}$, $[\mathbf{4}]^{0}$, $[\mathbf{4}]^{2+}$ and $[\mathbf{4}]^{4+}$.

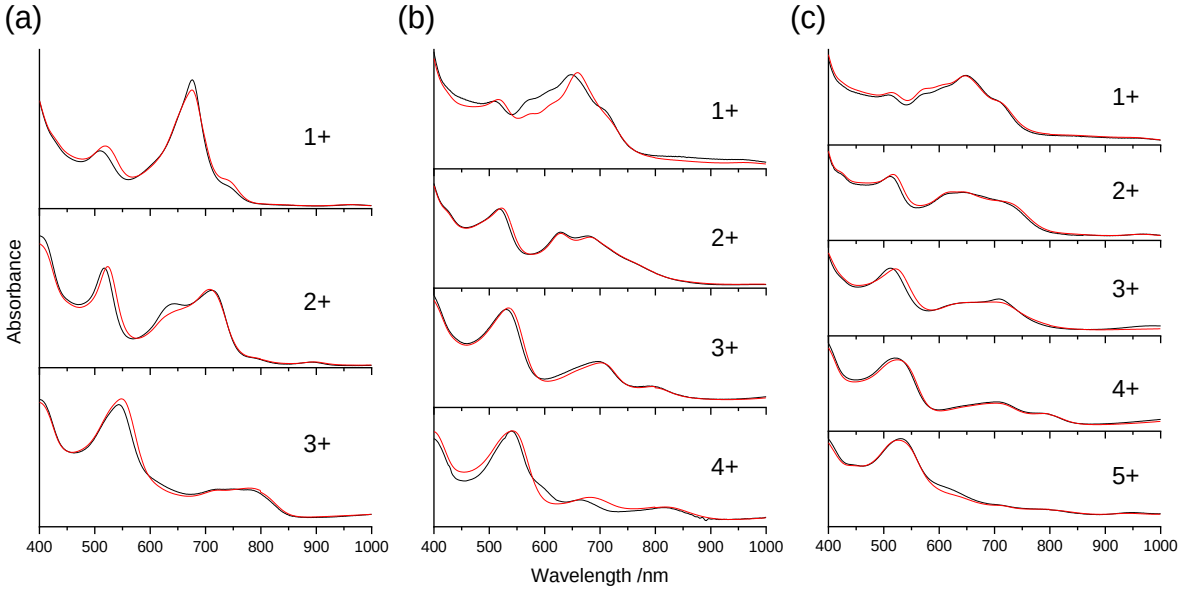

Fig. S319. Comparison of absorption spectra between oxidized Y(III) (black curves) and Tb(III) (red curves) complexes for (a) **[3]**, (b) **[4]** and (c) **[5]** series prepared by electrochemical oxidations in CH_2Cl_2.

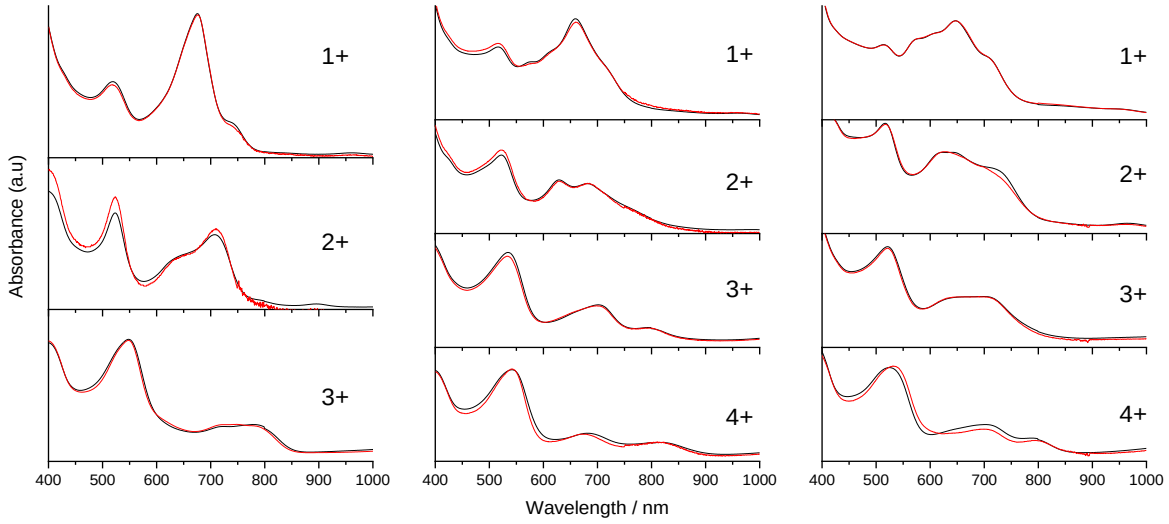

Fig. S320. Comparison of absorption spectra between the electrochemically (black curves) and chemically (red curves) oxidized (a) **[3]**, (b) **[4]** and (c) **[5]** series in CH_2Cl_2.

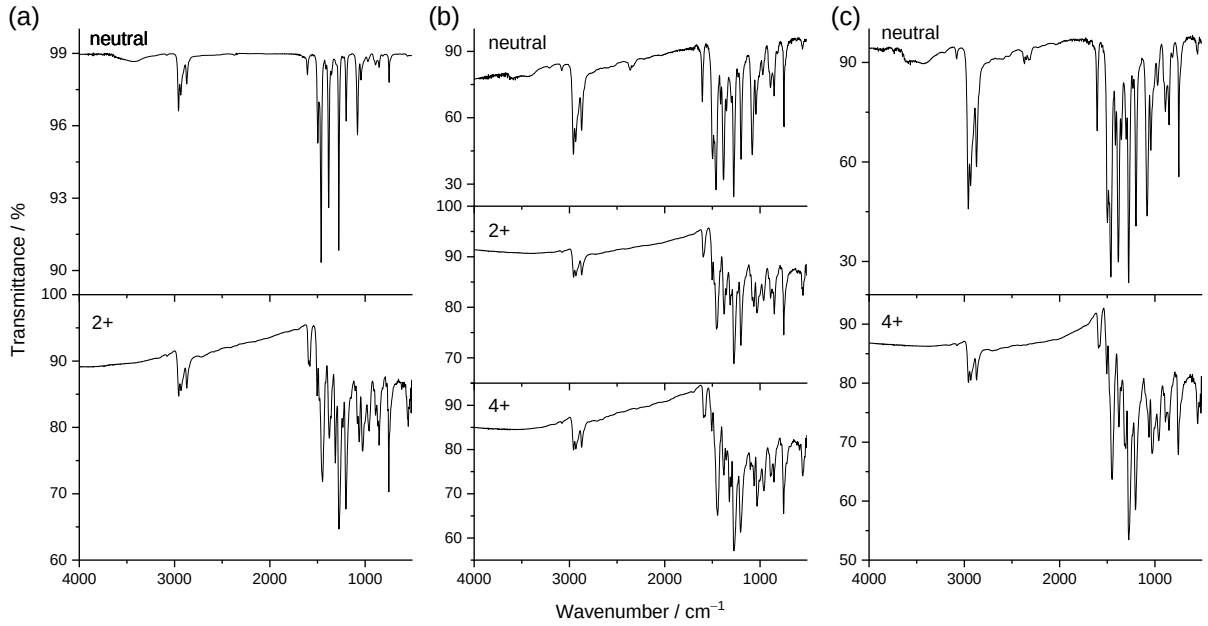

Fig. S321. IR spectra for (a) **[3]**, (b) **[4]** and (c) **[5]** series at room temperature.

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