CHEMISTRY
A European Journal

Supporting Information

Ab Initio Crystal Field for Lanthanides

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chem_201605102_sm_miscellaneous_information.pdf

Electronic Supplementary Information

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Molecular structure of the $[Tb(Pc)_2]^-$ anion was taken from the *J. Am. Chem. Soc.* 2009, *131*, 4387–4396 (DOI: 10.1021/ja808649g). Cartesian coordinates for the real and symmetrized anions are given in Table S5 and Table S6, respectively. Employed basis sets in *ab initio* calculations:

$[Tb(Pc)_2]^-$
Tb.ANO-RCC...8s7p5d4f2g1h.
N.ANO-RCC...3s2p1d. (close)
N.ANO-DK3.Tsuchiya.12s8p.2s1p. (distant)
C.ANO-DK3.Tsuchiya.12s8p.2s1p.
H.ANO-DK3.Tsuchiya.6s.1s.

Ab initio calculations performed were of CASSCF/RASSI/SINGLE_ANISO kind. Active space of the CASSCF method included the $4f^8$ configuration of Tb site only, CAS(8in7). 7 spin septet, 106 spin quintet, 283 spin triplet and 121 spin singlet states were mixed by spin-orbit coupling within RASSI, resulting in 1517 spin-orbit states.

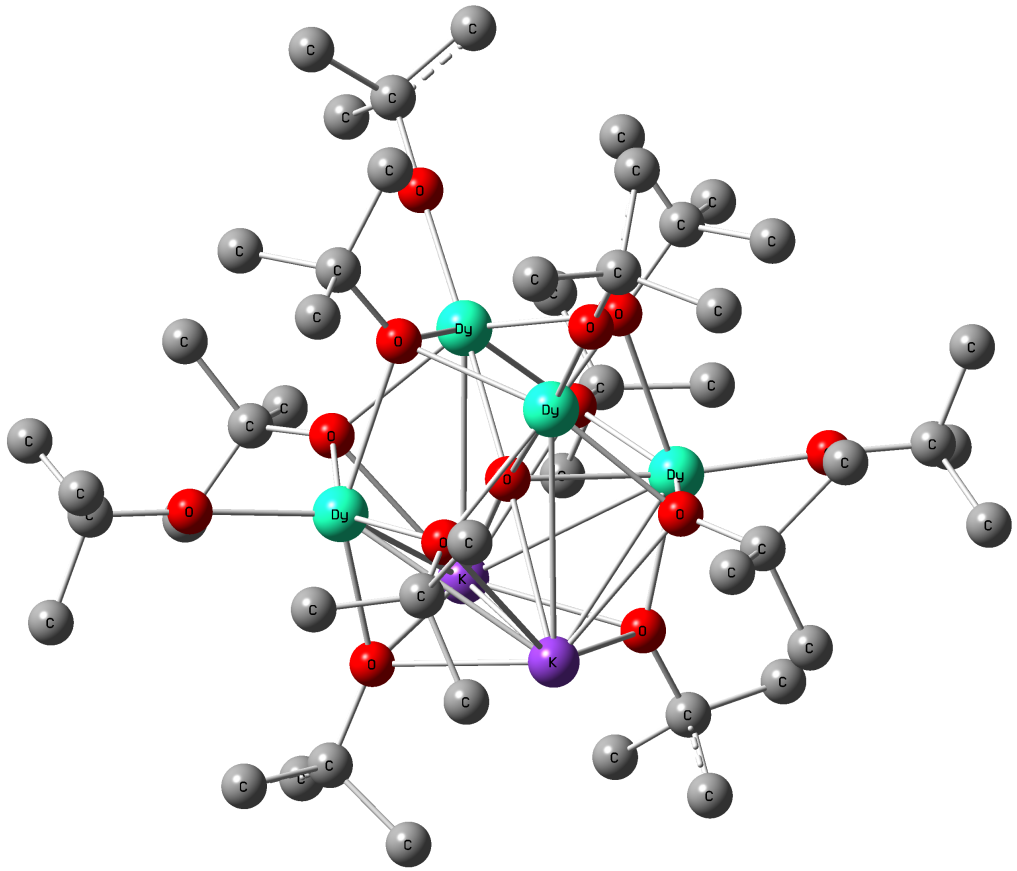

Figure S1. Structure of the investigated Dy_4K_2. Exact atomic coordinates of the individual Dy fragments are given in Tables S7-S10.

Table S1. Energy spectrum and composition of the wave functions of the $[Tb(Pc)_2]^-$ anion predicted by all computational models discussed in the paper. Quantization axis was chosen the (pseudo) C4 symmetry axis of the compound, perpendicular to the planes of the Pc ligands.

Ab initio, experimental geometry		Ab initio, D_{4d}-symm. geometry		Electrostatic (Mulliken point charges)		Fitting of Ishikawa [12]		Fitting of Reu [28]	
E (cm^{-1})	w.f.	E (cm^{-1})	w.f.	E (cm^{-1})	w.f.	E (cm^{-1})	w.f.	E (cm^{-1})	w.f.
0.000		0.000		0.0	*mixed*	0		0	
0.004	$\|\pm6\rangle$	0.000	$\|\pm6\rangle$	0.0		0	$\|\pm6\rangle$	0	$\|\pm6\rangle$
308.291		304.992		100.5		436		282	$\|0\rangle$
308.506	$\|\pm5\rangle$	304.992	$\|\pm5\rangle$	100.7		436	$\|\pm5\rangle$	344	
484.716		484.431		176.7		494	$\|0\rangle$	344	
491.493		484.431	$\|\pm4\rangle$	179.4		509		446	
512.300		560.055		222.7		509	$\|\pm1\rangle$	706	
545.831		560.055	$\|\pm3\rangle$	242.0		548		860	*not*
572.115	*mixed*	583.250		255.1		548	$\|\pm2\rangle$	860	
663.475		583.250	$\|\pm2\rangle$	304.0		581		882	*reported*
666.951		588.638		305.1		581	$\|\pm4\rangle$	882	
808.916		588.638	$\|\pm1\rangle$	379.2		589		1019	
809.479		589.465	$\|0\rangle$	379.2		589	$\|\pm3\rangle$	1037	

Table S2. Weights of M_J components in the wavefunctions of the ground J=6 of $[Tb(Pc)_2]^-$ anion (*ab initio*, experimental geometry).

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	50.0	50.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-5	0.0	0.0	49.5	49.6	0.0	0.0	0.1	0.0	0.5	0.0	0.3	0.0	0.0
-4	0.0	0.0	0.0	0.0	32.7	42.2	0.9	17.1	0.1	5.9	0.2	0.0	0.8
-3	0.0	0.0	0.5	0.4	0.4	0.5	14.8	0.0	41.5	1.7	32.5	7.5	0.2
-2	0.0	0.0	0.0	0.0	11.4	6.4	0.5	13.5	0.3	41.0	2.7	0.3	23.9
-1	0.0	0.0	0.0	0.0	0.5	0.3	33.2	0.7	7.5	1.4	14.2	42.0	0.3
0	0.0	0.0	0.0	0.0	10.0	1.2	0.9	37.4	0.3	0.0	0.3	0.3	49.5
1	0.0	0.0	0.0	0.0	0.5	0.3	33.2	0.7	7.5	1.4	14.2	42.0	0.3
2	0.0	0.0	0.0	0.0	11.4	6.4	0.5	13.5	0.3	41.0	2.7	0.3	23.9
3	0.0	0.0	0.5	0.4	0.4	0.5	14.8	0.0	41.5	1.7	32.5	7.5	0.2
4	0.0	0.0	0.0	0.0	32.7	42.2	0.9	17.1	0.1	5.9	0.2	0.0	0.8
5	0.0	0.0	49.5	49.6	0.0	0.0	0.1	0.0	0.5	0.0	0.3	0.0	0.0
6	50.0	50.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S3. Splitting of the J=6 produced by rank-specific (k-only) parameters for $[Tb(Pc)_2]^-$ anion (experimental geometry).

m_J	k=2	k=4	k=6	k=8	k=10	k=12
w.f. 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
w.f. 2	0.00183	0.15170	1.02129	0.41860	0.06161	0.05147
w.f. 3	196.93019	7.58773	1.50773	0.63198	0.15611	0.06149
w.f. 4	197.06756	10.42196	5.42905	0.85229	0.46144	0.07255
w.f. 5	353.63238	46.56382	6.15801	1.98023	0.48011	0.08045
w.f. 6	357.02547	60.75342	7.30264	2.71945	0.49475	0.08216
w.f. 7	458.93165	81.80692	10.42406	3.15271	0.51783	0.08275
w.f. 8	487.25422	98.37045	11.63305	3.25256	0.53779	0.08444
w.f. 9	527.33146	100.88083	13.19747	3.64401	0.54357	0.08720
w.f. 10	610.96279	141.94305	14.21675	3.85225	0.58444	0.09234
w.f. 11	616.90328	142.06945	18.41717	5.96032	0.88203	0.10754
w.f. 12	753.92189	151.47063	21.92269	6.48309	0.95363	0.11389
w.f. 13	754.14679	151.81670	25.16108	6.87865	1.04508	0.16643

Cumulative effect of various ranks:

m_J	k=2	k=2,4	k=2,4,6	k=2,4,6,8	k=2,4,6,8,10	k=2,4,6,8,10,12
w.f. 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

w.f. 2	0.00183	0.00018	0.01364	0.00784	0.00698	0.00480
w.f. 3	196.93019	319.32357	310.75398	308.25954	308.29236	308.29180
w.f. 4	197.06756	319.33777	311.02201	308.44146	308.50628	308.50600
w.f. 5	353.63238	479.47367	483.32774	484.74636	484.71239	484.71650
w.f. 6	357.02547	489.66592	489.42668	491.56332	491.50027	491.49310
w.f. 7	458.93165	513.84730	512.42721	512.27838	512.30174	512.30050
w.f. 8	487.25422	555.00932	544.92483	545.99939	545.85211	545.83140
w.f. 9	527.33146	574.61885	573.36591	571.94291	572.09253	572.11560
w.f. 10	610.96279	666.86956	665.98864	663.88023	663.49683	663.47510
w.f. 11	616.90328	667.77638	667.41827	666.51437	666.93649	666.95140
w.f. 12	753.92189	811.19185	809.18597	808.92908	808.85048	808.91650
w.f. 13	754.14679	811.41564	809.83660	809.45593	809.54722	809.47960

Electrostatic approach:

Structure of the Dy_4K_2 compound is taken from ref. [50]. Structure of the $[Tb(Pc)_2]^-$ is taken from *J. Am. Chem. Soc.* 2009, *131*, 4387–4396 (DOI: 10.1021/ja808649g). In this work we analyze the electrostatic effect of the ligands on the energy splitting of the ground *J* multiplet of the Ln(III) site in these compounds.

All atoms (except the Ln^{3+}) were replaced by point charges, placed at their original crystallographic position. The values of the point charges were the *ab initio* calculated Mulliken charges for the corresponding atoms in the previous CASSCF calculation (assuming the same computational details: basis sets, methods, thresholds, etc.). Ln^{3+} surrounded by these point charges (included as XFIELD in Seward) was calculated by the same computational methodology (CASSCF/RASSI/SINGLE_ANISO). Active space of the CASSCF method included the $4f^n$ shell of the Ln(III) site. State-Average CASSCF calculations on all available roots of all spin states were performed.

For Tb(III), 7 spin septet, 106 spin quintet, 283 spin triplet and 121 spin singlet states were mixed by spin-orbit coupling within RASSI, resulting in 1517 spin-orbit states. For Dy(III), 21 spin sextet, 128 spin quartet and 130 spin doublet states were mixed by spin-orbit coupling within RASSI, resulting in 898 spin-orbit states.

The *ab initio* obtained eigenstates of the ground *J* multiplet (J=6 for Tb^{3+} and J=15/2 for Dy^{3+}) were further employed for the computation of the parameters of the crystal field. All spin-orbit states were employed for the computation of the *ab initio* calculated magnetic susceptibility χT.

Employed basis sets in *ab initio* calculations of $[Tb(Pc)_2]^-$ and Dy_4K_2 compounds.

$[Tb(Pc)_2]^-$	Dy_4K_2
Tb.ANO-RCC...8s7p5d4f2g1h. N.ANO-RCC...3s2p1d. (close) N.ANO-DK3.Tsuchiya.12s8p.2s1p. (distant) C.ANO-DK3.Tsuchiya.12s8p.2s1p. H.ANO-DK3.Tsuchiya.6s.1s.	Dy.ANO-RCC...8s7p5d4f2g1h. Lu.ANO-RCC...7s6p4d3f1g. (replacing all other Dy) K.ANO-RCC...5s4p1d. O.ANO-RCC...4s3p2d. (close) O.ANO-DK3.Tsuchiya.12s8p.2s1p. (distant) C.ANO-RCC...3s2p1d. (close) C.ANO-DK3.Tsuchiya.12s8p.2s1p. (distant) H.ANO-DK3.Tsuchiya.6s.1s.

The quantization axis for the parameters of the crystal field was chosen the same as in the original *ab initio* calculation, for consistency.

Table S4 shows a comparison of energy spectra (in cm^{-1}) obtained *ab initio* and within the electrostatic approach for Dy_4K_2 compound.[50]

Dy1		Dy2		Dy3		Dy4	
Ab initio	Electrostatic	Ab initio	Electrostatic	Ab initio	Electrostatic	Ab initio	Electrostatic
0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
384	107	405	113	358	72	344	5
384	107	405	113	358	72	344	5
664	139	723	166	556	114	524	60
664	139	723	166	556	114	524	60
738	169	831	185	623	174	590	80
738	169	831	185	623	174	590	80
812	183	901	200	721	212	665	103
812	183	901	200	721	212	665	103
881	215	961	232	766	229	729	128
881	215	961	232	766	229	729	128
942	254	018	279	843	258	791	164
942	254	018	279	843	258	791	164
1043	318	1113	360	920	304	829	179
1043	318	1113	360	920	304	829	179

Tables S5 gives the atomic coordinates and corresponding Mulliken charge for each atom of the real geometry of the computed $[Tb(Pc)_2]^-$ anion.
Table S6 gives the atomic coordinates of the symmetrized structure.
Table S7-S10 give the coordinates and calculated Mulliken charges of all atoms in Dy_4K_2 molecule.

Table S5. Cartesian coordinates (in Å) and Mulliken charges of the real structure of the computed $[Tb(Pc)_2]^-$ anion.

Atom	Cartesian coordinates			Charge
	x	y	z	
Tb1	12.51390200	0.97301300	5.96085700	----
N2	14.57294900	2.16574800	6.87227200	-0.0038
N3	13.14251600	2.43151500	4.24333200	-0.1265
N4	10.71666100	2.56736000	5.23813300	-0.0332
N5	12.14944100	2.32935400	7.85473000	-0.1194
N6	13.52397000	-0.61926100	7.65478300	0.0185
N7	14.04571100	-0.50784600	5.06287000	-0.1575
N8	11.26025400	-0.27502100	4.09275400	0.0548
N9	10.74398100	-0.36274700	6.69947800	-0.1551
N10	15.59595000	2.47852400	4.89007600	-0.3813
N11	10.93969000	2.88235800	2.90294300	-0.3136
N12	9.72762700	2.78574900	7.24501400	-0.3730
N13	14.37237200	2.23422500	9.23461600	0.2927
N14	15.76895000	-0.89502300	7.03766100	-0.2952
N15	13.01644500	-0.54634100	2.72768000	-0.3329
N16	9.02303500	-0.41049600	4.72715600	-0.2915
N17	11.77970800	-0.69551200	9.02973100	-0.3323
C18	16.55493300	2.26531800	8.44469900	0.0065
C19	17.55457600	2.26902000	9.57033000	-0.2639
C20	18.88699800	2.41337800	9.43209500	-0.3191
C21	19.23413500	2.50221400	8.14354400	-0.2699
C22	18.25520300	2.47260200	7.01791300	-0.2683
C23	16.90897400	2.36525900	7.15614800	-0.0613
C24	15.07751400	2.18758700	8.21266100	0.0492
C25	15.65601100	2.31713900	6.20824900	0.0111
C26	14.41732400	2.95749800	2.62153500	-0.0577
C27	15.46699800	3.21290200	1.90073600	-0.3048
C28	15.06225800	3.54973900	0.57268900	-0.2370
C29	13.70720200	3.67188800	-0.01974800	-0.2985
C30	12.67545100	3.44609700	0.70845600	-0.3020
C31	13.07008300	3.07224500	2.03156600	-0.0178
C32	14.45082600	2.57254300	4.02857300	0.0224
C33	12.27682900	2.76502100	3.11029600	0.0613
C34	8.75804100	3.07224500	3.69532700	0.0019
C35	7.80208400	3.29803600	2.57957100	-0.2702
C36	6.47554600	3.53863400	2.74495900	-0.3156
C37	6.12109000	3.52012700	4.02116800	0.2734
C38	7.07478200	3.27952900	5.12705100	-0.2673
C39	8.40538100	3.04633500	4.98387800	-0.0581
C40	10.23095700	2.78723000	3.90021200	0.0652
C41	9.65102500	2.77612500	5.91943500	0.0144
C42	10.92870500	2.81314000	9.54070800	-0.0656
C43	9.94655000	3.14257400	10.29853400	-0.3002
C44	10.35803000	3.22770800	11.67101400	-0.2393
C45	11.68823400	2.97970800	12.26345100	-0.2966
C46	12.67911500	2.69839400	11.51056200	-0.3062
C47	12.27823800	2.63546800	10.13314500	-0.0041
C48	10.86907800	2.63805900	8.10404800	0.0270
C49	13.03203100	2.35711500	9.02232600	0.0483
C50	14.18801000	-0.91056900	9.93566600	-0.0551
C51	14.26436800	-0.95128500	11.32789400	-0.2465
C52	15.54838400	-1.08083800	12.09065700	-0.2833
C53	16.68996700	-1.16227100	11.53277800	-0.3245
C54	16.63655800	-1.11045000	10.15783000	-0.2541
C55	15.37195300	-0.98089700	9.37285100	-0.0065
C56	13.07678300	-0.72919500	8.86681100	-0.0123
C57	14.90319700	-0.83653900	7.93125400	0.0398
C58	16.24503400	-0.94758400	4.72221900	-0.0151
C59	17.63521700	-1.23630100	4.89748100	-0.3000
C60	18.17389100	-1.34734600	3.71260700	-0.2877
C61	17.37576900	-1.20298700	2.47836200	0.2507
C62	16.00254300	-0.94018100	2.32284800	-0.3012
C63	15.45287700	-0.82543400	3.49291100	-0.0652
C64	15.32867300	-0.76621000	5.73676700	0.0393
C65	14.06078600	-0.56781000	3.71260700	0.0037
C66	10.58638600	-0.73141600	1.85630300	-0.0562
C67	10.49522800	-1.02531600	0.48382400	-0.2494

C68	9.23275200	-1.25851000	-0.25425400	-0.2885
C69	8.08192000	-1.25110700	0.31596700	-0.3165
C70	8.14184500	-0.94388200	1.67116700	-0.2606
C71	9.40338200	-0.69958300	2.41418200	-0.0109
C72	11.71335200	-0.49229900	2.90047400	-0.0108
C73	9.87779700	-0.40716500	3.81875200	0.0264
C74	8.50428400	-0.54782200	7.00557000	-0.0226
C75	7.10998700	-0.55892600	6.82290200	-0.3050
C76	6.53731800	-0.72549400	7.99049700	-0.2835
C77	7.36396600	-0.82913600	9.22721000	-0.2562
C78	8.73713800	-0.80322500	9.39753600	-0.3059
C79	9.31715200	-0.64406100	8.23487800	-0.0628
C80	9.43981300	-0.40346300	6.03545400	0.0202
C81	10.72567600	-0.57373200	8.05221000	-0.0021
H82	17.21674700	2.16167600	10.45404900	0.2744
H83	19.50012900	2.44299000	10.15783000	0.2786
H84	20.15538000	2.59105000	7.93125400	0.2587
H85	18.59946600	2.53552800	6.13666200	0.2764
H86	16.36425100	3.17588700	2.20682900	0.2853
H87	15.77689800	3.72741100	-0.02715300	0.2407
H88	13.60422700	3.91618700	-0.93062000	0.2602
H89	11.77493900	3.51272300	0.41223800	0.2871
H90	8.14038300	3.26472300	1.69338300	0.2764
H91	5.87296300	3.70520100	2.02909800	0.2791
H92	5.20904100	3.67188800	4.23592600	0.2628
H93	6.72590700	3.29063400	6.01077000	0.2775
H94	9.06310400	3.30544000	9.99244200	0.2864
H95	9.67923400	3.48311200	12.28566700	0.2380
H96	11.80628800	3.02782700	13.20394500	0.2609
H97	13.56485400	2.54663200	11.81912300	0.2838
H98	13.45530900	-0.89576300	11.82159200	0.2759
H99	15.50854200	-1.09934500	13.04102500	0.2665
H100	17.50187700	-1.25110700	12.01907100	0.2816
H101	17.45522700	-1.15856900	9.67894300	0.2738
H102	18.08780800	-1.32513700	5.72689300	0.2885
H103	19.10243500	-1.53242100	3.64348900	0.2596
H104	17.86244200	-1.29552500	1.66869800	0.2463
H105	15.54904000	-0.86244900	1.49096700	0.2891
H106	11.30657900	-1.07713600	-0.00740500	0.2726
H107	9.27668200	-1.42507800	-1.18981100	0.2664
H108	7.27037100	-1.43248100	-0.14317200	0.2803
H109	7.32455600	-0.89206100	2.15005400	0.2754
H110	6.65877700	-0.46268700	5.99349000	0.2852
H111	5.59041000	-0.77731500	8.04727300	0.2533
H112	6.86580500	-0.92907600	10.03193700	0.2408
H113	9.18926000	-0.88836000	10.22941600	0.2829

Table S6. Cartesian coordinates (in Å) of the D_{4d}-symmetrized structure of the computed $[Tb(Pc)_2]^-$ anion.

Atom	Cartesian coordinates		
	x	y	z
Tb1	0.00000000	0.00000000	0.00000000
N2	0.75704728	-1.82767382	1.38325000
N3	3.08912759	-1.27955855	1.64635000
N4	1.82767382	-0.75704728	-1.38325000
N5	1.27955855	-3.08912759	-1.64635000
N6	-1.82767382	-0.75704728	1.38325000
N7	-1.27955855	-3.08912759	1.64635000
N8	1.82767382	0.75704728	1.38325000
N9	1.27955855	3.08912759	1.64635000
N10	-0.75704728	1.82767382	1.38325000
N11	-3.08912759	1.27955855	1.64635000
N12	-0.75704728	-1.82767382	-1.38325000
N13	-3.08912759	-1.27955855	-1.64635000
N14	0.75704728	1.82767382	-1.38325000
N15	3.08912759	1.27955855	-1.64635000
N16	-1.82767382	0.75704728	-1.38325000
N17	-1.27955855	3.08912759	-1.64635000
C18	2.10127099	-2.11677340	1.57902500
C19	2.21346595	-3.54992064	1.85100000
C20	3.33293440	-4.35625649	2.12577500
C21	3.10228222	-5.67578831	2.39612500
C22	1.81974361	-6.20703320	2.39612500
C23	0.72359799	-5.43707901	2.12577500
C24	0.94501618	-4.07532975	1.85100000
C25	0.01096186	-2.98260780	1.57902500
C26	2.11677340	-2.10127099	-1.57902500
C27	3.54992064	-2.21346595	-1.85100000
C28	4.35625649	-3.33293440	-2.12577500
C29	5.67578831	-3.10228222	-2.39612500
C30	6.20703320	-1.81974361	-2.39612500
C31	5.43707901	-0.72359799	-2.12577500
C32	4.07532975	-0.94501618	-1.85100000
C33	2.98260780	-0.01096186	-1.57902500
C34	-2.11677340	-2.10127099	1.57902500
C35	-3.54992064	-2.21346595	1.85100000
C36	-4.35625649	-3.33293440	2.12577500
C37	-5.67578831	-3.10228222	2.39612500
C38	-6.20703320	-1.81974361	2.39612500
C39	-5.43707901	-0.72359799	2.12577500
C40	-4.07532975	-0.94501618	1.85100000
C41	-2.98260780	-0.01096186	1.57902500
C42	2.11677340	2.10127099	1.57902500
C43	3.54992064	2.21346595	1.85100000
C44	4.35625649	3.33293440	2.12577500
C45	5.67578831	3.10228222	2.39612500
C46	6.20703320	1.81974361	2.39612500
C47	5.43707901	0.72359799	2.12577500
C48	4.07532975	0.94501618	1.85100000
C49	2.98260780	0.01096186	1.57902500
C50	-2.10127099	2.11677340	1.57902500
C51	-2.21346595	3.54992064	1.85100000
C52	-3.33293440	4.35625649	2.12577500
C53	-3.10228222	5.67578831	2.39612500
C54	-1.81974361	6.20703320	2.39612500
C55	-0.72359799	5.43707901	2.12577500
C56	-0.94501618	4.07532975	1.85100000
C57	-0.01096186	2.98260780	1.57902500
C58	-2.10127099	-2.11677340	-1.57902500
C59	-2.21346595	-3.54992064	-1.85100000
C60	-3.33293440	-4.35625649	-2.12577500
C61	-3.10228222	-5.67578831	-2.39612500
C62	-1.81974361	-6.20703320	-2.39612500
C63	-0.72359799	-5.43707901	-2.12577500
C64	-0.94501618	-4.07532975	-1.85100000
C65	-0.01096186	-2.98260780	-1.57902500
C66	2.10127099	2.11677340	-1.57902500
C67	2.21346595	3.54992064	-1.85100000

C68	3.33293440	4.35625649	-2.12577500
C69	3.10228222	5.67578831	-2.39612500
C70	1.81974361	6.20703320	-2.39612500
C71	0.72359799	5.43707901	-2.12577500
C72	0.94501618	4.07532975	-1.85100000
C73	0.01096186	2.98260780	-1.57902500
C74	-2.11677340	2.10127099	-1.57902500
C75	-3.54992064	2.21346595	-1.85100000
C76	-4.35625649	3.33293440	-2.12577500
C77	-5.67578831	3.10228222	-2.39612500
C78	-6.20703320	1.81974361	-2.39612500
C79	-5.43707901	0.72359799	-2.12577500
C80	-4.07532975	0.94501618	-1.85100000
C81	-2.98260780	0.01096186	-1.57902500
H82	4.19275633	-4.00629657	2.12410000
H83	3.81834238	-6.22902738	2.58582500
H84	1.70461171	-7.10456329	2.58582500
H85	-0.13184696	-5.79760591	2.12410000
H86	4.00629657	-4.19275633	-2.12410000
H87	6.22902738	-3.81834238	-2.58582500
H88	7.10456329	-1.70461171	-2.58582500
H89	5.79760591	0.13184696	-2.12410000
H90	-4.00629657	-4.19275633	2.12410000
H91	-6.22902738	-3.81834238	2.58582500
H92	-7.10456329	-1.70461171	2.58582500
H93	-5.79760591	0.13184696	2.12410000
H94	4.00629657	4.19275633	2.12410000
H95	6.22902738	3.81834238	2.58582500
H96	7.10456329	1.70461171	2.58582500
H97	5.79760591	-0.13184696	2.12410000
H98	-4.19275633	4.00629657	2.12410000
H99	-3.81834238	6.22902738	2.58582500
H100	-1.70461171	7.10456329	2.58582500
H101	0.13184696	5.79760591	2.12410000
H102	-4.19275633	-4.00629657	-2.12410000
H103	-3.81834238	-6.22902738	-2.58582500
H104	-1.70461171	-7.10456329	-2.58582500
H105	0.13184696	-5.79760591	-2.12410000
H106	4.19275633	4.00629657	-2.12410000
H107	3.81834238	6.22902738	-2.58582500
H108	1.70461171	7.10456329	-2.58582500
H109	-0.13184696	5.79760591	-2.12410000
H110	-4.00629657	4.19275633	-2.12410000
H111	-6.22902738	3.81834238	-2.58582500
H112	-7.10456329	1.70461171	-2.58582500
H113	-5.79760591	-0.13184696	-2.12410000

Table S7. Cartesian coordinates (in Å) and Mulliken charges of the Dy1 fragment of the computed Dy_4K_2 compound.[29]

Atom	Cartesian coordinates			Charge
	x	y	z	
Dy1	2.61115700	16.14127000	8.16963900	----
Lu2	3.82293700	16.01239000	11.41442700	2.3636
Lu3	4.57065800	18.67821200	9.36546100	2.2121
Lu4	0.50691100	16.69354800	10.82818300	2.2229
K5	1.27745100	19.40738400	8.80255100	1.8678
K6	2.46423900	19.22704400	12.06734000	1.9364
O7	2.62726700	17.49876300	10.08259900	-1.5208
O8	4.79614200	16.20077100	9.19812200	-0.8297
O9	2.09889300	14.89588800	10.12926800	-0.8147
O10	3.25679100	18.20863800	7.42916700	-0.7579
O11	0.39151500	16.81186100	8.46253900	-0.8599
O16	2.84002200	14.78791300	6.61802500	-0.3578
O12	4.92734200	18.06620300	11.64043500	-0.6130
O13	1.98130200	16.63726400	12.67825200	-0.6073
O14	3.39062000	20.48069700	9.97148400	-0.6235
O15	0.06660600	18.86337700	11.08930400	-0.6160
O17	4.79718700	14.56047800	12.52491300	-0.5909
O18	6.31507600	19.43541200	8.47587300	-0.5885
O19	-1.15445700	15.58508700	11.52265300	-0.5932
C20	6.04368300	15.56670800	8.80699600	1.5133
C24	1.75104800	13.49911100	10.12926800	1.5048
C28	3.39928200	18.72553700	6.11134000	1.3569
C32	-0.77874600	16.78199600	7.58695000	1.5340
C52	2.97441200	13.87127900	5.53131800	1.5968
C21	5.90714300	14.06425400	8.96033500	-0.9698
C22	7.14060300	16.05144500	9.70258500	-0.9739
C23	6.34884800	15.88374000	7.35360800	-0.9643
C25	2.89860700	12.61234200	9.68702900	-0.9754
C26	0.58147900	13.34748700	9.13812000	-0.9375
C27	1.28103900	13.00748200	11.44265000	-0.9934
C29	2.32016500	18.27066500	5.24019600	-0.9851
C30	3.37098800	20.32218100	6.11356200	-0.9306
C31	4.75808500	18.18796200	5.46242700	-0.9362
C33	-1.92622500	16.30185400	8.35586800	-0.9967
C34	-0.48603700	15.97563300	6.30690300	-0.9749
C35	-1.16365600	18.19255600	7.11359900	-0.9511
C36	5.91595000	18.53715600	12.49157800	0.1957
C37	6.46111900	17.48268100	13.44717000	-0.7810
C38	5.33484300	19.68122600	13.46717000	-0.7575
C39	7.05810900	19.20797600	11.78710800	-0.7791
C40	1.72541300	16.45347700	14.07608200	0.1819
C41	2.82547400	17.01862100	14.96056000	-0.7731
C42	1.54700100	14.98548400	14.33387000	-0.7722
C43	0.37395200	17.08983800	14.41387200	-0.7600
C44	3.45757100	21.90274400	10.00926300	0.1933
C45	2.63450400	22.54369900	9.01811500	-0.7833
C46	4.93263800	22.36450800	9.90037000	-0.7788
C47	2.93077200	22.38058900	11.36487000	-0.7586
C48	-0.99371000	19.82136300	11.46709600	0.1732
C49	-0.73614000	20.35664100	12.75603300	-0.7724
C50	-2.32321800	19.24932800	11.46487300	-0.7879
C51	-1.00783700	20.99529900	10.49817000	-0.7530
C53	1.71302000	13.09937600	5.40686900	-1.0210
C54	4.02447500	12.95004900	5.70021300	-1.0527
C55	3.37142400	14.62710000	4.26238200	-0.9997
C56	5.47597600	13.60249100	13.26716300	0.2411
C57	6.81880000	13.34978500	12.84492500	-0.8285
C58	5.54827400	14.13087700	14.75166300	-0.7956
C59	4.69092000	12.28152600	13.28494100	-0.8086
C60	7.47024400	20.01893400	7.88029500	0.2299
C61	8.25773700	20.72880900	8.92033400	-0.8067
C62	8.34274100	18.97594600	7.30027300	-0.8060
C63	7.04970900	20.92637900	6.76692000	-0.8024
C64	-2.28296100	14.91426600	11.99156000	0.2450
C65	-1.91128700	14.10101200	13.21605000	-0.8097
C66	-2.86907100	14.04128100	10.92040800	-0.8099
C67	-3.36358400	15.96414600	12.34046200	-0.7968

H68	5.70783900	13.84830500	9.89370300	0.0975
H69	6.74650800	13.63235600	8.69810300	0.1426
H70	5.18116200	13.74262800	8.38698000	0.1196
H71	7.21764900	17.02551300	9.62480400	0.0904
H72	7.98677500	15.63562800	9.43813100	0.1428
H73	6.93476600	15.81482000	10.63150900	0.0917
H74	5.62662300	15.54373500	6.78692100	0.1013
H75	7.19331300	15.46103100	7.09804300	0.1422
H76	6.42331700	16.85551000	7.24027100	0.1132
H77	3.16675000	12.85815600	8.77810600	0.1030
H78	2.61190600	11.67732800	9.70258500	0.1423
H79	3.65671200	12.73180300	10.29594100	0.1160
H80	-0.16764900	13.91033300	9.42701900	0.0883
H81	0.29381800	12.41247400	9.11145200	0.1401
H82	0.87181800	13.62776200	8.24475300	0.0719
H83	1.99121000	13.12464600	12.10712000	0.1154
H84	1.05294400	12.05638800	11.37153600	0.1366
H85	0.48822600	13.51289500	11.71599400	0.1085
H86	2.32323400	17.29200300	5.19797200	0.0958
H87	2.45095600	18.63823800	4.34016200	0.1361
H88	1.46087000	18.58080500	5.59576500	0.0763
H89	2.52278100	20.63232100	6.49357600	0.0680
H90	3.45693300	20.65069900	5.19352800	0.1491
H91	4.11444800	20.66218600	6.65358200	0.1245
H92	5.51748000	18.48202000	6.00689100	0.1270
H93	4.84885700	18.54634500	4.55572600	0.1465
H94	4.73930200	17.20929900	5.42909200	0.1325
H95	-1.73982600	15.40130000	8.69143600	0.1170
H96	-2.71783300	16.27658300	7.77806900	0.1327
H97	-2.08997000	16.90605100	9.10923000	0.0892
H98	0.25774400	16.39145000	5.82021800	0.1085
H99	-1.28329000	15.96414600	5.73577000	0.1453
H100	-0.24469800	15.05670100	6.54691200	0.1232
H101	-1.35257400	18.75769900	7.89140600	0.0676
H102	-1.96243300	18.14201500	6.54691200	0.1413
H103	-0.42415700	18.57850800	6.60024700	0.0707
H104	5.73305300	17.14497400	14.00941300	0.1677
H105	7.15379700	17.88241700	14.01385800	0.2395
H106	6.84614800	16.74294100	12.93159500	0.1790
H107	4.97942800	20.42096600	12.92937300	0.1175
H108	6.05392700	20.01433900	14.04497000	0.2168
H109	4.61922700	19.30676100	14.02052400	0.1178
H110	7.48464800	18.56931800	11.17597400	0.1816
H111	7.71339700	19.51581800	12.44713200	0.2378
H112	6.72309200	19.97298700	11.27597700	0.1510
H113	3.67834100	16.59591200	14.72944000	0.1664
H114	2.61381000	16.83713200	15.90059500	0.2381
H115	2.89163100	17.98579700	14.82055400	0.1254
H116	0.78660700	14.65237100	13.81385000	0.1947
H117	1.38036400	14.83845400	15.28946100	0.2344
H118	2.35968700	14.50534200	14.06719300	0.1649
H119	0.40746100	18.05012200	14.21831000	0.1297
H120	0.17669800	16.95659300	15.36279700	0.2276
H121	-0.32778300	16.67172400	13.87163000	0.1572
H122	2.91678500	22.25653300	8.12474800	0.1808
H123	2.72936700	23.51547000	9.09589600	0.2346
H124	1.69797200	22.29558800	9.16034300	0.1268
H125	5.44004500	22.01761100	10.66262100	0.1827
H126	4.97024300	23.34317000	9.90037000	0.2301
H127	5.32125200	22.02220500	9.06700600	0.1771
H128	2.00473200	22.08193600	11.48042900	0.1227
H129	2.96558100	23.35925100	11.40042600	0.2219
H130	3.48709200	22.00612400	12.08045200	0.1342
H131	-0.71860900	19.62838800	13.41161300	0.1905
H132	-1.44279900	20.99300200	12.99159700	0.2350
H133	0.12895300	20.81381000	12.75158800	0.1261
H134	-2.52971000	18.90932300	10.56928400	0.1885
H135	-2.97661000	19.93623000	11.71154900	0.2391
H136	-2.36307500	18.51418200	12.11156400	0.2033
H137	-0.13550300	21.44327800	10.51372700	0.1283

H138	-1.70493200	21.63165900	10.76262500	0.2193
H139	-1.19104300	20.66907800	9.59147000	0.1215
H140	1.54734900	12.61463900	6.24023300	0.1334
H141	1.79689000	12.46071800	4.66906400	0.1279
H142	0.97356000	13.71276300	5.22908400	0.1348
H143	4.88003800	13.43708300	5.76466000	0.1230
H144	4.05983400	12.34125700	4.93351800	0.1209
H145	3.88611800	12.43544700	6.52246600	0.1230
H146	2.68964200	15.29792000	4.05348500	0.1340
H147	3.44759900	13.99533400	3.51568700	0.1354
H148	4.23464300	15.07048500	4.40238700	0.1398
H149	6.81207600	13.00748200	11.92489100	0.2360
H150	7.22844300	12.68355900	13.43605800	0.2604
H151	7.33441400	14.18141800	12.88048200	0.2315
H152	6.00686400	14.99467300	14.76944100	0.2142
H153	6.03064100	13.48762400	15.30501700	0.2405
H154	4.63418600	14.24114900	15.10056500	0.2140
H155	3.81091500	12.43085300	13.68717900	0.2277
H156	5.18243500	11.61759800	13.81162800	0.2474
H157	4.58069100	11.95530500	12.36712900	0.2242
H158	7.71116700	21.44098100	9.31368200	0.2242
H159	9.05877600	21.11935500	8.51142900	0.2472
H160	8.52200300	20.09474600	9.61813800	0.2313
H161	8.62016500	18.35336900	8.00474400	0.2270
H162	9.13642900	19.39635700	6.90692500	0.2483
H163	7.85266400	18.48891200	6.60691400	0.2315
H164	6.53821600	20.41407400	6.10467300	0.2255
H165	7.84475900	21.30773600	6.34023700	0.2482
H166	6.49250400	21.64774100	7.12471100	0.2191
H167	-1.21537200	13.45316400	12.98048600	0.2319
H168	-2.70234100	13.62546400	13.54495100	0.2480
H169	-1.57727400	14.70061500	13.91607600	0.2246
H170	-3.12505900	14.59264000	10.15149100	0.2336
H171	-3.66103400	13.58181500	11.27153300	0.2469
H172	-2.20482600	13.37735300	10.63817600	0.2256
H173	-3.02267500	16.56604700	13.03604300	0.2098
H174	-4.16797800	15.50927500	12.66714000	0.2414
H175	-3.58463400	16.48564000	11.53820900	0.2193

Table S8. Cartesian coordinates (in Å) and Mulliken charges of the Dy2 fragment of the computed Dy_4K_2 compound.[29]

Atom	Cartesian coordinates			Charge
	x	y	z	
Dy2	3.82293700	16.01239000	11.41442700	----
Lu1	2.61115700	16.14127000	8.16963900	2.3795
Lu3	4.57065800	18.67821200	9.36546100	2.2201
Lu4	0.50691100	16.69354800	10.82818300	2.2078
K5	1.27745100	19.40738400	8.80255100	1.9621
K6	2.46423900	19.22704400	12.06734000	1.8411
O7	2.62726700	17.49876300	10.08259900	-1.5211
O8	4.79614200	16.20077100	9.19812200	-0.8298
O9	2.09889300	14.89588800	10.12926800	-0.8107
O12	4.92734200	18.06620300	11.64043500	-0.7494
O13	1.98130200	16.63726400	12.67825200	-0.7822
O17	4.79718700	14.56047800	12.52491300	-0.2765
O10	3.25679100	18.20863800	7.42916700	-0.6101
O11	0.39151500	16.81186100	8.46253900	-0.6051
O14	3.39062000	20.48069700	9.97148400	-0.6235
O15	0.06660600	18.86337700	11.08930400	-0.6158
O16	2.84002200	14.78791300	6.61802500	-0.5861
O18	6.31507600	19.43541200	8.47587300	-0.5883
O19	-1.15445700	15.58508700	11.52265300	-0.5934
C20	6.04368300	15.56670800	8.80699600	1.5181
C24	1.75104800	13.49911100	10.12926800	1.5043
C36	5.91595000	18.53715600	12.49157800	1.3945
C40	1.72541300	16.45347700	14.07608200	1.4616
C56	5.47597600	13.60249100	13.26716300	1.4255
C21	5.90714300	14.06425400	8.96033500	-0.9679
C22	7.14060300	16.05144500	9.70258500	-0.9718
C23	6.34884800	15.88374000	7.35360800	-0.9702
C25	2.89860700	12.61234200	9.68702900	-0.9770
C26	0.58147900	13.34748700	9.13812000	-0.9416
C27	1.28103900	13.00748200	11.44265000	-0.9906
C28	3.39928200	18.72553700	6.11134000	0.1873
C29	2.32016500	18.27066500	5.24019600	-0.7738
C30	3.37098800	20.32218100	6.11356200	-0.7630
C31	4.75808500	18.18796200	5.46242700	-0.7705
C32	-0.77874600	16.78199600	7.58695000	0.1855
C33	-1.92622500	16.30185400	8.35586800	-0.7794
C34	-0.48603700	15.97563300	6.30690300	-0.7813
C35	-1.16365600	18.19255600	7.11359900	-0.7580
C37	6.46111900	17.48268100	13.44717000	-0.9779
C38	5.33484300	19.68122600	13.46717000	-0.9211
C39	7.05810900	19.20797600	11.78710800	-0.9827
C41	2.82547400	17.01862100	14.96056000	-0.9716
C42	1.54700100	14.98548400	14.33387000	-0.9719
C43	0.37395200	17.08983800	14.41387200	-0.9553
C44	3.45757100	21.90274400	10.00926300	0.1923
C45	2.63450400	22.54369900	9.01811500	-0.7853
C46	4.93263800	22.36450800	9.90037000	-0.7788
C47	2.93077200	22.38058900	11.36487000	-0.7570
C48	-0.99371000	19.82136300	11.46709600	0.1738
C49	-0.73614000	20.35664100	12.75603300	-0.7704
C50	-2.32321800	19.24932800	11.46487300	-0.7885
C51	-1.00783700	20.99529900	10.49817000	-0.7547
C52	2.97441200	13.87127900	5.53131800	0.2223
C53	1.71302000	13.09937600	5.40686900	-0.8098
C54	4.02447500	12.95004900	5.70021300	-0.8091
C55	3.37142400	14.62710000	4.26238200	-0.7994
C57	6.81880000	13.34978500	12.84492500	-1.0539
C58	5.54827400	14.13087700	14.75166300	-0.9705
C59	4.69092000	12.28152600	13.28494100	-0.9967
C60	7.47024400	20.01893400	7.88029500	0.2302
C61	8.25773700	20.72880900	8.92033400	-0.8064
C62	8.34274100	18.97594600	7.30027300	-0.8059
C63	7.04970900	20.92637900	6.76692000	-0.8029
C64	-2.28296100	14.91426600	11.99156000	0.2446
C65	-1.91128700	14.10101200	13.21605000	-0.8087
C66	-2.86907100	14.04128100	10.92040800	-0.8107
C67	-3.36358400	15.96414600	12.34046200	-0.7970

H68	5.70783900	13.84830500	9.89370300	0.0903
H69	6.74650800	13.63235600	8.69810300	0.1425
H70	5.18116200	13.74262800	8.38698000	0.1213
H71	7.21764900	17.02551300	9.62480400	0.0863
H72	7.98677500	15.63562800	9.43813100	0.1420
H73	6.93476600	15.81482000	10.63150900	0.0831
H74	5.62662300	15.54373500	6.78692100	0.1109
H75	7.19331300	15.46103100	7.09804300	0.1430
H76	6.42331700	16.85551000	7.24027100	0.1166
H77	3.16675000	12.85815600	8.77810600	0.1093
H78	2.61190600	11.67732800	9.70258500	0.1427
H79	3.65671200	12.73180300	10.29594100	0.1126
H80	-0.16764900	13.91033300	9.42701900	0.0947
H81	0.29381800	12.41247400	9.11145200	0.1414
H82	0.87181800	13.62776200	8.24475300	0.0833
H83	1.99121000	13.12464600	12.10712000	0.1123
H84	1.05294400	12.05638800	11.37153600	0.1362
H85	0.48822600	13.51289500	11.71599400	0.1049
H86	2.32323400	17.29200300	5.19797200	0.1604
H87	2.45095600	18.63823800	4.34016200	0.2409
H88	1.46087000	18.58080500	5.59576500	0.1395
H89	2.52278100	20.63232100	6.49357600	0.1080
H90	3.45693300	20.65069900	5.19352800	0.2269
H91	4.11444800	20.66218600	6.65358200	0.1674
H92	5.51748000	18.48202000	6.00689100	0.1761
H93	4.84885700	18.54634500	4.55572600	0.2321
H94	4.73930200	17.20929900	5.42909200	0.1846
H95	-1.73982600	15.40130000	8.69143600	0.1859
H96	-2.71783300	16.27658300	7.77806900	0.2372
H97	-2.08997000	16.90605100	9.10923000	0.1461
H98	0.25774400	16.39145000	5.82021800	0.1638
H99	-1.28329000	15.96414600	5.73577000	0.2381
H100	-0.24469800	15.05670100	6.54691200	0.1856
H101	-1.35257400	18.75769900	7.89140600	0.1195
H102	-1.96243300	18.14201500	6.54691200	0.2267
H103	-0.42415700	18.57850800	6.60024700	0.1246
H104	5.73305300	17.14497400	14.00941300	0.1078
H105	7.15379700	17.88241700	14.01385800	0.1393
H106	6.84614800	16.74294100	12.93159500	0.1096
H107	4.97942800	20.42096600	12.92937300	0.0736
H108	6.05392700	20.01433900	14.04497000	0.1421
H109	4.61922700	19.30676100	14.02052400	0.0729
H110	7.48464800	18.56931800	11.17597400	0.1161
H111	7.71339700	19.51581800	12.44713200	0.1355
H112	6.72309200	19.97298700	11.27597700	0.0980
H113	3.67834100	16.59591200	14.72944000	0.1106
H114	2.61381000	16.83713200	15.90059500	0.1448
H115	2.89163100	17.98579700	14.82055400	0.0720
H116	0.78660700	14.65237100	13.81385000	0.1286
H117	1.38036400	14.83845400	15.28946100	0.1337
H118	2.35968700	14.50534200	14.06719300	0.0994
H119	0.40746100	18.05012200	14.21831000	0.0805
H120	0.17669800	16.95659300	15.36279700	0.1397
H121	-0.32778300	16.67172400	13.87163000	0.1096
H122	2.91678500	22.25653300	8.12474800	0.1820
H123	2.72936700	23.51547000	9.09589600	0.2386
H124	1.69797200	22.29558800	9.16034300	0.1307
H125	5.44004500	22.01761100	10.66262100	0.1830
H126	4.97024300	23.34317000	9.90037000	0.2292
H127	5.32125200	22.02220500	9.06700600	0.1766
H128	2.00473200	22.08193600	11.48042900	0.1196
H129	2.96558100	23.35925100	11.40042600	0.2182
H130	3.48709200	22.00612400	12.08045200	0.1320
H131	-0.71860900	19.62838800	13.41161300	0.1893
H132	-1.44279900	20.99300200	12.99159700	0.2311
H133	0.12895300	20.81381000	12.75158800	0.1216
H134	-2.52971000	18.90932300	10.56928400	0.1886
H135	-2.97661000	19.93623000	11.71154900	0.2402
H136	-2.36307500	18.51418200	12.11156400	0.2047
H137	-0.13550300	21.44327800	10.51372700	0.1311

H138	-1.70493200	21.63165900	10.76262500	0.2231
H139	-1.19104300	20.66907800	9.59147000	0.1237
H140	1.54734900	12.61463900	6.24023300	0.2296
H141	1.79689000	12.46071800	4.66906400	0.2487
H142	0.97356000	13.71276300	5.22908400	0.2256
H143	4.88003800	13.43708300	5.76466000	0.2310
H144	4.05983400	12.34125700	4.93351800	0.2562
H145	3.88611800	12.43544700	6.52246600	0.2306
H146	2.68964200	15.29792000	4.05348500	0.2168
H147	3.44759900	13.99533400	3.51568700	0.2463
H148	4.23464300	15.07048500	4.40238700	0.2247
H149	6.81207600	13.00748200	11.92489100	0.1283
H150	7.22844300	12.68355900	13.43605800	0.1238
H151	7.33441400	14.18141800	12.88048200	0.1281
H152	6.00686400	14.99467300	14.76944100	0.1405
H153	6.03064100	13.48762400	15.30501700	0.1378
H154	4.63418600	14.24114900	15.10056500	0.1330
H155	3.81091500	12.43085300	13.68717900	0.1416
H156	5.18243500	11.61759800	13.81162800	0.1349
H157	4.58069100	11.95530500	12.36712900	0.1362
H158	7.71116700	21.44098100	9.31368200	0.2244
H159	9.05877600	21.11935500	8.51142900	0.2457
H160	8.52200300	20.09474600	9.61813800	0.2348
H161	8.62016500	18.35336900	8.00474400	0.2279
H162	9.13642900	19.39635700	6.90692500	0.2487
H163	7.85266400	18.48891200	6.60691400	0.2297
H164	6.53821600	20.41407400	6.10467300	0.2267
H165	7.84475900	21.30773600	6.34023700	0.2483
H166	6.49250400	21.64774100	7.12471100	0.2181
H167	-1.21537200	13.45316400	12.98048600	0.2320
H168	-2.70234100	13.62546400	13.54495100	0.2474
H169	-1.57727400	14.70061500	13.91607600	0.2247
H170	-3.12505900	14.59264000	10.15149100	0.2299
H171	-3.66103400	13.58181500	11.27153300	0.2485
H172	-2.20482600	13.37735300	10.63817600	0.2273
H173	-3.02267500	16.56604700	13.03604300	0.2122
H174	-4.16797800	15.50927500	12.66714000	0.2417
H175	-3.58463400	16.48564000	11.53820900	0.2170

Table S9. Cartesian coordinates (in Å) and Mulliken charges of the Dy3 fragment of the computed Dy_4K_2 compound.[29]

Atom	Cartesian coordinates			Charge
	x	y	z	
Dy3	4.57065800	18.67821200	9.36546100	----
Lu1	2.61115700	16.14127000	8.16963900	2.4390
Lu2	3.82293700	16.01239000	11.41442700	2.4067
Lu4	0.50691100	16.69354800	10.82818300	2.0979
K5	1.27745100	19.40738400	8.80255100	1.9248
K6	2.46423900	19.22704400	12.06734000	1.9000
O7	2.62726700	17.49876300	10.08259900	-1.5250
O8	4.79614200	16.20077100	9.19812200	-0.8338
O10	3.25679100	18.20863800	7.42916700	-0.7693
O12	4.92734200	18.06620300	11.64043500	-0.7578
O14	3.39062000	20.48069700	9.97148400	-0.8401
O18	6.31507600	19.43541200	8.47587300	-0.3426
O9	2.09889300	14.89588800	10.12926800	-0.6001
O11	0.39151500	16.81186100	8.46253900	-0.6058
O13	1.98130200	16.63726400	12.67825200	-0.6078
O15	0.06660600	18.86337700	11.08930400	-0.6181
O16	2.84002200	14.78791300	6.61802500	-0.5863
O17	4.79718700	14.56047800	12.52491300	-0.5905
O19	-1.15445700	15.58508700	11.52265300	-0.5956
C20	6.04368300	15.56670800	8.80699600	1.5185
C28	3.39928200	18.72553700	6.11134000	1.3613
C36	5.91595000	18.53715600	12.49157800	1.3958
C44	3.45757100	21.90274400	10.00926300	1.5463
C60	7.47024400	20.01893400	7.88029500	1.5336
C21	5.90714300	14.06425400	8.96033500	-0.9734
C22	7.14060300	16.05144500	9.70258500	-0.9683
C23	6.34884800	15.88374000	7.35360800	-0.9640
C24	1.75104800	13.49911100	10.12926800	0.1722
C25	2.89860700	12.61234200	9.68702900	-0.7757
C26	0.58147900	13.34748700	9.13812000	-0.7532
C27	1.28103900	13.00748200	11.44265000	-0.7748
C29	2.32016500	18.27066500	5.24019600	-0.9882
C30	3.37098800	20.32218100	6.11356200	-0.9269
C31	4.75808500	18.18796200	5.46242700	-0.9298
C32	-0.77874600	16.78199600	7.58695000	0.1842
C33	-1.92622500	16.30185400	8.35586800	-0.7811
C34	-0.48603700	15.97563300	6.30690300	-0.7811
C35	-1.16365600	18.19255600	7.11359900	-0.7560
C37	6.46111900	17.48268100	13.44717000	-0.9792
C38	5.33484300	19.68122600	13.46717000	-0.9200
C39	7.05810900	19.20797600	11.78710800	-0.9798
C40	1.72541300	16.45347700	14.07608200	0.1816
C41	2.82547400	17.01862100	14.96056000	-0.7721
C42	1.54700100	14.98548400	14.33387000	-0.7735
C43	0.37395200	17.08983800	14.41387200	-0.7607
C45	2.63450400	22.54369900	9.01811500	-1.0159
C46	4.93263800	22.36450800	9.90037000	-0.9691
C47	2.93077200	22.38058900	11.36487000	-0.9546
C48	-0.99371000	19.82136300	11.46709600	0.1722
C49	-0.73614000	20.35664100	12.75603300	-0.7699
C50	-2.32321800	19.24932800	11.46487300	-0.7887
C51	-1.00783700	20.99529900	10.49817000	-0.7522
C52	2.97441200	13.87127900	5.53131800	0.2219
C53	1.71302000	13.09937600	5.40686900	-0.8099
C54	4.02447500	12.95004900	5.70021300	-0.8093
C55	3.37142400	14.62710000	4.26238200	-0.7998
C56	5.47597600	13.60249100	13.26716300	0.2408
C57	6.81880000	13.34978500	12.84492500	-0.8278
C58	5.54827400	14.13087700	14.75166300	-0.7957
C59	4.69092000	12.28152600	13.28494100	-0.8083
C61	8.25773700	20.72880900	8.92033400	-1.0159
C62	8.34274100	18.97594600	7.30027300	-1.0183
C63	7.04970900	20.92637900	6.76692000	-1.0085
C64	-2.28296100	14.91426600	11.99156000	0.2467
C65	-1.91128700	14.10101200	13.21605000	-0.8102
C66	-2.86907100	14.04128100	10.92040800	-0.8116
C67	-3.36358400	15.96414600	12.34046200	-0.7978

H68	5.70783900	13.84830500	9.89370300	0.1006
H69	6.74650800	13.63235600	8.69810300	0.1438
H70	5.18116200	13.74262800	8.38698000	0.1232
H71	7.21764900	17.02551300	9.62480400	0.0774
H72	7.98677500	15.63562800	9.43813100	0.1423
H73	6.93476600	15.81482000	10.63150900	0.0850
H74	5.62662300	15.54373500	6.78692100	0.1071
H75	7.19331300	15.46103100	7.09804300	0.1427
H76	6.42331700	16.85551000	7.24027100	0.1068
H77	3.16675000	12.85815600	8.77810600	0.1642
H78	2.61190600	11.67732800	9.70258500	0.2430
H79	3.65671200	12.73180300	10.29594100	0.1736
H80	-0.16764900	13.91033300	9.42701900	0.1417
H81	0.29381800	12.41247400	9.11145200	0.2302
H82	0.87181800	13.62776200	8.24475300	0.1241
H83	1.99121000	13.12464600	12.10712000	0.1772
H84	1.05294400	12.05638800	11.37153600	0.2449
H85	0.48822600	13.51289500	11.71599400	0.1685
H86	2.32323400	17.29200300	5.19797200	0.1027
H87	2.45095600	18.63823800	4.34016200	0.1369
H88	1.46087000	18.58080500	5.59576500	0.0794
H89	2.52278100	20.63232100	6.49357600	0.0652
H90	3.45693300	20.65069900	5.19352800	0.1491
H91	4.11444800	20.66218600	6.65358200	0.1162
H92	5.51748000	18.48202000	6.00689100	0.1118
H93	4.84885700	18.54634500	4.55572600	0.1467
H94	4.73930200	17.20929900	5.42909200	0.1325
H95	-1.73982600	15.40130000	8.69143600	0.1880
H96	-2.71783300	16.27658300	7.77806900	0.2385
H97	-2.08997000	16.90605100	9.10923000	0.1509
H98	0.25774400	16.39145000	5.82021800	0.1653
H99	-1.28329000	15.96414600	5.73577000	0.2365
H100	-0.24469800	15.05670100	6.54691200	0.1819
H101	-1.35257400	18.75769900	7.89140600	0.1155
H102	-1.96243300	18.14201500	6.54691200	0.2215
H103	-0.42415700	18.57850800	6.60024700	0.1200
H104	5.73305300	17.14497400	14.00941300	0.1104
H105	7.15379700	17.88241700	14.01385800	0.1399
H106	6.84614800	16.74294100	12.93159500	0.1172
H107	4.97942800	20.42096600	12.92937300	0.0696
H108	6.05392700	20.01433900	14.04497000	0.1420
H109	4.61922700	19.30676100	14.02052400	0.0730
H110	7.48464800	18.56931800	11.17597400	0.1092
H111	7.71339700	19.51581800	12.44713200	0.1355
H112	6.72309200	19.97298700	11.27597700	0.0873
H113	3.67834100	16.59591200	14.72944000	0.1642
H114	2.61381000	16.83713200	15.90059500	0.2347
H115	2.89163100	17.98579700	14.82055400	0.1216
H116	0.78660700	14.65237100	13.81385000	0.1962
H117	1.38036400	14.83845400	15.28946100	0.2359
H118	2.35968700	14.50534200	14.06719300	0.1654
H119	0.40746100	18.05012200	14.21831000	0.1293
H120	0.17669800	16.95659300	15.36279700	0.2264
H121	-0.32778300	16.67172400	13.87163000	0.1604
H122	2.91678500	22.25653300	8.12474800	0.1055
H123	2.72936700	23.51547000	9.09589600	0.1277
H124	1.69797200	22.29558800	9.16034300	0.0625
H125	5.44004500	22.01761100	10.66262100	0.1210
H126	4.97024300	23.34317000	9.90037000	0.1380
H127	5.32125200	22.02220500	9.06700600	0.1078
H128	2.00473200	22.08193600	11.48042900	0.0689
H129	2.96558100	23.35925100	11.40042600	0.1348
H130	3.48709200	22.00612400	12.08045200	0.0781
H131	-0.71860900	19.62838800	13.41161300	0.1860
H132	-1.44279900	20.99300200	12.99159700	0.2304
H133	0.12895300	20.81381000	12.75158800	0.1210
H134	-2.52971000	18.90932300	10.56928400	0.1895
H135	-2.97661000	19.93623000	11.71154900	0.2398
H136	-2.36307500	18.51418200	12.11156400	0.2065
H137	-0.13550300	21.44327800	10.51372700	0.1247

H138	-1.70493200	21.63165900	10.76262500	0.2180
H139	-1.19104300	20.66907800	9.59147000	0.1183
H140	1.54734900	12.61463900	6.24023300	0.2278
H141	1.79689000	12.46071800	4.66906400	0.2490
H142	0.97356000	13.71276300	5.22908400	0.2257
H143	4.88003800	13.43708300	5.76466000	0.2313
H144	4.05983400	12.34125700	4.93351800	0.2567
H145	3.88611800	12.43544700	6.52246600	0.2289
H146	2.68964200	15.29792000	4.05348500	0.2189
H147	3.44759900	13.99533400	3.51568700	0.2456
H148	4.23464300	15.07048500	4.40238700	0.2249
H149	6.81207600	13.00748200	11.92489100	0.2339
H150	7.22844300	12.68355900	13.43605800	0.2599
H151	7.33441400	14.18141800	12.88048200	0.2325
H152	6.00686400	14.99467300	14.76944100	0.2186
H153	6.03064100	13.48762400	15.30501700	0.2396
H154	4.63418600	14.24114900	15.10056500	0.2126
H155	3.81091500	12.43085300	13.68717900	0.2258
H156	5.18243500	11.61759800	13.81162800	0.2478
H157	4.58069100	11.95530500	12.36712900	0.2232
H158	7.71116700	21.44098100	9.31368200	0.1334
H159	9.05877600	21.11935500	8.51142900	0.1260
H160	8.52200300	20.09474600	9.61813800	0.1382
H161	8.62016500	18.35336900	8.00474400	0.1293
H162	9.13642900	19.39635700	6.90692500	0.1275
H163	7.85266400	18.48891200	6.60691400	0.1344
H164	6.53821600	20.41407400	6.10467300	0.1320
H165	7.84475900	21.30773600	6.34023700	0.1303
H166	6.49250400	21.64774100	7.12471100	0.1285
H167	-1.21537200	13.45316400	12.98048600	0.2309
H168	-2.70234100	13.62546400	13.54495100	0.2492
H169	-1.57727400	14.70061500	13.91607600	0.2277
H170	-3.12505900	14.59264000	10.15149100	0.2322
H171	-3.66103400	13.58181500	11.27153300	0.2490
H172	-2.20482600	13.37735300	10.63817600	0.2286
H173	-3.02267500	16.56604700	13.03604300	0.2132
H174	-4.16797800	15.50927500	12.66714000	0.2422
H175	-3.58463400	16.48564000	11.53820900	0.2202

Table S10. Cartesian coordinates (in Ångstrom) and Mulliken charges of the Dy4 fragment of the computed Dy_4K_2 compound.[29]

Atom	Cartesian coordinates			Charge
	x	y	z	
Dy4	0.50691100	16.69354800	10.82818300	----
Lu1	2.61115700	16.14127000	8.16963900	2.4484
Lu2	3.82293700	16.01239000	11.41442700	2.4142
Lu3	4.57065800	18.67821200	9.36546100	2.1067
K5	1.27745100	19.40738400	8.80255100	1.9237
K6	2.46423900	19.22704400	12.06734000	1.8904
O7	2.62726700	17.49876300	10.08259900	-1.5229
O9	2.09889300	14.89588800	10.12926800	-0.8193
O11	0.39151500	16.81186100	8.46253900	-0.8696
O13	1.98130200	16.63726400	12.67825200	-0.7985
O15	0.06660600	18.86337700	11.08930400	-0.9116
O19	-1.15445700	15.58508700	11.52265300	-0.2893
O8	4.79614200	16.20077100	9.19812200	-0.5988
O10	3.25679100	18.20863800	7.42916700	-0.6102
O12	4.92734200	18.06620300	11.64043500	-0.6140
O14	3.39062000	20.48069700	9.97148400	-0.6255
O16	2.84002200	14.78791300	6.61802500	-0.5862
O17	4.79718700	14.56047800	12.52491300	-0.5909
O18	6.31507600	19.43541200	8.47587300	-0.5903
C24	1.75104800	13.49911100	10.12926800	1.5077
C32	-0.77874600	16.78199600	7.58695000	1.5380
C40	1.72541300	16.45347700	14.07608200	1.4664
C48	-0.99371000	19.82136300	11.46709600	1.7302
C64	-2.28296100	14.91426600	11.99156000	1.3856
C20	6.04368300	15.56670800	8.80699600	0.1770
C21	5.90714300	14.06425400	8.96033500	-0.7712
C22	7.14060300	16.05144500	9.70258500	-0.7683
C23	6.34884800	15.88374000	7.35360800	-0.7684
C25	2.89860700	12.61234200	9.68702900	-0.9809
C26	0.58147900	13.34748700	9.13812000	-0.9364
C27	1.28103900	13.00748200	11.44265000	-0.9832
C28	3.39928200	18.72553700	6.11134000	0.1871
C29	2.32016500	18.27066500	5.24019600	-0.7729
C30	3.37098800	20.32218100	6.11356200	-0.7628
C31	4.75808500	18.18796200	5.46242700	-0.7721
C33	-1.92622500	16.30185400	8.35586800	-0.9942
C34	-0.48603700	15.97563300	6.30690300	-0.9759
C35	-1.16365600	18.19255600	7.11359900	-0.9504
C36	5.91595000	18.53715600	12.49157800	0.1949
C37	6.46111900	17.48268100	13.44717000	-0.7805
C38	5.33484300	19.68122600	13.46717000	-0.7556
C39	7.05810900	19.20797600	11.78710800	-0.7804
C41	2.82547400	17.01862100	14.96056000	-0.9731
C42	1.54700100	14.98548400	14.33387000	-0.9742
C43	0.37395200	17.08983800	14.41387200	-0.9486
C44	3.45757100	21.90274400	10.00926300	0.1921
C45	2.63450400	22.54369900	9.01811500	-0.7828
C46	4.93263800	22.36450800	9.90037000	-0.7799
C47	2.93077200	22.38058900	11.36487000	-0.7558
C49	-0.73614000	20.35664100	12.75603300	-1.0191
C50	-2.32321800	19.24932800	11.46487300	-1.0324
C51	-1.00783700	20.99529900	10.49817000	-0.9649
C52	2.97441200	13.87127900	5.53131800	0.2221
C53	1.71302000	13.09937600	5.40686900	-0.8091
C54	4.02447500	12.95004900	5.70021300	-0.8096
C55	3.37142400	14.62710000	4.26238200	-0.7992
C56	5.47597600	13.60249100	13.26716300	0.2401
C57	6.81880000	13.34978500	12.84492500	-0.8280
C58	5.54827400	14.13087700	14.75166300	-0.7953
C59	4.69092000	12.28152600	13.28494100	-0.8083
C60	7.47024400	20.01893400	7.88029500	0.2317
C61	8.25773700	20.72880900	8.92033400	-0.8074
C62	8.34274100	18.97594600	7.30027300	-0.8064
C63	7.04970900	20.92637900	6.76692000	-0.8036
C65	-1.91128700	14.10101200	13.21605000	-0.9989
C66	-2.86907100	14.04128100	10.92040800	-1.0067
C67	-3.36358400	15.96414600	12.34046200	-0.9786

H68	5.70783900	13.84830500	9.89370300	0.1494
H69	6.74650800	13.63235600	8.69810300	0.2408
H70	5.18116200	13.74262800	8.38698000	0.1811
H71	7.21764900	17.02551300	9.62480400	0.1430
H72	7.98677500	15.63562800	9.43813100	0.2425
H73	6.93476600	15.81482000	10.63150900	0.1424
H74	5.62662300	15.54373500	6.78692100	0.1652
H75	7.19331300	15.46103100	7.09804300	0.2418
H76	6.42331700	16.85551000	7.24027100	0.1711
H77	3.16675000	12.85815600	8.77810600	0.1119
H78	2.61190600	11.67732800	9.70258500	0.1438
H79	3.65671200	12.73180300	10.29594100	0.1178
H80	-0.16764900	13.91033300	9.42701900	0.0817
H81	0.29381800	12.41247400	9.11145200	0.1404
H82	0.87181800	13.62776200	8.24475300	0.0774
H83	1.99121000	13.12464600	12.10712000	0.1130
H84	1.05294400	12.05638800	11.37153600	0.1356
H85	0.48822600	13.51289500	11.71599400	0.0889
H86	2.32323400	17.29200300	5.19797200	0.1586
H87	2.45095600	18.63823800	4.34016200	0.2378
H88	1.46087000	18.58080500	5.59576500	0.1360
H89	2.52278100	20.63232100	6.49357600	0.1065
H90	3.45693300	20.65069900	5.19352800	0.2241
H91	4.11444800	20.66218600	6.65358200	0.1684
H92	5.51748000	18.48202000	6.00689100	0.1794
H93	4.84885700	18.54634500	4.55572600	0.2339
H94	4.73930200	17.20929900	5.42909200	0.1837
H95	-1.73982600	15.40130000	8.69143600	0.1089
H96	-2.71783300	16.27658300	7.77806900	0.1325
H97	-2.08997000	16.90605100	9.10923000	0.0772
H98	0.25774400	16.39145000	5.82021800	0.1127
H99	-1.28329000	15.96414600	5.73577000	0.1462
H100	-0.24469800	15.05670100	6.54691200	0.1272
H101	-1.35257400	18.75769900	7.89140600	0.0639
H102	-1.96243300	18.14201500	6.54691200	0.1415
H103	-0.42415700	18.57850800	6.60024700	0.0716
H104	5.73305300	17.14497400	14.00941300	0.1679
H105	7.15379700	17.88241700	14.01385800	0.2382
H106	6.84614800	16.74294100	12.93159500	0.1757
H107	4.97942800	20.42096600	12.92937300	0.1144
H108	6.05392700	20.01433900	14.04497000	0.2120
H109	4.61922700	19.30676100	14.02052400	0.1138
H110	7.48464800	18.56931800	11.17597400	0.1827
H111	7.71339700	19.51581800	12.44713200	0.2394
H112	6.72309200	19.97298700	11.27597700	0.1562
H113	3.67834100	16.59591200	14.72944000	0.1137
H114	2.61381000	16.83713200	15.90059500	0.1451
H115	2.89163100	17.98579700	14.82055400	0.0743
H116	0.78660700	14.65237100	13.81385000	0.1271
H117	1.38036400	14.83845400	15.28946100	0.1338
H118	2.35968700	14.50534200	14.06719300	0.1067
H119	0.40746100	18.05012200	14.21831000	0.0771
H120	0.17669800	16.95659300	15.36279700	0.1390
H121	-0.32778300	16.67172400	13.87163000	0.0913
H122	2.91678500	22.25653300	8.12474800	0.1772
H123	2.72936700	23.51547000	9.09589600	0.2337
H124	1.69797200	22.29558800	9.16034300	0.1260
H125	5.44004500	22.01761100	10.66262100	0.1843
H126	4.97024300	23.34317000	9.90037000	0.2300
H127	5.32125200	22.02220500	9.06700600	0.1811
H128	2.00473200	22.08193600	11.48042900	0.1156
H129	2.96558100	23.35925100	11.40042600	0.2166
H130	3.48709200	22.00612400	12.08045200	0.1288
H131	-0.71860900	19.62838800	13.41161300	0.1089
H132	-1.44279900	20.99300200	12.99159700	0.1245
H133	0.12895300	20.81381000	12.75158800	0.0559
H134	-2.52971000	18.90932300	10.56928400	0.1118
H135	-2.97661000	19.93623000	11.71154900	0.1299
H136	-2.36307500	18.51418200	12.11156400	0.1277
H137	-0.13550300	21.44327800	10.51372700	0.0768

H138	-1.70493200	21.63165900	10.76262500	0.1382
H139	-1.19104300	20.66907800	9.59147000	0.0702
H140	1.54734900	12.61463900	6.24023300	0.2272
H141	1.79689000	12.46071800	4.66906400	0.2474
H142	0.97356000	13.71276300	5.22908400	0.2286
H143	4.88003800	13.43708300	5.76466000	0.2308
H144	4.05983400	12.34125700	4.93351800	0.2566
H145	3.88611800	12.43544700	6.52246600	0.2300
H146	2.68964200	15.29792000	4.05348500	0.2182
H147	3.44759900	13.99533400	3.51568700	0.2462
H148	4.23464300	15.07048500	4.40238700	0.2224
H149	6.81207600	13.00748200	11.92489100	0.2343
H150	7.22844300	12.68355900	13.43605800	0.2609
H151	7.33441400	14.18141800	12.88048200	0.2303
H152	6.00686400	14.99467300	14.76944100	0.2146
H153	6.03064100	13.48762400	15.30501700	0.2404
H154	4.63418600	14.24114900	15.10056500	0.2143
H155	3.81091500	12.43085300	13.68717900	0.2288
H156	5.18243500	11.61759800	13.81162800	0.2469
H157	4.58069100	11.95530500	12.36712900	0.2224
H158	7.71116700	21.44098100	9.31368200	0.2270
H159	9.05877600	21.11935500	8.51142900	0.2474
H160	8.52200300	20.09474600	9.61813800	0.2328
H161	8.62016500	18.35336900	8.00474400	0.2300
H162	9.13642900	19.39635700	6.90692500	0.2494
H163	7.85266400	18.48891200	6.60691400	0.2301
H164	6.53821600	20.41407400	6.10467300	0.2290
H165	7.84475900	21.30773600	6.34023700	0.2485
H166	6.49250400	21.64774100	7.12471100	0.2207
H167	-1.21537200	13.45316400	12.98048600	0.1412
H168	-2.70234100	13.62546400	13.54495100	0.1316
H169	-1.57727400	14.70061500	13.91607600	0.1329
H170	-3.12505900	14.59264000	10.15149100	0.1401
H171	-3.66103400	13.58181500	11.27153300	0.1285
H172	-2.20482600	13.37735300	10.63817600	0.1310
H173	-3.02267500	16.56604700	13.03604300	0.1285
H174	-4.16797800	15.50927500	12.66714000	0.1327
H175	-3.58463400	16.48564000	11.53820900	0.1373

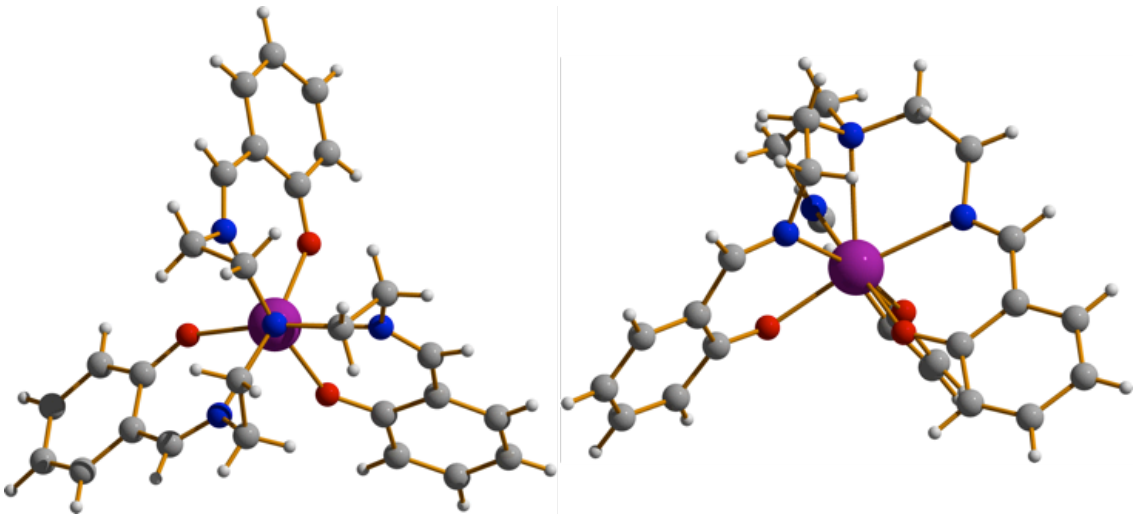

Figure S2. Experimental structure of Er-trensal (two views) possessing a near-C_3 symmetry. Color scheme: Er- purple, O- red, N-blue, C-grey, H-white.

Table S11. Cartesian coordinates (in Å) and calculated atomic charges of the *trensal*$^{3-}$ ligand (computed alone) in various computational models.

Atom	Cartesian coordinates			Charge						
	x	y	z	B3LYP		M06		M062X		CASPT2
				LoProp	Mulliken	LoProp	Mulliken	LoProp	Mulliken	Mulliken
Er1	6.489149	3.745763	3.383046	not included in these calculations						
O2	4.649010	3.972779	2.219125	-0.5255	-0.4263	-0.5380	-0.4681	-0.5425	-0.4445	-0.5688
N3	4.887787	2.167890	4.368643	-0.1903	-0.0560	-0.2042	-0.0907	-0.1926	-0.0520	-0.1738
N4	6.489149	3.745763	6.098864	-0.1684	-0.2021	-0.1890	-0.2441	-0.1845	-0.2080	-0.3845
C5	3.518065	3.398496	1.978816	0.2624	0.0693	0.2800	0.1357	0.2708	0.0600	0.1324
C6	2.698567	3.813193	0.906543	-0.2231	0.1199	-0.2302	0.0747	-0.2291	0.0945	0.1003
C7	1.496248	3.205195	0.644690	-0.1740	0.0266	-0.1703	0.0144	-0.1713	-0.0177	0.0103
C8	1.033618	2.131927	1.403733	-0.2776	-0.0551	-0.2860	-0.0932	-0.2884	-0.0857	-0.1728
C9	1.794070	1.727344	2.472692	-0.1684	0.1551	-0.1656	0.1271	-0.1656	0.1080	0.2195
C10	3.021046	2.317360	2.777635	-0.0844	-0.1658	-0.0927	-0.1797	-0.1009	-0.1627	-0.3125
C11	3.721804	1.829613	3.974205	-0.0218	-0.0431	-0.0108	-0.0103	-0.0174	-0.0679	0.0028
C12	5.333547	1.609341	5.669623	-0.1365	0.0456	-0.1352	0.0379	-0.1369	-0.0204	-0.0217
C13	5.474996	2.780383	6.594397	-0.1348	0.0264	-0.1311	0.0262	-0.1327	-0.0304	-0.0250
H14	2.987305	4.529080	0.353005	0.1080	-0.1206	0.1086	-0.0956	0.1106	-0.0822	-0.0579
H15	0.964840	3.525490	-0.074579	0.0847	-0.1299	0.0849	-0.1088	0.0872	-0.0960	-0.0762
H16	0.218662	1.693629	1.188284	0.0802	-0.1422	0.0800	-0.1225	0.0815	-0.1086	-0.0857
H17	1.476783	1.020448	3.022915	0.0817	-0.1247	0.0838	-0.0989	0.0872	-0.0856	-0.0671
H18	3.257876	1.196891	4.509513	0.0330	-0.0944	0.0351	-0.0860	0.0413	-0.0563	-0.0102
H19	4.687941	0.999095	6.006055	0.0533	-0.0747	0.0596	-0.0564	0.0627	-0.0280	0.0082
H20	6.166022	1.165423	5.570185	0.1241	0.0765	0.1237	0.0739	0.1251	0.0985	0.1236
H21	5.740376	2.466831	7.451221	0.0576	-0.0778	0.0635	-0.0582	0.0643	-0.0342	-0.0044
H22	4.636682	3.220929	6.665661	0.1078	0.0586	0.1079	0.0597	0.1084	0.0805	0.1070
O23	7.211968	2.039772	2.219125	-0.5255	-0.4263	-0.5377	-0.4678	-0.5425	-0.4446	-0.5688
C24	8.274784	1.347486	1.978816	0.2624	0.0691	0.2801	0.1362	0.2708	0.0602	0.1324
C25	8.325394	0.430431	0.906543	-0.2231	0.1200	-0.2301	0.0749	-0.2291	0.0946	0.1003
C26	9.453096	-0.306809	0.644690	-0.1740	0.0266	-0.1703	0.0140	-0.1713	-0.0178	0.0103
C27	10.613888	-0.170824	1.403733	-0.2776	-0.0551	-0.2860	-0.0931	-0.2884	-0.0857	-0.1728
C28	10.584041	0.690038	2.472692	-0.1684	0.1551	-0.1656	0.1270	-0.1656	0.1082	0.2195
C29	9.459584	1.457622	2.777635	-0.0844	-0.1657	-0.0927	-0.1798	-0.1010	-0.1628	-0.3125
C30	9.531607	2.308370	3.974205	-0.0218	-0.0431	-0.0107	-0.0102	-0.0174	-0.0681	0.0028
N31	8.655659	3.149003	4.368643	-0.1903	-0.0561	-0.2045	-0.0904	-0.1926	-0.0521	-0.1738
O32	7.604522	5.225861	2.219125	-0.5255	-0.4263	-0.5379	-0.4681	-0.5424	-0.4445	-0.5688
C33	7.672651	6.492430	1.978816	0.2624	0.0692	0.2801	0.1358	0.2708	0.0601	0.1324
C34	8.441539	6.994787	0.906543	-0.2231	0.1200	-0.2302	0.0746	-0.2291	0.0945	0.1003
C35	8.516156	8.340025	0.644690	-0.1740	0.0265	-0.1703	0.0142	-0.1713	-0.0178	0.0103
C36	7.817994	9.277309	1.403733	-0.2776	-0.0551	-0.2861	-0.0932	-0.2884	-0.0857	-0.1728
C37	7.087389	8.821029	2.472692	-0.1684	0.1551	-0.1656	0.1269	-0.1656	0.1083	0.2195
C38	6.984870	7.463429	2.777635	-0.0844	-0.1658	-0.0926	-0.1795	-0.1010	-0.1629	-0.3125

C39	6.212090	7.100428	3.974205	-0.0218	-0.0430	-0.0108	-0.0101	-0.0174	-0.0681	0.0028
N40	5.922054	5.921519	4.368643	-0.1903	-0.0561	-0.2041	-0.0903	-0.1926	-0.0520	-0.1738
C41	7.831620	3.351294	6.594397	-0.1347	0.0266	-0.1310	0.0266	-0.1326	-0.0301	-0.0247
C42	8.916497	3.814317	5.669623	-0.1366	0.0455	-0.1352	0.0372	-0.1369	-0.0203	-0.0217
H43	9.767788	3.560329	6.006055	0.0533	-0.0747	0.0596	-0.0563	0.0627	-0.0280	0.0082
H44	8.884703	4.757220	5.570185	0.1241	0.0765	0.1236	0.0739	0.1250	0.0985	0.1236
H45	7.970473	3.737896	7.451221	0.0575	-0.0779	0.0634	-0.0584	0.0642	-0.0343	-0.0045
H46	7.869253	2.405020	6.665661	0.1078	0.0585	0.1079	0.0596	0.1083	0.0805	0.1070
C47	6.158884	5.106734	6.594397	-0.1349	0.0263	-0.1311	0.0261	-0.1327	-0.0306	-0.0250
C48	5.215456	5.814754	5.669623	-0.1365	0.0457	-0.1352	0.0375	-0.1369	-0.0200	-0.0217
H49	5.009771	6.678988	6.006055	0.0533	-0.0747	0.0596	-0.0565	0.0627	-0.0280	0.0082
H50	4.414775	5.315769	5.570185	0.1241	0.0765	0.1236	0.0740	0.1250	0.0984	0.1236
H51	5.754651	5.033685	7.451221	0.0576	-0.0777	0.0635	-0.0580	0.0643	-0.0341	-0.0043
H52	6.959565	5.612463	6.665661	0.1078	0.0585	0.1079	0.0597	0.1083	0.0805	0.1070
H53	5.896100	7.818563	4.509513	0.0330	-0.0944	0.0351	-0.0860	0.0413	-0.0563	-0.0102
H54	6.633842	9.449257	3.022915	0.0817	-0.1247	0.0838	-0.0989	0.0872	-0.0856	-0.0671
H55	7.845894	10.202230	1.188284	0.0802	-0.1422	0.0800	-0.1225	0.0815	-0.1087	-0.0857
H56	9.059244	8.640091	-0.074579	0.0847	-0.1299	0.0849	-0.1088	0.0872	-0.0960	-0.0762
H57	8.917146	6.386789	0.353005	0.1080	-0.1206	0.1086	-0.0955	0.1106	-0.0822	-0.0579
H58	10.311524	2.222958	4.509513	0.0330	-0.0944	0.0351	-0.0860	0.0413	-0.0562	-0.0102
H59	11.354875	0.768707	3.022915	0.0817	-0.1247	0.0838	-0.0989	0.0872	-0.0856	-0.0671
H60	11.400943	-0.657447	1.188284	0.0802	-0.1422	0.0800	-0.1225	0.0815	-0.1086	-0.0857
H61	9.441416	-0.927169	-0.074579	0.0847	-0.1299	0.0849	-0.1088	0.0872	-0.0960	-0.0762
H62	7.561049	0.322542	0.353005	0.1080	-0.1206	0.1086	-0.0955	0.1106	-0.0822	-0.0579

Table S12. Calculated energy splitting of the ground J=15/2 multiplet for the Er^{3+} free ion (in cm^{-1}) inserted in the field created by the atomic charges of the *trensal*$^{3-}$ ligand listed in Table S11. These energies are included in Figure 7 of the main text.

B3LYP		M06		M062X		CASPT2	FAIEMP
LoProp	Mulliken	LoProp	Mulliken	LoProp	Mulliken	Mulliken	Mulliken
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
10.427	8.999	9.734	7.242	10.195	7.654	4.492	6.291
10.427	8.999	9.734	7.242	10.195	7.654	4.492	6.291
25.529	23.171	24.695	20.714	25.508	20.631	18.979	43.846
25.529	23.171	24.695	20.714	25.508	20.631	18.979	43.846
35.341	33.205	34.468	30.174	35.555	29.969	30.133	90.055
35.341	33.205	34.468	30.174	35.555	29.969	30.133	90.055
39.006	37.045	38.088	33.519	39.302	33.492	34.005	160.604
39.006	37.045	38.088	33.519	39.302	33.492	34.005	160.604
79.087	63.972	79.573	64.831	80.350	62.008	74.801	188.873
79.087	63.972	79.573	64.831	80.350	62.008	74.801	188.873
80.913	65.487	81.439	66.379	82.235	63.499	76.867	201.133
80.913	65.487	81.439	66.379	82.235	63.499	76.867	201.133
81.850	66.797	82.324	67.477	83.210	64.642	78.156	243.337
81.850	66.797	82.324	67.477	83.210	64.642	78.156	243.337
g tensor of the ground Kramers doublet							
0.00111	0.00079	0.00014	0.00102	0.00135	0.00152	0.00507	7.71259
0.00134	0.00089	0.00058	0.00150	0.00165	0.00176	0.00703	7.34849
17.41775	17.59741	17.37042	17.45758	17.40149	17.47573	17.16437	4.03559

Table S13. *Ab initio* derived parameters of the crystal-field of the ground J=15/2 multiplet of the Er3+ ion for all computed models, given in the initial coordinate system. The quantization axis is the Cartesian z, parallel to the near-C_3 symmetry axis of the compound. Labeling of the computational models is the same as used in the main text, Table 2.
The following parameters are given in terms of Extended Stevens Operators, as defined in Rudowicz, C.; J.Phys.C: Solid State Phys.,18(1985) 1415-1430 ; and also as implemented in the EasySpin function in MATLAB.

CASSCF active space: CAS(11in7), ($4f^{11}$ shell).

rank	projection	A1	A2	A3	A4
2	-2	0.33554262E-02	0.15645289E-01	0.33345663E-02	0.12232506E-01
	-1	-0.36575708E-02	-0.71215221E-02	-0.32564856E-02	-0.60183532E-02
	0	-0.90653805E+00	-0.11157454E+01	-0.82297164E+00	-0.10087775E+01
	1	0.71216399E-02	0.35419525E-02	0.58486274E-02	0.65691850E-02
	2	-0.43492087E-03	-0.15352024E-02	-0.28702990E-03	-0.67885416E-03
4	-4	0.29142247E-04	0.19223775E-04	0.28036259E-04	-0.22497330E-04
	-3	0.81224359E-01	0.11570903E+00	0.80461697E-01	0.11477811E+00
	-2	0.14295448E-03	0.76468927E-04	0.12379629E-03	0.34338044E-04
	-1	-0.58483508E-04	-0.96725773E-04	-0.57593441E-04	-0.51321157E-04
	0	-0.97975997E-03	-0.79585241E-03	-0.96843667E-03	-0.78992258E-03
	1	0.70531652E-04	-0.15437009E-04	0.70166736E-04	0.92980189E-05
	2	0.40349870E-04	-0.12817141E-03	0.30828449E-04	-0.98031208E-04
	3	0.15024025E+00	0.22071505E+00	0.15006666E+00	0.22013795E+00
	4	-0.15842003E-03	-0.19713933E-03	-0.13579482E-03	-0.18295369E-03
6	-6	0.73098120E-03	0.11236492E-02	0.74245288E-03	0.11461311E-02
	-5	0.15204626E-04	0.16076653E-04	0.13843057E-04	0.13436269E-04
	-4	0.55612800E-07	-0.15959983E-05	0.13230370E-06	-0.13124124E-05
	-3	-0.48296823E-03	-0.68841563E-03	-0.52220068E-03	-0.76896062E-03
	-2	-0.27719567E-05	-0.41532771E-05	-0.25000966E-05	-0.36755528E-05
	-1	0.26819451E-05	0.45957250E-05	0.21431996E-05	0.42064100E-05
	0	0.10007000E-03	0.15608498E-03	0.98806083E-04	0.15384815E-03
	1	-0.38045270E-05	-0.72216437E-05	-0.28024667E-05	-0.55034449E-05
	2	-0.11348259E-05	-0.32008631E-05	-0.91964300E-06	-0.29221533E-05
	3	-0.73927805E-03	-0.12122852E-02	-0.72528556E-03	-0.11929779E-02
	4	0.10713150E-05	0.22305062E-05	0.77593494E-06	0.19750662E-05
	5	-0.36930260E-05	-0.42195506E-05	-0.39388129E-05	-0.37301717E-05
	6	0.49889355E-03	0.77162632E-03	0.48780699E-03	0.75363479E-03
		Energy spectra recovered with the above CF parameters (in cm-1)			
		0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000
		62.175	86.146	53.813	77.562
		62.175	86.146	53.813	77.562
		102.801	148.759	95.140	137.216
		102.801	148.759	95.140	137.216
		104.073	153.522	98.466	149.017
		104.073	153.522	98.466	149.017
		213.001	363.960	214.919	366.768
		213.001	363.960	214.919	366.768
		414.728	614.628	406.126	604.778
		414.728	614.628	406.126	604.778
		456.237	680.945	448.484	672.207
		456.237	680.945	448.484	672.207
		483.249	723.535	474.204	712.479
		483.249	723.535	474.204	712.479
		Recovery factor of the initial ab initio energy matrix (in %)			
		98.964	97.898	98.953	97.935

CASSCF active space: CAS(11in14), ($4f^{11}$ + $5f^{0}$ shell).

rank	projection	B1	B2	B3	B4
2	-2	0.33069178E-02	0.23038309E-02	0.33310800E-02	0.30468557E-02
	-1	-0.95502602E-03	0.12014236E-02	-0.10467050E-02	0.11733037E-04
	0	-0.94948136E+00	-0.11122607E+01	-0.85842293E+00	-0.10041023E+01
	1	0.24641221E-02	0.56794895E-03	0.20612143E-02	0.21784022E-02
	2	-0.16004134E-03	-0.22246278E-02	-0.65267510E-04	-0.17501442E-02
4	-4	0.21576694E-04	0.54909958E-04	0.20657079E-04	0.51336617E-04
	-3	0.85321862E-01	0.10677587E+00	0.84163015E-01	0.10557887E+00
	-2	0.65929659E-04	0.27349370E-04	0.58632709E-04	0.14664862E-04
	-1	-0.25131011E-04	-0.46727343E-04	-0.25698349E-04	-0.48661380E-04
	0	-0.61163434E-03	-0.55875272E-03	-0.62693453E-03	-0.54548295E-03
	1	0.23023772E-04	0.60357855E-04	0.24226914E-04	0.66598107E-04
	2	0.46524906E-05	-0.19816623E-04	0.77404715E-06	-0.28068185E-04
	3	0.15563386E+00	0.19528516E+00	0.15556920E+00	0.19564818E+00
	4	-0.63903694E-04	-0.22169983E-03	-0.54414840E-04	-0.23000073E-03
6	-6	0.78845565E-03	0.96671484E-03	0.80161396E-03	0.98726158E-03
	-5	0.10199452E-04	0.12967029E-04	0.96357228E-05	0.11937595E-04
	-4	-0.26590448E-07	-0.42284782E-06	0.18053210E-07	-0.40008169E-06
	-3	-0.50563217E-03	-0.63971423E-03	-0.55387512E-03	-0.70026556E-03
	-2	-0.15365696E-05	-0.56767376E-06	-0.14244673E-05	-0.40496514E-06
	-1	0.10816614E-05	0.14077862E-05	0.87626958E-06	0.12214450E-05
	0	0.10796431E-03	0.13367383E-03	0.10598665E-03	0.13213951E-03
	1	-0.12427450E-05	-0.19056907E-05	-0.82329473E-06	-0.15741555E-05
	2	-0.59419596E-06	0.34740060E-07	-0.49731259E-06	0.19863233E-06
	3	-0.82856714E-03	-0.10575970E-02	-0.81231828E-03	-0.10403104E-02
	4	0.34130667E-06	0.12036835E-05	0.22808297E-06	0.55684369E-06
	5	-0.32601874E-05	-0.29561071E-05	-0.34078573E-05	-0.28996589E-05
	6	0.55059999E-03	0.67345254E-03	0.53828039E-03	0.66057440E-03
		Energy spectra recovered with the above CF parameters (in cm-1)			
		0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000
		70.751	80.867	61.191	70.658
		70.751	80.867	61.191	70.658
		110.768	131.844	102.916	122.497
		110.768	131.844	102.916	122.497
		113.629	133.980	105.488	126.733
		113.629	133.980	105.488	126.733
		241.350	305.772	241.595	309.146
		241.350	305.772	241.595	309.146
		443.362	547.964	433.095	538.045
		443.362	547.964	433.095	538.045
		487.769	600.829	478.367	592.274
		487.769	600.829	478.367	592.274
		518.252	635.896	507.060	625.663
		518.252	635.896	507.060	625.663
		Recovery factor of the initial ab initio energy matrix (in %)			
		98.993	98.249	98.982	98.234

RASSCF active space: CAS(17in25) (Ras1 - $5p^6$, Ras2 - $4f^{11}$, Ras3 - $5f^0$, $5d^0$ and $6p^0$).**

rank	projection	C1	C2	C3	C4
2	-2	0.37161614E-02	0.19477249E-02	0.37270342E-02	0.32696935E-02
	-1	-0.11642244E-03	0.12483490E-02	-0.40324710E-03	-0.62862203E-03
	0	-0.96314591E+00	-0.10350985E+01	-0.87201558E+00	-0.93000927E+00
	1	0.20747581E-03	-0.57326387E-03	0.14328311E-03	0.31450400E-02
	2	0.48010450E-03	-0.21397901E-02	0.59988302E-03	-0.13686190E-02
4	-4	0.62593058E-05	0.30461207E-04	0.50686335E-05	0.21434324E-04
	-3	0.93771115E-01	0.10981953E+00	0.92928921E-01	0.10892142E+00
	-2	0.29534389E-04	-0.35791517E-04	0.24173669E-04	-0.50491923E-04
	-1	-0.20859188E-04	-0.41862102E-04	-0.21473783E-04	-0.45341670E-04
	0	-0.10259560E-02	-0.76100932E-03	-0.10205064E-02	-0.72985689E-03
	1	0.15593511E-04	0.62443399E-04	0.16614608E-04	0.70230944E-04
	2	-0.15570700E-04	-0.57538921E-04	-0.18253292E-04	-0.68712939E-04
	3	0.16669852E+00	0.19583799E+00	0.16649319E+00	0.19581988E+00
	4	-0.29255367E-04	-0.23075849E-03	-0.21808970E-04	-0.25913977E-03
6	-6	0.81240748E-03	0.93827335E-03	0.82575013E-03	0.95771529E-03
	-5	0.76897235E-05	0.97470867E-05	0.72655385E-05	0.84758760E-05
	-4	-0.55515534E-07	-0.45073183E-06	-0.45802385E-07	-0.57607889E-06
	-3	-0.52766122E-03	-0.62862186E-03	-0.57538716E-03	-0.68429371E-03
	-2	-0.88057342E-06	0.66533114E-06	-0.78250255E-06	0.84816061E-06
	-1	-0.56410440E-07	0.60690602E-07	-0.18591026E-06	-0.54403895E-09
	0	0.10936137E-03	0.12928833E-03	0.10743452E-03	0.12778959E-03
	1	0.65946364E-06	0.17612388E-06	0.94701458E-06	0.23848257E-06
	2	-0.43710069E-06	0.63153221E-06	-0.38698741E-06	0.80548106E-06
	3	-0.82668986E-03	-0.99737382E-03	-0.81079827E-03	-0.98020590E-03
	4	-0.38589039E-06	-0.12659347E-06	-0.48019368E-06	-0.10932861E-05
	5	-0.29282828E-05	-0.18807030E-05	-0.30156413E-05	-0.16118854E-05
	6	0.55243139E-03	0.63532438E-03	0.54057162E-03	0.62331888E-03
		Energy spectra recovered with the above CF parameters (in cm-1)			
		0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000
		62.783	68.535	53.224	58.839
		62.783	68.535	53.224	58.839
		108.766	122.287	98.193	111.569
		108.766	122.287	98.193	111.569
		109.130	122.870	103.961	117.773
		109.130	122.870	103.961	117.773
		235.425	291.842	236.346	295.601
		235.425	291.842	236.346	295.601
		455.642	531.100	445.690	521.411
		455.642	531.100	445.690	521.411
		500.786	581.642	491.597	573.206
		500.786	581.642	491.597	573.206
		529.233	613.391	518.376	603.491
		529.233	613.391	518.376	603.491
		Recovery factor of the initial ab initio energy matrix (in %)			
		99.021	98.160	99.013	98.122

The difference between the energy spectra reported here and the ab initio spectra reported in Table 2 in the main text lies in the non-crystal field contributions, i.e. parameters of ranks 8, 10, 12 and 14. Their cumulative weight of the operators of these ranks is smaller than 2% for the entire energy matrix.

Table S14. *Ab initio* derived parameters of the crystal-field of the ground J=15/2 multiplet of the Dy^{3+} ions in Dy_4K_2 compound [50] in ab initio calculation and also using the point-charge electrostatic model for each Dy sites as given in Tables S7-S10. The quantization axis is the Cartesian z, parallel to the near-C_3 symmetry axis of the compound. Labeling of the computational models is the same as used in the main text, Table 2. The following parameters are given in terms of Extended Stevens Operators, as defined in Rudowicz, C.; J.Phys.C: Solid State Phys.,18(1985) 1415-1430 ; and also as implemented in the EasySpin function in MATLAB.

Ab initio parameters and electrostatic ones for each Dy site are given for the same coordinate frame and the same quantization axis.

Ab initio calculations:

rank	projection	Dy1 - ab initio	Dy2 - ab initio	Dy3 - ab initio	Dy4 - ab initio
2	-2	-0.66718516E+00	0.53279367E+00	0.15435940E+01	-0.51936442E+00
	-1	0.10348958E+01	0.58360115E+00	-0.13125250E+01	-0.66457378E+00
	0	-0.48813073E+01	-0.54321866E+01	-0.40756737E+01	-0.37079134E+01
	1	-0.10999643E+01	0.44884449E-01	-0.11925241E+01	0.10868966E+01
	2	0.63932035E+00	0.10044601E+01	-0.54056855E-01	-0.64100939E+00
4	-4	-0.14378849E-01	0.97717170E-02	-0.25007381E-01	-0.40626414E-01
	-3	0.13485933E-02	0.26286126E-03	-0.94897668E-02	0.12692108E-01
	-2	0.37485571E-02	-0.16164622E-02	-0.51973117E-02	0.21858655E-02
	-1	-0.10080913E-01	-0.70654092E-02	0.52266524E-02	0.27415675E-02
	0	-0.12185249E-01	-0.12766939E-01	-0.11673534E-01	-0.11450944E-01
	1	0.15161117E-01	-0.44868919E-02	0.16033833E-01	-0.15470680E-01
	2	-0.46280268E-02	-0.44872590E-02	-0.20524489E-02	0.45785840E-03
	3	0.15717383E-01	-0.29371876E-02	0.59584903E-02	0.66039401E-03
	4	0.37572026E-01	0.36386403E-01	0.31154893E-01	-0.21640662E-02
6	-6	-0.52531068E-04	0.41366402E-04	0.45212184E-04	0.25679190E-04
	-5	0.80399071E-04	0.28655934E-04	-0.29844555E-03	0.16049990E-03
	-4	-0.26866690E-04	0.14025759E-04	-0.82770308E-04	-0.12113469E-03
	-3	0.21040554E-04	0.92014634E-07	-0.26895116E-04	0.62509037E-04
	-2	-0.10623470E-04	-0.18016589E-05	-0.52527731E-04	0.13628256E-04
	-1	0.68612317E-04	0.53498272E-04	0.45468389E-04	0.12372396E-04
	0	0.34081734E-04	0.40899697E-04	0.24597881E-04	0.21580367E-04
	1	-0.14738757E-03	0.59731918E-04	-0.12851649E-03	0.13872552E-03
	2	0.13009913E-04	-0.76207812E-05	0.19393678E-04	0.45844056E-04
	3	0.73147554E-04	-0.40257426E-04	0.29020181E-04	0.13013637E-04
	4	0.81025900E-04	0.76739488E-04	0.77169680E-04	0.87902847E-05
	5	0.58029131E-04	-0.16315516E-03	-0.20141690E-03	-0.17408223E-03
	6	0.28109209E-04	0.51983626E-04	0.21446188E-04	-0.14474849E-04
		Energy spectra recovered with the above CF parameters (in cm-1)			
		0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000
		381.342	401.090	356.907	343.898
		381.342	401.090	356.907	343.898
		667.158	727.523	556.476	524.722
		667.158	727.523	556.476	524.722
		738.143	830.304	624.752	591.419
		738.143	830.304	624.752	591.419
		810.865	900.277	720.818	664.537
		810.865	900.277	720.818	664.537
		879.361	959.587	765.962	729.095
		879.361	959.587	765.962	729.095
		941.854	1016.185	843.747	791.590
		941.854	1016.185	843.747	791.590
		1041.397	1112.102	918.926	827.831
		1041.397	1112.102	918.926	827.831
		Recovery factor of the initial ab initio energy matrix (in %)			
		98.183	98.428	98.435	98.487

Electrostatic model for Dy^{3+} ions calculations where ligand atoms were described using point charges listed in Table S7-S10.

rank	projection	Dy1 - electrostatic	Dy2 - electrostatic	Dy3 - electrostatic	Dy4 - electrostatic
2	-2	0.14477657E+00	0.33562921E+00	0.14826950E+01	-0.54748283E+00
	-1	0.46966225E+00	-0.72354165E+00	-0.17644033E+01	-0.65532405E+00
	0	-0.10241267E+01	-0.11961196E+01	-0.85129759E+00	-0.94444708E-01
	1	0.18860709E+01	-0.22486758E+01	0.16684996E+01	-0.13337186E+01
	2	0.10536347E+01	0.12446014E+01	-0.12091653E+00	-0.34031560E+00
4	-4	-0.57637913E-02	0.35645245E-02	-0.10515862E-01	-0.17588368E-01
	-3	-0.45000458E-03	-0.61003894E-03	0.15796369E-03	0.18106265E-01
	-2	0.11726387E-02	-0.62462308E-03	-0.15758051E-02	0.47399433E-03
	-1	-0.42136218E-02	-0.26951109E-02	-0.83441095E-03	-0.89542337E-04
	0	-0.37256711E-02	-0.38045623E-02	-0.38926796E-02	-0.36245124E-02
	1	0.69615169E-02	-0.25077102E-02	0.92659181E-02	-0.10929104E-01
	2	-0.11046525E-02	-0.83165939E-03	-0.11628389E-02	-0.64977864E-03
	3	0.11008779E-01	-0.51291562E-02	0.11710696E-01	0.43607663E-02
	4	0.14498509E-01	0.13898750E-01	0.12665981E-01	-0.86343404E-03
6	-6	-0.32664740E-05	0.46526041E-05	0.12511739E-04	0.93867378E-05
	-5	-0.36720644E-04	-0.26194044E-04	-0.32695072E-04	0.47545904E-04
	-4	0.83482806E-05	-0.65178019E-05	0.49091807E-05	0.12568539E-04
	-3	-0.20333080E-05	-0.65192942E-05	0.13476013E-04	0.19666947E-04
	-2	-0.58505114E-05	0.35089888E-06	-0.60553328E-05	0.13136086E-06
	-1	0.16666167E-04	0.14188091E-04	-0.67128599E-05	-0.42602832E-05
	0	0.81369677E-05	0.85027927E-05	0.65810588E-05	0.59486270E-05
	1	-0.31561175E-04	0.12266516E-04	-0.31621268E-04	0.24971113E-04
	2	0.34502680E-05	-0.31333099E-06	0.64509327E-05	0.75154471E-05
	3	0.27200402E-05	-0.88962848E-05	0.12898660E-04	0.13363164E-04
	4	-0.17402226E-04	-0.18317873E-04	-0.12347987E-04	0.34751755E-05
	5	0.47797405E-04	-0.36982815E-04	0.25197143E-04	0.49415570E-05
	6	0.93836697E-05	0.11061790E-04	0.87020893E-05	-0.80197003E-05
		Energy spectra recovered with the above CF parameters (in cm-1)			
		0.000	0.000	0.000	0.000
		0.000	0.000	0.000	0.000
		106.395	112.678	72.383	5.173
		106.395	112.678	72.383	5.173
		138.712	165.853	113.481	59.952
		138.712	165.853	113.481	59.952
		169.211	185.198	173.774	80.248
		169.211	185.198	173.774	80.248
		183.416	199.709	211.586	102.813
		183.416	199.709	211.586	102.813
		215.193	231.307	228.470	128.074
		215.193	231.307	228.470	128.074
		253.341	279.176	257.875	163.563
		253.341	279.176	257.875	163.563
		318.061	359.808	304.115	178.412
		318.061	359.808	304.115	178.412
		Recovery factor of the initial ab initio energy matrix (in %)			
		99.564	99.689	99.588	99.378