Pushing Boundaries in Single Molecule Magnets: An Ab Initio Perspective on Harnessing Higher Oxidation States for Unprecedented Lanthanide SMM Performance

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Table S1: *Ab initio* SINGLE_ANISO computed crystal field parameters for $[EuO2]^{2-}$, $[GdO2]^{-}$, $[TbO_2]$ and $[DyO2]^{+}$.

k	q	B_k^q			
		$[EuO_2]^{2-}$	**$[GdO_2]^{-}$**	**[TbO2]**	**$[DyO2]^{+}$**
2	−2	1.38E+02	−4.90E−03	−1.79E+00	−5.07E+01
	−1	2.65E−02	2.74E+01	−9.17E+00	−2.97E+01
	0	9.98E+02	1.29E+01	6.09E+02	2.71E+02
	1	5.09E−02	1.10E+02	−6.33E+01	8.53E+00
	2	7.05E+02	−8.65E−03	−7.06E+01	1.57E+02
4	−4	1.36E−03	−4.58E−06	5.25E−01	−3.24E−01
	−3	5.90E−03	9.33E−04	−7.30E−01	−8.66E−02
	−2	−1.25E+01	2.05E−04	8.12E−01	1.45E+00
	−1	−2.04E−03	1.25E+00	−5.61E−01	−2.85E+00
	0	−2.86E+01	−1.12E+00	−2.47E+01	−3.05E+00
	1	−3.74E−03	5.02E+00	1.76E+01	−7.30E−01
	2	−6.41E+01	3.21E−04	−3.17E−01	−4.47E+00
	3	6.86E−03	9.34E−04	−7.68E+00	−9.07E−02
	4	−1.80E−03	−3.10E−06	−6.56E+00	1.20E−01
6	−6	−1.21E−05	1.31E−09	1.90E−01	1.75E−04
	−5	−1.39E+00	−5.98E−07	5.55E−02	−1.49E−03
	−4	2.38E−04	1.33E−07	−1.07E−01	9.85E−03
	−3	−1.48E−03	4.47E−05	1.82E−01	3.99E−03
	−2	3.65E+00	−7.00E−06	−8.79E−02	−6.42E−02
	−1	−2.93E−04	4.15E−02	−2.56E−02	6.61E−03
	0	1.78E+00	−5.46E−02	4.46E+00	6.53E−02
	1	−5.44E−04	1.67E−01	1.97E+00	1.75E−02
	2	1.87E+01	−1.14E−05	−1.45E+00	1.99E−01
	3	−1.71E−03	4.47E−05	1.92E+00	3.04E−03
	4	−2.98E−04	1.24E−07	−3.24E+00	−3.67E−03
	5	8.42E+00	−5.17E−07	−1.80E+01	−2.26E−04
	6	−8.63E−06	−2.27E−09	−1.94E+00	6.20E−05

Table S2: Structure parameters of CASSCF optimized $[LnO_2]^{-}$.

Metal Ion	Ln−O1 bond distance (Å)	Ln−O2 bond distance (Å)	O−Ln−O angle (°)
Ce(III)	1.890	1.851	180.0
Pr(III)	1.837	1.874	180.0
Nd(III)	1.839	1.839	180.0
Pm(III)	2.024	2.099	180.0
Sm(III)	2.014	2.086	179.9
Eu(III)	2.009	2.009	180.0
Gd(III)	1.996	2.117	180.0

Tb(III)	1.921	1.875	179.9
Dy(III)	1.861	2.228	112.8
Ho(III)	1.853	2.214	112.8
Er(III)	1.957	2.085	180.0
Tm(III)	1.952	2.084	179.9
Yb(III)	1.952	2.082	180.0
Lu(III)	2.007	2.007	180.0

Table S3: Structure parameters of CASSCF optimized [LnO_2]

Metal Ion	Ln−O1 bond distance (Å)	Ln−O2 bond distance(Å)	O−Ln−O angle(°)
Ce(IV)	1.813	1.813	180.0
Pr(IV)	1.812	1.812	179.9
Nd(IV)	1.805	1.805	180.0
Pm(IV)	1.823	1.823	179.9
Sm(IV)	1.844	1.844	179.9
Eu(IV)	1.853	1.852	179.9
Gd(IV)	1.885	1.885	179.9
Tb(IV)	1.839	1.839	179.9
Dy(IV)	1.865	1.865	179.9
Ho(IV)	1.892	1.892	180.0
Er(IV)	1.867	1.867	179.9
Tm(IV)	1.865	1.864	179.9
Yb(IV)	1.778	2.128	179.9
Lu(IV)	1.902	1.902	179.9

Table S4: |V(r)|/G(r) ratio of casscf optimised $[LnO2]^-$ where Ln ranges from Ce to Lu.

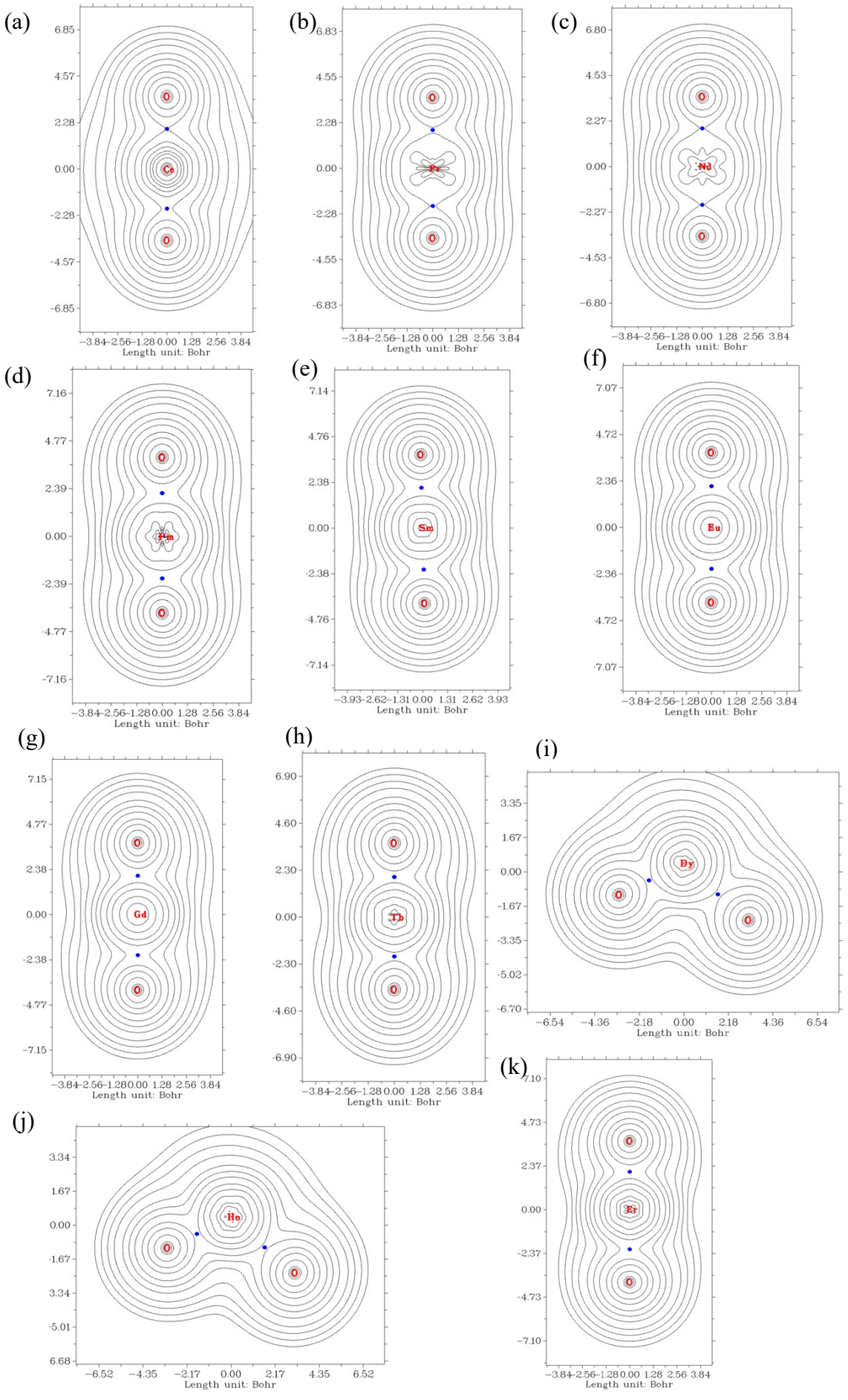
Metal (III)		V(r)	G(r)	|V(r)/G(r)|
Ce	BCP−1	−0.297	0.175	1.694
	BCP−2	−0.337	0.192	1.750

Pr	BCP−1	−0.306	0.197	1.553
	BCP−2	−0.341	0.212	1.609
Nd	BCP−1	−0.344	0.216	1.588
	BCP−2	−0.344	0.217	1.588
Pm	BCP−1	−0.164	0.128	1.286
	BCP−2	−0.207	0.154	1.342
Sm	BCP−1	−0.150	0.118	1.270
	BCP−2	−0.191	0.146	1.312
Eu	BCP−1	−0.191	0.154	1.244
	BCP−2	−0.191	0.154	1.244
Gd	BCP−1	−0.224	0.176	1.277
	BCP−2	−0.154	0.130	1.187
Tb	BCP−1	−0.279	0.216	1.293
	BCP−2	−0.324	0.242	1.337
Dy	BCP−1	−0.091	0.077	1.179
	BCP−2	−0.327	0.242	1.352
Ho	BCP−1	−0.093	0.079	1.183
	BCP−2	−0.331	0.248	1.335
Er	BCP−1	−0.214	0.176	1.215
	BCP−2	−0.137	0.117	1.168
Tm	BCP−1	−0.140	0.118	1.184
	BCP−2	−0.219	0.178	1.230
Yb	BCP−1	−0.137	0.116	1.180
	BCP−2	−0.215	0.175	1.225
Lu	BCP−1	−0.195	0.167	1.168
	BCP−2	−0.195	0.167	1.168

Table S5: |V(r)/G(r)| ratio of CASSCF optimised [LnO_2] where Ln ranges from Ce to Lu.

Metal (IV)		V(r)	G(r)	|V(r)/G(r)|
Ce	BCP−1	−0.383	0.206	1.859
	BCP−2	−0.383	0.206	1.859
Pr	BCP−1	−0.393	0.233	1.685
	BCP−2	−0.393	0.233	1.685
Nd	BCP−1	−0.400	0.248	1.611
	BCP−2	−0.400	0.248	1.611
Pm	BCP−1	−0.377	0.249	1.515
	BCP−2	−0.377	0.249	1.515
Sm	BCP−1	−0.348	0.245	1.422
	BCP−2	−0.349	0.245	1.423
Eu	BCP−1	−0.336	0.249	1.350
	BCP−2	−0.337	0.249	1.350
Gd	BCP−1	−0.292	0.216	1.349
	BCP−2	−0.292	0.216	1.350

Tb	BCP−1	−0.370	0.277	1.335
	BCP−2	−0.370	0.277	1.335
Dy	BCP−1	−0.324	0.250	1.296
	BCP−2	−0.324	0.250	1.296
Ho	BCP−1	−0.282	0.223	1.263
	BCP−2	−0.282	0.223	1.263
Er	BCP−1	−0.305	0.243	1.253
	BCP−2	−0.305	0.243	1.254
Tm	BCP−1	−0.302	0.244	1.239
	BCP−2	−0.302	0.244	1.239
Yb	BCP−1	−0.127	0.109	1.167
	BCP−2	−0.389	0.296	1.312
Lu	BCP−1	−0.252	0.206	1.220
	BCP−2	−0.252	0.206	1.220


(a)
6.85
4.57
2.28
0.00
-2.28
-4.57
-6.85
O
Ce
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(b)
6.83
4.55
2.28
0.00
-2.28
-4.55
-6.83
O
Pr
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(c)
6.80
4.53
2.27
0.00
-2.27
-4.53
-6.80
O
Nd
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(d)
7.16
4.77
2.39
0.00
-2.39
-4.77
-7.16
O
Pm
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(e)
7.14
4.76
2.38
0.00
-2.38
-4.76
-7.14
O
Sm
O
−3.93 −2.62 −1.31 0.00 1.31 2.62 3.93
Length unit: Bohr
(f)
7.07
4.72
2.36
0.00
-2.36
-4.72
-7.07
O
Eu
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(g)
7.15
4.77
2.38
0.00
-2.38
-4.77
-7.15
O
Gd
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(h)
6.90
4.60
2.30
0.00
-2.30
-4.60
-6.90
O
Tb
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr
(i)
3.35
1.67
0.00
-1.67
-3.35
-5.02
-6.70
Dy
O
O
−6.54 −4.36 −2.18 0.00 2.18 4.36 6.54
Length unit: Bohr
(j)
3.34
1.67
0.00
-1.67
3.34
-5.01
6.68
Ho
O
O
−6.52 −4.35 −2.17 0.00 2.17 4.35 6.52
Length unit: Bohr
(k)
7.10
4.73
2.37
0.00
-2.37
-4.73
-7.10
O
Er
O
−3.84 −2.56 −1.28 0.00 1.28 2.56 3.84
Length unit: Bohr

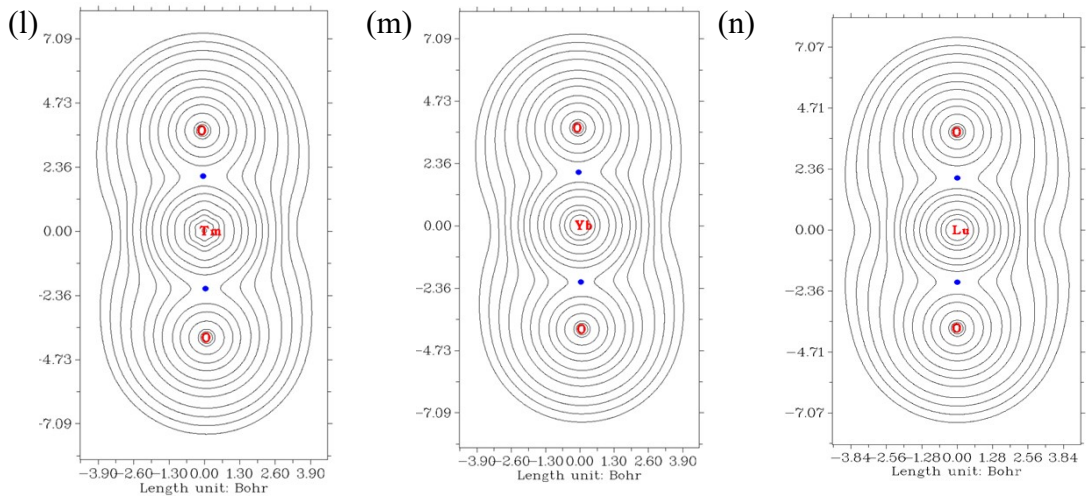
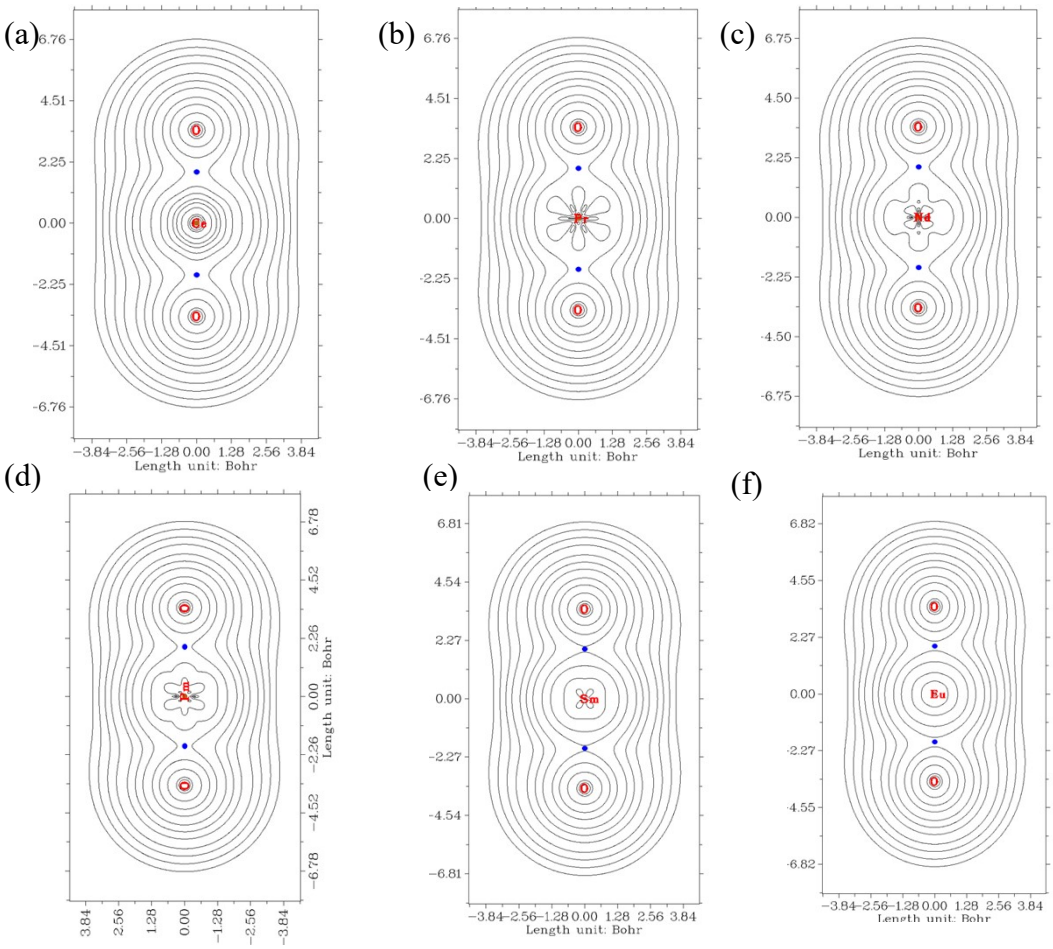


Figure S1: Contour plots depicting the Laplacian of electron density for CASSCF-optimized $[LnO_2]^-$ models where (a) $[CeO_2]^-$, (b) $[PrO_2]^-$, (c) $[NdO_2]^-$, (d) $[PmO_2]^-$, (e) $[SmO_2]^-$, (f) $[EuO_2]^-$, (g) $[GdO_2]^-$, (h) $[TbO_2]^-$, (i) $[DyO_2]^-$, (j) $[HoO_2]^-$, (k) $[ErO_2]^-$, (l) $[TmO_2]^-$, (m) $[YbO_2]^-$, (n) $[LuO_2]^-$. The contour lines' concentration and gradient indicate variations in electron density, with darker/more concentrated regions potentially representing areas of higher electron localization or bonding interactions. The blue dot shows the bond critical point (3,−1) between the two atoms.


(a)
(b)
(c)
(d)
(e)
(f)
Length unit: Bohr

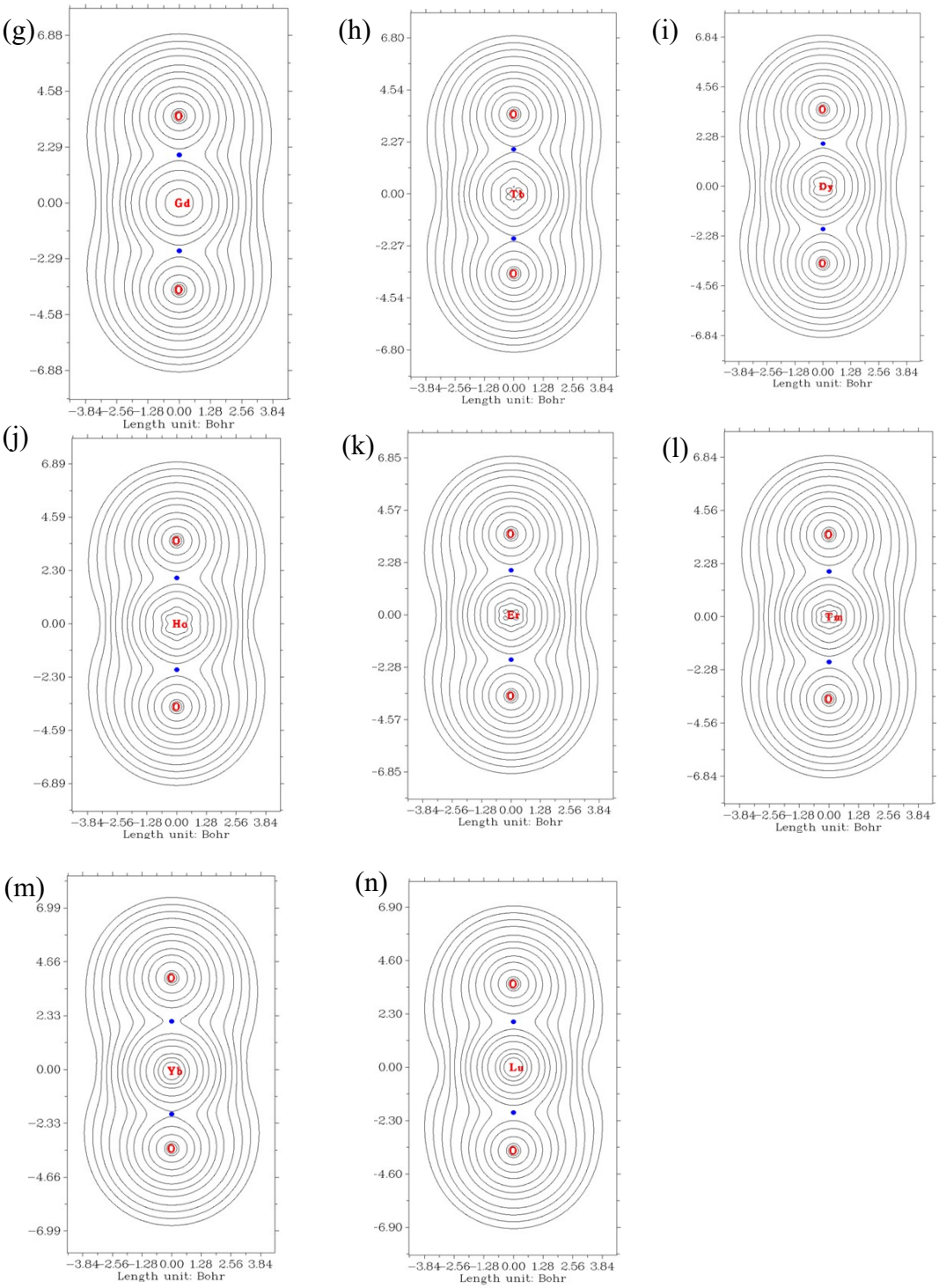


Figure S2: Contour plots depicting the Laplacian of electron density for CASSCF-optimized [LnO_2] models where (a) [CeO_2], (b) [PrO_2], (c) [NdO_2], (d) [PmO_2], (e) [SmO_2], (f) [EuO_2], (g) [GdO_2], (h) [TbO_2], (i) [DyO_2], (j) [HoO_2], (k) [ErO_2], (l) [TmO_2], (m) [YbO_2], (n) [LuO_2]. The contour lines' concentration and gradient indicate variations in electron density, with darker/more concentrated regions potentially representing areas of higher electron localization or bonding interactions. The blue dot shows the bond critical point (3,−1) between the two atoms.

Table S6: Wiberg Bond order computed using NBO Analysis for casscf optimised $[LnO_2]$ and $[LnO_2]^-$.

Metal	Ln^{III} (Ln-O1,Ln-O2)	Ln^{IV} (Ln-O1,Ln-O2)
Ce	1.460,1.423	1.551,1.551
Pr	1.248,1.310	1.414,1.414
Nd	1.226,1.227	1.375,1.375
Pm	1.121,1.219	1.366,1.366
Sm	0.885,0.939	1.263,1.263
Eu	0.755,0.755	0.942,0.942
Gd	0.971,1.157	1.053,1.053
Tb	1.073,1.188	1.104,1.104
Dy	1.159,1.351	1.053,1.053
Ho	1.171, 1.341	1.004,1.004
Er	0.618,0.618	1.023,1.023
Tm	0.830,0.898	1.052,1.052
Yb	0.501,0.601	0.970,0.402
Lu	0.954,0.954	0.878,0.878

Table S7: $|V(r)|/G(r)$ ratio of DFT optimised $[LnO_2]^-$ where Ln ranges from Ce to Yb.

Metal (III)		V(r)	G(r)	$\|V(r)/G(r)\|$
Ce	BCP−1	−0.260	0.182	1.432
	BCP−2	−0.244	0.163	1.498
Pr	BCP−1	−0.246	0.169	1.455
	BCP−2	−0.246	0.169	1.455
Nd	BCP−1	−0.251	0.183	1.372
	BCP−2	−0.251	0.183	1.372
Pm	BCP−1	−0.248	0.181	1.372
	BCP−2	−0.248	0.181	1.372
Sm	BCP−1	−0.240	0.187	1.283
	BCP−2	−0.240	0.187	1.283
Eu	BCP−1	−0.232	0.187	1.239
	BCP−2	−0.232	0.187	1.239
Gd	BCP−1	−0.237	0.184	1.286
	BCP−2	−0.237	0.184	1.286
Tb	BCP−1	−0.229	0.178	1.286
	BCP−2	−0.229	0.178	1.286
Dy	BCP−1	−0.223	0.175	1.275
	BCP−2	−0.223	0.175	1.275
Ho	BCP−1	−0.221	0.176	1.260
	BCP−2	−0.221	0.176	1.260

Er	BCP−1	−0.215	0.173	1.244
	BCP−2	−0.220	0.177	1.241
Tm	BCP−1	−0.205	0.163	1.260
	BCP−2	−0.209	0.167	1.257
Yb	BCP−1	−0.204	0.167	1.218
	BCP−2	−0.208	0.172	1.213
Lu	BCP−1	−0.207	0.170	1.219
	BCP−2	−0.207	0.170	1.219

Table S8: |V(r)|/G(r) ratio of DFT optimised [LnO_2] where Ln ranges from Ce to Yb.

Metal (IV)		V(r)	G(r)	|V(r)/G(r)|
Ce	BCP−1	−0.416	0.217	1.914
	BCP−2	−0.416	0.217	1.914
Pr	BCP−1	−0.425	0.242	1.754
	BCP−2	−0.425	0.242	1.754
Nd	BCP−1	−0.426	0.255	1.671
	BCP−2	−0.426	0.255	1.671
Pm	BCP−1	−0.427	0.266	1.607
	BCP−2	−0.427	0.266	1.607
Sm	BCP−1	−0.416	0.271	1.535
	BCP−2	−0.416	0.271	1.535
Eu	BCP−1	−0.422	0.298	1.416
	BCP−2	−0.422	0.298	1.416
Gd	BCP−1	−0.404	0.275	1.468
	BCP−2	−0.405	0.275	1.471
Tb	BCP−1	−0.460	0.334	1.378
	BCP−2	−0.460	0.334	1.378
Dy	BCP−1	−0.436	0.323	1.352
	BCP−2	−0.437	0.323	1.352
Ho	BCP−1	−0.420	0.316	1.331
	BCP−2	−0.422	0.317	1.33
Er	BCP−1	−0.415	0.318	1.303
	BCP−2	−0.415	0.318	1.303
Tm	BCP−1	−0.407	0.317	1.283
	BCP−2	−0.407	0.317	1.283
Yb	BCP−1	−0.400	0.311	1.284
	BCP−2	−0.400	0.311	1.284
Lu	BCP−1	−0.389	0.305	1.277
	BCP−2	−0.389	0.305	1.277

Table S9: |V(r)|/G(r) ratio of DFT optimised $[LnO_2]^+$ where Ln ranges from Ce to Yb.

Metal (V)		V(r)	G(r)	|V(r)/G(r)|
Pr	BCP−1	−0.428	0.221	1.939
	BCP−2	−0.428	0.221	1.939
Nd	BCP−1	−0.448	0.252	1.779
	BCP−2	−0.448	0.252	1.779
Pm	BCP−1	−0.421	0.271	1.557
	BCP−2	−0.421	0.271	1.557
Sm	BCP−1	−0.445	0.284	1.566
	BCP−2	−0.445	0.284	1.566
Eu	BCP−1	−0.433	0.290	1.493
	BCP−2	−0.433	0.290	1.493
Gd	BCP−1	−0.439	0.299	1.468
	BCP−2	−0.439	0.299	1.468
Tb	BCP−1	−0.489	0.347	1.408
	BCP−2	−0.489	0.347	1.408
Dy	BCP−1	−0.478	0.350	1.367
	BCP−2	−0.478	0.350	1.367
Ho	BCP−1	−0.461	0.343	1.342
	BCP−2	−0.461	0.343	1.342
Er	BCP−1	−0.451	0.343	1.317
	BCP−2	−0.451	0.343	1.317
Tm	BCP−1	−0.441	0.340	1.298
	BCP−2	−0.441	0.340	1.298
Yb	BCP−1	−0.431	0.333	1.296
	BCP−2	−0.431	0.333	1.296
Lu	BCP−1	−0.421	0.327	1.290
	BCP−2	−0.421	0.327	1.290

Energy (cm^{-1})	g_{xx}	g_{yy}	g_{zz}
$[CeO_2]^-$			
0.0	0.000	0.000	4.152
1273.4	0.000	0.000	2.054
2159.5	0.010	0.012	8.002
$[NdO_2]^-$			
0.0	0.000	0.000	6.044
1996.6	0.000	0.000	10.035
3018.4	0.027	0.028	1.032
3039.3	0.026	0.029	4.051
3914.7	0.000	0.000	14.0121
$[SmO_2]^-$			
0.0	0.386	0.387	0.641
294.8	0.000	0.000	3.074
862.5	1.345	1.346	2.133
$[DyO_2]^-$			
0.0	0.000	0.000	19.954
590.5	0.000	0.000	16.871
1102.4	0.014	0.016	13.950
1494.4	0.318	0.354	11.345
1765.2	2.685	2.969	8.546
1948.8	3.305	6.049	9.513
2123.2	0.783	1.590	15.881
2262.8	0.109	0.211	19.632
$[ErO_2]^-$			
0.0	9.564	9.503	1.233
122.1	0.018	0.078	3.678

ions for casscf optimised toy models.

(a)

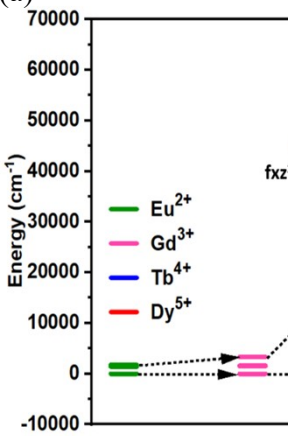


Figure S3: (a) Relative $[EuO_2]^{2-}$, $[GdO_2]^-$, [Tb lanthanide ions from C

Table S10: Energy of the states (cm^{-1}) along with g_{xx}, g_{yy} and g_{zz} for all the Kramers

317.7	0.009	0.105	6.069
502.5	0.054	0.059	8.417
613.3	0.002	0.002	10.784
707.9	0.000	0.000	13.226
1051.7	0.000	0.000	15.686
2349.5	0.000	0.0000	17.966
$[YbO_2]^-$			
0.0	4.559	4.553	1.263
1252.0	0.000	0.006	3.553
2794.7	0.000	0.005	5.791
4479.7	0.002	8.002	8.002
$[PrO_2]$			
0.0	0.000	0.000	4.181
1385.8	0.000	0.001	2.028
2815.4	0.000	0.000	8.002
$[PmO_2]$			
0.0	0.000	0.000	6.025
2453.8	0.000	0.000	10.015
4095.6	0.001	0.002	0.676
4338.9	0.001	0.001	4.226
4750.1	0.000	0.000	13.990
$[EuO_2]$			
0.0	0.098	0.143	1.551
281.5	0.006	0.056	2.087
412.3	0.118	0.135	5.044
$[HoO_2]$			
0.0	0.000	0.000	20.012
1680.9	0.000	0.000	16.275
3456.5	0.000	0.000	12.577
5330.7	0.000	0.000	9.011
5680.4	10.205	10.197	1.649
5988.7	0.002	0.006	4.895
6474.3	0.000	0.000	17.743
6620.7	0.002	0.002	7.886
$[TmO_2]$			
0.0	9.288	9.243	1.277
239.3	0.001	0.001	13.162
285.5	0.021	0.066	3.806
452.1	0.000	0.000	15.793
646.6	0.000	0.000	10.619
701.9	0.007	0.079	6.123
907.1	0.035	0.036	8.311
4178.6	0.000	0.000	17.966
$[LuO_2]$			
0.0	4.238	4.235	1.405
2888.9	0.001	0.001	3.625
5622.6	0.003	0.004	5.789
7505.8	0.003	0.003	8.002

$[NdO_2]^+$			
0.0	0.000	0.000	4.105
2945.8	0.001	0.001	2.010
3232.0	0.000	0.000	8.002
$[SmO_2]^+$			
0.0	0.000	0.000	0.289
314.4	0.000	0.000	6.006
658.2	0.000	0.000	4.201
2331.3	0.000	0.000	8.123
3048.0	0.000	0.000	10.002
$[GdO_2]^+$			
0.0	1.982	2.069	3.986
94.7	0.045	0.048	7.984
165.1	2.625	1.491	0.063
$[ErO_2]^+$			
0.0	0.000	0.000	20.011
2352.3	0.000	0.000	16.047
4788.7	0.000	0.000	12.072
7317.7	0.000	0.000	8.085
8424.4	9.238	9.177	1.873
8886.8	0.029	0.029	5.603
9951.7	0.000	0.000	4.079
9963.0	0.000	0.000	9.248
$[YbO_2]^+$			
0.0	0.008	0.008	3.758
2430.7	0.005	0.005	4.238
2745.2	0.008	0.008	0.229

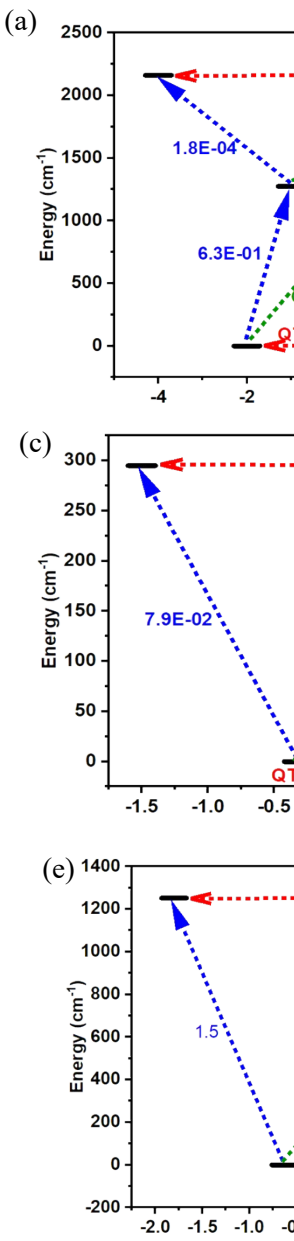


Figure S4: Relaxation
$[SmO_2]^-$, (d) $[ErO_2]^-$
through Orbach/Rama
QTM/TA-QTM betwe
the mean absolute va
magnetic moment. colo
Hydrogens have been

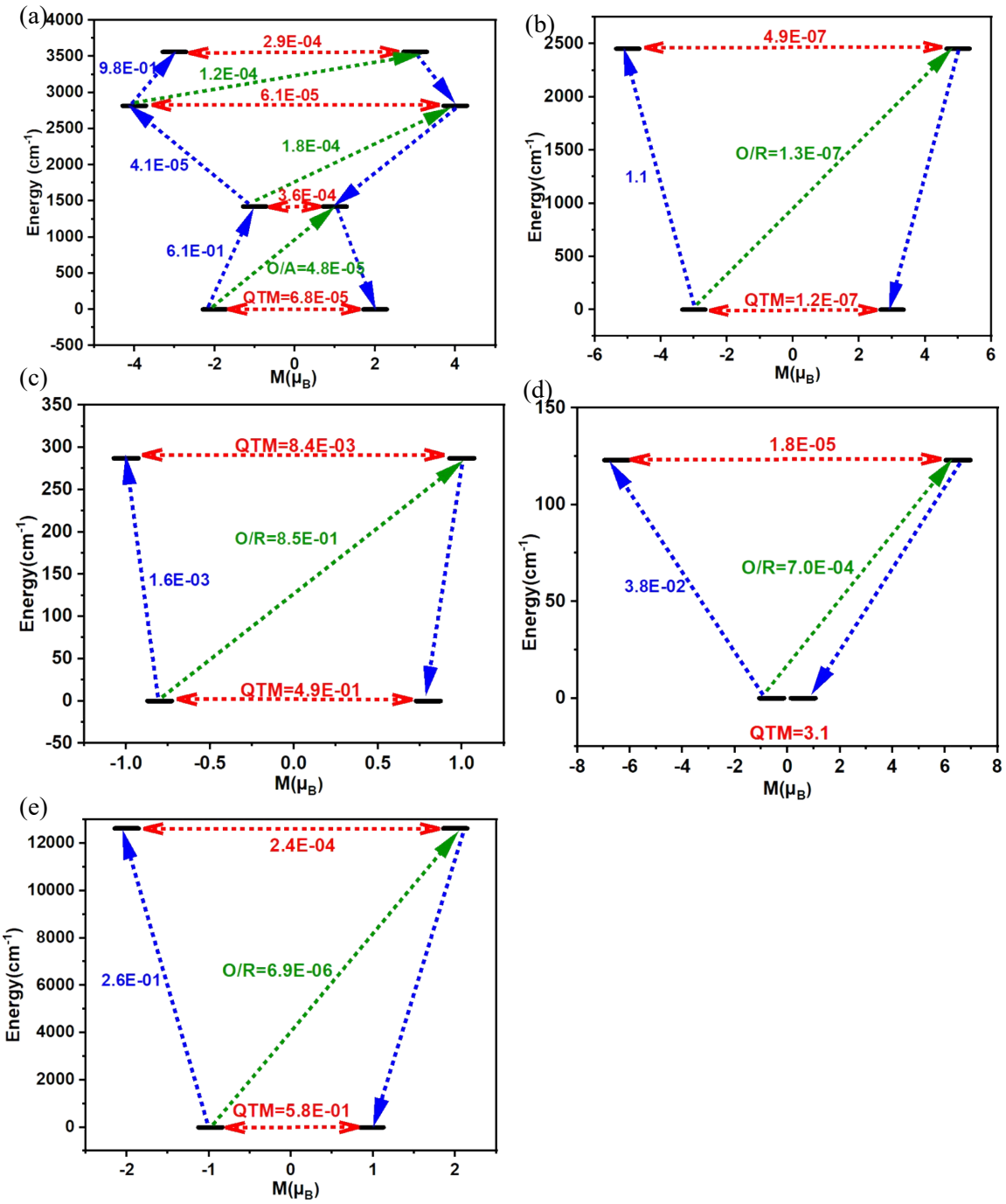


Figure S5: Relaxation mechanism in CASSCF optimised (a) [PrO_2], (b) [PmO_2], (c) [EuO_2], (d) [TmO_2] and (e) [LuO_2]. The green/blue arrows sshow the possible pathway through Orbach/Raman relaxation. The dotted red lines represent the presence of QTM/TA-QTM between the connecting pairs. The numbers provided at each arrow are the mean absolute values for the corresponding matrix element of the transition magnetic moment.

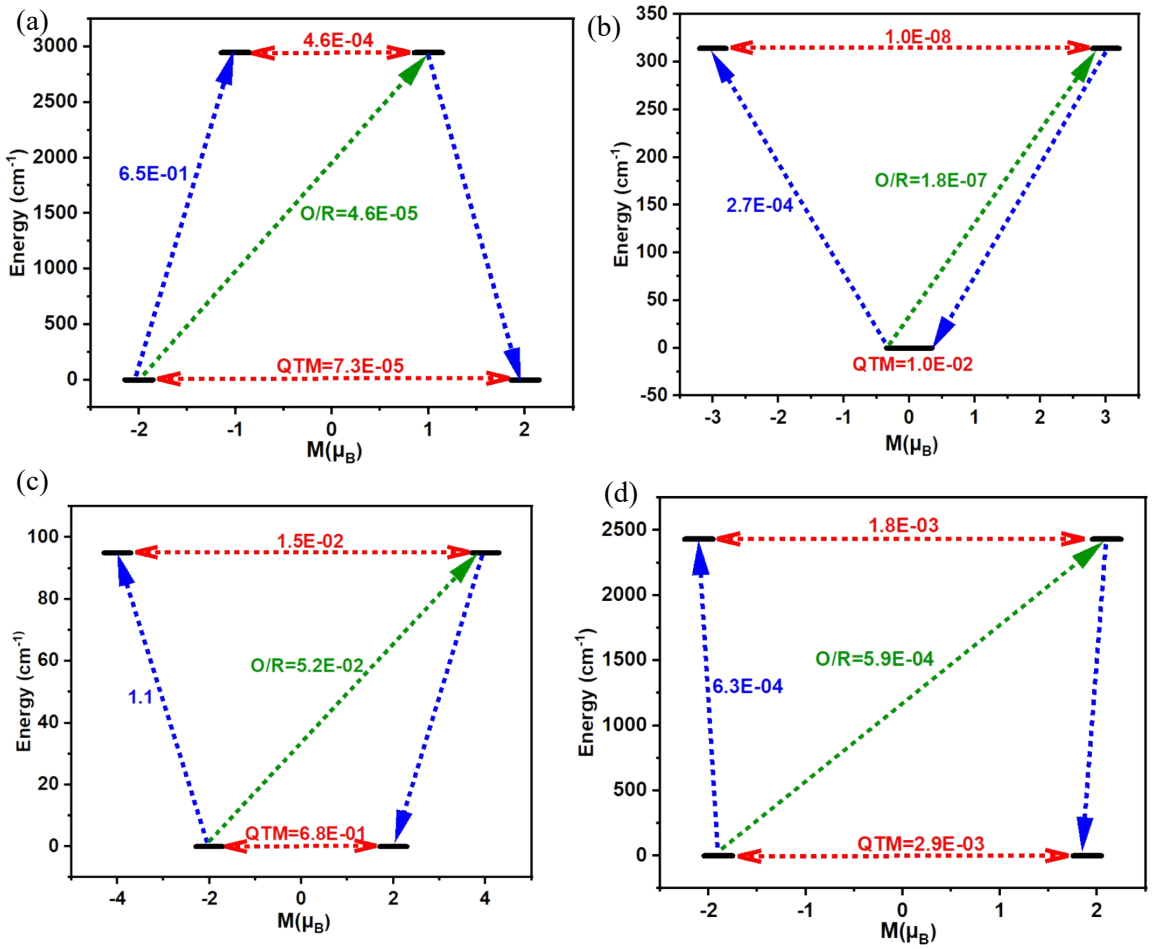


Figure S6: Relaxation mechanism in DFT optimised (a) $[NdO_2]^+$, (b)$[SmO_2]^+$, (c) $[GdO_2]^+$ and (d) $[YbO_2]^+$. The green/blue arrows show the possible pathway through Orbach/Raman relaxation. The dotted red lines represent the presence of QTM/TA-QTM between the connecting pairs. The numbers provided at each arrow are the mean absolute values for the corresponding matrix element of the transition magnetic moment.

Table S11: Energies of different states, along with tunnel splitting for various CASSCF optimised non−Kramers small models.

Energy states (cm^{-1})	Energy states (cm^{-1})	Tunnel splitting
$[PrO_2]^-$		
0.000	0.005	0.005
2092.763	2092.776	0.013

3424.330	4076.005	651.675
$[PmO_2]^-$		
0.000		
207.565	207.879	0.314
429.887	431.12	1.233
$[TbO_2]^-$		
0.000	0.000	0.000
582.889	582.889	0.000
1211.077	1211.077	0.000
1886.420	1887.260	0.840
$[HoO_2]^-$		
0.000	0.000	0.000
370.581	370.594	0.013
557.614	557.782	0.168
681.755	682.912	1.157
$[TmO_2]^-$		
0.000		
25.153	25.987	0.834
$[NdO_2]$		
0.000	0.004	0.004
2621.244	2621.317	0.073
4642.09	5107.262	465.172
$[SmO_2]$		
0.000	0.149	0.149
734.681	1176.596	441.915
$[DyO_2]$		
0.000	0.000	0.000
46.255	46.255	0.000
482.546	582.547	0.001
1142.678	1144.724	2.046
$[ErO_2]$		
0.000	0.000	0.000
2602.491	2602.491	0.000
3623.733	3623.734	0.001
3800.126	3800.129	0.003
3802.638	3802.791	0.153
$[YbO_2]$		
0.000	5.157	5.157
232.258	233.263	1.005
$[EuO_2]^+$		
0	––	––
375.813	376.563	0.75
$[HoO_2]^+$		
0.000	0.000	0.000
89.578	89.578	0.000
574.680	574.680	0.000
1323.757	1323.931	0.174
$[TmO_2]^+$		

0.000		
260.225	283.297	23.072
$[LuO_2]^+$		
0.000	––	––
6712.857	6712.857	0.000

Table S12: U_{cal} value and mode of relaxation in CASSCF optimised $[LnO_2]^-$ complexes.

Metal	U_{cal} Value (cm^{-1}) and mode of relaxation in Ln(III)
Ce	1274 cm^{-1}, TA−QTM from first excited state
Pr	2092.7, Tunnel splitting from ground state
Nd	1997 cm^{-1}, TA−QTM from first excited state
Pm	No SMM properties, Tunnel splitting from ground state
Sm	295 cm^{-1}, TA−QTM from first excited state
Tb	1886 cm^{-1}, Tunnel splitting from third excited state
Dy	1765 cm^{-1}, TA−QTM from fourth excited state
Ho	371 cm^{-1}, Tunnel splitting from first excited state
Er	No SMM properties, QTM from ground state
Tm	No SMM properties, Tunnel splitting from ground state
Yb	No SMM properties, QTM from ground state.

Table S13: U_{cal} value and mode of relaxation in CASSCF $[LnO_2]$ complexes.

Metal	U_{cal} Value (cm−1) and mode of relaxation in Ln(IV)
Pr	1386 cm^{-1}, TA−QTM from first excited state
Nd	2621 cm^{-1}, tunnel splitting from first excited state.

Pm	2454 cm^{-1}, QTM from first excited state
Sm	No SMM properties, Tunnel splitting from ground state.
Eu	No SMM properties, QTM from ground state.
Dy	1144 cm^{-1}, tunnel splitting from fourth excited state
Ho	5680 cm^{-1}, QTM from fourth excited state
Er	4070.2 cm^{-1}, TS from second excited state
Tm	No SMM Properties, QTM from ground state.
Yb	No SMM properties, Tunnel splitting from ground state.
Lu	No SMM Properties, QTM from ground excited state.

Table S14: U_{cal} value and mode of relaxation in DFT optimised $[LnO_2]^+$ complexes.

Metal	U_{cal} Value (cm^{-1}) and mode of relaxation in Ln(IV)
Nd	2945 cm^{-1}, TA−QTM from first excited state
Pm	3015.4 cm^{-1}, tunnel splitting from first excited state.
Sm	No SMM properties, QTM from ground state
Eu	No SMM properties, Tunnel splitting from ground state.
Gd	No SMM properties, QTM from ground state
Ho	1323.7 cm^{-1}, tunnel splitting from third excited state
Er	8424 cm^{-1}, QTM from fourth excited state
Tm	No SMM properties, Tunnel splitting from ground state.
Yb	No SMM Properties, QTM from ground state.

Lu	No SMM properties, Tunnel splitting from ground state.

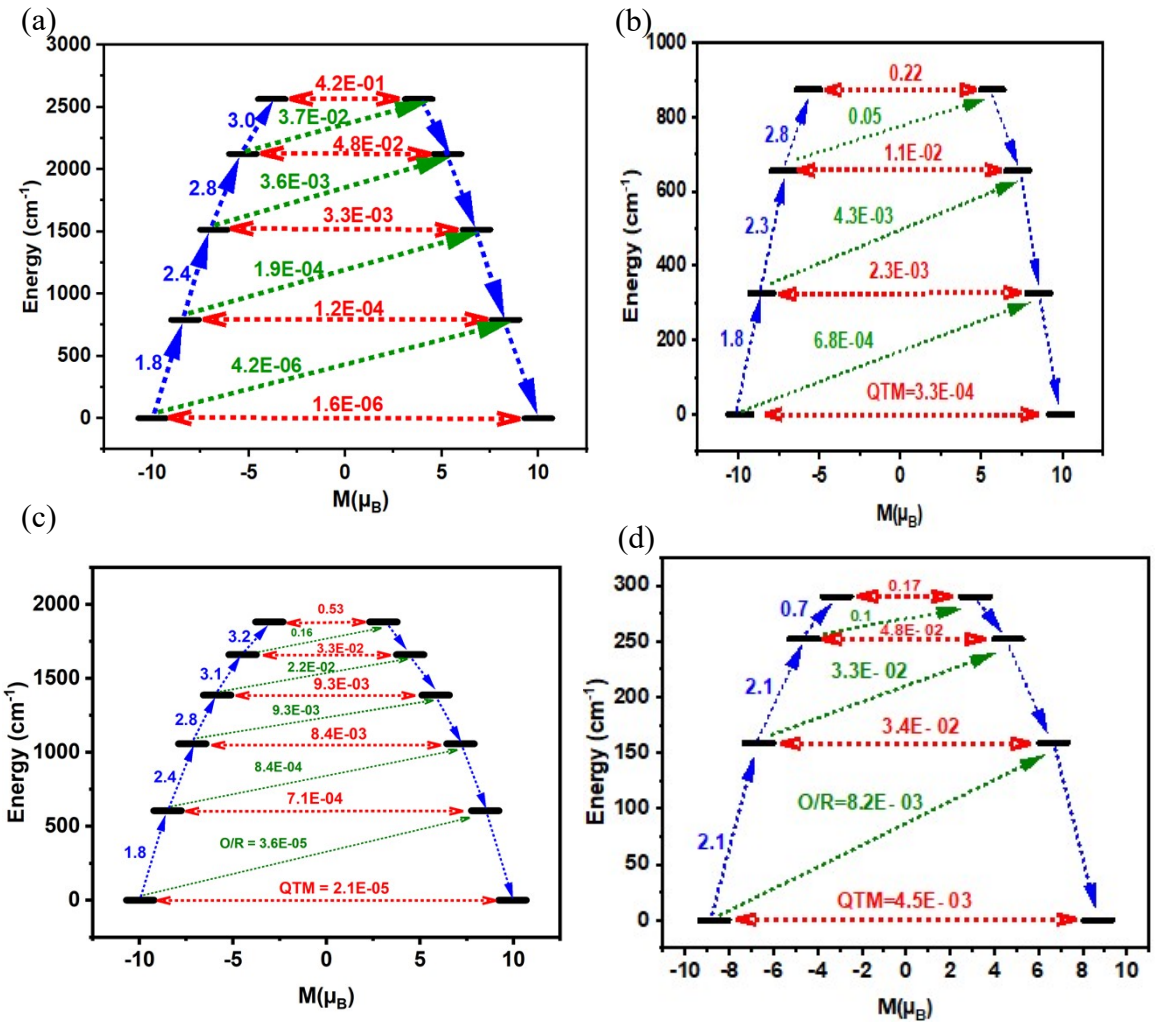


Figure S7: (a) magnetic relaxation mechanism for (a) **m1** (b) **m3** (c) **m4** and (d) **m5**. The green/blue arrows show the possible pathway through Orbach/Raman relaxation. The dotted red lines represent the presence of QTM/TA-QTM between the connecting pairs. The numbers provided at each arrow are the mean absolute values for the corresponding matrix element of the transition magnetic moment.

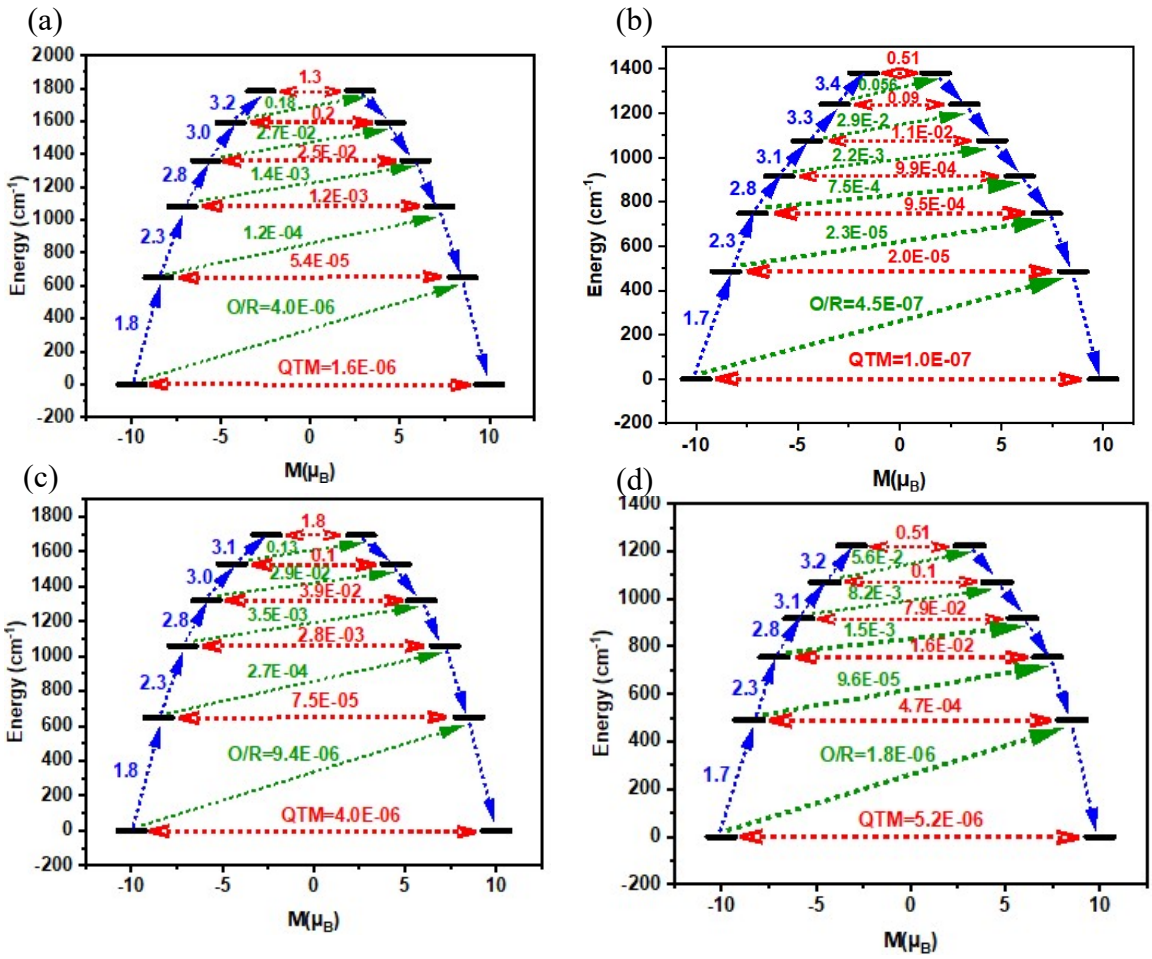


Figure S8: (a) magnetic relaxation mechanism for (a) **4**-Ho (b) **4**-Dy (c) **5**-Ho and (d) **5**-Dy. The green/blue arrows show the possible pathway through Orbach/Raman relaxation. The dotted red lines represent the presence of QTM/TA-QTM between the connecting pairs. The numbers provided at each arrow are the mean absolute values for the corresponding matrix element of the transition magnetic moment.

Table S15. The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of 28 selected normal modes of **4**-Dy.

C	Energy	oscillator strength	population	Q_k	S_j
1	36.4	3.97	0.005	0.37	0.223
2	43.2	0.53	0.005	0.46	0.077
	48.2	0.40	0.006		
	54.4	0.47	0.007		
	57.4	0.38	0.007		
	60.1	0.28	0.007		

	66.5	0.47	0.008		
	67.2	0.40	0.008		
3	71.2	0.58	0.009	0.38	0.133
4	80.2	1.39	0.010	0.33	0.104
5	84.7	1.25	0.011	0.33	0.169
6	91.8	1.18	0.011	0.32	0.136
	99.8	0.08	0.012		
7	114.9	0.43	0.014	0.33	0.129
	116.6	0.13	0.014		
8	126.5	0.29	0.016	0.32	0.129
	134.3	0.11	0.017		
	135.5	0.22	0.017		
	140.5	0.02	0.017		
9	143.0	0.58	0.018	0.31	0.159
	145.7	0.03	0.018		
10	151.4	0.66	0.019	0.30	0.181
	158.0	0.18	0.020		
11	164.4	1.17	0.020	0.28	0.116
	165.8	0.22	0.021		
	170.8	0.22	0.021		
12	178.0	1.54	0.022	0.29	0.165
13	182.1	1.44	0.023	0.29	0.245
	183.3	0.23	0.023		
14	187.8	1.91	0.023	0.29	0.251
15	191.1	2.10	0.024	0.30	0.197
	192.5	0.49	0.024		
16	195.9	3.78	0.024	0.32	0.169
	200.1	0.40	0.025		
17	204.1	1.19	0.025	0.32	0.184
	204.5	1.40	0.025		
	205.2	0.35	0.025		
18	208.2	1.79	0.026	0.31	0.319
19	215.8	20.23	0.027	0.24	0.167
	218.1	0.48	0.027		
	220.7	0.44	0.027		
20	227.4	0.90	0.028	0.32	0.227
21	229.5	1.16	0.028	0.31	0.102
	232.6	0.20	0.029		
	235.9	0.34	0.029		
	237.3	0.42	0.029		
	239.4	0.45	0.030		
	240.6	0.47	0.030		
22	243.7	2.62	0.030	0.32	0.124
	246.4	0.48	0.031		
	249.0	0.46	0.031		
	251.7	0.43	0.031		
23	253.8	1.12	0.031	0.30	0.052
	257.8	0.41	0.032		

	259.1	0.48	0.032		
24	261.6	0.47	0.032	0.30	0.218
	265.5	0.30	0.033		
	272.2	0.49	0.034		
25	274.8	0.49	0.034	0.24	0.170
	276.4	0.28	0.034		
	285.5	0.11	0.035		
	288.4	0.08	0.036		
	290.6	0.10	0.036		
	294.6	0.13	0.037		
	297.6	0.01	0.037		
26	302.3	0.50	0.037	0.28	0.122
	306.5	0.22	0.038		
27	335.0	0.23	0.042	0.29	0.119
	340.6	0.12	0.042		
	359.7	0.03	0.045		
28	361.3	0.11	0.045	0.20	0.157

Table S16: The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of 27 selected normal modes of **4**-Ho.

C	Energy	oscillator strength	population	Q_k	S_j
1	42.7	1.12	0.005	0.42	0.142
	46.4	0.09	0.006		
	55.7	0.03	0.007		
	62.4	0.11	0.008		
2	63.7	0.59	0.008	0.41	0.109
	72.4	0.34	0.009		
	78.4	0.06	0.010		
	80.8	0.36	0.010		
	88.2	0.42	0.011		
	92.0	0.23	0.011		
	99.2	0.20	0.012		
3	108.1	0.54	0.013	0.32	0.198
	114.7	0.05	0.014		
	118.5	0.07	0.015		
	123.7	0.17	0.015		
	132.3	0.19	0.016		
	133.3	0.01	0.017		
4	135.7	0.52	0.017	0.32	0.032
	146.0	0.09	0.018		
	149.0	0.15	0.018		
	150.4	0.11	0.019		
	154.1	0.02	0.019		
5	164.1	1.93	0.020	0.30	0.181

	167.1	0.03	0.021		
	168.6	0.13	0.021		
	174.3	0.17	0.022		
	180.3	0.72	0.022		
	182.8	0.23	0.023		
6	186.2	1.14	0.023	0.30	0.217
7	188.9	1.11	0.023	0.35	0.208
8	190.5	0.95	0.024	0.29	0.184
	192.8	0.38	0.024		
	198.2	0.96	0.025	0.29	
9	198.6	3.30	0.025	0.29	0.154
	200.8	0.50	0.025		
	205.9	1.74	0.026	0.30	0.121
10	211.4	0.04	0.026		
	215.5	0.70	0.027		
	220.7	0.11	0.027		
11	224.6	1.25	0.028	0.31	0.022
	226.9	0.43	0.028		
12	230.0	0.90	0.029	0.28	0.016
	233.0	0.82	0.029		
	238.4	0.08	0.030		
	238.9	0.83	0.030		
13	242.9	2.89	0.030	0.23	0.122
	246.7	0.18	0.031		
	247.5	0.45	0.031		
	249.2	0.49	0.031		
	251.9	0.83	0.031		
14	256.3	1.33	0.032	0.30	0.196
15	258.1	0.97	0.032	0.30	0.029
16	263.9	1.59	0.033	0.29	0.169
17	265.8	1.16	0.033	0.27	0.264
	267.6	0.25	0.033		
	272.3	0.27	0.034		
	276.3	0.48	0.034		
	279.8	0.51	0.035		
	284.7	0.42	0.035		
	291.1	0.21	0.036		
18	293.2	0.99	0.036	0.25	0.201
	294.7	0.23	0.037		
19	304.0	1.34	0.038	0.28	0.095
	306.1	0.37	0.038		
	315.9	0.45	0.039		
	319.1	0.16	0.040		
20	325.5	3.01	0.040	0.27	0.151
21	341.4	0.96	0.042	0.23	0.104
	351.8	0.37	0.044		
	358.9	0.77	0.045		
22	368.2	0.92	0.046	0.20	0.080

23	392.2	0.75	0.049	0.23	0.167
	398.4	0.32	0.049		
	437.4	0.04	0.054		
	441.1	0.15	0.055		
24	452.3	0.95	0.056	0.17	0.102
	455.3	0.67	0.056		
25	457.8	1.51	0.057	0.17	0.150
26	464.9	1.27	0.058	0.16	0.148
27	489.1	1.31	0.061	0.16	0.181

Table S17: The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of 24 selected normal modes of **5**-Dy.

C	Energy	oscillator strength	population	Q_k	S_j
1	22.6	0.39	0.003	0.65	0.201
2	32.9	3.12	0.004	0.46	0.160
	45.5	0.03	0.006		
3	50.7	1.80	0.006	0.42	0.179
	54.5	0.44	0.007		
	64.7	0.04	0.008		
4	72.5	0.78	0.009	0.38	0.115
	85.4	0.40	0.011		
	93.1	0.23	0.012		
	99.4	0.25	0.012		
5	116.7	0.54	0.014	0.44	0.052
	120.2	0.16	0.015		
	120.8	0.19	0.015		
6	128.8	1.13	0.016	0.43	0.046
	129.6	0.12	0.016		
	137.2	0.17	0.017		
7	140.1	0.57	0.017	0.34	0.103
	143.7	0.07	0.018		
	152.2	0.30	0.019		
	154.8	0.42	0.019		
	160.9	0.10	0.020		
	166.7	0.40	0.021		
	171.2	0.20	0.021		
	174.7	0.29	0.022		
8	175.2	1.66	0.022	0.30	0.205
9	183.8	1.70	0.023	0.32	0.246
10	191.8	1.77	0.024	0.30	0.205
11	193.7	1.26	0.024	0.34	0.168
12	206.6	1.55	0.026	0.26	0.193
13	208.7	1.12	0.026	0.28	0.160
	219.0	0.08	0.027		

14	222.3	1.66	0.028	0.24	0.102
	235.8	0.21	0.029		
15	241.4	0.95	0.030	0.29	0.165
	246.7	0.33	0.031		
	250.8	0.17	0.031		
	253.4	0.49	0.031		
16	256.7	0.67	0.032	0.28	0.135
	264.9	0.36	0.033		
17	270.1	0.75	0.033	0.23	0.133
18	275.2	0.78	0.034	0.28	0.210
19	282.5	0.75	0.035	0.22	0.263
	284.0	0.01	0.035		
	286.8	0.49	0.036		
	290.8	0.25	0.036		
	293.0	0.02	0.036		
20	296.3	0.25	0.037	0.25	0.112
	297.0	0.29	0.037		
21	303.0	0.52	0.038	0.28	0.218
22	326.5	58.05	0.040	0.16	0.311
23	336.4	8.04	0.042	0.24	0.132
24	356.1	0.53	0.044	0.21	0.186

Table S18: The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of 30 selected normal modes of **5**-Ho.

C	Energy	oscillator strength	population	Q_k	S_j
1	34.4	0.03	0.004	0.56	0.040
	52.3	0.21	0.006		
	57.0	0.27	0.007		
2	64.2	0.66	0.008	0.35	0.119
	75.0	0.04	0.009		
3	83.0	0.54	0.010	0.37	0.163
	88.1	0.40	0.011		
	94.0	0.09	0.012		
	105.9	0.19	0.013		
4	113.2	0.54	0.014	0.32	0.137
	123.8	0.14	0.015		
	126.7	0.05	0.016		
5	131.6	0.53	0.016	0.46	0.040
	137.6	0.38	0.017		
	139.4	0.22	0.017		
	143.4	0.05	0.018		
6	144.9	0.52	0.018	0.41	0.016
	150.0	0.18	0.019		
	155.8	0.04	0.019		

7	163.5	0.84	0.020	0.29	0.067
	166.9	0.20	0.021		
	170.6	0.14	0.021		
	175.7	0.21	0.022		
8	178.1	0.67	0.022	0.32	0.212
9	186.8	1.11	0.023	0.30	0.155

Metal	Term Symbol Ln(III)	Number of roots	Term Symbol Ln(IV)	Number of roots	
		191.6	0.35	0.024	
		194.9	0.47	0.024	
10		198.3	0.97	0.025	0.28	0.193
11		209.0	0.82	0.026	0.30	0.160
12		211.5	0.56	0.026	0.27	0.168
13		228.1	0.59	0.028	0.29	0.132
		230.8	0.19	0.029		
		235.4	0.05	0.029		
14		241.9	1.28	0.030	0.25	0.131
		247.7	0.39	0.031		
		256.2	0.23	0.032		
		259.8	0.23	0.032		
		260.9	0.18	0.032		
15		267.8	0.40	0.033	0.27	0.128
		273.7	0.39	0.034		
16		277.1	0.95	0.034	0.28	0.184
		279.7	0.27	0.035		
17		285.5	0.68	0.035	0.26	0.193
		289.3	0.18	0.036		
		294.3	0.48	0.036		
		294.8	0.42	0.037		
		304.9	0.02	0.038		
18		309.8	2.21	0.038	0.27	0.184
19		328.3	3.58	0.041	0.26	0.191
20		347.5	5.74	0.043	0.22	0.140
21		359.0	15.91	0.045	0.16	0.209
22		370.4	1.24	0.046	0.22	0.228
23		379.4	1.77	0.047	0.22	0.202
24		410.3	9.08	0.051	0.15	0.226
		421.4	0.47	0.052	0.15	
25		438.5	2.06	0.054	0.18	0.105
26		458.4	3.74	0.057	0.17	0.298
27		464.2	1.43	0.058	0.21	0.190
28		480.5	1.57	0.059	0.22	0.207
29		512.4	2.95	0.063	0.19	0.183
30		526.2	11.65	0.065	0.17	0.205

Ce	$^2F_{5/2}$	7 doublets	^1S	-
Pr	$^3H_4$	21 triplets, 28 singlets	$^2F_{5/2}$	7 doublets
Nd	$^4I_{9/2}$	35 quartets, 112	$^3H_4$	21 triplets, 28 singlets
Pm	$^5I_4$	35 quintets, 210 triplets	$^4I_{9/2}$	35 quartets, 112
Sm	$^6H_{5/2}$	21 sextets, 224 quartets	$^5I_4$	35 quintets, 210 triplets
Eu	$^7F_0$	7 heptets, 140 quintets	$^6H_{5/2}$	21 sextets, 224 quartets
Gd	$^8S_{7/2}$	-	$^7F_0$	7 heptets, 140 quintets
Tb	$^7F_6$	7 heptets, 140 quintets	$^8S_{7/2}$	-
Dy	$^6H_{15/2}$	21 sextets, 224 quartets	$^7F_6$	7 heptets, 140 quintets
Ho	$^5I_8$	35 quintets, 210 triplets	$^6H_{15/2}$	21 sextets, 224 quartets
Er	$^4I_{15/2}$	35 quartets, 112	$^5I_8$	35 quintets, 210 triplets
Tm	$^3H_6$	21 triplets, 28 singlets	$^4I_{15/2}$	35 quartets, 112
Yb	$^2F_{7/2}$	7 doublets	$^3H_6$	21 triplets, 28 singlets
Lu	^1S	-	$^2F_{7/2}$	7 doublets

Table S19: Term symbols and a number of roots computed in CASSCF calculations for different lanthanides in +3 and +4 oxidation states.

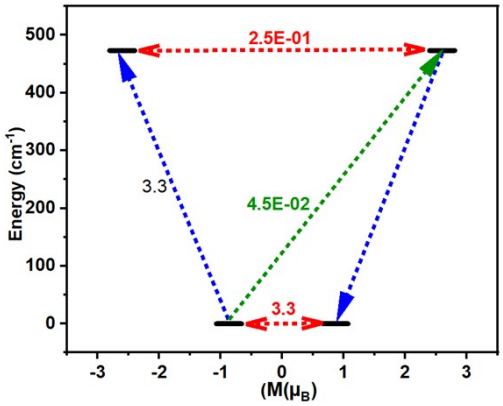


Figure S9: *ab initio* computed magnetization relaxation mechanism of **6**-Er. The green/blue arrows show the possible pathway through Orbach/Raman relaxation. The dotted red lines represent the presence of QTM/TA-QTM between the connecting pairs. The numbers provided at each arrow are the mean absolute values for the corresponding matrix element of the transition magnetic moment.

Table S20: Different parameters measured using different methodologies for CASSCF optimised [HoO_2].

Orbitals employed	**Notation**	**KD1−KD2 gap (cm^{-1})**	**KD1−KD8 gap (cm^{-1})**	**U_{cal} (cm^{-1})**	**g_{zz}, g_{xx}, g_{yy}**
4f	CAS(9,7)	1680.9	6620.6	5680.4	20.012, 0.000, 0.000

4f+6s+3*6p	CAS(9,11)	1714.7	7849.6	4903.6	19.383, 0.000, 0.000
Seven 4f+ $5d_z^2$, $5d_{x^2-y^2}$	CAS(9,9)	1982.9	9680.5	8366.2	20.012, 0.000, 0.000
Seven 4f+ $5d_z^2$, $5d_{x^2-y^2}$,$5d_{xy}$	CAS(9,10)	1788.8	8225.4	5587.2	19.868, 0.000, 0.000
Seven 4f+ $5d_z^2$, $5d_{x^2-y^2}$, $5d_{xy,}$ $5d_{yz,}$ 5_{xz}	CAS(9,12)	1797.2	8405.9	5565.4	19.493, 0.000, 0.000
CASPT2	21 states in pt2	1680.9	6620.7	5680.4	20.012, 0.000, 0.000

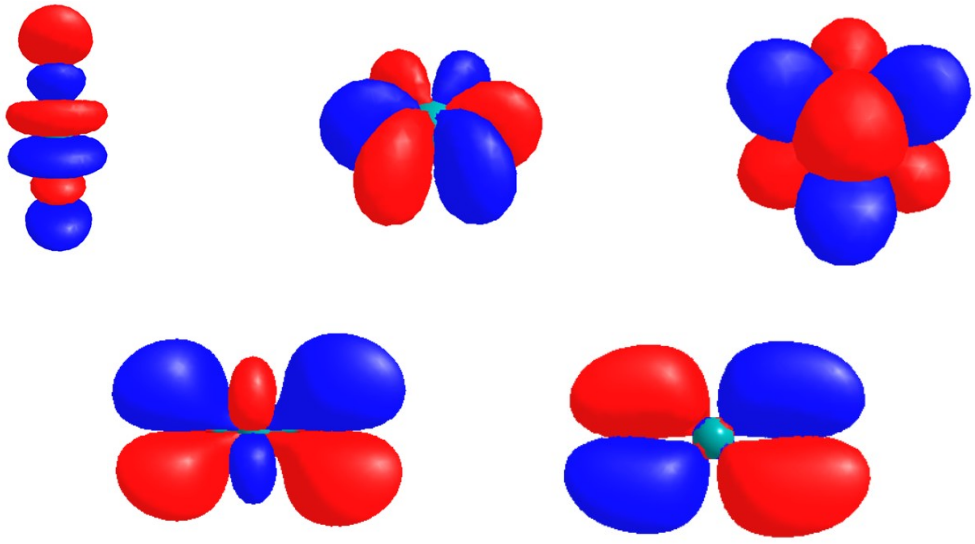


Figure S10: Representative orbitals used in the CASSCF optimization calculations of all the models.

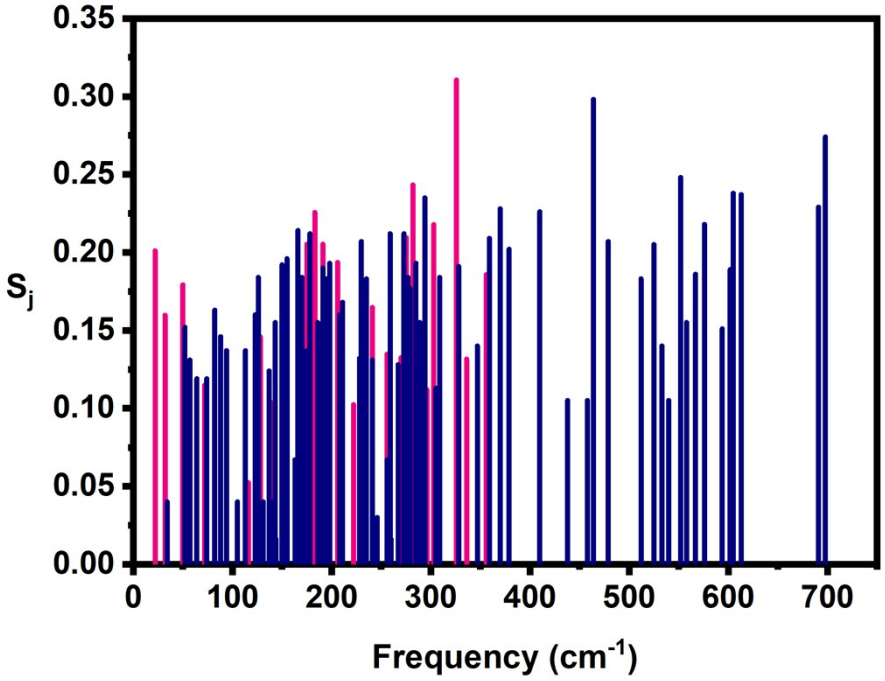


Figure S11: The coupling strength for all the vibrational modes of **5**-Ho and **5**-Dy.

Table S21: The vibrational mode numbers (ω), energy (cm^{-1}), oscilator strength (km mol^{-1}), population (at 100 K), maximum displacement (Q_k) and coupling strength (S_j in cm^{-1}) of all normal modes of **5**-Ho.

c	Energy	oscillator strength	population	Q_k	S_j
1	34.4	0.03	0.004	0.56	0.04
2	52.3	0.21	0.006	0.45	0.152
3	57.0	0.27	0.007	0.44	0.131
4	64.2	0.66	0.008	0.35	0.119
5	75.0	0.04	0.009	0.45	0.119
6	83.0	0.44	0.010	0.37	0.163
7	88.1	0.40	0.011	0.36	0.146
8	94.0	0.09	0.012	0.34	0.137
9	105.9	0.19	0.013	0.36	0.04
10	113.2	0.44	0.014	0.32	0.137
11	123.8	0.14	0.015	0.49	0.16
12	126.7	0.05	0.016	0.35	0.184
13	131.6	0.53	0.016	0.46	0.04

14	137.6	0.38	0.017	0.38	0.124
15	139.4	0.22	0.017	0.36	0.04
16	143.4	0.05	0.018	0.43	0.155
17	144.9	0.52	0.018	0.41	0.016
18	150.0	0.18	0.019	0.33	0.192
19	155.8	0.04	0.019	0.37	0.196
20	163.5	0.84	0.020	0.29	0.067
21	166.9	0.20	0.021	0.29	0.214
22	170.6	0.14	0.021	0.30	0.184
23	175.7	0.21	0.022	0.29	0.137
24	178.1	0.67	0.022	0.32	0.212
25	186.8	1.11	0.023	0.30	0.155
26	191.6	0.35	0.024	0.31	0.19
27	194.9	0.47	0.024	0.28	0.183
28	198.3	0.97	0.025	0.28	0.193
29	209.0	0.82	0.026	0.30	0.16
30	211.5	0.56	0.026	0.27	0.168
31	228.1	0.59	0.028	0.29	0.132
32	230.8	0.19	0.029	0.31	0.207
33	235.4	0.05	0.029	0.31	0.183
34	241.9	1.28	0.030	0.25	0.131
35	247.7	0.39	0.031	0.25	0.03
36	256.2	0.23	0.032	0.29	0.067
37	259.8	0.23	0.032	0.28	0.212
38	260.9	0.18	0.032	0.28	0.016
39	267.8	0.40	0.033	0.27	0.128
40	273.7	0.39	0.034	0.28	0.212
41	277.1	0.95	0.034	0.28	0.184
42	279.7	0.27	0.035	0.24	0.177
43	285.5	0.68	0.035	0.26	0.193
44	289.3	0.18	0.036	0.23	0.155
45	294.3	0.48	0.036	0.25	0.235
46	294.8	0.42	0.037	0.22	0.207
47	304.9	0.02	0.038	0.23	0.113
48	309.8	2.21	0.038	0.27	0.184
49	328.3	3.58	0.041	0.26	0.191
50	347.5	5.74	0.043	0.22	0.14
51	359.0	15.91	0.045	0.16	0.209
52	370.4	1.24	0.046	0.22	0.228
53	379.4	1.77	0.047	0.22	0.202
54	410.3	9.08	0.051	0.15	0.226
55	421.4	4.67	0.052	0.15	0.105
56	438.5	2.06	0.054	0.18	0.105
57	458.4	3.74	0.057	0.17	0.298
58	464.3	1.43	0.058	0.17	0.19
59	479.6	1.57	0.059	0.16	0.207
60	512.1	2.95	0.063	0.15	0.183
61	525.7	11.65	0.065	0.13	0.205

62	533.0	0.37	0.066	0.12	0.14
63	540.7	0.13	0.067	0.12	0.105
64	552.3	2.30	0.068	0.15	0.248
65	558.5	0.09	0.069	0.16	0.155
66	567.8	1.76	0.070	0.15	0.186
67	576.2	10.25	0.071	0.12	0.218
68	594.3	1.97	0.074	0.12	0.151
69	602.1	1.25	0.075	0.11	0.189
70	605.9	8.42	0.075	0.10	0.238
71	613.3	5.49	0.076	0.11	0.237
72	691.4	3.52	0.086	0.10	0.229
73	698.8	3.28	0.087	0.09	0.274

Table S22: Structure parameters of DFT optimized $[LnO_2]^-$ and $[LnO_2]$.

Models	Ln−O1 bond distance (Å)	Ln−O2 bond distance (Å)	O−Ln−O angle (°)
$[LnO_2]^-$	1.964	1.964	117.1
$[LnO_2]$	1.819	1.819	179.9

Table S23: Complexes with g-tensor values and their theoretically predicted $\tau_{QTM.}$

complexes	g_x	g_y	g_z	τ_{QTM}
m3	0.2273	0.1132	19.2594	2.13E-06
m4	2.84E-04	3.53E-04	19.9787	0.695
m5	5.86E-05	6.82E-05	19.9023	17.598
1	2.75E-03	0.01698	19.7969	0.0005
2	1.6816	1.1677	0.3878	3.55E-09
3	2.38E-05	2.76E-05	19.9696	107.478
4-Dy	2.27E-07	4.77E-07	20.0055	512067.6
4-Ho	4.55E-06	5.28E-06	19.9812	2940.95
5-Dy	1.46E-06	1.68E-06	20	28839.27
5-Ho	1.07E-05	1.33E-05	19.9703	491.818
6-Er	10.7946	9.30421	1.7315	5.05E-10
m1	0.00014	1.61E-04	16.79	2.653
m2	1.2E-06	1.2E-06	20.0115	49631.64
7-Er	0.2261	0.2261	14.38	1.01E-06
8-Er	0.180	0.317	16.966	9.12E-07

Table S24: Complexes with their theoretically predicted U_{cal} values computed using CASSCF/RASSI-SO/Single_Aniso methods.

complexes	U_{cal} (cm^{-1})	Mode of relaxation
m1	2564	TA-QTM from fourth excited state

m2	5394	TA-QTM from fourth excited state
m3	875	TA-QTM from third excited state
m4	1881	TA-QTM from fifth excited state
m5	280	TA-QTM from third excited state
1-Ho	Non-SMM	-
2-Ho	725	TA-QTM from second excited state
3-Ho	1299	TA-QTM from third excited state
4-Dy	1384	TA-QTM from sixth excited state
4-Ho	1785	TA-QTM from fifth excited state
5-Dy	1223	TA-QTM from fifth excited state
5-Ho	1694	TA-QTM from fifth excited state
6-Er	Non-SMM	-
7-Er	6243	TA-QTM from third excited state
8-Er	1232	TA-QTM from first excited state

Input files

DFT Optimisation

CASSCF optimisation

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%pal nprocs 4 end
!UKS BP86 DKH autoaux Notrah Largeprint UNO UCO SLOWCONV TIGHTSCF
%basis  newgto Yb "SARC-DKH-TZVP" end
       newgto O "DKH-TZVP" end
end
%SCF
 MAXITER 2500
 end
%maxcore 10000
*xyz -1 2
Yb       0.000000000      0.000000000     -0.040515000
O        0.000000000      0.000000000      2.076678000
O        0.000000000      0.000000000     -2.036163000
*
%pal nprocs 4 end
!CASSCF DKH autoaux Largeprint VERYSLOWCONV MOREAD TIGHTSCF OPT FREQ
%moinp ""
```

```
%basis  newgto Yb "SARC-DKH-TZVP" end
       newgto O "DKH-TZVP" end
end
%casscf
nel 19
norb 15
mult 2
nroots 1
end
%scf
Lshift 1
MAXITER 4000
end
%maxcore 12000
*xyz -1 2
Yb       0.000000000      0.000000000     -0.040515000
O        0.000000000      0.000000000      2.076678000
O        0.000000000      0.000000000     -2.036163000
*
```

Input file for magnetic properties

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   Charge
    0
   Coord
   Dy+4-O2.xyz
   Group
   NoSym
   Basis set
```

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  ANGM
   -0.003730000      0.004457000      0.045960000
  SDIPolar
  AMFI
  Douglas-Kroll
 &SEWARD
  Cholesky
 &GUESSORB
  PRMO
   3
  PRPOpulation

> export MOLCAS_MOLDEN=ON
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  Spin
   7
  Inactive
   37
  Nactel
   8 0 0
  Ras2
   7
  CiRoot
   7 7 1
 >>>COPY Dy+4-O2.JobIph RAS1-Dy+4-O2.JobIph

 > export MOLCAS_MOLDEN=ON
 &RASSCF
  Spin
```

```
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 Inactive
  37
 Nactel
  8 0 0
 Ras2
  7
 CiRoot
  140 140 1


>>>COPY RAS1-Dy+4-O2.JobIph JOB001
>>>COPY Dy+4-O2.JobIph JOB002
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 Nr of JobIph
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  1 2 3 4 5 6 7
  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62
63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92
93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115
116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136
137 138 139 140
 Spin
 MEES
 Properties
  3
 'AngMom' 1 'AngMom' 2 'AngMom' 3
 SOProperties
  3
 'AngMom' 1 'AngMom' 2 'AngMom' 3


 &SINGLE_ANISO
```

MLTP

8

2 2 1 1 1 1 1 1

CRYS

Dy

UBAR

TINT

0.0 300 50 1

Coordinates of all the structures

$[EuO_2]^{2-}$

Eu	0.000000000	0.000000000	0.040925000
O	0.000000000	0.000000000	−2.224855000
O	0.000000000	0.000000000	1.902572000

$[CeO_2]^-$

Ce	−0.000022000	−0.000005000	0.013149000
O	0.000011000	0.000003000	1.864081000
O	0.000011000	0.000003000	−1.877230000

$[PrO_2]^-$

Pr	0.000009000	0.000005000	−0.012239000
O	−0.000005000	−0.000003000	1.861791000
O	−0.000005000	−0.000003000	−1.849551000

$[NdO_2]^-$

Nd	−0.000006000	0.000005000	−0.000102000
O	0.000003000	−0.000003000	1.838814000
O	0.000003000	−0.000003000	−1.838712000

$[PmO_2]^-$

Pm	0.000011000	0.000040000	−0.025015000
O	−0.000006000	−0.000020000	2.073539000
O	−0.000006000	−0.000020000	−2.048523000

$[SmO_2]^-$

Sm	−0.000614000	−0.000177000	−0.024186000
O	0.000307000	0.000089000	2.062214000
O	0.000307000	0.000088000	−2.038028000

$[EuO_2]^-$

Eu	0.000001000	−0.000001000	0.000034000
O	−0.000001000	0.000000000	2.008537000
O	−0.000001000	0.000000000	−2.008571000

$[GdO_2]^-$

Gd	0.000000000	0.000000000	−0.040515000
O	0.000000000	0.000000000	2.076678000
O	0.000000000	0.000000000	−2.036163000

$[TbO_2]^-$

Tb	−0.000058000	−0.000011000	0.015397000
O	0.000029000	0.000006000	1.890628000
O	0.000029000	0.000006000	−1.906025000

$[DyO_2]^-$

Dy	0.494366000	−0.560570000	−0.142835000
O	−0.257281000	0.282421000	1.777238000
O	−0.237085000	0.278149000	−1.634403000

$[HoO_2]^-$

Ho	0.267676000	−0.694005000	−0.140387000
O	−0.138554000	0.353963000	1.766928000
O	−0.129122000	0.340042000	−1.626541000

$[ErO_2]^-$

Er	−0.000001000	−0.000002000	−0.042921000
O	0.000000000	0.000001000	2.042502000
O	0.000000000	0.000001000	−1.999580000

$[TmO_2]^-$

Tm	0.000902000	−0.000024000	−0.043996000
O	−0.000452000	0.000012000	2.040239000
O	−0.000450000	0.000012000	−1.996243000

$[LuO_2]^-$

Lu	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	2.006771000
O	0.000000000	0.000000000	−2.006771000

$[CeO_2]$

Ce	−0.000002000	−0.000003000	−0.000014000
O	0.000001000	0.000002000	1.813043000
O	0.000001000	0.000002000	−1.813029000

$[PrO_2]$

Pr	−0.000013000	−0.000001000	0.000010000
O	0.000007000	0.000001000	1.812399000
O	0.000007000	0.000001000	−1.812409000

$[NdO_2]$

Nd	−0.000002000	−0.000003000	0.000033000
O	0.000001000	0.000002000	1.805028000
O	0.000001000	0.000002000	−1.805062000

$[PmO_2]$

Pm	0.000580000	0.000197000	0.000005000
O	−0.000290000	−0.000098000	1.823914000
O	−0.000290000	−0.000098000	−1.823919000

[SmO_2]

Sm	−0.000119000	−0.000027000	−0.000098000
O	0.000060000	0.000014000	1.843786000
O	0.000060000	0.000014000	−1.843688000

[EuO_2]

Eu	0.000234000	0.000074000	0.000219000
O	−0.000117000	−0.000036000	1.852667000
O	−0.000117000	−0.000036000	−1.852886000

[GdO_2]

Gd	0.000013000	−0.000032000	0.000083000
O	−0.000006000	0.000017000	1.884718000
O	−0.000006000	0.000017000	−1.884801000

[TbO_2]

Tb	0.000007000	−0.000018000	0.000044000
O	−0.000004000	0.000009000	1.839676000
O	−0.000004000	0.000009000	−1.839720000

[DyO_2]

Dy	−0.000004000	−0.000006000	0.000032000
O	0.000002000	0.000003000	1.865460000
O	0.000002000	0.000003000	−1.865492000

[HoO_2]

Ho	−0.000002000	−0.000004000	0.000019000
O	0.000001000	0.000002000	1.892886000
O	0.000001000	0.000002000	−1.892905000

[ErO_2]

Er	−0.000011000	−0.000018000	−0.000059000
O	0.000005000	0.000009000	1.867622000
O	0.000005000	0.000009000	−1.867563000

[TmO_2]

Tm	0.000144000	−0.000069000	0.000043000
O	−0.000072000	0.000035000	1.864968000
O	−0.000072000	0.000035000	−1.865011000

[YbO_2]

Yb	−0.000074000	−0.000024000	0.116589000
O	0.000036000	0.000012000	1.895067000
O	0.000038000	0.000013000	−2.011656000

$LnO_2@C_{82}$ (**m1**)

Zr	−0.004203000	−0.520069000	−0.393989000
O	1.711503000	0.139702000	0.276809000
O	−1.708369000	0.179073000	0.268328000
C	−3.282674000	−1.397762000	−1.943040000
C	−4.178878000	−0.991707000	−0.919286000
C	−4.502245000	0.393153000	−0.699197000

C	−2.760485000	−0.375654000	−2.862041000
C	−3.151893000	0.969885000	−2.647642000
C	−3.969700000	1.356710000	−1.540927000
C	−0.787716000	−1.812941000	−3.372277000
C	−1.476788000	−0.592530000	−3.553144000
C	−0.644371000	0.519619000	−3.890343000
C	−1.023115000	1.852555000	−3.500941000
C	−2.222368000	2.067065000	−2.878944000
C	0.786191000	0.463261000	−3.820392000
C	1.477324000	−0.731212000	−3.525407000
C	0.643265000	−1.890466000	−3.410138000
C	−4.033895000	1.807820000	1.260593000
C	−3.426177000	2.789299000	0.384199000
C	−4.590108000	0.644724000	0.732149000
C	−3.441974000	2.601477000	−0.991421000
C	−2.326475000	3.013023000	−1.778140000
C	−2.234967000	3.294711000	1.005972000
C	−1.105497000	3.677497000	0.262888000
C	−1.156813000	3.560102000	−1.195905000
C	1.312479000	3.600398000	−1.258585000
C	0.096020000	3.421325000	−1.936393000
C	0.151417000	2.577984000	−3.085055000
C	−3.669675000	−0.673248000	2.595059000
C	−3.046908000	0.528709000	3.116898000
C	−4.399083000	−0.618012000	1.408717000
C	−3.222570000	1.744141000	2.457032000
C	−2.107982000	2.631793000	2.303340000
C	−1.758448000	0.188591000	3.634611000
C	−0.665113000	1.060947000	3.535968000
C	−0.846525000	2.335179000	2.838244000
C	1.350558000	3.822504000	0.183570000
C	0.182556000	3.672150000	0.955407000
C	0.305410000	3.009139000	2.255186000
C	1.575868000	2.595271000	2.688666000
C	−3.358179000	−2.706792000	0.644894000
C	−2.631265000	−2.792279000	1.898009000
C	−4.189090000	−1.635392000	0.388841000
C	−2.754803000	−1.767714000	2.835403000
C	−1.575692000	−1.255603000	3.461404000
C	−1.353865000	−3.366033000	1.633489000
C	−0.182279000	−2.924021000	2.285970000
C	−0.303297000	−1.808434000	3.228115000
C	1.756786000	1.324998000	3.397789000
C	0.665729000	0.482808000	3.653480000

C	0.850709000	−0.962167000	3.505370000
C	2.114513000	−1.444826000	3.131352000
C	−1.281880000	−2.808816000	−2.427388000
C	−2.476148000	−2.603018000	−1.690913000
C	−2.511123000	−3.219834000	−0.401922000
C	−1.313897000	−3.714968000	0.216196000
C	−0.095654000	−3.815131000	−0.480375000
C	−0.150830000	−3.478519000	−1.869456000
C	2.226109000	−2.924921000	−1.876508000
C	1.023971000	−2.968768000	−2.534285000
C	2.238700000	−2.552282000	2.185957000
C	1.108225000	−3.198791000	1.650571000
C	1.160462000	−3.655808000	0.257090000
C	2.331092000	−3.373512000	−0.494334000
C	4.039001000	−1.086813000	1.844345000
C	3.431228000	−2.329090000	1.414909000
C	3.445905000	−2.688006000	0.072423000
C	4.589466000	−0.217533000	0.904092000
C	3.669213000	1.716866000	2.111156000
C	3.047660000	0.810498000	3.055530000
C	3.226772000	−0.565709000	2.923281000
C	4.399806000	1.209023000	1.038416000
C	3.353665000	2.834672000	−0.471599000
C	2.628536000	3.398972000	0.650460000
C	2.753092000	2.820137000	1.910695000
C	4.191622000	1.753831000	−0.295118000
C	1.280468000	1.747281000	−3.340100000
C	2.471823000	1.840854000	−2.582792000
C	2.507485000	2.907509000	−1.635926000
C	3.975797000	−1.754743000	−0.918305000
C	3.157620000	−1.825913000	−2.089393000
C	2.760113000	−0.664515000	−2.803130000
C	4.502485000	−0.538929000	−0.513362000
C	4.178159000	0.654233000	−1.251645000
C	3.279589000	0.633995000	−2.350247000

LnO_2@SWCNT(4,4) (**m2**)

Zr	0.000000000	−0.000034000	−0.000042000
O	1.870303000	0.008314000	0.006221000
O	−1.870301000	−0.008360000	−0.006311000
C	−4.966709000	3.449741000	−0.117194000
C	−4.813641000	3.284157000	1.224589000
C	−2.375297000	3.254591000	0.990530000
C	−3.520756000	2.950679000	1.784501000
C	−3.358426000	2.019562000	2.852148000

C	−4.465643000	1.255069000	3.372437000
C	−4.307081000	−0.070023000	3.660905000
C	0.083314000	3.284732000	0.702346000
C	−1.071414000	3.046990000	1.524613000
C	−0.907375000	2.214982000	2.662339000
C	−2.054594000	1.524150000	3.150429000
C	−1.892366000	0.140179000	3.513312000
C	−3.027444000	−0.708719000	3.492347000
C	−2.878248000	−2.009678000	2.876638000
C	−3.988571000	−2.643035000	2.250001000
C	−3.840920000	−3.240957000	1.002628000
C	−4.967837000	−3.448040000	0.117224000
C	−4.814731000	−3.282461000	−1.224548000
C	2.531531000	3.361160000	0.429095000
C	1.403104000	3.159132000	1.260580000
C	1.571345000	2.425400000	2.476182000
C	0.416273000	1.752989000	2.995076000
C	0.579158000	0.428212000	3.459453000
C	−0.579063000	−0.427526000	3.459301000
C	−0.416178000	−1.752378000	2.995156000
C	−1.571337000	−2.424918000	2.476527000
C	−1.403106000	−3.158854000	1.261059000
C	−2.531543000	−3.361046000	0.429624000
C	−2.376339000	−3.253991000	−0.990613000
C	−3.521720000	−2.949544000	−1.784487000
C	−3.359076000	−2.018533000	−2.852128000
C	−4.466051000	−1.253690000	−3.372412000
C	−4.307074000	0.071332000	−3.660920000
C	4.967820000	3.448154000	0.116637000
C	3.840920000	3.241175000	1.002084000
C	3.988582000	2.643403000	2.249519000
C	2.878262000	2.010140000	2.876249000
C	3.027459000	0.709291000	3.492153000
C	1.892371000	−0.139593000	3.513400000
C	2.054580000	−1.523655000	3.150770000
C	0.907443000	−2.214674000	2.662819000
C	1.071439000	−3.046845000	1.525206000
C	−0.083282000	−3.284606000	0.702911000
C	0.082096000	−3.284798000	−0.702462000
C	−1.072495000	−3.047055000	−1.524885000
C	−0.908207000	−2.215123000	−2.662629000
C	−2.055059000	−1.523652000	−3.150493000
C	−1.892403000	−0.139662000	−3.513222000
C	−3.027225000	0.709575000	−3.492286000

C	−2.877641000	2.010483000	−2.876601000
C	−3.987772000	2.644200000	−2.249978000
C	−3.839923000	3.242179000	−1.002658000
C	4.307095000	0.070640000	3.660857000
C	4.465648000	−1.254509000	3.372678000
C	3.358415000	−2.019081000	2.852535000
C	3.520748000	−2.950331000	1.785024000
C	2.375296000	−3.254456000	0.991133000
C	2.530490000	−3.361883000	−0.429070000
C	1.402069000	−3.159446000	−1.260511000
C	1.570580000	−2.425756000	−2.476072000
C	0.415543000	−1.753030000	−2.994769000
C	0.578926000	−0.428283000	−3.459011000
C	−0.579012000	0.427773000	−3.459314000
C	−0.415631000	1.752601000	−2.995282000
C	−1.570586000	2.425377000	−2.476560000
C	−1.402071000	3.159281000	−1.261114000
C	−2.530485000	3.361828000	−0.429694000
C	4.813634000	−3.283852000	1.225150000
C	4.966715000	−3.449708000	−0.116595000
C	3.839915000	−3.242334000	−1.002088000
C	3.987758000	−2.644620000	−2.249543000
C	2.877631000	−2.011015000	−2.876287000
C	3.027218000	−0.710201000	−3.492206000
C	1.892408000	0.139039000	−3.513157000
C	2.055079000	1.523064000	−3.150659000
C	0.908142000	2.214510000	−2.662896000
C	1.072468000	3.046685000	−1.525335000
C	−0.082132000	3.284680000	−0.703021000
C	4.307066000	−0.071970000	−3.660899000
C	4.466049000	1.253096000	−3.372568000
C	3.359087000	2.018042000	−2.852418000
C	3.521722000	2.949301000	−1.784974000
C	2.376335000	3.253809000	−0.991126000
C	4.814728000	3.282380000	−1.225113000
H	−5.955487000	3.595843000	−0.544822000
H	−5.686553000	3.305178000	1.870155000
H	−5.460639000	1.688145000	3.395045000
H	−5.178451000	−0.667175000	3.913300000
H	−4.995183000	−2.424503000	2.592114000
H	−5.956659000	−3.593734000	0.544891000000
H	−5.687681000	−3.303062000	−1.870079000
H	−5.461186000	−1.686453000	−3.395052000
H	−5.178229000	0.668770000	−3.913387000

H	5.956641000	3.593951000	0.544273000
H	4.995199000	2.424906000	2.591645000
H	−4.994449000	2.425956000	−2.592076000
Ho	10.914605000	3.804332000	3.937070000
O	9.520171000	5.597924000	3.475156000
C	10.973651000	1.701329000	2.419337000
H	10.464560000	0.960526000	3.016726000
C	12.479945000	2.051963000	2.759405000
H	12.956550000	1.557563000	3.597466000
C	8.575661000	5.739369000	2.304482000
H	7.742763000	5.053517000	2.481266000
H	9.131619000	5.450489000	1.419537000
C	9.184294000	6.678227000	4.485800000
H	10.098867000	7.256326000	4.620150000
H	8.920862000	6.180880000	5.413523000
C	8.153505000	7.200190000	2.351859000
H	8.919582000	7.834615000	1.891236000
H	7.211447000	7.365001000	1.821207000
C	8.037450000	7.480663000	3.864030000
H	7.074336000	7.121513000	4.242493000
H	8.117183000	8.545088000	4.102525000
B	10.199573000	2.969028000	1.671627000
H	9.019678000	3.076007000	1.834840000
B	12.281179000	1.871201000	-0.019833000
H	12.615217000	1.362308000	-1.035558000
B	12.745242000	3.544333000	0.453985000
H	13.415947000	4.234697000	-0.240475000
B	11.434387000	4.231257000	1.454756000
H	11.196424000	5.390414000	1.311120000
B	11.027124000	3.161899000	0.085077000
H	10.460997000	3.568082000	-0.875785000
B	12.884485000	3.582078000	2.246800000
H	13.767887000	4.155477000	2.800495000
B	13.447102000	2.155697000	1.314363000
H	14.581817000	1.825227000	1.359482000
B	12.199381000	0.897068000	1.450788000
H	12.405573000	-0.245825000	1.659916000
B	10.691191000	1.529147000	0.722635000
H	9.881512000	0.748495000	0.357108000
O	12.309000000	5.597942000	4.399001000
C	10.855671000	1.701311000	5.454798000
H	11.364793000	0.960536000	4.857401000
C	9.349358000	2.051872000	5.114739000
H	8.872773000	1.557452000	4.276679000

C	13.253407000	5.739439000	5.569753000
H	14.086269000	5.053505000	5.393123000
H	12.697339000	5.450694000	6.454674000
C	12.645039000	6.678127000	3.388289000
H	11.730524000	7.256292000	3.253820000
H	12.908498000	6.180673000	2.460632000
C	13.675678000	7.200224000	5.522264000
H	12.909606000	7.834758000	5.982745000
H	14.617699000	7.365017000	6.052989000
C	13.791901000	7.480523000	4.010075000
H	14.755016000	7.121236000	3.631741000
H	13.712294000	8.544929000	3.771453000
B	11.629692000	2.969046000	6.202504000
H	12.809581000	3.076077000	6.039293000
B	9.548147000	1.871113000	7.893975000
H	9.214140000	1.362200000	8.909701000
B	9.084000000	3.544223000	7.420165000
H	8.413263000	4.234552000	8.114629000
B	10.394817000	4.231216000	6.419388000
H	10.632723000	5.390385000	6.563022000
B	10.802138000	3.161873000	7.789061000
H	11.368252000	3.568080000	8.749921000
B	8.944747000	3.581965000	5.627351000
H	8.061311000	4.155315000	5.073660000
B	8.382204000	2.155555000	6.559787000
H	7.247505000	1.825031000	6.514672000
B	9.629985000	0.896986000	6.423351000
H	9.423848000	-0.245915000	6.214223000
B	11.138147000	1.529138000	7.151497000
H	11.947869000	0.748527000	7.517018000
H	5.460638000	−1.687596000	3.395398000
H	5.686555000	−3.304709000	1.870708000
H	5.955492000	−3.595863000	−0.544202000
H	4.994433000	−2.426458000	−2.591695000
H	5.178223000	−0.669449000	−3.913256000
H	5.461191000	1.685836000	−3.395236000
H	5.687667000	3.302929000	−1.870661000

$[(C_2B_9H_{11})_2Ho^{IV}(THF)_2]$ (**m3**)

Ho	10.914605000	3.804332000	3.937070000
O	9.520171000	5.597924000	3.475156000
C	10.973651000	1.701329000	2.419337000
H	10.464560000	0.960526000	3.016726000
C	12.479945000	2.051963000	2.759405000
H	12.956550000	1.557563000	3.597466000

C	8.575661000	5.739369000	2.304482000
H	7.742763000	5.053517000	2.481266000
H	9.131619000	5.450489000	1.419537000
C	9.184294000	6.678227000	4.485800000
H	10.098867000	7.256326000	4.620150000
H	8.920862000	6.180880000	5.413523000
C	8.153505000	7.200190000	2.351859000
H	8.919582000	7.834615000	1.891236000
H	7.211447000	7.365001000	1.821207000
C	8.037450000	7.480663000	3.864030000
H	7.074336000	7.121513000	4.242493000
H	8.117183000	8.545088000	4.102525000
B	10.199573000	2.969028000	1.671627000
H	9.019678000	3.076007000	1.834840000
B	12.281179000	1.871201000	-0.019833000
H	12.615217000	1.362308000	-1.035558000
B	12.745242000	3.544333000	0.453985000
H	13.415947000	4.234697000	-0.240475000
B	11.434387000	4.231257000	1.454756000
H	11.196424000	5.390414000	1.311120000
B	11.027124000	3.161899000	0.085077000
H	10.460997000	3.568082000	-0.875785000
B	12.884485000	3.582078000	2.246800000
H	13.767887000	4.155477000	2.800495000
B	13.447102000	2.155697000	1.314363000
H	14.581817000	1.825227000	1.359482000
B	12.199381000	0.897068000	1.450788000
H	12.405573000	-0.245825000	1.659916000
B	10.691191000	1.529147000	0.722635000
H	9.881512000	0.748495000	0.357108000
O	12.309000000	5.597942000	4.399001000
C	10.855671000	1.701311000	5.454798000
H	11.364793000	0.960536000	4.857401000
C	9.349358000	2.051872000	5.114739000
H	8.872773000	1.557452000	4.276679000
C	13.253407000	5.739439000	5.569753000
H	14.086269000	5.053505000	5.393123000
H	12.697339000	5.450694000	6.454674000
C	12.645039000	6.678127000	3.388289000
H	11.730524000	7.256292000	3.253820000
H	12.908498000	6.180673000	2.460632000
C	13.675678000	7.200224000	5.522264000
H	12.909606000	7.834758000	5.982745000
H	14.617699000	7.365017000	6.052989000

C	13.791901000	7.480523000	4.010075000
H	14.755016000	7.121236000	3.631741000
H	13.712294000	8.544929000	3.771453000
B	11.629692000	2.969046000	6.202504000
H	12.809581000	3.076077000	6.039293000
B	9.548147000	1.871113000	7.893975000
H	9.214140000	1.362200000	8.909701000
B	9.084000000	3.544223000	7.420165000
H	8.413263000	4.234552000	8.114629000
B	10.394817000	4.231216000	6.419388000
H	10.632723000	5.390385000	6.563022000
B	10.802138000	3.161873000	7.789061000
H	11.368252000	3.568080000	8.749921000
B	8.944747000	3.581965000	5.627351000
H	8.061311000	4.155315000	5.073660000
B	8.382204000	2.155555000	6.559787000
H	7.247505000	1.825031000	6.514672000
B	9.629985000	0.896986000	6.423351000
H	9.423848000	-0.245915000	6.214223000
B	11.138147000	1.529138000	7.151497000
H	11.947869000	0.748527000	7.517018000

$[(C_2B_9H_{11})_2Ho^{IV}]$ (**m4**)

Ho	10.913138000	3.131952000	3.937461000
C	11.088029000	1.307618000	2.244872000
H	10.712827000	0.410114000	2.724995000
C	12.551840000	1.815257000	2.635291000
H	13.113455000	1.257281000	3.378129000
B	10.114373000	2.555773000	1.695557000
H	8.941649000	2.513308000	1.929564000
B	12.315544000	2.130167000	-0.121101000
H	12.698981000	1.861631000	-1.207220000
B	12.526888000	3.759846000	0.633938000
H	13.071398000	4.650764000	0.076262000
B	11.147604000	4.004895000	1.730687000
H	10.685967000	5.077903000	2.048760000
B	10.872223000	3.173991000	0.189992000
H	10.231944000	3.647724000	-0.685902000
B	12.705801000	3.468736000	2.387611000
H	13.350591000	4.090084000	3.192001000
B	13.464107000	2.354532000	1.239692000
H	14.631908000	2.179080000	1.220638000
B	12.407028000	0.902621000	1.154137000
H	12.802384000	-0.207469000	1.134469000
B	10.799984000	1.411611000	0.526490000

H	10.135484000	0.588137000	0.001741000
C	10.738039000	1.303284000	5.625987000
H	11.110917000	0.406151000	5.143436000
C	9.274545000	1.814105000	5.238657000
H	8.711079000	1.258542000	4.495348000
B	11.715004000	2.548199000	6.176486000
H	12.887333000	2.504252000	5.941536000
B	9.515189000	2.123241000	7.995268000
H	9.132792000	1.852932000	9.081329000
B	9.305657000	3.754798000	7.244107000
H	8.763297000	4.645460000	7.804284000
B	10.683962000	3.999259000	6.146137000
H	11.147218000	5.071640000	5.827931000
B	10.960127000	3.165069000	7.684531000
H	11.602442000	3.635697000	8.560597000
B	9.123630000	3.467126000	5.490029000
H	8.480097000	4.091626000	4.686917000
B	8.364785000	2.352321000	6.636814000
H	7.196735000	2.178760000	6.657098000
B	9.419738000	0.898498000	6.717762000
H	9.022504000	-0.210957000	6.735655000
B	11.028562000	1.403045000	7.344319000
H	11.692198000	0.577397000	7.866704000

[{μ-1,2-[o-$C_6H_4(CH_2)_2$]-1,2-$C_2B_{10}H_{10}$}$_2$$Ho^{IV}$]$^{4-}$ (**m5**)

Ho	-2.942706000	4.018064000	1.567388000
C	-1.871467000	6.274248000	1.540186000
C	-1.450859000	5.510464000	2.841840000
C	-4.454550000	2.270670000	0.708554000
C	-3.910212000	3.064512000	-0.527515000
C	-5.961124000	2.466235000	0.988711000
H	-6.302782000	1.657199000	1.647908000
H	-6.142271000	3.411755000	1.523773000
C	2.159276000	6.548441000	3.001433000
H	2.437475000	6.037767000	3.922342000
C	1.411158000	7.870856000	0.673743000
H	1.102766000	8.396330000	-0.229028000
C	0.954952000	6.193660000	2.375248000
C	-4.973875000	3.937126000	-1.228374000
H	-5.156410000	4.859582000	-0.654565000
H	-4.591092000	4.243069000	-2.210927000
C	-0.724661000	6.456614000	0.522633000
H	-0.544610000	5.520693000	-0.029676000
H	-1.023322000	7.210872000	-0.217276000
C	0.039065000	5.106517000	2.900730000

H	0.297815000	4.873711000	3.942212000
H	0.222466000	4.192237000	2.314566000
C	2.997004000	7.542869000	2.473020000
H	3.928810000	7.800073000	2.979072000
C	2.620265000	8.208718000	1.301033000
H	3.254437000	8.991824000	0.882603000
C	0.572777000	6.869532000	1.186544000
C	-6.294774000	3.213530000	-1.390306000
C	-6.788922000	2.478401000	-0.280677000
C	-8.016873000	1.810514000	-0.400334000
H	-8.381263000	1.234397000	0.449115000
C	-8.770237000	1.864528000	-1.583323000
H	-9.722654000	1.336474000	-1.650916000
C	-8.283101000	2.589473000	-2.676929000
H	-8.850793000	2.632890000	-3.607708000
C	-7.049489000	3.250490000	-2.572438000
H	-6.655591000	3.802412000	-3.424752000
B	-1.503680000	1.767961000	-1.209443000
H	-0.746198000	1.648943000	-2.144980000
B	-1.890444000	6.598156000	4.029193000
H	-1.005883000	6.988469000	4.756690000
B	-4.260950000	4.959437000	3.579785000
H	-5.007001000	4.153925000	4.091525000
B	-4.751936000	5.821546000	2.062355000
H	-5.837179000	5.614726000	1.561171000
B	-1.096510000	2.681090000	0.314845000
H	0.011266000	3.174161000	0.350435000
B	-2.510754000	7.696331000	2.103702000
H	-2.006367000	8.723941000	1.709673000
B	-3.453697000	6.475872000	1.055661000
B	-3.250984000	1.889358000	-1.493897000
H	-3.680790000	1.795128000	-2.621705000
B	-2.573410000	0.397318000	-0.704864000
H	-2.548391000	-0.615546000	-1.366325000
B	-3.480809000	6.175653000	4.695038000
H	-3.663372000	6.221804000	5.890350000
B	-4.276993000	7.574817000	2.216958000
H	-4.970619000	8.494556000	1.847975000
B	-4.052639000	0.701785000	0.305867000
H	-4.968138000	-0.085000000	0.223108000
B	-1.730537000	1.742906000	1.731048000
H	-1.058332000	1.621214000	2.731368000
B	-1.113021000	0.873666000	0.265728000
H	-0.090629000	0.228742000	0.292367000

B	-2.290454000	3.335630000	-0.813477000
B	-4.809588000	6.685265000	3.649803000
H	-5.858104000	6.999103000	4.163694000
B	-2.530588000	4.853840000	3.926543000
B	-3.305566000	7.701070000	3.739646000
H	-3.327480000	8.750629000	4.341357000
B	-2.533552000	0.231977000	1.095444000
H	-2.434104000	-0.860671000	1.605790000
B	-3.484110000	1.556754000	1.858309000
H	-4.056523000	1.325006000	2.894975000
H	-3.576737000	6.701732000	-0.125422000
H	-2.044230000	4.010879000	4.639952000
H	-2.074662000	4.279069000	-1.537540000

$[Tb(OSi(O^tBu)_3)_4]$ (**1**)

Tb	5.841224078	6.735304212	25.314820288
Si	3.909163308	7.412886936	23.074205237
Si	4.441747800	8.337646668	28.248187843
Si	6.280182492	3.229860348	25.613622946
Si	9.055924296	8.179862652	24.433392936
O	4.802819730	8.511182160	23.941461731
O	4.405848685	6.134997960	23.914334661
O	4.252595073	7.370883000	21.496381447
O	2.365052902	7.819194240	23.230084672
O	5.131586681	7.547245680	27.029898958
O	2.967676142	8.901603360	27.871647908
O	5.376234046	9.640711080	28.511360915
O	4.264349570	7.412617680	29.564458087
O	6.218076309	4.819682400	25.841571315
O	4.971897446	2.419265160	26.029841282
O	6.657081021	3.078942360	24.029321049
O	6.560741776	2.524275000	27.054191857
O	7.684690911	7.418002800	24.795357131
O	8.928844919	8.595997800	22.872169293
O	10.365523442	7.287413640	24.772278877
O	9.242253452	9.574743360	25.240322065
C	4.814980455	9.996129000	23.889231998
C	5.951622043	10.430977440	24.793737605
H	6.789019871	10.169193294	24.403836576
H	5.931137812	11.384911060	24.897468283
H	5.854530657	10.013374847	25.652855978
C	3.511571538	10.503676560	24.430558765
H	3.512179025	11.463870382	24.415173262
H	2.790990670	10.175197703	23.889029558
C	5.074717893	10.421553480	22.462024182

H	4.365510260	10.104167970	21.898874295
H	5.116953214	11.379175907	22.415867674
H	5.909555118	10.050168679	22.164638610
C	5.225209027	6.662739720	20.704432939
C	6.527819107	6.456758880	21.467229968
H	6.365634881	5.896948730	22.230796272
H	7.171195613	6.035319389	20.893067300
H	6.865677922	7.305871139	21.759068661
C	4.630815450	5.315113440	20.341254099
H	3.774011085	5.443400461	19.929125067
H	5.215961032	4.860555461	19.732433562
H	4.526012564	4.787573622	21.138263627
C	5.443446733	7.510896120	19.497480740
H	5.726765063	8.387108995	19.769075351
H	6.122030635	7.112787661	18.945950957
H	4.625891319	7.577819699	19.000448027
C	1.159949284	7.374921840	22.577820334
C	0.041899925	7.759957920	23.483135703
H	0.015900163	8.714928175	23.570711604
H	−0.787802391	7.448092158	23.115948535
H	0.179733356	7.362549527	24.346464846
C	1.059890824	8.065563480	21.248188995
H	1.834800169	7.859865359	20.722652613
H	0.271550063	7.764844916	20.791887375
H	1.007936887	9.014744731	21.386091685
C	1.223352351	5.912861760	22.357564716
H	1.239414083	5.461386762	23.204739081
H	0.454490362	5.629873704	21.858183689
H	2.020703318	5.697187704	21.866240834
C	1.664560477	8.280968280	27.824681637
C	1.748268600	6.940073400	27.169178246
H	2.359720718	6.382982736	27.656372335
H	0.878994864	6.531450494	27.163428926
H	2.058650562	7.043211911	26.266737536
C	0.800877042	9.236827080	27.011679284
H	1.143713295	9.293815112	26.116404979
H	−0.101434121	8.913504475	26.989653722
H	0.820103571	10.107695224	27.416601422
C	1.135597662	8.157110520	29.246625992
H	1.020959948	9.032300222	29.623125438
H	0.292767322	7.699052213	29.236058581
H	1.763192012	7.660198572	29.778195110
C	5.120544378	10.833515160	29.276587234
C	4.519905177	11.872843320	28.351027782

H	3.690728270	11.543758637	27.996229992
H	4.359066444	12.682792294	28.840934579
H	5.128413491	12.050390726	27.630257469
C	4.190459502	10.562912880	30.456817244
H	4.573093619	9.883445364	31.017173448
H	4.074863051	11.368917253	30.964903227
H	3.338058286	10.265209984	30.130320681
C	6.475227229	11.299328040	29.791596693
H	7.058570936	11.472607739	29.048355448
H	6.364539918	12.102060953	30.305229554
H	6.859986107	10.615283172	30.345717719
C	5.155630795	6.510610080	30.265308224
C	4.914280957	5.140097040	29.696044624
H	3.976866430	4.936768372	29.737787922
C	6.598597452	6.936034560	30.084326126
H	6.712299448	7.831916586	30.411915869
H	7.171966263	6.341921196	30.573909017
H	6.827353973	6.905770186	29.152329056
C	4.743629977	6.571192680	31.717213821
H	3.823265802	6.309354683	31.799769189
H	5.292952974	5.975652259	32.231292052
H	4.850835185	7.467922862	32.043507942
C	3.545609146	2.545815480	25.805536848
C	3.053925841	3.744004680	26.584529143
H	3.393445110	4.547424196	26.184182167
H	2.094328104	3.761237064	26.573799779
H	3.732794021	3.744422027	27.476200001
C	2.370986371	2.867576400	24.811147516
H	2.426685818	2.272305235	24.053978342
H	1.531515740	2.733810019	25.255383662
C	2.956318221	1.276273440	26.276819089
H	3.141073230	1.163509027	27.210557150
H	2.006304664	1.293371196	26.136770526
H	3.337591362	0.544610648	25.783673239
C	7.111643255	1.966915080	23.265714257
C	6.686278383	2.287329720	21.832838098
H	7.038329066	3.143873444	21.578248516
H	7.025001802	1.613193473	21.239969898
H	5.681782353	1.632754921	21.850936308
H	5.523582954	0.737007523	23.679503304
C	6.767636305	0.686602800	24.009481848
H	5.927733499	0.799138345	24.463718572
H	7.454511018	0.496710006	24.650976335
C	8.632998154	1.888830840	23.349524759

H	8.891476854	1.643336682	24.240466830
H	8.957013537	1.119458746	22.956020283
H	8.944646769	2.655618077	22.643532626
C	7.786420650	2.311562760	27.816179122
C	8.335650735	3.613415520	28.366008403
H	8.555832678	3.500381851	29.294240074
H	9.533154064	1.506527708	28.456377987
C	9.298521703	1.992494400	27.726295396
H	9.800148958	2.810076781	27.770872866
H	9.482447527	1.549204784	26.895154345
C	6.606018358	1.851135000	28.612986210
H	6.874962777	1.691439266	29.519516224
H	5.924473131	2.526806006	28.594159213
C	9.731637162	9.477811200	22.057952295
C	9.481226329	9.055079280	20.636007940
H	8.542351607	9.110209446	20.445956494
H	9.963113970	9.634208548	20.040386545
H	9.780439325	8.150958020	20.513936123
C	11.214927306	9.353953440	22.397648000
H	11.489191321	8.439129254	22.305294495
H	11.727249888	9.903841506	21.799799755
H	11.361496736	9.642676649	23.301667748
C	9.273287694	10.914291960	22.284281138
H	9.408479180	11.152462355	23.204212735
H	9.778869579	11.504662666	21.722224431
H	8.339556002	10.989279756	22.069167517
C	10.714818146	5.910169200	24.509915568
C	10.055106158	5.040472320	25.546817474
H	9.103198345	5.074452427	25.434179399
H	10.358439406	4.135381739	25.444301440
H	10.286026527	5.357696276	26.423264782
C	10.287877501	5.525133120	23.103761597
H	10.709055484	6.110670680	22.470283768
H	10.553015147	4.618978978	22.926463923
H	9.334896690	5.600713279	23.026388714
C	12.224589007	5.848240320	24.662151068
H	12.462804262	6.037311883	25.572446482
H	12.533951338	4.969765694	24.426631413
H	12.631731597	6.496191421	24.083008356
C	9.650152074	9.869578680	26.576431510
C	11.165235074	9.800918400	26.649715089
H	11.544835990	10.388098422	25.991822895
H	11.456525006	10.069285855	27.524218964
H	11.454028883	8.900835980	26.479057473

C	9.207133221	11.308752000	26.831102068
H	8.253824814	11.371259780	26.734051936
H	9.455844050	11.567170446	27.721153399
H	9.632113010	11.890789232	26.197421797
C	8.978037908	8.940645480	27.559079275
H	9.233397264	8.034747131	27.370121008
H	9.247103034	9.169418840	28.451762337
H	8.024780609	9.027036268	27.480532234
H	9.214196103	3.865076402	28.012137188
H	5.664770266	1.910490291	28.879311159
H	1.805238545	2.072652895	24.719354170
H	4.045890750	5.036551640	29.211094320
H	5.353606463	5.829593694	29.120208307
H	7.384938925	3.706392370	28.461414694
H	3.414481286	9.927218697	25.192050600

$[Pr^{IV}(OSiPh_3)_4(MeCN)_2]$ (**2**)

Pr	8.023000000	1.953000000	10.587000000
Si	5.686000000	4.040000000	8.652000000
Si	8.873000000	4.307000000	13.243000000
Si	5.882000000	−0.515000000	12.309000000
Si	9.292000000	−0.285000000	7.931000000
O	6.577000000	3.115000000	9.608000000
O	8.211000000	3.171000000	12.306000000
O	6.775000000	0.534000000	11.479000000
O	8.522000000	0.636000000	9.001000000
N	9.668000000	3.556000000	9.369000000
N	10.392000000	1.139000000	11.325000000
C	4.572000000	5.095000000	9.726000000
C	3.507000000	5.839000000	9.197000000
H	3.338000000	5.811000000	8.262000000
C	2.693000000	6.615000000	10.013000000
H	1.983000000	7.119000000	9.633000000
C	2.918000000	6.654000000	11.365000000
H	2.357000000	7.182000000	11.923000000
C	3.945000000	5.941000000	11.917000000
H	4.094000000	5.971000000	12.853000000
C	4.759000000	5.178000000	11.116000000
H	5.470000000	4.690000000	11.516000000
C	6.759000000	5.136000000	7.581000000
C	7.454000000	4.593000000	6.508000000
H	7.373000000	3.667000000	6.310000000
C	8.281000000	5.415000000	5.718000000
H	8.747000000	5.043000000	4.980000000
C	8.418000000	6.746000000	6.002000000

H	8.959000000	7.298000000	5.449000000
C	7.775000000	7.286000000	7.088000000
H	7.896000000	8.202000000	7.308000000
C	6.946000000	6.484000000	7.858000000
H	6.491000000	6.868000000	8.598000000
C	4.662000000	2.950000000	7.536000000
C	4.230000000	3.318000000	6.274000000
H	4.494000000	4.160000000	5.920000000
C	3.408000000	2.475000000	5.504000000
H	3.122000000	2.746000000	4.640000000
C	3.019000000	1.246000000	6.012000000
H	2.453000000	0.679000000	5.500000000
C	3.444000000	0.851000000	7.244000000
H	3.186000000	0.001000000	7.585000000
C	4.264000000	1.697000000	8.012000000
H	4.554000000	1.412000000	8.870000000
C	9.758000000	5.570000000	12.181000000
C	11.131000000	5.578000000	11.987000000
H	11.668000000	4.943000000	12.448000000
C	11.736000000	6.489000000	11.141000000
H	12.676000000	6.453000000	11.005000000
C	10.990000000	7.444000000	10.492000000
H	11.414000000	8.094000000	9.941000000
C	9.603000000	7.449000000	10.648000000
H	9.074000000	8.089000000	10.185000000
C	8.994000000	6.521000000	11.484000000
H	8.049000000	6.527000000	11.583000000
C	7.546000000	5.175000000	14.248000000
C	7.703000000	6.511000000	14.646000000
H	8.449000000	7.014000000	14.340000000
C	6.762000000	7.102000000	15.492000000
H	6.886000000	7.996000000	15.786000000
C	5.649000000	6.392000000	15.902000000
H	5.001000000	6.808000000	16.458000000
C	5.478000000	5.090000000	15.509000000
H	4.719000000	4.601000000	15.804000000
C	6.424000000	4.482000000	14.671000000
H	6.294000000	3.583000000	14.391000000
C	10.048000000	3.491000000	14.467000000
C	10.895000000	4.218000000	15.283000000
H	10.941000000	5.161000000	15.181000000
C	11.682000000	3.600000000	16.250000000
H	12.253000000	4.121000000	16.803000000
C	11.635000000	2.225000000	16.406000000

H	12.181000000	1.798000000	17.055000000
C	10.799000000	1.488000000	15.618000000
H	10.748000000	0.548000000	15.734000000
C	10.030000000	2.099000000	14.653000000
H	9.470000000	1.564000000	14.102000000
C	4.565000000	0.427000000	13.276000000
C	3.880000000	−0.158000000	14.344000000
H	4.099000000	−1.037000000	14.630000000
C	2.877000000	0.558000000	14.981000000
H	2.417000000	0.166000000	15.714000000
C	2.533000000	1.828000000	14.563000000
H	1.820000000	2.294000000	14.984000000
C	3.230000000	2.412000000	13.543000000
H	3.024000000	3.300000000	13.277000000
C	4.237000000	1.711000000	12.894000000
H	4.706000000	2.123000000	12.177000000
C	6.993000000	−1.486000000	13.442000000
C	7.573000000	−2.676000000	13.027000000
H	7.308000000	−3.046000000	12.194000000
C	8.519000000	−3.338000000	13.772000000
H	8.894000000	−4.151000000	13.455000000
C	8.917000000	−2.819000000	14.966000000
H	9.590000000	−3.262000000	15.470000000
C	8.346000000	−1.648000000	15.454000000
H	8.598000000	−1.306000000	16.303000000
C	7.407000000	−0.987000000	14.679000000
H	7.035000000	−0.171000000	14.995000000
C	5.058000000	−1.699000000	11.108000000
C	4.116000000	−2.654000000	11.541000000
H	3.882000000	−2.688000000	12.461000000
C	3.527000000	−3.532000000	10.678000000
H	2.903000000	−4.170000000	11.003000000
C	3.835000000	−3.493000000	9.338000000
H	3.413000000	−4.092000000	8.734000000
C	4.774000000	−2.565000000	8.863000000
H	4.996000000	−2.534000000	7.940000000
C	5.379000000	−1.690000000	9.761000000
H	6.025000000	−1.071000000	9.443000000
C	10.288000000	−1.607000000	8.792000000
C	11.410000000	−2.206000000	8.178000000
H	11.646000000	−1.957000000	7.292000000
C	12.172000000	−3.149000000	8.842000000
H	12.918000000	−3.545000000	8.406000000
C	11.869000000	−3.515000000	10.111000000

H	12.417000000	−4.138000000	10.573000000
C	10.740000000	−2.969000000	10.741000000
H	10.508000000	−3.245000000	11.620000000
C	9.965000000	−2.034000000	10.084000000
H	9.199000000	−1.675000000	10.518000000
C	8.043000000	−1.040000000	6.758000000
C	6.991000000	−0.257000000	6.262000000
H	6.888000000	0.632000000	6.578000000
C	6.098000000	−0.742000000	5.325000000
H	5.408000000	−0.183000000	4.989000000
C	6.218000000	−2.043000000	4.879000000
H	5.618000000	−2.384000000	4.226000000
C	7.225000000	−2.851000000	5.401000000
H	7.285000000	−3.759000000	5.128000000
C	8.142000000	−2.351000000	6.315000000
H	8.841000000	−2.909000000	6.637000000
C	10.468000000	0.812000000	6.959000000
C	11.702000000	1.176000000	7.521000000
H	11.966000000	0.794000000	8.349000000
C	12.536000000	2.077000000	6.896000000
H	13.360000000	2.319000000	7.303000000
C	12.188000000	2.630000000	5.690000000
H	12.775000000	3.238000000	5.255000000
C	10.981000000	2.300000000	5.116000000
H	10.725000000	2.688000000	4.287000000
C	10.142000000	1.396000000	5.756000000
H	9.313000000	1.175000000	5.348000000
C	10.275000000	4.249000000	8.739000000
C	11.082000000	5.173000000	7.918000000
H	11.175000000	4.807000000	7.014000000
H	11.969000000	5.276000000	8.322000000
H	10.638000000	6.045000000	7.875000000
C	11.419000000	0.681000000	11.368000000
C	12.734000000	0.095000000	11.373000000
H	12.731000000	−0.721000000	10.829000000
H	12.989000000	−0.129000000	12.293000000
H	13.379000000	0.732000000	11.002000000

$[Ce(O)(NR_2)_3]^+$ (**3**)

Ce	1.420105000	4.567286000	7.198787000
C	3.953820000	1.527653000	8.744377000
H	3.717633000	0.626892000	8.437886000
H	4.698802000	1.473829000	9.378209000
H	4.217553000	2.075392000	7.975022000
C	3.017957000	3.940236000	10.383166000

H	3.128021000	4.622535000	9.688870000
H	3.869448000	3.807259000	10.850200000
H	2.337077000	4.233102000	11.025338000
C	2.043436000	1.185712000	11.031593000
H	1.271476000	1.554565000	11.513221000
H	2.808709000	1.127139000	11.640405000
H	1.821769000	0.291283000	10.697997000
C	0.551637000	−0.231127000	7.776950000
H	1.181664000	−0.150391000	7.030529000
H	−0.200952000	−0.799445000	7.507988000
H	1.005866000	−0.634807000	8.546305000
C	−1.226985000	1.239536000	9.734739000
H	−0.704525000	0.918175000	10.499925000
H	−1.920105000	0.582566000	9.513732000
H	−1.648775000	2.094388000	9.964086000
C	−1.214242000	2.023151000	6.836627000
H	−1.532249000	2.934993000	7.007595000
H	−1.980714000	1.415256000	6.776163000
H	−0.714551000	2.002571000	5.994298000
C	−1.005123000	4.958144000	9.724315000
H	−1.255928000	4.624118000	8.836116000
H	−1.805248000	5.024632000	10.285172000
H	−0.367170000	4.339167000	10.137139000
C	0.523784000	7.112689000	11.221325000
H	1.306471000	6.552285000	11.396463000
H	−0.145289000	6.965464000	11.921876000
H	0.791522000	8.056192000	11.219240000
C	−1.644970000	7.840896000	9.257281000
H	−1.313130000	8.762237000	9.226006000
H	−2.294229000	7.753828000	9.989106000
H	−2.080801000	7.620851000	8.408697000
C	3.510228000	7.994453000	8.792332000
H	3.310917000	8.022948000	9.751419000
H	4.019203000	8.792315000	8.542135000
H	4.037231000	7.193425000	8.592174000
C	2.340811000	7.840896000	6.004723000
H	2.774712000	6.981295000	5.819160000
H	2.949533000	8.572270000	5.767036000
H	1.520437000	7.913717000	5.473054000
C	1.100988000	9.620256000	8.100121000
H	0.252766000	9.655083000	7.610152000
H	1.696884000	10.329467000	7.774865000
H	0.931723000	9.750067000	9.057123000
C	−1.435467000	6.279999000	5.723251000

H	−1.796697000	5.700599000	6.427972000
H	−2.157363000	6.830904000	5.354211000
H	−0.742584000	6.859399000	6.100631000
C	−2.120212000	4.155533000	3.784226000
H	−1.829107000	3.603045000	3.029466000
H	−2.865099000	4.728600000	3.502755000
H	−2.413674000	3.577716000	4.518137000
C	−0.267629000	6.362318000	2.941897000
H	0.483783000	6.936969000	3.200434000
H	−1.044519000	6.917972000	2.722975000
H	−0.015729000	5.827244000	2.160032000
C	0.679339000	2.507567000	2.599961000
H	−0.024654000	1.974076000	3.023211000
H	1.285543000	1.917086000	2.103738000
H	0.275197000	3.151872000	1.982809000
C	2.927255000	4.486392000	3.031551000
H	2.472328000	5.132281000	2.451928000
H	3.508324000	3.911741000	2.491543000
H	3.468867000	4.967642000	3.692487000
C	2.581364000	2.097555000	4.874667000
H	3.196104000	2.523398000	5.508499000
H	3.090997000	1.541900000	4.247090000
H	1.943195000	1.537151000	5.364636000
N	0.640713000	4.342334000	4.943471000
N	0.931278000	6.601360000	8.275258000
N	1.169144000	2.580388000	8.490010000
O	3.249117000	4.665278000	7.026359000
Si	1.914373000	7.946961000	7.828032000
Si	−0.209333000	6.665474000	9.552096000
Si	−0.697242000	5.224098000	4.361972000
Si	1.644930000	3.425742000	3.919332000
Si	2.474545000	2.306518000	9.584413000
Si	−0.087439000	1.476362000	8.247945000

4−Dy

Y	−0.005006000	0.086180000	−0.268107000
C	−2.397140000	1.206498000	0.019063000
C	−2.192801000	0.435037000	1.225598000
C	−2.231565000	−0.970982000	0.860794000
C	−2.417901000	−1.061768000	−0.561372000
C	−2.514068000	0.275066000	−1.079422000
C	−2.691785000	2.701851000	−0.185151000
H	−2.992844000	2.774370000	−1.229447000
C	−2.142026000	0.871237000	2.697374000
H	−1.598405000	0.074954000	3.216349000

C	−3.542700000	0.915228000	3.350571000
H	−4.178386000	1.682890000	2.903102000
H	−3.447757000	1.138749000	4.419554000
H	−4.061591000	−0.041744000	3.255741000
C	−1.360733000	2.152041000	3.035018000
H	−0.366142000	2.166769000	2.572227000
H	−1.215045000	2.207671000	4.119720000
H	−1.887663000	3.061134000	2.738328000
C	−2.445242000	−2.096261000	1.885407000
H	−2.256305000	−1.655681000	2.867792000
C	−3.925085000	−2.551122000	1.902090000
H	−4.614494000	−1.702498000	1.945442000
H	−4.109378000	−3.182038000	2.779145000
H	−4.177582000	−3.141150000	1.016021000
C	−1.530319000	−3.334244000	1.817959000
H	−1.720068000	−3.963393000	0.943393000
H	−1.706497000	−3.959045000	2.701298000
H	−0.473340000	−3.061589000	1.817199000
C	−2.698204000	−2.366503000	−1.316727000
H	−2.577334000	−3.163942000	−0.582698000
C	−4.158600000	−2.471238000	−1.812895000
H	−4.869330000	−2.210221000	−1.023012000
H	−4.367908000	−3.499977000	−2.128123000
H	−4.357315000	−1.822521000	−2.670443000
C	−1.716704000	−2.711404000	−2.456573000
H	−1.775216000	−2.016647000	−3.300789000
H	−1.938678000	−3.710320000	−2.849912000
H	−0.677736000	−2.736450000	−2.106311000
C	−2.879783000	0.590259000	−2.536111000
H	−2.853959000	−0.366595000	−3.059063000
C	−4.330107000	1.100092000	−2.705640000
H	−5.036474000	0.455179000	−2.174309000
H	−4.600063000	1.093234000	−3.768080000
H	−4.474096000	2.121170000	−2.341269000
C	−1.874849000	1.483885000	−3.291457000
H	−1.788972000	2.490758000	−2.871697000
H	−2.178150000	1.593657000	−4.339111000
H	−0.870660000	1.034121000	−3.308321000
C	2.494785000	0.823886000	−0.726475000
C	2.420178000	−0.582172000	−1.044563000
C	2.239559000	−1.322274000	0.174980000
C	2.198137000	−0.372907000	1.258650000
C	2.350579000	0.959501000	0.706759000
H	2.984517000	1.276621000	−2.710872000

C	2.643665000	−1.232271000	−2.415853000
H	2.495511000	−2.301394000	−2.260972000
C	4.093480000	−1.094233000	−2.935238000
H	4.238943000	−1.751714000	−3.800236000
H	4.340864000	−0.077759000	−3.254313000
H	4.814489000	−1.385955000	−2.165626000
C	1.620480000	−0.836460000	−3.502854000
H	0.586415000	−1.036571000	−3.183412000
H	1.686190000	0.215552000	−3.797151000
H	1.776956000	−1.435048000	−4.407803000
C	2.388536000	−2.837327000	0.369952000
H	2.194703000	−3.018657000	1.429274000
C	3.839470000	−3.300810000	0.105533000
H	3.967655000	−4.337347000	0.438479000
H	4.088287000	−3.266510000	−0.959509000
C	1.403933000	−3.753627000	−0.385664000
H	1.596732000	−3.799235000	−1.461923000
H	1.494441000	−4.777872000	−0.005494000
C	2.322225000	−0.673227000	2.760320000
H	2.319902000	0.296815000	3.262467000
C	3.679897000	−1.324910000	3.119066000
H	3.839554000	−1.269938000	4.201892000
C	1.181110000	−1.467358000	3.421741000
H	0.200094000	−1.031940000	3.205626000
H	1.161232000	−2.516378000	3.113603000
H	1.312858000	−1.457607000	4.510077000
C	2.586248000	2.170401000	1.626499000
H	2.014614000	1.966761000	2.538893000
C	4.069805000	2.258333000	2.057136000
H	4.202896000	3.077484000	2.773158000
H	4.411004000	1.337803000	2.536309000
H	4.723716000	2.450537000	1.202065000
C	2.103398000	3.559053000	1.177355000
H	2.708584000	3.981605000	0.373444000
H	2.065879000	3.476052000	−3.028723000
H	1.058911000	3.558340000	0.856587000
C	2.852009000	1.861538000	−1.802033000
C	4.217060000	2.544641000	−1.582047000
H	4.994459000	1.804515000	−1.365799000
H	4.508479000	3.081884000	−2.492155000
H	4.206495000	3.270186000	−0.766397000
C	1.755942000	2.883900000	−2.159395000
H	1.536649000	3.582493000	−1.351433000
H	2.179227000	4.247711000	2.026454000

H	0.817553000	2.387686000	−2.448057000
H	4.565525000	−2.681768000	0.640162000
H	0.363794000	−3.449491000	−0.239339000
H	3.714724000	−2.381461000	2.838875000
H	4.519184000	−0.822075000	2.629475000
C	−3.910076000	3.208947000	0.611903000
C	−1.506469000	3.675253000	−0.059369000
H	−1.129474000	3.761628000	0.960396000
H	−3.692420000	3.341545000	1.674013000
H	−4.758378000	2.522801000	0.520813000
H	−4.222158000	4.184316000	0.220886000
H	−1.814242000	4.678255000	−0.378404000
H	−0.673772000	3.382971000	−0.711471000

5−Dy

Y	0.720375000	−0.056221000	−0.266543000
C	−2.356005000	3.227251000	−2.105401000
C	−1.350870000	2.060496000	−2.109742000
C	0.107459000	2.541836000	−2.287696000
C	−1.504194000	1.034283000	−0.979882000
C	−1.489133000	1.235304000	0.449135000
C	−3.388515000	−0.718437000	2.832825000
C	−1.616624000	−0.386784000	−1.234196000
C	0.021066000	−1.467722000	−2.856651000
C	−1.434253000	−0.983011000	−2.640183000
C	−1.643363000	−0.064098000	1.067187000
C	−1.937634000	−0.258140000	2.561808000
C	−1.707723000	−1.067266000	0.037608000
C	3.054825000	1.030664000	0.305610000
C	3.292933000	0.044345000	−0.705750000
C	−2.448725000	−2.034640000	−3.119797000
C	3.052742000	−1.244512000	−0.130535000
C	2.663750000	0.352721000	1.504859000
C	−0.926216000	−1.112271000	3.350920000
C	2.663546000	−1.057424000	1.234730000
H	0.758553000	−0.640922000	−2.802993000
H	0.316215000	−2.262845000	−2.158387000
H	0.165293000	−1.876835000	−3.863359000
H	−3.378572000	2.849409000	−2.004889000
H	−2.184323000	3.952377000	−1.309462000
H	−2.290954000	3.765598000	−3.057981000
H	−0.899277000	−2.161197000	3.039020000
H	0.084916000	−0.706035000	3.250349000
H	−1.182467000	−1.098967000	4.416566000
H	0.473219000	3.119577000	−1.435094000

H	0.803021000	1.696617000	−2.457657000
H	0.210992000	3.171923000	−3.178879000
H	−3.551390000	−1.770474000	2.585297000
H	−3.617528000	−0.595049000	3.897275000
H	−4.109251000	−0.122351000	2.263348000
H	−2.334197000	−2.175699000	−4.200821000
H	−2.319225000	−3.011324000	−2.651357000
H	−3.472733000	−1.697229000	−2.934292000
H	−1.871305000	0.732995000	3.015548000
H	−1.561542000	−0.155262000	−3.340199000
H	−1.584277000	1.525848000	−3.033085000
C	−2.009179000	−2.536641000	0.360907000
H	−1.937351000	−2.599416000	1.446556000
C	−1.000940000	−3.583622000	−0.153565000
H	−1.020252000	−3.708963000	−1.238951000
H	0.029695000	−3.340441000	0.145409000
H	−1.230925000	−4.561984000	0.283266000
C	−3.460690000	−2.950333000	0.027871000
H	−3.680593000	−3.919808000	0.490248000
H	−4.178042000	−2.222348000	0.416943000
H	−3.637750000	−3.049795000	−1.043445000
C	−1.529535000	2.521971000	1.285067000
H	−1.229074000	2.218354000	2.292323000
C	−2.969354000	3.065187000	1.421671000
H	−2.990871000	3.910602000	2.119005000
H	−3.371154000	3.408411000	0.464955000
H	−3.644829000	2.294878000	1.807425000
C	−0.535497000	3.648216000	0.945554000
H	−0.563880000	4.398652000	1.743466000
H	0.495922000	3.276670000	0.892436000
H	−0.756712000	4.169980000	0.013093000
C	3.376241000	2.500357000	0.184891000
H	4.439408000	2.675385000	0.398997000
H	3.189631000	2.891068000	−0.821224000
H	2.806912000	3.111024000	0.891979000
C	2.537094000	0.998977000	2.862116000
H	3.528242000	1.110461000	3.322303000
H	2.097350000	2.000266000	2.809550000
H	1.930942000	0.406239000	3.552361000
C	2.545519000	−2.164687000	2.253470000
H	3.543980000	−2.471111000	2.593696000
H	1.984372000	−1.859357000	3.139592000
H	2.062074000	−3.060068000	1.847535000
C	3.864466000	0.312255000	−2.077371000

H	3.544846000	1.278637000	−2.482679000
H	4.961804000	0.335873000	−2.037633000
H	3.593053000	−0.462147000	−2.802900000
C	3.331806000	−2.574448000	−0.787620000
H	3.230494000	−2.532087000	−1.877101000
H	4.361009000	−2.896250000	−0.578470000
H	2.673955000	−3.369224000	−0.419518000

4−Ho

Zr	0.034776000	0.163980000	−0.427247000
C	−2.250044000	1.135192000	0.152659000
C	−1.793696000	0.412019000	1.324390000
C	−1.792977000	−1.012112000	0.985741000
C	−2.160572000	−1.149436000	−0.395908000
C	−2.421566000	0.175491000	−0.920030000
C	−2.777442000	2.573886000	−0.006437000
H	−3.174288000	2.591532000	−1.019025000
C	−1.620126000	0.879011000	2.780173000
H	−0.898671000	0.183178000	3.216413000
C	−2.921371000	0.729566000	3.607831000
H	−3.729323000	1.351097000	3.216770000
H	−2.725381000	1.048707000	4.636775000
H	−3.280063000	−0.299515000	3.648651000
C	−1.026891000	2.274107000	3.024888000
H	−0.131110000	2.461196000	2.427177000
H	−0.739097000	2.350415000	4.078388000
H	−1.743517000	3.075788000	2.837453000
C	−1.854103000	−2.114614000	2.056601000
H	−1.559539000	−1.635768000	2.991381000
C	−3.323874000	−2.576902000	2.248172000
H	−4.032058000	−1.744019000	2.267767000
H	−3.408727000	−3.112370000	3.199475000
H	−3.635446000	−3.266301000	1.459311000
C	−0.953335000	−3.354306000	1.926022000
H	−1.271864000	−4.040070000	1.136615000
H	−0.998438000	−3.916465000	2.864807000
H	0.087728000	−3.088711000	1.751239000
C	−2.505159000	−2.492671000	−1.057899000
H	−2.226604000	−3.248454000	−0.324516000
C	−4.031642000	−2.646270000	−1.277458000
H	−4.610421000	−2.308024000	−0.413869000
H	−4.260563000	−3.704743000	−1.439530000
H	−4.382389000	−2.102127000	−2.157869000
C	−1.752015000	−2.875768000	−2.347257000
H	−1.956767000	−2.203877000	−3.186403000

H	−2.071326000	−3.876046000	−2.657619000
H	−0.669207000	−2.924254000	−2.195318000
C	−3.063414000	0.414938000	−2.297696000
H	−3.004941000	−0.546399000	−2.809452000
C	−4.576456000	0.734354000	−2.180678000
H	−5.079773000	0.070860000	−1.472606000
H	−5.045049000	0.595438000	−3.160652000
H	−4.771290000	1.765270000	−1.874316000
C	−2.365820000	1.420869000	−3.237673000
H	−2.320394000	2.437423000	−2.835865000
H	−2.921603000	1.474232000	−4.179451000
H	−1.346883000	1.108145000	−3.496765000
C	2.333471000	0.858475000	−0.874654000
C	2.258671000	−0.548673000	−1.156674000
C	2.144970000	−1.271499000	0.082557000
C	2.165966000	−0.295215000	1.151598000
C	2.250450000	1.030394000	0.564362000
H	2.500427000	1.296874000	−2.912182000
C	2.184873000	−1.202550000	−2.538031000
H	2.066245000	−2.268387000	−2.350822000
C	3.442169000	−1.068946000	−3.420134000
H	3.327303000	−1.693559000	−4.312618000
H	3.635683000	−0.047606000	−3.758357000
H	4.329945000	−1.416358000	−2.883845000
C	0.903143000	−0.757914000	−3.277502000
H	−0.009206000	−0.743997000	−2.624444000
H	0.981722000	0.226479000	−3.744774000
H	0.617185000	−1.474536000	−4.054277000
C	2.432534000	−2.767513000	0.272481000
H	2.312742000	−2.955314000	1.340133000
C	3.914610000	−3.056500000	−0.075119000
H	4.169525000	−4.075398000	0.234794000
H	4.089922000	−2.989915000	−1.153571000
C	1.539868000	−3.799798000	−0.451202000
H	1.828391000	−3.954901000	−1.495049000
H	1.652158000	−4.770750000	0.042290000
C	2.466177000	−0.547683000	2.636400000
H	2.399089000	0.427276000	3.122346000
C	3.934298000	−1.022598000	2.818729000
H	4.233872000	−0.855804000	3.858302000
C	1.549016000	−1.471160000	3.455260000
H	0.497437000	−1.192533000	3.375515000
H	1.647943000	−2.524922000	3.185639000
H	1.831346000	−1.388142000	4.509948000

C	2.531340000	2.280934000	1.413469000
H	2.103792000	2.069538000	2.397182000
C	4.055834000	2.459969000	1.621728000
H	4.231942000	3.324039000	2.270701000
H	4.514647000	1.591518000	2.097331000
H	4.574460000	2.640736000	0.676417000
C	1.911559000	3.626734000	0.998514000
H	2.402520000	4.081320000	0.136821000
H	0.987529000	3.105259000	−3.140493000
H	0.840808000	3.559504000	0.792805000
C	2.419500000	1.889262000	−2.003509000
C	3.670801000	2.783868000	−2.019027000
H	4.578983000	2.173708000	−1.985084000
H	3.691842000	3.356878000	−2.952555000
H	3.709745000	3.496169000	−1.195111000
C	1.107138000	2.683646000	−2.136347000
H	1.022325000	3.492475000	−1.412863000
H	2.030195000	4.329147000	1.829796000
H	0.194438000	2.043983000	−2.016317000
H	4.603508000	−2.370490000	0.422978000
H	0.479382000	−3.543586000	−0.419255000
H	4.038214000	−2.092135000	2.618912000
H	4.640499000	−0.488679000	2.177677000
C	−3.995042000	2.835439000	0.909872000
C	−1.798990000	3.761341000	0.041681000
H	−1.340609000	3.911402000	1.018438000
H	−3.704356000	3.036244000	1.942894000
H	−4.699430000	1.997932000	0.904397000
H	−4.526188000	3.720493000	0.544045000
H	−2.352887000	4.675204000	−0.197633000

5−Ho

Zr	0.718405000	−0.073560000	−0.333231000
C	−1.796652000	3.245437000	−2.450105000
C	−0.893036000	2.015656000	−2.259619000
C	0.607490000	2.373349000	−2.171233000
C	−1.268841000	1.048829000	−1.131174000
C	−1.324861000	1.294537000	0.295976000
C	−3.674158000	−0.348947000	2.352841000
C	−1.411343000	−0.372067000	−1.353747000
C	0.416981000	−1.519637000	−2.607340000
C	−1.053647000	−1.038704000	−2.695392000
C	−1.608900000	0.020334000	0.934304000
C	−2.145098000	−0.084605000	2.370067000
C	−1.618353000	−1.014745000	−0.066238000

C	2.863012000	0.922367000	0.545692000
C	3.203869000	−0.158350000	−0.342404000
C	−1.992310000	−2.107591000	−3.275854000
C	2.774060000	−1.379573000	0.270593000
C	2.185700000	0.374056000	1.681150000
C	−1.454300000	−1.035317000	3.364090000
C	2.132059000	−1.059693000	1.512593000
H	1.162212000	−0.689532000	−2.597404000
H	0.608628000	−2.204434000	−1.758893000
H	0.722167000	−2.087475000	−3.494098000
H	−2.842236000	2.935812000	−2.543584000
H	−1.728609000	3.975166000	−1.644069000
H	−1.519186000	3.752728000	−3.380452000
H	−1.535521000	−2.093620000	3.102824000
H	−0.397253000	−0.795643000	3.479900000
H	−1.925959000	−0.913621000	4.344412000
H	0.835267000	3.079778000	−1.372741000
H	1.275861000	1.480660000	−2.024761000
H	0.980713000	2.787156000	−3.114775000
H	−3.909950000	−1.395682000	2.146993000
H	−4.083206000	−0.110701000	3.339698000
H	−4.196685000	0.270245000	1.617333000
H	−1.702648000	−2.297994000	−4.314928000
H	−1.960814000	−3.060269000	−2.748404000
H	−3.024840000	−1.747368000	−3.282798000
H	−2.025933000	0.907507000	2.807346000
H	−1.053776000	−0.247880000	−3.446497000
H	−1.009505000	1.456556000	−3.189065000
C	−2.031342000	−2.456735000	0.255301000
H	−2.098758000	−2.480469000	1.341429000
C	−1.023995000	−3.567798000	−0.101006000
H	−0.925994000	−3.745953000	−1.174407000
H	−0.025612000	−3.360003000	0.308611000
H	−1.355777000	−4.511129000	0.344375000
C	−3.452071000	−2.792201000	−0.257643000
H	−3.791634000	−3.718827000	0.217165000
H	−4.168356000	−2.006369000	−0.004410000
H	−3.489412000	−2.944056000	−1.336076000
C	−1.413258000	2.615094000	1.076905000
H	−1.230547000	2.339640000	2.118562000
C	−2.851022000	3.183198000	1.021888000
H	−2.923196000	4.060799000	1.672442000
H	−3.130942000	3.491483000	0.011463000
H	−3.589278000	2.453734000	1.366004000

C	−0.375569000	3.717668000	0.803659000
H	−0.465797000	4.478357000	1.585597000
H	0.649966000	3.334872000	0.847018000
H	−0.513163000	4.233133000	−0.147802000
C	3.351778000	2.338257000	0.393405000
H	4.384215000	2.396543000	0.763930000
H	3.373925000	2.672194000	−0.647907000
H	2.766202000	3.053705000	0.973915000
C	1.866864000	1.131256000	2.943205000
H	2.747512000	1.126538000	3.598893000
H	1.618864000	2.177281000	2.747990000
H	1.042616000	0.688513000	3.504633000
C	1.823665000	−2.082619000	2.579395000
H	2.729331000	−2.666938000	2.781742000
H	1.530877000	−1.610544000	3.517271000
H	1.039164000	−2.792191000	2.301333000
C	4.053096000	−0.038845000	−1.582503000
H	3.887118000	0.899836000	−2.120149000
H	5.114604000	−0.056880000	−1.302401000
H	3.896699000	−0.867040000	−2.279680000
C	3.095274000	−2.770107000	−0.209556000
H	3.187704000	−2.833257000	−1.297746000
H	4.064165000	−3.078253000	0.206704000
H	2.360014000	−3.508714000	0.121199000

$[Er^{V}O_2(NO_2)_2]^-$ (**6**-Er)

Pr	0.000002000	0.000167000	−0.000526000
N	−3.051956000	0.002520000	0.000735000
O	−4.314529000	−0.004654000	−0.000368000
O	−2.349748000	−0.057892000	−1.121213000
O	−2.351862000	0.070947000	1.123137000
N	3.051924000	−0.003082000	0.000660000
O	4.314510000	0.002909000	0.003590000
O	2.348183000	0.058409000	1.121651000
O	2.353342000	−0.070750000	−1.122642000
O	−0.011627000	−1.817980000	0.078880000
O	0.011747000	1.818276000	−0.080375000

$[NEr^{V}O]^-$ (**7**-Er)

Pr	0.000000000	0.000000000	0.036987000
O	0.000000000	0.000000000	−1.267732000
N	0.000000000	0.000000000	1.137088000

$[(Cp^{iPr5})Er(Cp^*)]^{2+}$ (**8**-Er)

Nb	0.065339000	−0.292439000	−0.376136000
C	1.406566000	−0.390569000	1.612762000
C	1.582934000	1.003805000	1.249068000

C	2.202321000	1.044194000	−0.057099000
C	2.520232000	−0.340103000	−0.448615000
C	2.114873000	−1.203575000	0.625553000
C	1.024167000	−0.877283000	2.987731000
H	0.492482000	−0.113415000	3.548200000
H	1.933855000	−1.116933000	3.549323000
H	0.411675000	−1.777635000	2.966967000
C	1.599804000	2.186136000	2.221589000
H	1.873562000	3.064390000	1.635148000
C	2.775173000	1.944866000	3.215829000
H	2.522214000	1.202715000	3.977121000
H	2.984720000	2.887126000	3.731129000
H	3.696785000	1.631227000	2.716896000
C	0.332830000	2.587645000	2.990826000
H	−0.448978000	2.935704000	2.313909000
H	0.585320000	3.427059000	3.645579000
H	−0.068983000	1.797605000	3.628715000
C	2.775002000	2.326845000	−0.670445000
H	2.321561000	3.148312000	−0.114104000
C	4.301612000	2.389466000	−0.366877000
H	4.538576000	2.131313000	0.668866000
H	4.640062000	3.416099000	−0.536969000
H	4.876864000	1.738884000	−1.029565000
C	2.521408000	2.669714000	−2.151846000
H	2.902537000	1.930473000	−2.861246000
H	3.041209000	3.607223000	−2.370754000
H	1.462272000	2.848059000	−2.353542000
C	3.396226000	−0.707055000	−1.651537000
H	3.495826000	0.211516000	−2.229230000
C	4.833161000	−1.100255000	−1.207763000
H	5.239003000	−0.428320000	−0.447407000
H	5.488028000	−1.044771000	−2.083085000
H	4.885359000	−2.123263000	−0.828525000
C	2.841713000	−1.770768000	−2.624627000
H	2.712097000	−2.754780000	−2.164854000
H	3.555172000	−1.897446000	−3.444618000
H	1.893044000	−1.471951000	−3.084178000
C	2.584294000	−2.643801000	0.786346000
H	2.995440000	−2.941893000	−0.178204000
C	3.771962000	−2.644581000	1.798713000
H	4.515145000	−1.874503000	1.579344000
H	4.268025000	−3.618483000	1.732658000
H	3.428091000	−2.520407000	2.828247000
C	1.567560000	−3.727707000	1.188586000

H	1.187317000	−3.603679000	2.204668000
H	2.074363000	−4.697137000	1.159117000
H	0.723013000	−3.796850000	0.495782000
C	−2.305122000	−0.901730000	0.296987000
C	−2.069305000	−0.785354000	−1.142370000
C	−1.854779000	0.598887000	−1.452683000
C	−1.874959000	1.354455000	−0.224052000
C	−2.212685000	0.427011000	0.862563000
H	−2.729900000	−2.927560000	0.058984000
C	−1.968340000	−1.929904000	−2.156789000
H	−1.710654000	−1.462632000	−3.105792000
C	−3.254863000	−2.728169000	−2.448746000
H	−3.078456000	−3.377465000	−3.312907000
H	−3.585059000	−3.362688000	−1.624335000
H	−4.074573000	−2.051289000	−2.709201000
C	−0.768351000	−2.815242000	−1.760625000
H	0.168291000	−2.232257000	−1.483874000
H	−0.977005000	−3.477113000	−0.916920000
H	−0.400837000	−3.420738000	−2.597065000
C	−1.448202000	1.163714000	−2.806686000
H	−1.346163000	2.240007000	−2.673458000
C	−2.432495000	0.959058000	−3.971621000
H	−2.063093000	1.495937000	−4.851755000
H	−2.573066000	−0.085586000	−4.258762000
C	−0.036200000	0.619721000	−3.074066000
H	−0.007282000	−0.428498000	−3.383610000
H	0.504838000	1.199171000	−3.830498000
C	−2.000820000	2.878942000	−0.136910000
H	−2.207592000	3.103989000	0.910291000
C	−3.236690000	3.362885000	−0.945945000
H	−3.462669000	4.393052000	−0.654084000
C	−0.765693000	3.719037000	−0.514235000
H	0.126413000	3.396978000	0.027493000
H	−0.548623000	3.707800000	−1.586350000
H	−0.956057000	4.763119000	−0.247636000
C	−2.706876000	0.956939000	2.202922000
H	−2.144954000	1.872133000	2.385055000
C	−4.197079000	1.391699000	2.032148000
H	−4.521924000	1.846341000	2.973177000
H	−4.340533000	2.131137000	1.243501000
H	−4.850001000	0.540746000	1.829290000
C	−2.579039000	0.117421000	3.482924000
H	−3.311347000	−0.689551000	3.536614000
H	−2.118202000	−2.309600000	2.979987000

H	−1.583207000	−0.303226000	3.625870000
C	−2.819468000	−2.218586000	0.879477000
C	−4.343561000	−2.130305000	1.166740000
H	−4.896087000	−1.670502000	0.341476000
H	−4.722356000	−3.149608000	1.294063000
H	−4.562140000	−1.582167000	2.083733000
C	−2.061705000	−2.872336000	2.050969000
H	−1.009655000	−3.044990000	1.806501000
H	−2.781202000	0.775555000	4.333444000
H	−2.507948000	−3.854476000	2.236033000
H	−3.412198000	1.376715000	−3.720820000
H	0.666293000	0.760760000	−2.189407000
H	−3.050641000	3.367559000	−2.023833000
H	−4.130596000	2.762029000	−0.758189000