Supporting Information

Periodic trends and hidden dynamics of magnetic properties in three series of triazacyclononane lanthanide complexes

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Computational results

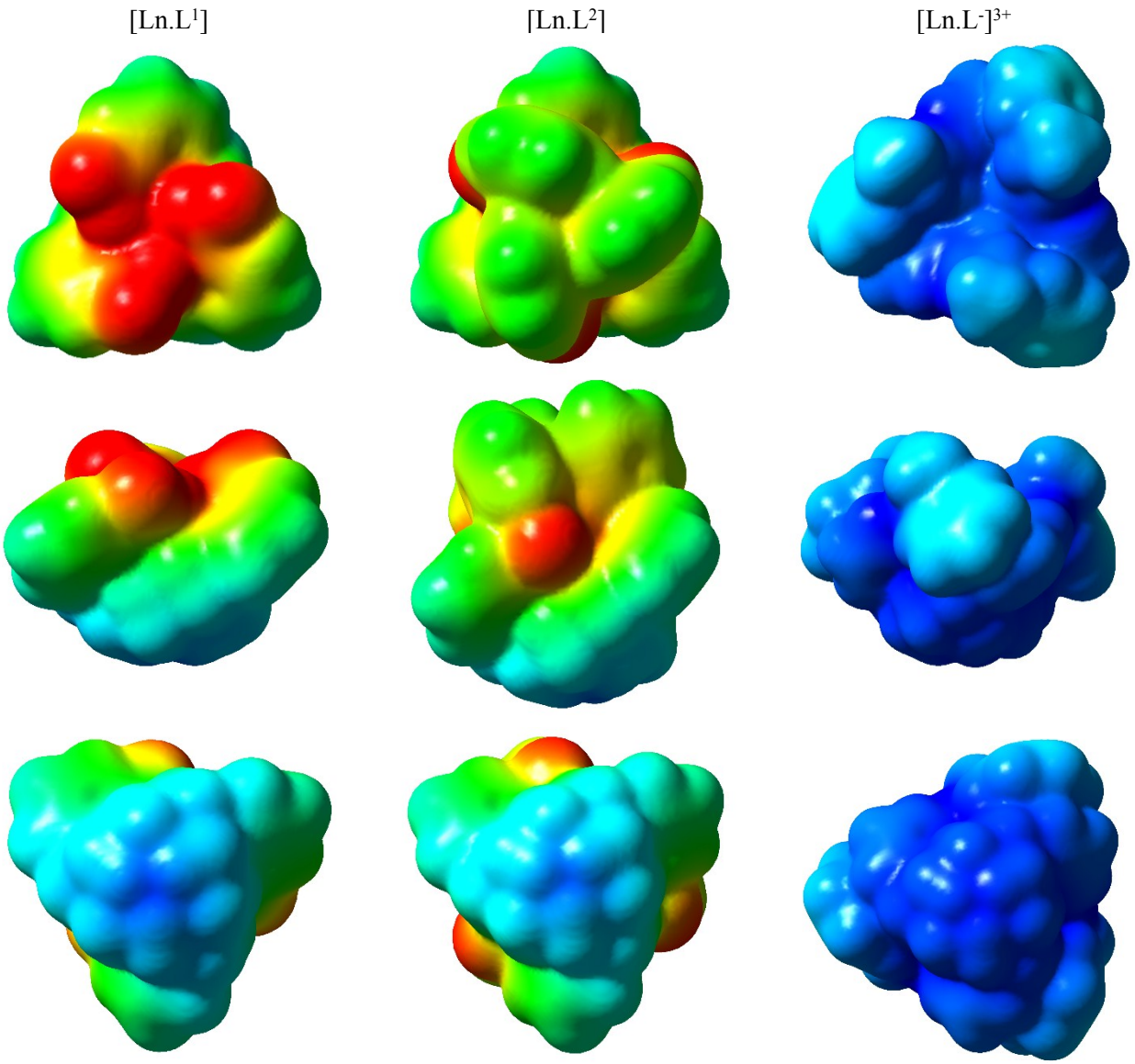


Figure S1. Electrostatic potential plotted on the electron density iso-value surface for [Tb.L[1]], [Tb.L[2]] and [Tb.L[3]]$^{3+}$. (blue and red colour correspond to ±0.109 for complexes of L[1] and L[2] and ±0.3 for L[3]). Nucleophilic site (red) is the most exposed to the interaction with solvent molecules in the case of L[1]. Figures are made with GaussView5.

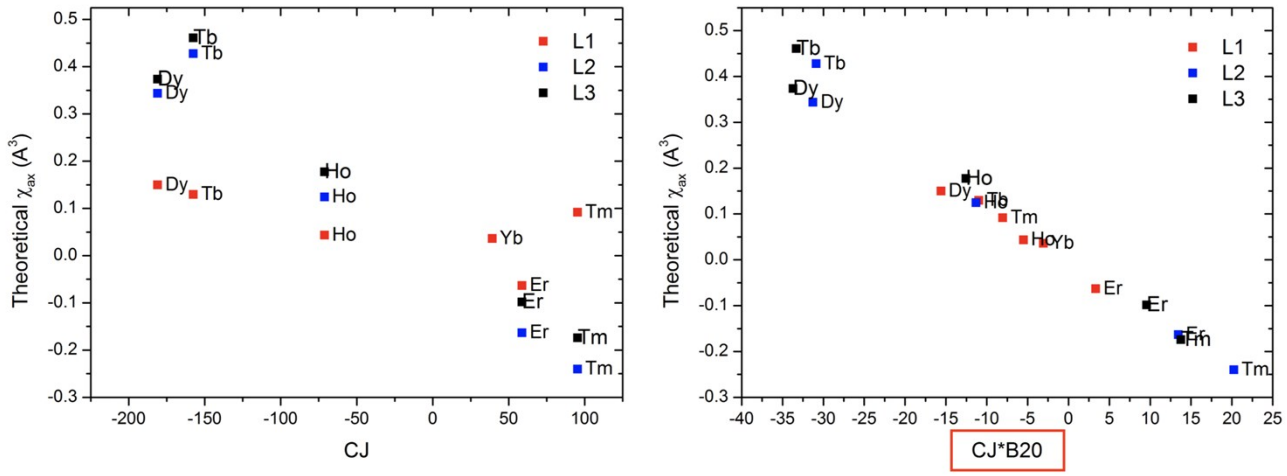
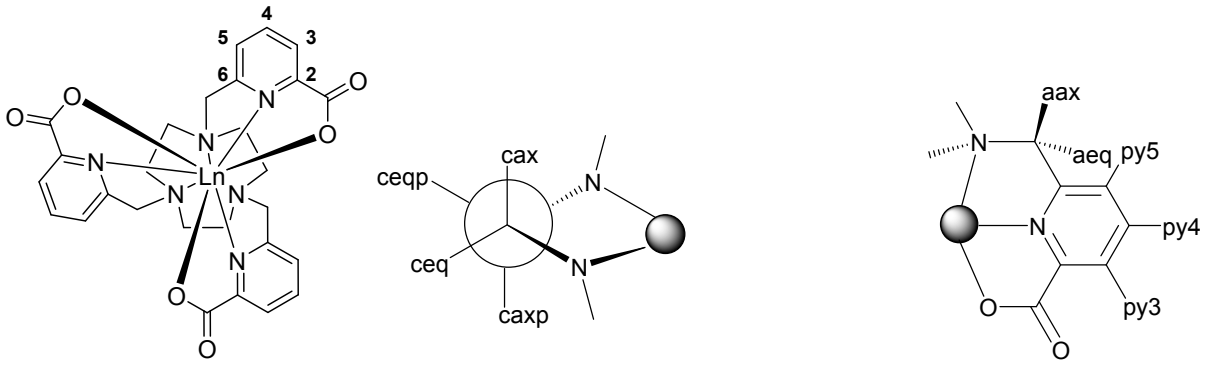


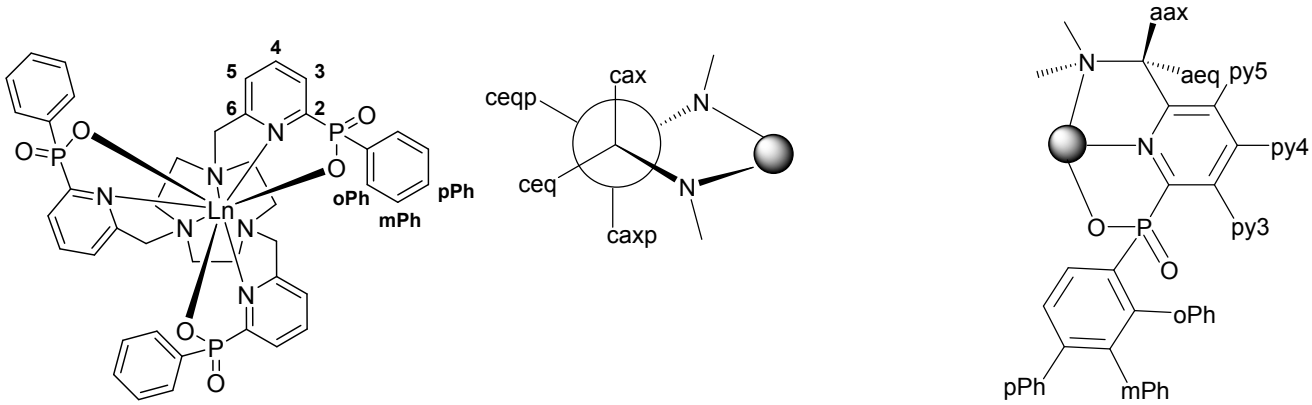
Figure S2. On the left - CASSCF computed axiality of magnetic susceptibility vs. C_J for C_3 symmetric DFT optimised structures (BP86 solvent SMD water for L1 and methanol for L2 and L3). On the right panel, the same axiality is plotted against the product of C_J and the ab initio ligand field parameter B^2_0. Figure shows that Bleaney's model works if we account for ligand field variation within each series. The biggest deviation from linear trend is found for Tb and Dy.

Experimental results: NMR

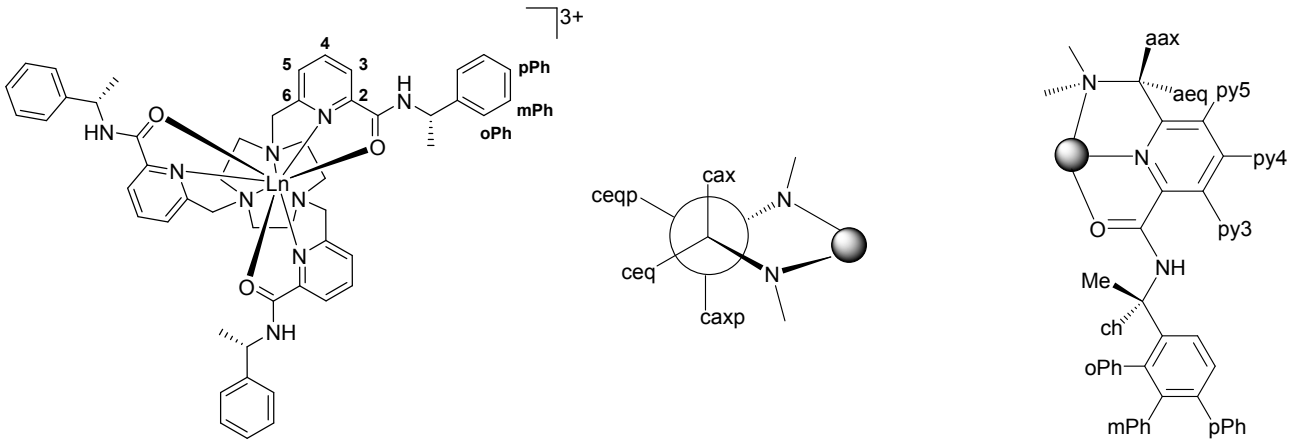
[Ln.**L**^{1}]



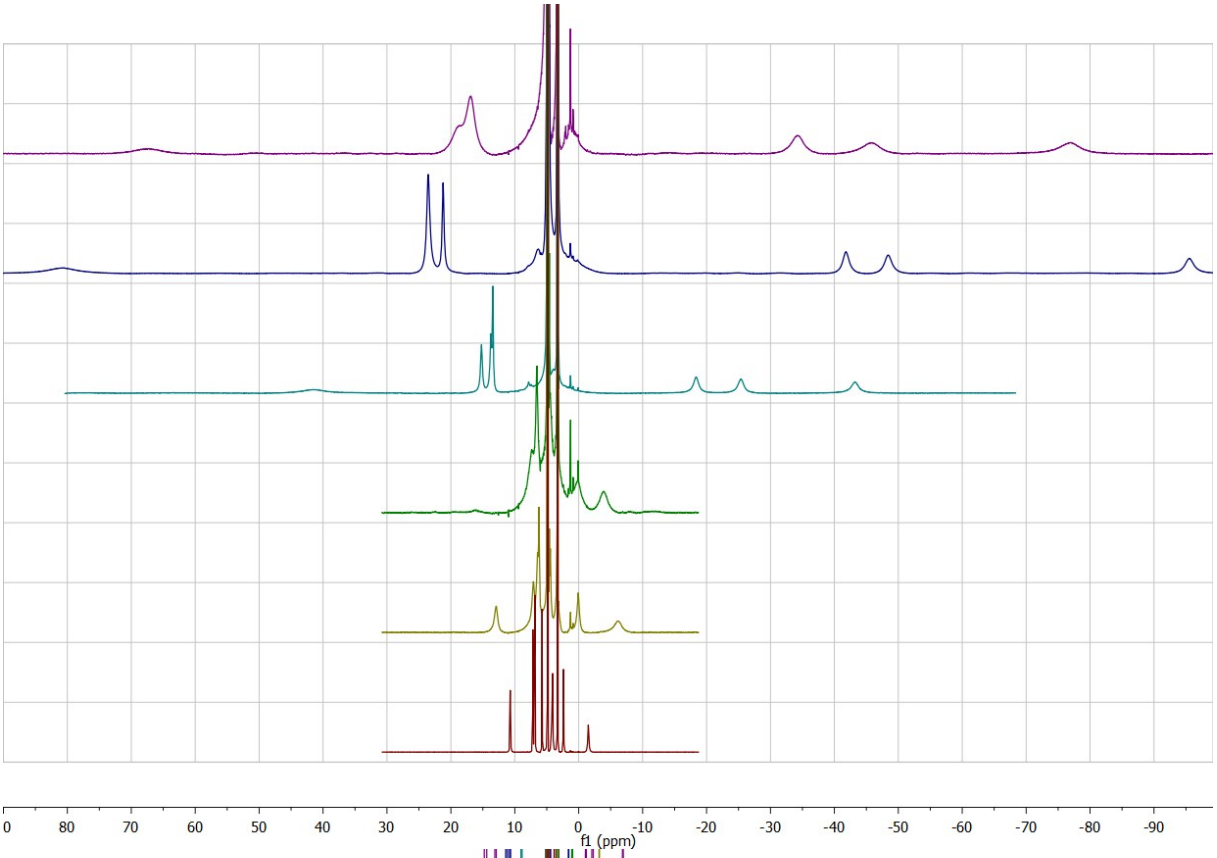
[Ln.**L**^{2}]

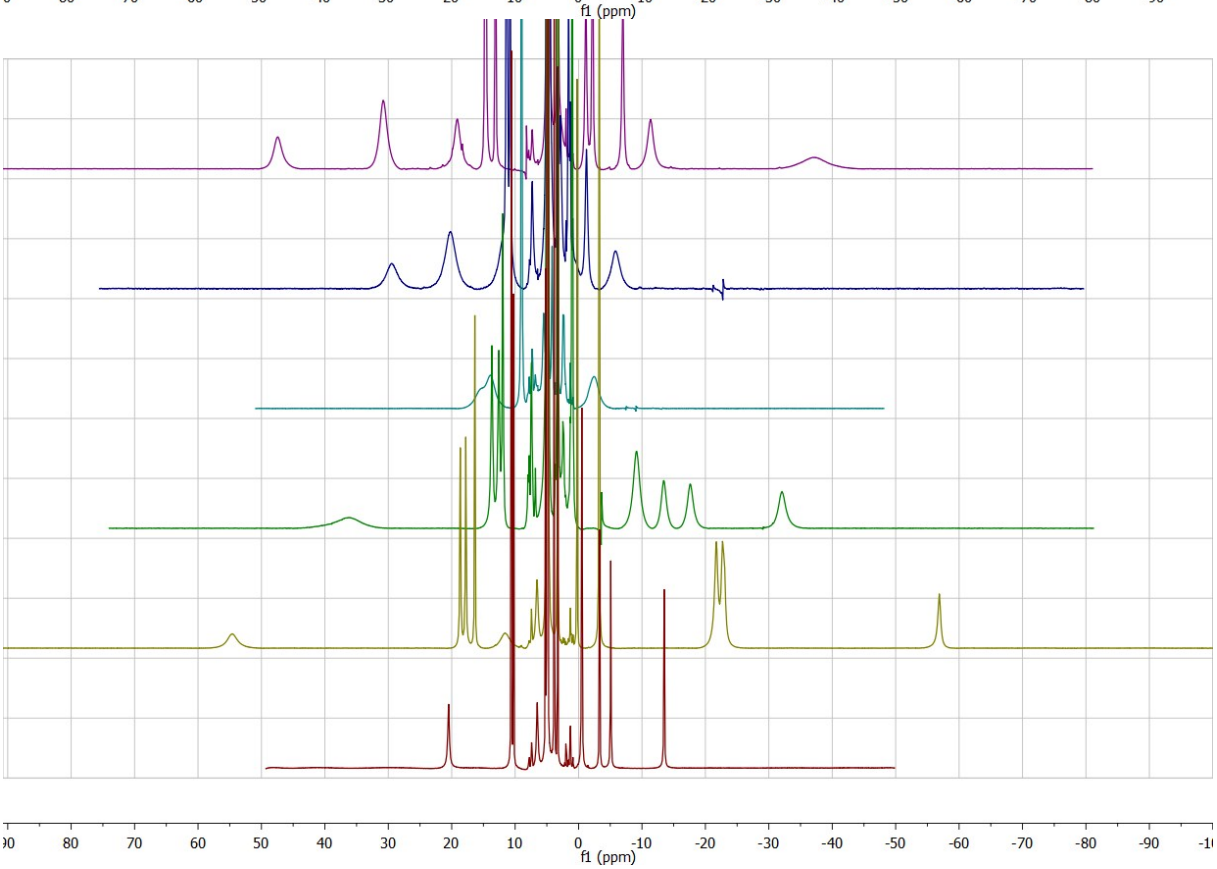


[Ln.**L**^{3}]$(CF_3SO_3)_3$
(major diastereoisomer)



Scheme S1. Labels used to assign NMR spectra.


0 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90
f1 (ppm)


90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -10
f1 (ppm)

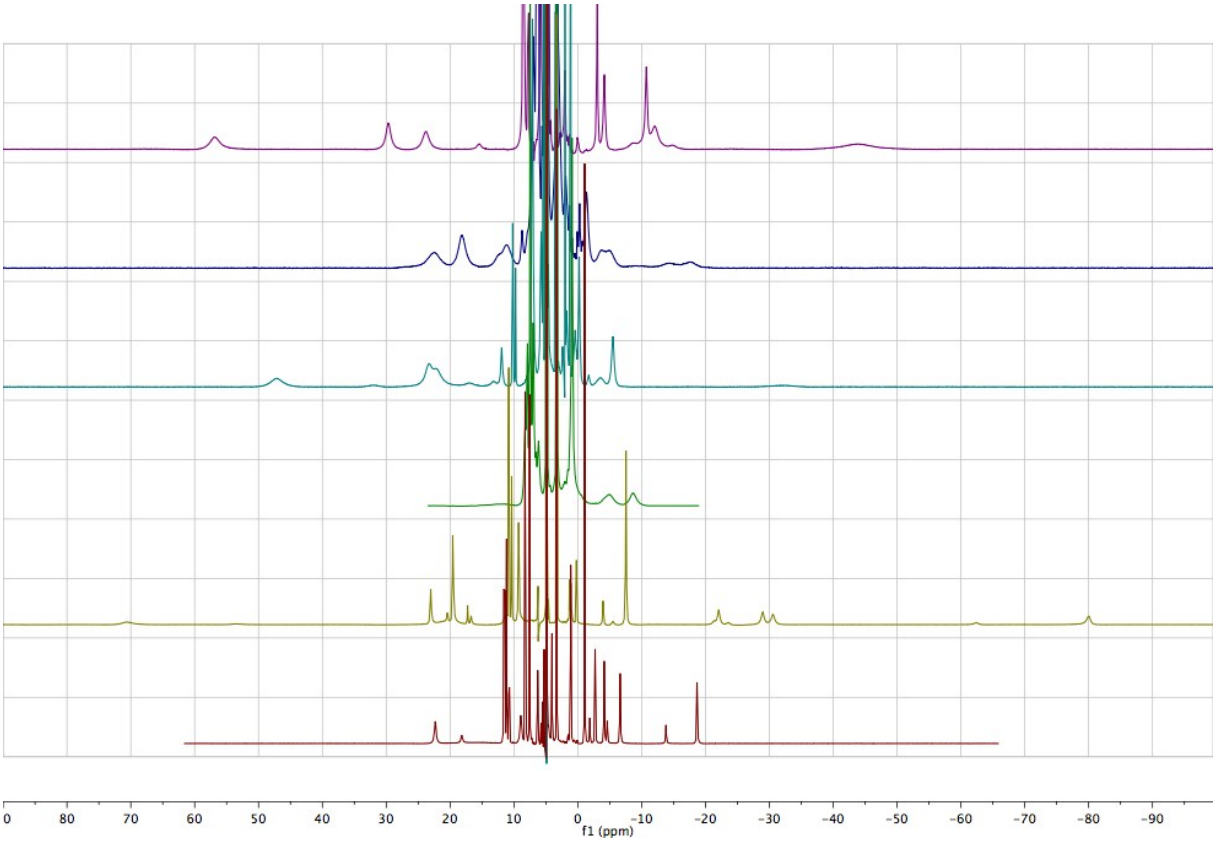


Figure S3. 1H NMR spectra measured in 700MHz spectrometer in deuterated methanol at 22 C of LnL1 (top), LnL2 (middle), LnL3(bottom), Ln=Tb, Dy, Ho, Er, Tm, Yb (from top to bottom in each panel).

Table S1. Assigned 1H NMR resonances. δ_{dia} *- diamagnetic reference Ln=Y,* δ_{fit} *– shift predicted by fit,* δ *and* ν *observed shift and the linewidth.*

LnL1		Tb			Dy			Ho			Er			Tm			Yb		
H	δ_{dia} (ppm)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)
aax	4.15	73.7	67.5	3377	88.8	80.8	3609	45.0	41.5	2616	-4.8	-3.8	269	-5.2	-6.4	433	-1.6	-1.5	120
aeq	4.08	11.6			13.9	6.4	902	8.7	3.9	785	3.0	0.0	304	3.0			3.4	4.1	47
cax	3.67	-76.5	-76.9	2635	-93.0	-95.5	1090	-42.8	-43.2	893	13.7			14.3	12.9	154	10.1	10.7	56
caxp	2.27	7.1			9.5			5.3			1.5			1.4	0.0	149	1.7	2.4	40
ceq	2.87	-28.5	-34.2	1553	-34.4	-41.8	799	-15.2	-18.3	608	6.7			6.9			5.3	4.2	120
ceqp	2.66	-32.5	-45.7	2117	-39.2	-48.4	894	-17.6	-25.4	686	7.0	7.2	109	7.3	7.1	106	5.4	5.7	25
py3	8.09	25.1	18.9	1633	28.8	23.5	392	18.1	15.2	230	5.9	4.3	98	5.8	4.4	59	6.7	6.8	22
py4	8.19	21.2	16.9	1058	23.7	21.2	229	15.8	13.4	103	6.6	6.4	55	6.5	6.5	69	7.2	7.2	29
py5	7.75	22.3	16.9	1058	24.7	23.5	392	16.0	13.7	215	6.0	5.8	310	5.9	6.2	46	6.6	6.9	37

LnL2		Tb			Dy			Ho			Er			Tm			Yb		
H	δ_{dia} (ppm)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)
aax	4.95	-34.8	-37.2	3288	-18.9	-23.1		-14.8			37.3	36.4	3165	57.4	54.6	1214	20.3	20.5	198
aeq	4.1	-0.1	-11.4	769	1.5	-5.9	944	2.1	-1.0	480	7.7			10.0	6.5	301	5.9	4.9	60
cax	3.62	50.0	47.4	993	31.1	29.5	1407	15.0	15.4	206	-32.7	-32.1	952	-55.3	-56.9	364	-13.5	-13.5	68
caxp	2.65	-0.8			0.4	0.6	864	-3.3	-2.8	121	5.6			7.4	11.6	1158	4.2	6.5	188
ceq	2.86	20.8			13.4	7.3	251	-2.2	-2.2	180	-11.0	-13.5	583	-19.6	-22.7	287	-3.6	-3.3	49
ceqp	2.65	22.7	19.1	814	14.5	12.0	1051	2.7	4.2	40	-13.1	-17.6	706	-22.9	-23.0	291	-4.8	-5.1	58
py3	7.34	-0.7	-2.2	127	2.7	1.6	150	2.3	2.4	56	13.6	12.6	228	17.5	17.8	95	10.3	10.3	26
py4	7.9	0.8	-1.2	214	3.7	2.9	276	4.4	5.5	47	13.4	11.9	124	16.9	16.4	58	10.5	10.6	36
py5	7.6	-1.8	-7.0	229	2.0	-1.3	287	5.8	6.6	165	15.1	13.7	214	19.7	18.7	100	11.1	10.6	36
mPh	6.7	21.5			15.3			9.8			-4.7			-11.8			1.4		

oPh	7.9	63.4			40.3			16.6			-36.7			-64.5			-12.6		
pPh	7.25	13.9	13.1	68	11.1	10.8	55	9.5	9.0	26	2.2	1.0	103	-0.9	0.2	34	4.9	5.2	25

LnL3		Tb			Dy			Ho			Er			Tm			Yb		
H	δ_{dia} (ppm)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)	δ_{fit} (ppm)	δ (ppm)	ν (Hz)
aax	3.99	-45.9	-44.0	3191	-33.5			-35.2	-32.2	3001	15.7			75.6	70.7	1355	23.4	22.3	208
aeq	3.71	-2.7	-12.0	787	-1.3	3.0	248	-1.6	-3.5	856	5.2			13.5	11.3	376	6.5	6.3	59
cax	3.65	59.7	56.9	987	45.4			47.3	47.2	1409	-9.3	-8.6	738	-76.3	-80.0	480	-18.0	-18.7	79
caxp	2.36	-3.6			-2.4			-2.7			3.8			12.2	20.6	2290	5.4	8.9	231
ceq	2.62	23.6	23.8	751	18.1	18.2	861	18.8	22.1	1262	-2.2	-4.4	1001	-26.6	-29.0	356	-5.1	-4.1	57
ceqp	2.86	26.5	29.7	567	20.4	22.5	1445	21.2	23.3	756	-2.6	-5.1	845	-30.6	-30.6	444	-6.1	-6.6	68
py3	8.5	-3.3	-10.7	253	-0.3	-1.4	412	-0.8	-5.5	308	11.2	8.3	200	25.5	23.0	134	13.1	11.6	32
py4	8.16	-0.5	2.0	156	1.7	2.8	462	1.4	1.7	213	10.2	8.2	197	20.4	19.6	71	11.4	11.4	32
py5	7.34	-1.7	-4.2	224	0.7	1.9	321	0.5	0.4	326	9.4	7.9	108	19.5	19.5	137	10.5	11.2	32
mPh	7.3	1.8			3.3			3.1			8.6			14.9	10.8	37	9.3		
oPh	6.95	0.3			2.1			1.9	5.7	204	8.5			16.2	9.3	90	9.3		
pPh	7.3	2.4	-3.1	111	3.7	6.5	100	3.6			8.4			14.0	10.4	32	9.0	8.1	26
Me	1.51	4.3			3.7			3.9			0.8			-3.2	-7.6	81	0.1		
ch	4.71	20.2			16.4			17.1			1.0			-18.8	-22.1	288	-2.0	-2.7	51

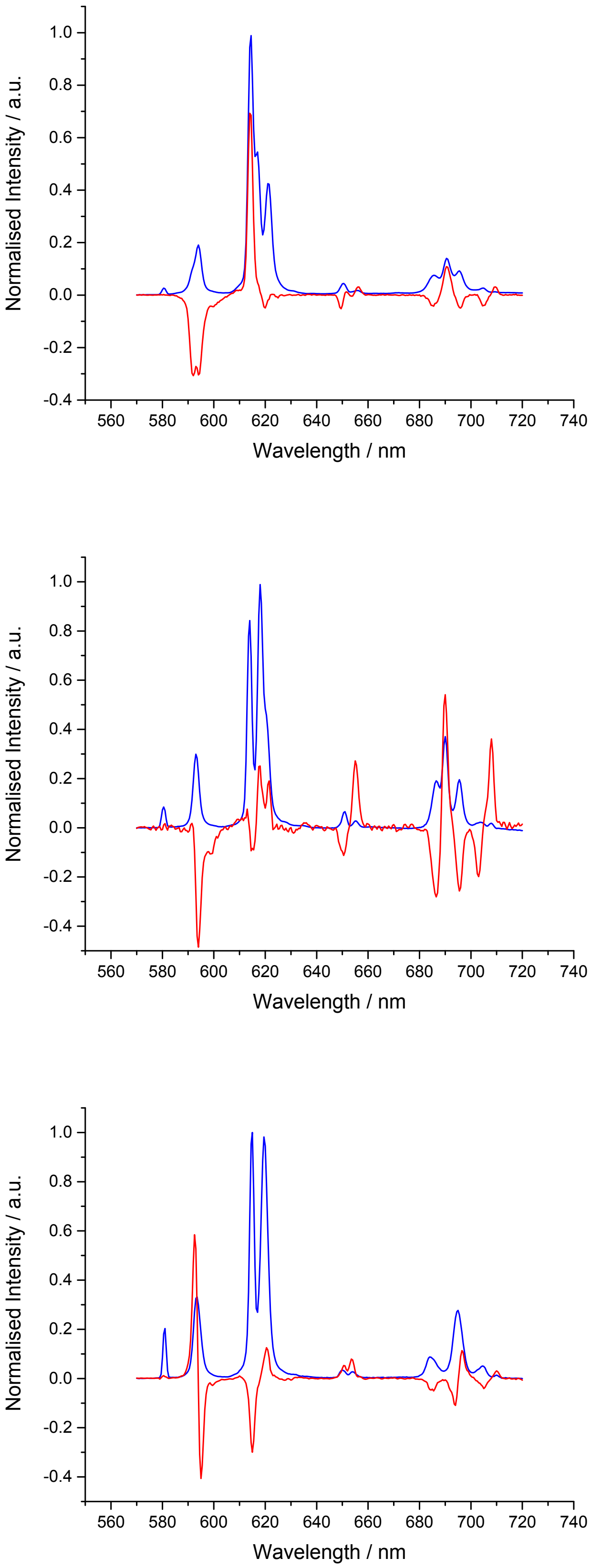


Figure S4. CPL (blue) plotted with total emission (red) for [EuL^1], [EuL^2] and [EuL^3] , (top, middle and bottom respectively).

DFT Geometries

Table S2. DFT optimised geometries of LnL[1] complexes

	Tb			Dy			Ho			Er			Tm			Yb		
	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z
Ln	0.012087	0.02263	-0.236779	0.006857	-0.008695	0.057882	0.008068	-0.009142	0.044888	0.011602	-0.005015	0.082191	0.016836	-0.026473	0.134404	0.016613	-0.029071	0.12549
O	1.300472	-1.274707	-1.77263	-0.302027	-1.830532	-1.419955	-0.313843	-1.836544	-1.405102	-0.284111	-1.788461	-1.423107	-0.324406	-1.864533	-1.280214	-0.33519	-1.844596	-1.279489
O	-1.808068	-0.428671	-1.696126	-1.421572	1.175692	-1.42229	-1.408886	1.175324	-1.429477	-1.421568	1.180928	-1.369309	-1.277325	1.026687	-1.48506	-1.249229	1.045819	-1.479462
O	0.484079	1.863589	-1.647403	1.749501	0.631576	-1.405317	1.751294	0.621854	-1.403321	1.623447	0.656027	-1.484141	1.745569	0.596075	-1.296017	1.736344	0.567001	-1.305051
O	-0.020515	3.813927	-2.631597	0.37101	-3.709201	-2.441562	0.358618	-3.708674	-2.43937	0.370466	-3.682013	-2.432826	0.350216	-3.704364	-2.373309	0.316538	-3.69156	-2.373987
O	3.223634	-1.859871	-2.766325	-3.395665	1.573815	-2.408402	-3.383002	1.586421	-2.410416	-3.381882	1.561154	-2.393066	-3.236415	1.54478	-2.44929	-3.207605	1.611086	-2.418581
O	-3.322286	-1.77475	-2.657308	3.066362	2.152547	-2.393889	3.066264	2.13963	-2.399456	2.981668	2.154982	-2.45417	3.035669	2.103451	-2.34208	3.048509	2.05937	-2.345791
N	-1.641309	0.150705	1.872351	1.677607	-0.008754	2.131025	1.67605	-0.007243	2.122784	1.672638	0.001097	2.152302	1.666954	-0.029802	2.186244	1.66518	-0.027832	2.167025
N	1.036372	1.308728	1.869565	-0.843693	-1.449175	2.132149	-0.840829	-1.449985	2.122305	-0.830118	-1.442707	2.150036	-0.85842	-1.446114	2.208205	-0.845045	-1.45103	2.182553
N	0.700079	-1.584674	1.830996	-0.838461	1.453493	2.129045	-0.840516	1.450016	2.120042	-0.832634	1.451082	2.155085	-0.843059	1.432151	2.193056	-0.851784	1.414356	2.155869
N	-1.713632	1.887237	-0.212856	1.889226	-1.691301	0.016201	1.882794	-1.688642	0.012149	1.888016	-1.661034	0.023872	1.881023	-1.707651	0.09059	1.86691	-1.707735	0.085584
N	2.498621	0.535695	-0.28277	-2.403829	-0.782665	0.017119	-2.395984	-0.777319	0.009591	-2.386725	-0.786265	0.038391	-2.377389	-0.75554	0.07735	-2.356501	-0.731731	0.068511
N	-0.78578	-2.399335	-0.289246	0.512716	2.467123	0.016552	0.511837	2.458179	0.009271	0.503844	2.463302	0.033883	0.493632	2.435435	0.075582	0.499079	2.412068	0.057689
C	-1.228136	1.145059	2.902422	1.388674	-1.051509	3.155166	1.389603	-1.051265	3.146185	1.396142	-1.041474	3.180535	1.383975	-1.075187	3.211484	1.387146	-1.072704	3.194539
C	-0.080051	2.05542	2.478931	-1.602271	-0.679189	3.15723	-1.600705	-0.682213	3.148001	-1.59876	-0.683155	3.176319	-1.602134	-0.682768	3.247083	-1.5995	-0.694571	3.219741
C	1.707797	0.436992	2.874267	0.210929	1.728028	3.150359	0.207532	1.72638	3.142198	0.209528	1.73036	3.182109	0.20875	1.71679	3.210033	0.195887	1.712771	3.176246
C	1.919779	-1.00142	2.415873	0.349952	-2.080411	2.724242	0.351567	-2.081214	2.716004	0.360876	-2.073791	2.750057	0.331507	-2.095137	2.787902	0.340119	-2.098557	2.772115
C	-0.362157	-1.75023	2.860351	-1.978465	0.732834	2.724694	-1.979461	0.729394	2.71691	-1.974947	0.730988	2.748281	-1.981307	0.726839	2.812181	-1.986898	0.712737	2.785237
C	-2.954535	0.521088	1.318103	1.622671	1.340697	2.723084	1.62015	1.340975	2.716716	1.621991	1.348363	2.75229	1.618299	1.319883	2.783034	1.610282	1.322095	2.760836
C	-2.845271	1.774185	0.488343	3.0129	-0.237982	1.554704	3.011188	-0.234379	1.546501	3.008094	-0.222538	1.572558	3.008141	-0.252351	1.617874	3.005703	-0.249413	1.598608
C	-3.854933	2.733124	0.400099	-1.711124	-2.487906	1.551347	-1.70828	-2.487573	1.540819	-1.687083	-2.489142	1.566395	-1.746516	-2.464706	1.624946	-1.728843	-2.466338	1.588047
C	-3.674508	3.818206	-0.455157	-1.311353	2.719107	1.546985	-1.313549	2.714865	1.537969	-1.305236	2.717432	1.575708	-1.324751	2.692234	1.605285	-1.336681	2.670932	1.562165
C	-1.547645	2.912989	-1.053029	3.011522	-1.487697	0.712959	3.008437	-1.482502	0.70317	3.003564	-1.476339	0.738139	3.013059	-1.496043	0.76841	3.005491	-1.494288	0.751542
C	2.012192	2.258847	1.308286	-2.792311	-1.855265	0.713582	-2.786601	-1.851665	0.702509	-2.772415	-1.863051	0.730342	-2.811569	-1.798243	0.79217	-2.792124	-1.786793	0.764918
C	3.012325	1.529439	0.448979	-0.228617	3.340474	0.704336	-0.230914	3.333324	0.693655	-0.216917	3.338932	0.741596	-0.245209	3.313544	0.759846	-0.251249	3.292699	0.725644
C	4.363532	1.866552	0.372182	4.100166	-2.353457	0.609131	4.099154	-2.344988	0.593526	4.073642	-2.367123	0.667982	4.114789	-2.340906	0.634643	4.107238	-2.337462	0.607023
C	5.181956	1.153987	-0.502555	-4.090623	-2.355398	0.61663	-4.085406	-2.350034	0.60296	-4.067115	-2.371416	0.631786	-4.131349	-2.239806	0.708459	-4.113376	-2.222902	0.676641
C	3.27381	-0.132353	-1.141266	-0.022604	4.715666	0.596268	-0.026152	4.708419	0.58177	0.008292	4.712327	0.65608	-0.03669	4.688018	0.651177	-0.04782	4.667041	0.606069
C	1.012228	-2.885047	1.219861	4.010931	-3.439383	-0.259915	4.009744	-3.430674	-0.275534	3.975691	-3.464512	-0.185453	4.030498	-3.415443	-0.248571	4.016208	-3.412316	-0.27505
C	-0.156477	-3.360374	0.395601	-4.988202	-1.724653	-0.243025	-4.981984	-1.716259	-0.25531	-4.967917	-1.746073	-0.228184	-5.003163	-1.582177	-0.158213	-4.986711	-1.546154	-0.173468
C	-0.551101	-4.69535	0.309763	0.96996	5.17746	-0.265821	0.966276	5.169301	-0.280695	0.999471	5.175905	-0.206633	0.957007	5.14702	-0.210674	0.952378	5.122177	-0.250401
C	-1.790754	-2.717623	-1.110204	2.850395	-3.62226	-1.00971	2.845898	-3.616759	-1.019242	2.825148	-3.631424	-0.95362	2.859642	-3.608433	-0.979505	2.839437	-3.605426	-0.996471
C	-2.375302	-1.554798	-1.895711	-4.564452	-0.626242	-0.988737	-4.556216	-0.616534	-0.997812	-4.549112	-0.644413	-0.971493	-4.529001	-0.527151	-0.935589	-4.511479	-0.478836	-0.933141
C	-2.502984	3.911855	-1.204501	1.717669	4.260169	-1.001965	1.715326	4.250589	-1.013622	1.718454	4.26089	-0.972856	1.702681	4.226683	-0.945287	1.706961	4.198472	-0.971802
C	-0.255688	2.884695	-1.853596	1.811887	-2.712726	-0.84068	1.805512	-2.710831	-0.844246	1.804929	-2.69629	-0.818367	1.808569	-2.721308	-0.777283	1.790039	-2.718804	-0.784673
C	4.630781	0.138879	-1.282307	-3.252412	-0.193021	-0.829114	-3.243809	-0.18553	-0.836252	-3.241067	-0.202138	-0.807653	-3.196351	-0.15606	-0.791714	-3.176843	-0.116542	-0.788284
C	2.558853	-1.187032	-1.971974	1.446994	2.906539	-0.83121	1.446148	2.897315	-0.839073	1.426634	2.90931	-0.824886	1.430642	2.874283	-0.77122	1.438204	2.846804	-0.788205
C	-1.617135	-5.026364	-0.524629	0.522848	-2.779727	-1.642952	0.512677	-2.781663	-1.638562	0.524938	-2.749075	-1.637403	0.504553	-2.792009	-1.553608	0.483918	-2.78089	-1.555604
C	-2.248262	-4.023023	-1.256897	-2.662272	0.95673	-1.629424	-2.651216	0.963624	-1.634736	-2.652862	0.952859	-1.601362	-2.535643	0.908343	-1.655292	-2.51088	0.951716	-1.640212
C	-1.72541	-1.204011	2.450022	2.164454	1.821142	-1.618161	2.165179	1.810821	-1.622005	2.086655	1.829222	-1.666757	2.147415	1.780488	-1.546527	2.15209	1.746746	-1.555426
H	-0.028852	-5.456253	0.890194	2.31528	-1.587822	3.415912	2.317226	-1.586474	3.405764	2.326839	-1.57159	3.43922	2.309925	-1.618967	3.457642	2.31618	-1.609988	3.44326
H	-0.960992	0.609068	3.822542	-2.527794	-1.216233	3.419855	-2.524993	-1.221343	3.410979	-2.524303	-1.224701	3.429387	-2.522826	-1.221413	3.52343	-2.515785	-1.241994	3.493456
H	-2.08522	1.783662	3.170789	0.214285	2.80021	3.404525	0.208974	2.798588	3.396477	0.2073	2.802098	3.438202	0.215568	2.791583	3.453022	0.193006	2.788953	3.412685
H	-0.424043	2.790777	1.740288	1.063935	-0.55658	4.07935	1.065138	-0.557519	4.071135	1.069715	-0.54797	4.104826	1.074302	-0.581061	4.14146	1.073586	-0.577828	4.122847
H	0.261263	2.619472	3.367221	-1.01028	-0.642445	4.080704	-1.008413	-0.644665	4.071243	-1.012566	-0.649506	4.103772	-0.99668	-0.643409	4.16161	-0.996395	-0.650573	4.135398
H	1.121025	0.452419	3.801756	-0.055828	1.205465	4.078062	-0.059218	1.203456	4.069733	-0.056144	1.204289	4.108159	-0.056557	1.203614	4.143463	-0.070933	1.203176	4.111076
H	2.690965	0.858465	3.139437	0.077557	-2.691814	3.604836	0.07848	-2.691394	3.597351	0.083614	-2.683778	3.629884	0.06142	-2.707396	3.66856	0.06451	-2.704839	3.655098
H	2.706797	-1.050383	1.651742	-2.371831	1.275332	3.604759	-2.371761	1.271275	3.597942	-2.369417	1.272315	3.628462	-2.357189	1.281235	3.692179	-2.352938	1.269936	3.667342
H	2.266779	-1.595141	3.282687	2.284755	1.410156	3.606479	2.281062	1.409666	3.601159	2.287392	1.412064	3.633353	2.281949	1.382763	3.665414	2.266372	1.388519	3.648605
H	-0.48362	-2.817935	3.105743	0.769145	-2.762295	1.972916	0.771189	-2.764152	1.965961	0.784421	-2.758025	2.002547	0.738016	-2.777825	2.029919	0.750696	-2.78595	2.021081
H	-0.031739	-1.270089	3.790484	-2.778561	0.706362	1.973668	-2.780766	0.702671	1.967261	-2.774376	0.706447	1.995918	-2.794134	0.697901	2.074626	-2.806808	0.684066	2.056373
H	-3.711162	0.646997	2.111929	2.007054	2.044642	1.973765	2.005049	2.046305	1.968952	2.003957	2.057425	2.005945	2.007079	2.023468	2.035065	2.002853	2.025573	2.01507
H	-3.289818	-0.296284	0.658462	3.789806	-0.294535	2.336465	3.788666	-0.29257	2.327679	3.789389	-0.270353	2.350209	3.780342	-0.308244	2.404047	3.778833	-0.30546	2.383876
H	-4.76403	2.623029	0.991539	3.253224	0.612921	0.896256	3.251374	0.617571	0.889311	3.239086	0.626382	0.907591	3.248666	0.60148	0.963212	3.246572	0.603456	0.942871
H	-4.446922	4.583966	-0.539466	-2.149835	-3.135409	2.329992	-2.149724	-3.134422	2.31856	-2.11803	-3.145485	2.34184	-2.196628	-3.109715	2.398878	-2.179866	-3.119343	2.354633
H	2.522983	2.833028	2.100279	-1.094164	-3.119474	0.891154	-1.092068	-3.120029	0.880899	-1.063119	-3.11012	0.902309	-1.145687	-3.099813	0.953547	-1.126872	-3.093009	0.910098
H	1.468725	2.972403	0.667851	-1.65281	3.423591	2.32501	-1.653138	3.421069	2.315359	-1.654751	3.418978	2.352635	-1.673862	3.398546	2.378166	-1.695561	3.376294	2.331182
H	4.760622	2.672917	0.989175	-2.169392	2.495622	0.892255	-2.172904	2.49177	0.884666	-2.155351	2.493716	0.910744	-2.181265	2.457118	0.95077	-2.186308	2.429653	0.900169
H	1.285637	-3.639041	1.978349	4.99888	-2.172676	1.199166	4.999957	-2.161225	1.179432	4.96373	-2.198011	1.274241	5.020976	-2.151005	1.210204	5.018788	-2.145529	1.173399
H	1.874216	-2.749396	0.546189	4.845914	-4.134774	-0.355802	4.84657	-4.123169	-0.376104	4.794853	-4.181793	-0.252989	4.876791	-4.092751	-0.371091	4.862181	-4.088519	-0.405549
H	-2.321601	4.731661	-1.898054	2.73878	-4.443619	-1.716171	2.732777	-4.437923	-1.725688	2.706049	-4.462018	-1.647934	2.750167	-4.420328	-1.697222	2.724945	-4.415674	-1.715315
H	6.243694	1.393109	-0.576851	-4.385361	-3.224578	1.204937	-4.381054	-3.220583	1.18878	-4.35647	-3.243256	1.218783	-4.463265	-3.085317	1.311281	-4.44526	-3.078809	1.264585
H	5.224579	-0.436986	-1.99073	-6.011081	-2.092533	-0.334059	-6.005257	-2.082673	-0.34781	-5.988333	-2.120277	-0.321282	-6.043514	-1.901121	-0.235299	-6.028494	-1.859972	-0.252108
H	-1.950049	-6.062098	-0.604441	-5.222768	-0.110891	-1.686717	-5.213001	-0.098425	-1.695199	-5.208835	-0.132503	-1.670691	-5.162348	-0.001991	-1.649269	-5.144659	0.061742	-1.635405
H	-3.076264	-4.23081	-1.93318	-0.633023	5.40561	1.179275	-0.638018	5.398914	1.1626	-0.587651	5.400157	1.256224	-0.645526	5.379193	1.234382	-0.665897	5.361013	1.176075
H	-2.385282	-1.211825	3.33788	1.155636	6.247781	-0.365238	1.150886	6.239546	-0.382884	1.202134	6.244759	-0.286839	1.145803	6.216807	-0.310204	1.137853	6.191787	-0.357803
H	-2.189795	-1.852496	1.696106	2.493193	4.572044	-1.700048	2.491002	4.560939	-1.712217	2.485603	4.573048	-1.680021	2.479749	4.536156	-1.642724	2.486884	4.504988	-1.667452

Table S3. DFT optimised geometries of LnL[2] complexes

	Tb			Dy			Ho			Er			Tm			Yb		
	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z
Ln	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
P	-2.851050	1.113710	-1.836550	-2.828540	1.138530	-1.842310	-2.816860	1.150020	-1.833120	-2.791320	1.177780	-1.852670	-2.797550	1.178370	-1.831630	-2.752530	1.217510	-1.842130
P	0.469950	-3.039130	-1.807830	2.429590	1.869410	-1.814290	0.436840	-3.027490	-1.798350	0.445290	-3.022840	-1.808470	2.417620	1.827310	-1.799860	0.419710	-3.006600	-1.801340
P	2.419920	1.935910	-1.785360	0.446210	-3.029970	-1.803620	2.432350	1.865710	-1.789900	2.435850	1.830830	-1.798390	0.408470	-3.027580	-1.796620	2.442250	1.785240	-1.780700
O	-0.394890	-1.810570	-1.394490	-0.396330	-1.784340	-1.393470	-0.405580	-1.782340	-1.389460	1.695490	0.513380	-1.436770	1.677960	0.511480	-1.428360	1.660540	0.487970	-1.429260
O	-1.364900	1.268440	-1.395890	1.771320	0.521360	-1.398920	-1.329250	1.274060	-1.388640	-0.388900	-1.776890	-1.398120	-1.308680	1.269560	-1.396990	-0.385740	-1.741650	-1.389550
O	1.806540	0.572780	-1.346720	-1.341560	1.273020	-1.399450	1.766520	0.520870	-1.372200	-1.310060	1.289390	-1.396370	-0.413560	-1.775190	-1.382030	-1.266920	1.284250	-1.390890
O	-3.795240	2.298680	-1.653600	-3.758420	2.334070	-1.652030	-3.740140	2.349940	-1.640550	-3.715670	2.379830	-1.676330	-3.700700	2.396070	-1.650870	-3.643030	2.442940	-1.652270
O	-0.102720	-4.437750	-1.592730	3.929910	2.052670	-1.600510	-0.156010	-4.415080	-1.566210	-0.150450	-4.410380	-1.580260	-0.196430	-4.410680	-1.565690	-0.206210	-4.379520	-1.566040
O	3.913920	2.165540	-1.573240	-0.147380	-4.416530	-1.568310	3.931620	2.042760	-1.565250	3.938670	1.933550	-1.548010	3.919000	1.932470	-1.542450	3.943120	1.845890	-1.505150
N	-2.511030	-0.836920	-0.015770	-2.509470	-0.818790	-0.031650	-2.500240	-0.808620	-0.023680	-2.489070	-0.785410	-0.047010	-2.498710	-0.772590	-0.013110	-2.479720	-0.755930	-0.051860
N	0.534360	2.611740	0.004620	0.568420	2.576390	-0.009770	0.565770	2.574430	0.002910	1.970320	-1.753190	-0.003840	1.953800	-1.761520	-0.010280	1.958850	-1.759210	-0.003750

N	1.990950	-1.763120	0.005170	1.976440	-1.763840	0.001900	1.968990	-1.762260	0.007820	0.596340	2.554790	0.011400	0.577780	2.555110	0.003770	0.607810	2.540130	0.011800
N	-0.844860	1.455410	2.074860	-0.843830	-1.451460	2.055090	-0.840420	-1.449570	2.060170	-0.841790	-1.442340	2.037390	1.670830	0.000000	2.043540	-0.838210	-1.438160	2.010730
N	1.685080	0.000000	2.085570	-0.835290	1.451460	2.054780	-0.838180	1.449570	2.063850	1.670930	0.000000	2.062180	-0.837980	-1.440540	2.052810	1.667900	0.000000	2.041520
N	-0.840220	-1.455410	2.080570	1.679120	0.000000	2.072100	1.678600	0.000000	2.075070	-0.829130	1.442340	2.061250	-0.832850	1.440540	2.054560	-0.829700	1.438160	2.039820
H	-0.727650	1.929330	-5.600370	-0.718520	1.954210	-5.623030	-0.692490	1.965050	-5.617300	-1.174680	-1.607670	-5.600770	-1.220260	-1.616590	-5.587100	-1.183580	-1.559940	-5.612510
H	-1.277670	-1.682560	-5.604960	-1.306360	-1.669720	-5.622690	-1.303290	-1.655720	-5.618340	-0.621410	2.020630	-5.665820	-0.626470	2.003070	-5.679080	-0.552340	2.071300	-5.689840
H	-2.728700	-0.551230	-7.288850	-2.739920	-0.508440	-7.301060	-2.734400	-0.487820	-7.294250	-2.697670	-0.566720	-7.278450	-2.776260	-0.596960	-7.247860	-2.704640	-0.495260	-7.277110
H	0.993480	2.639930	-7.260700	2.127530	-0.418310	-5.653450	2.141930	-0.415620	-5.637380	2.197730	-0.416580	-5.627550	2.170030	-0.436340	-5.621080	2.212740	-0.452790	-5.636640
H	2.163820	-0.358900	-5.602990	1.005050	2.681010	-7.274220	1.048570	2.666270	-7.261460	1.888650	-2.265510	-7.272690	1.851450	-2.286530	-7.262990	1.867360	-2.304900	-7.271330
H	1.837790	-2.180100	-7.275200	1.793760	-2.269320	-7.291090	1.807140	-2.262180	-7.279930	1.139340	2.770110	-7.265610	1.145990	2.718310	-7.280810	1.259000	2.732560	-7.271120
H	-0.098170	1.638700	-3.212450	-0.085280	1.620430	-3.239950	-0.076590	1.633590	-3.229470	-1.228710	-0.833560	-3.231970	-1.246590	-0.829180	-3.221580	-1.218310	-0.795560	-3.238460
H	-1.351940	-0.965040	-3.225110	-1.363170	-0.956200	-3.240540	-1.357670	-0.946250	-3.234890	-0.035000	1.635190	-3.272700	-0.051370	1.636840	-3.279590	-0.014410	1.681660	-3.284960
H	1.583650	-0.749640	-3.216990	1.551990	-0.764940	-3.258730	1.555480	-0.764430	-3.245890	1.572520	-0.765350	-3.241240	1.541380	-0.777110	-3.234590	1.580850	-0.775760	-3.248420
H	-4.244700	1.291830	-6.590710	-4.222370	1.358820	-6.595380	-4.211570	1.382210	-6.584940	-4.263260	1.238010	-6.592020	-4.346180	1.198550	-6.548210	-4.248640	1.321250	-6.574180
H	0.933870	-4.383030	-6.559110	3.348170	3.069610	-6.540820	0.888050	-4.447040	-6.528860	0.957140	-4.448850	-6.533950	0.907750	-4.463450	-6.520670	0.893320	-4.465290	-6.519960
H	3.333050	3.055690	-6.530030	0.885920	-4.456240	-6.532390	3.391640	3.031360	-6.516120	3.467930	3.134670	-6.477570	3.475900	3.067560	-6.489670	3.590400	3.005710	-6.454630
H	-4.317170	2.006830	-4.199130	-4.279710	2.067190	-4.201410	-4.266060	2.086900	-4.189790	-4.320810	1.999810	-4.213290	-4.374260	1.974320	-4.173830	-4.287580	2.071310	-4.191210
H	0.357620	-4.773540	-4.162190	3.976500	2.738080	-4.148330	0.307730	-4.795250	-4.126650	0.340310	-4.795180	-4.140180	0.289160	-4.802340	-4.126150	0.272190	-4.786340	-4.123680
H	3.958620	2.769110	-4.130590	0.315780	-4.802030	-4.127480	4.002430	2.702840	-4.118510	4.046450	2.752330	-4.078770	4.043360	2.705810	-4.085480	4.120540	2.620780	-4.045540
H	-5.434010	-0.397690	-1.646390	-5.419700	-0.371520	-1.682890	-5.410270	-0.350790	-1.673100	-5.404930	-0.289750	-1.677380	2.453860	4.837740	-1.631420	-5.393220	-0.213210	-1.670830
H	2.355480	4.935350	-1.631780	3.063030	-4.499510	-1.651990	3.048610	-4.499960	-1.647660	3.064030	-4.492690	-1.649260	3.015090	-4.526460	-1.633660	3.036580	-4.498810	-1.659020
H	3.078670	-4.510900	-1.626970	2.445930	4.865770	-1.630140	2.435760	4.865420	-1.624720	2.509260	4.834190	-1.585090	-5.424370	-0.262720	-1.621740	2.533570	4.798260	-1.598690
H	0.884230	6.456790	-0.264700	-6.038900	-2.386520	-0.302630	-6.035250	-2.367100	-0.296550	-6.045800	-2.304170	-0.305360	5.084390	-4.028350	-0.285750	-6.051580	-2.236180	-0.319350
H	-6.045410	-2.400040	-0.244750	5.116960	-4.011400	-0.277430	5.107050	-4.014250	-0.278570	5.123940	-3.987960	-0.289040	1.008100	6.394510	-0.276580	5.107180	-3.996440	-0.314310
H	5.122470	-4.026200	-0.236360	1.006900	6.414600	-0.259060	0.985930	6.414010	-0.264150	1.082050	6.391690	-0.211620	-6.067200	-2.269250	-0.239280	1.101170	6.372400	-0.249630
H	-0.846450	5.427100	1.231980	-4.300320	-3.390170	1.203030	-4.297440	-3.378540	1.205450	-4.309620	-3.340950	1.182190	5.093740	-1.995030	1.188110	-4.320270	-3.311010	1.147380
H	-4.297160	-3.392890	1.256810	-0.758610	5.417140	1.219700	-0.776070	5.414470	1.217370	5.107990	-1.968850	1.204090	-0.764690	5.404200	1.198950	5.107660	-1.973370	1.173740
H	5.104100	-2.013990	1.263910	5.103600	-2.002540	1.228060	5.099450	-2.004210	1.225860	-0.708910	5.405430	1.244350	-4.322700	-3.319190	1.229540	-0.702750	5.405150	1.203280
H	-2.185700	2.501570	0.844580	-2.153660	2.510120	0.809180	-1.084300	-3.128520	0.821780	-1.089240	-3.113420	0.787080	3.238400	0.641520	0.798160	-1.095210	-3.103490	0.751690
H	-1.079210	-3.136190	0.845670	-1.086040	-3.132010	0.818940	-2.159940	2.507060	0.821370	-2.128330	2.507180	0.801090	-1.103330	-3.108990	0.802940	-2.125380	2.508540	0.779140
H	3.267460	0.631470	0.859040	3.260210	0.632890	0.843940	3.263000	0.632180	0.849740	3.240770	0.652750	0.827130	-2.150610	2.494360	0.803580	3.243010	0.647770	0.809250
H	-2.098690	-3.167330	2.309520	-2.107140	-3.159700	2.281250	-2.106350	-3.156580	2.283650	-2.111780	-3.149300	2.248630	3.786270	-0.208010	2.266040	-2.112180	-3.142320	2.217140
H	-1.710120	3.394760	2.312450	-1.681160	3.400510	2.280500	-1.684630	3.398550	2.290840	-1.671460	3.395390	2.279080	-2.112390	-3.142840	2.274050	-1.669060	3.392480	2.260500
H	3.794760	-0.233050	2.326870	3.789120	-0.230790	2.311090	3.788010	-0.235570	2.315830	3.785760	-0.205330	2.290850	-1.685320	3.388980	2.274600	3.781600	-0.207480	2.277090
H	-2.777890	0.692650	1.910510	-2.774460	0.705060	1.880840	-2.777990	0.704230	1.897290	0.764590	-2.763180	1.885400	0.764820	-2.764760	1.893010	0.761330	-2.768680	1.867320
H	1.990560	2.053380	1.915200	0.772650	-2.757980	1.906660	0.774380	-2.758470	1.912070	-2.776680	0.711970	1.888950	-2.783420	0.709000	1.919230	-2.782460	0.717760	1.878860
H	0.782980	-2.753200	1.923890	2.000370	2.053580	1.923810	1.998950	2.053530	1.927270	2.006750	2.056190	1.955100	2.008440	2.055350	1.921090	2.013410	2.055380	1.946290
H	0.200710	2.801840	3.356790	-2.538730	-1.218260	3.330070	-2.533500	-1.223350	3.338980	2.320360	-1.600120	3.316400	2.331990	-1.589060	3.305910	-2.533720	-1.233800	3.292910
H	-2.528070	-1.223420	3.364490	2.312940	-1.585060	3.350640	2.315430	-1.583790	3.353890	-2.536910	-1.229450	3.317510	0.200660	2.793120	3.342430	2.318350	-1.600600	3.295350
H	2.319650	-1.578190	3.371600	0.195520	2.794490	3.352410	0.195680	2.793390	3.358360	0.190330	2.781990	3.372640	-2.518620	-1.225410	3.351540	0.187110	2.779180	3.352340
H	-2.382560	1.265180	3.543090	-2.380820	1.273330	3.515520	-2.377690	1.269310	3.531340	0.063830	-2.690080	3.513560	0.079070	-2.682360	3.527080	0.054850	-2.686930	3.492620
H	2.278510	1.431970	3.553050	0.072740	-2.685040	3.535700	0.073930	-2.684330	3.540860	-2.374320	1.268950	3.524810	-2.353240	1.276960	3.543940	-2.365420	1.268360	3.512930
H	0.088360	-2.686950	3.555570	2.274230	1.413460	3.556500	2.274570	1.412730	3.559470	2.270460	1.381620	3.574300	2.280540	1.390650	3.542940	2.265520	1.371360	3.563150
H	-0.062560	1.204310	4.025030	-1.025490	-0.646850	4.002930	-1.020480	-0.649640	4.010110	-1.024110	-0.661050	3.995510	1.090500	-0.564300	3.998940	-1.021910	-0.664140	3.971860
H	-1.012670	-0.645630	4.026900	1.061400	-0.556130	4.017290	1.063680	-0.555770	4.021400	1.076280	-0.578000	4.008770	-0.058280	1.193810	4.008840	1.072350	-0.580710	3.987420
H	1.066430	-0.548000	4.032920	-0.070290	1.193240	4.011010	-0.067480	1.192190	4.017660	-0.074950	1.176260	4.021080	-0.999820	-0.648770	4.008510	-0.077740	1.173570	4.000820
C	-1.947570	-0.874360	-5.300670	-1.961380	-0.850740	-5.315020	-1.956150	-0.835620	-5.309070	-1.867850	-0.818030	-5.299770	-1.915560	-0.831060	-5.280260	-1.867860	-0.765570	-5.303870
C	0.301160	2.115800	-5.282350	0.311960	2.128950	-5.303690	0.338070	2.129600	-5.292850	0.402420	2.184980	-5.320680	0.397660	2.161010	-5.332060	0.472480	2.195890	-5.331620
C	1.769940	-1.329170	-5.290480	1.732800	-1.381940	-5.322050	1.741940	-1.378270	-5.309460	1.793230	-1.379130	-5.304310	1.759690	-1.395890	-5.296390	1.789800	-1.405500	-5.308020
C	-2.760820	-0.238830	-6.243490	-2.764900	-0.198430	-6.254790	-2.758220	-0.179550	-6.247440	-2.721460	-0.232810	-6.239520	-2.787570	-0.257810	-6.210420	-2.720280	-0.166890	-6.236270
C	1.266750	2.513690	-6.211550	1.278890	2.535900	-6.227690	1.314760	2.522150	-6.212810	1.618070	-2.415760	-6.225960	1.579380	-2.433320	-6.216170	1.594230	-2.443810	-6.223700
C	1.586110	-2.350850	-6.226920	1.544320	-2.420070	-6.239220	1.552930	-2.413920	-6.229350	1.390510	2.604790	-6.216390	1.392440	2.561560	-6.229160	1.489080	2.566230	-6.217240
C	-1.986420	-0.473180	-3.966700	-1.991000	-0.452480	-3.979950	-1.984350	-0.439680	-3.973290	-1.896100	-0.388670	-3.974360	-1.928090	-0.394500	-3.956950	-1.885610	-0.342820	-3.976190
C	0.651540	1.951990	-3.943590	0.663730	1.941110	-3.968530	0.679970	1.943410	-3.954930	0.726080	1.969830	-3.982620	0.714990	1.956880	-3.990750	0.768840	1.979270	-3.987530
C	1.445580	-1.546430	-3.952830	1.411730	-1.574190	-3.979820	1.414930	-1.571910	-3.968900	1.445730	-1.571540	-3.968680	1.410690	-1.584010	-3.960570	1.439530	-1.583620	-3.971220
C	-3.612290	0.795850	-5.852380	-3.597550	0.849820	-5.859480	-3.587910	0.870280	-5.850090	-3.601740	0.780140	-5.854550	-3.670460	0.750040	-5.817930	-3.588720	0.852740	-5.842030
C	1.079410	-3.587920	-5.825860	2.594770	2.754950	-5.816660	1.037830	-3.640960	-5.808580	1.095780	-3.642190	-5.812040	1.050410	-3.656200	-5.800210	1.048220	-3.657460	-5.802710
C	2.580430	2.748030	-5.802070	1.035520	-3.648280	-5.814200	2.630660	2.728030	-5.795090	2.698680	2.810510	-5.774590	2.701310	2.758690	-5.785700	2.798800	2.720710	-5.759560
C	-2.844100	0.562760	-3.571870	-2.830030	0.597030	-3.580790	-2.820460	0.611390	-3.572180	-2.786270	0.621200	-3.585120	-2.820110	0.610810	-3.560200	-2.764280	0.673580	-3.577810
C	0.941820	-2.790300	-3.547950	1.983320	2.166410	-3.553460	0.903580	-2.805930	-3.543810	0.927120	-2.805060	-3.550710	0.885740	-2.814110	-3.540510	0.897650	-2.804670	-3.546110
C	1.968840	2.193100	-3.530000	0.906840	-2.809440	-3.550560	1.999610	2.155720	-3.533260	2.038020	2.181500	-3.537490	2.027800	2.160350	-3.544020	2.082720	2.139800	-3.526720
C	-3.656460	1.197150	-4.515080	-3.632830	1.247840	-4.520890	-3.621700	1.266180	-4.510850	-3.637440	1.207340	-4.525070	-3.689840	1.184770	-4.490600	-3.614000	1.273370	-4.510260
C	0.758040	-3.810340	-4.484670	2.948950	2.572230	-4.477840	0.713950	-3.839700	-4.464260	0.751310	-3.839810	-4.472590	0.704760	-3.849620	-4.460460	0.700950	-3.840890	-4.461990
C	2.933190	2.589990	-4.459710	0.717450	-3.845700	-4.468310	2.975130	2.546790	-4.453520	3.024790	2.600350	-4.432710	3.021290	2.559680	-4.440640	3.098030	2.508720	-4.411690
C	-3.429840	-0.327900	-0.847790	-3.422290	-0.304950	-0.866620	-3.413080	-0.291510	-0.857510	-3.402790	-0.256140	-0.874090	-3.415190	-0.240730	-0.835450	-3.389170	-0.209630	-0.872140
C	2.011230	-2.813580	-0.826300	1.481540	3.106570	-0.834610	1.984960	-2.809810	-0.827910	1.992180	-2.805670	-0.835250	1.962320	-2.821170	-0.832160	1.973110	-2.810450	-0.836040
C	1.434290	3.158080	-0.823820	1.995000	-2.810880	-0.834080	1.478170	3.105820	-0.821780	1.520170	3.081670	-0.805530	1.492020	3.083030	-0.823190	1.536990	3.055970	-0.805220
C	-4.715750	-0.853120	-0.962650	-4.706540	-0.830860	-0.996390	-4.698560	-0.813740	-0.987540	-4.694720	-0.763650	-0.997790	3.060680	-3.669180	-0.960160	-4.686640	-0.701850	-0.997990
C	1.601680	4.535690	-0.951620	3.098390	-3.651950	-0.965720	3.087060	-3.652290	-0.961680	3.099050	-3.641780	-0.967080	1.689730	4.456120	-0.952340	3.077460	-3.648270	-0.976710
C	3.112200	-3.660120	-0.944640	1.681170	4.480750	-0.953740	1.671670	4.480100	-0.947770	1.737410	4.453830	-0.914070	-4.711750	-0.739390	-0.946590	1.757770	4.426260	-0.927520
C	0.782360	5.372750	-0.198200	-5.042140	-1.948280	-0.236370	-5.037280	-1.931710	-0.229910	-5.042430	-1.880570	-0.243140	4.205050	-3.386270	-0.218660	-5.043570	-1.824010	-0.255350
C	-5.047210	-1.963400	-0.190560	4.234030	-3.374500	-0.208770	4.225050	-3.376270	-0.207960	4.238070	-3.355280	-0.218780	0.882940	5.313040	-0.207810	4.222800	-3.362450	-0.237410
C	4.242000	-3.384840	-0.178410	0.878930	5.332950	-0.199330	0.863690	5.332000	-0.199060	0.940970	5.311240	-0.159450	-5.060310	-1.852660	-0.186930	0.957860	5.292820	-0.186710
C	-0.176180	4.805390	0.637750	-4.081760	-2.505220	0.604650	-4.077660	-2.492700	0.608890	-4.083910	-2.455370	0.587450	4.212650	-2.263270	0.604400	-4.087980	-2.419660	0.563950
C	-4.081450	-2.514370	0.648090	-0.098080	4.783470	0.627260	-0.111460	4.781410	0.628830	4.231610	-2.240260	0.614770	-0.097420	4.767680	0.617150	4.225350	-2.245590	0.593700
C	4.234130	-2.272490	0.659510	4.228950	-2.264490	0.631940	4.223120	-2.265840	0.632070	-0.049500	4.767870	0.654810	-4.097390	-2.434180	0.633800	-0.039770	4.760070	0.626040
C	-2.817240	-1.927460	0.701800	-2.819240	-1.916090	0.673270	-2.813540	-1.907340	0.678330	-2.813700	-1.883860	0.651940	3.067790	-1.470130	0.674900	-2.812430	-1.860750	0.632450
C	-0.276030	3.415580	0.705960	-0.229180	3.396320	0.688880	-0.236160	3.393820	0.696900	3.079130	-1.458160	0.688180	-2.823180	-1.870240	0.686880	3.073820	-1.462800	0.676330
C	3.089410	-1.477520	0.717680	3.080840	-1.475340	0.703120	3.076160	-1.475400	0.705970	-0.197150	3.382130	0.706700	-0.225010	3.380760	0.689520	-0.189800	3.375130	0.691710
C	-1.340360	2.724090	1.516810	-1.699230	-2.507300	1.489350	-1.696270	-2.503740	1.493240	-1.699860	-2.492220	1.463070	3.014140	-0.198420	1.476970	-1.700180	-2.483470	1.433280
C	-1.693770	-2.513600	1.517080	-1.312910	2.723990	1.489570	-1.317590	2.720990	1.499900	-1.295890	2.716840	1.493210	-1.704520	-2.486190	1.485840	-1.294140	2.714710	1.473800
C	3.030730	-0.210710	1.529900	3.023920	-0.209390	1.515280	3.023440	-0.210340	1.519470	3.015830	-0.192660	1.499440	-1.312570	2.710670	1.487150	3.014330	-0.194990	1.483130
C	-1.981610	0.723530	2.665700	-1.981420	0.729180	2.639300	-1.981350	0.727450	2.652070	0.347510	-2.079620	2.635990	0.354390	-2.076910	2.643320	0.345260	-2.081080	2.614240
C	1.615060	1.351800	2.671200	0.350330	-2.075560	2.655170	0.352520	-2.075460	2.660200	-1.980120	0.727750	2.644430	1.619330	1.341340	2.657810	-1.980430	0.728070	2.628090
C	0.359520	-2.074260	2.675140	1.616030	1.346480	2.669890	1.615480	1.346080	2.673360	1.614480	1.336770	2.684930	-1.974330	0.729510	2.660830	1.614400	1.333900	2.669950
C	0.201940	1.730750	3.098710	-1.610320	-0.682510	3.074840	-1.607000	-0.684560	3.083090	-1.610210	-0.688320	3.067930	1.400760	-1.051640	3.065490	-1.608880	-0.688990	3.044920
C	-1.602540	-0.685840	3.102140	1.387190	-1.046850	3.090900	1.388950	-1.046500	3.094840	1.391980	-1.058610	3.073540	0.207380	1.722130	3.084230	1.389350	-1.060470	3.052270
C	1.393640	-1.041880	3.108680	0.201620	1.724640	3.089940	0.201330	1.723460	3.095540	0.199510	1.713480	3.104120	-1.596310	-0.683270	3.087800	0.198360	1.710670	3.084370

Table 4. DFT optimised geometries of LnL^3 complexes

	Tb			Dy			Ho			Er			Tm			Yb		
	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z	x	y	z
Ln	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
O	1.810310	0.684350	-1.472470	1.801230	0.656300	-1.494450	1.794780	0.646890	-1.481300	1.806170	0.649630	-1.447360	-0.350850	-1.871600	-1.465300	1.719450	0.641270	-1.505550
O	-1.482900	1.131330	-1.529620	-1.440870	1.142720	-1.538620	-1.404120	1.151360	-1.562840	-1.433730	1.132990	-1.527760	-1.386100	1.116700	-1.578600	-1.353280	1.171210	-1.547140
O	-0.267070	-1.820930	-1.573370	-0.290280	-1.791840	-1.578110	-0.295650	-1.779510	-1.580480	-0.285620	-1.778710	-1.569380	1.671500	0.617580	-1.567900	-0.336530	-1.716680	-1.585300
N	1.667820	0.000000	2.070170	1.666580	0.000000	2.050050	1.667620	0.000000	2.037510	3.159480	2.090180	-2.521230	0.226500	-3.734600	-2.586200	2.945970	2.078370	-2.723440
N	-0.833660	-1.455060	2.026390	-0.831120	-1.447220	2.016800	-0.831890	-1.443020	2.009010	0.241720	-3.766550	-2.485780	-3.357000	1.635700	-2.535500	-3.290230	1.687950	-2.576450
N	-0.834160	1.455060	2.010220	-0.835460	1.447220	1.987000	-0.835730	1.443020	1.987790	-3.341840	1.512650	-2.650840	2.977000	2.061000	-2.693400	0.186310	-3.638070	-2.635260
N	1.893300	-1.681760	-0.079260	1.873160	-1.677240	-0.094300	1.869990	-1.670750	-0.105710	1.660350	0.000000	2.057460	-0.834030	-1.439500	2.032600	-0.838370	1.434100	1.964520
N	0.516100	2.505260	-0.129720	-2.397010	-0.830860	-0.128660	-2.386480	-0.803450	-0.134140	-0.825040	-1.441790	2.013930	-0.827570	1.439500	1.988500	1.662730	0.000000	1.957030
N	-2.406580	-0.869660	-0.135650	0.530470	2.483780	-0.139710	0.531670	2.475950	-0.134450	-0.835320	1.441790	1.977200	1.661600	0.000000	1.955300	-0.824350	-1.434100	1.958860
N	0.285650	-3.813580	-2.461000	0.245660	-3.780040	-2.486490	0.242170	-3.757860	-2.510130	-2.390390	-0.828960	-0.119980	1.866300	-1.707500	-0.144220	0.520260	2.467920	-0.133830
N	3.154590	2.151240	-2.518250	3.154410	2.114880	-2.541660	3.120880	2.099610	-2.570700	0.533100	2.480900	-0.130430	-2.383400	-0.790300	-0.097710	-2.383680	-0.749340	-0.133270
N	-3.393320	1.468240	-2.658660	-3.353680	1.515920	-2.654040	-3.329060	1.561880	-2.647370	1.864130	-1.676950	-0.078770	0.492180	2.457700	-0.153720	1.848240	-1.650070	-0.176400
H	1.029190	-0.538600	4.013930	1.038560	-0.537350	3.997990	1.046730	-0.545930	3.985870	-5.051490	-5.998670	-0.253600	-5.131200	-5.929200	-0.456100	7.622730	-1.578300	-1.047860
H	-0.094440	1.226540	3.978740	-1.038390	-0.628750	3.958620	-1.029970	-0.633630	3.955560	7.650710	-1.498610	-0.275020	-2.689000	7.319500	-0.251340	-2.453640	7.439750	-0.509400
H	-1.045750	-0.636230	3.967960	-0.092670	1.225780	3.956100	-0.086950	1.217850	3.954480	-2.411010	7.294850	-0.705640	7.552100	-1.584300	-0.732350	-5.007750	-5.950980	-0.263760
H	2.264240	1.441740	3.530710	0.062300	-2.677740	3.515170	2.265200	1.429540	3.508650	6.773470	-2.523360	-2.372480	-5.567300	-4.643400	-2.548000	-5.570040	-4.715880	-2.356060
H	0.062620	-2.683020	3.524940	2.262810	1.439500	3.512510	0.064510	-2.682530	3.498590	-5.528810	-4.792220	-2.383330	-1.397600	7.158800	-2.378700	6.531100	-2.549360	-3.068600
H	-2.405620	1.274020	3.445870	-2.391080	1.284290	3.440500	-2.383780	1.282620	3.449870	-0.991100	6.874270	-2.711730	6.498200	-2.618100	-2.742200	-1.089170	7.118020	-2.572010
H	2.302460	-1.561970	3.377810	2.307790	-1.561610	3.354870	2.311450	-1.569240	3.332500	-3.944660	5.510610	0.113730	-1.772200	-4.696900	-5.134700	-3.164700	3.882930	-5.140810
H	0.181980	2.818900	3.298500	-2.541670	-1.216030	3.273940	-2.535980	-1.220460	3.276540	-2.705480	-6.161700	0.569550	-3.306500	3.918300	-5.026500	-1.883990	-4.658860	-5.103380
H	-2.548310	-1.217730	3.276360	0.178730	2.816940	3.272540	0.180850	2.810840	3.274170	6.721390	0.673360	0.516270	4.757600	0.846900	-5.295300	4.537630	0.843610	-5.435820
H	3.780590	-0.294230	2.267550	3.779260	-0.299640	2.240550	3.779670	-0.303300	2.229810	5.095280	0.874870	-5.007990	-0.558500	-5.684200	-4.280800	-4.609730	3.353820	-4.242320
H	-2.098460	-3.173680	2.223410	-2.106400	-3.158920	2.207580	-2.120890	-3.145790	2.191760	5.316240	2.400240	-4.112580	-4.729900	3.294800	-4.154600	4.876630	2.371980	-4.583460
H	-1.684340	3.415240	2.171600	-1.675610	3.411230	2.147890	-1.671920	3.408390	2.152770	-1.737370	-4.876770	-4.989340	5.051800	2.359200	-4.399000	-0.613280	-5.609220	-4.292400
H	0.797180	-2.757280	1.913150	0.792090	-2.758290	1.901530	0.787560	-2.757540	1.881150	-0.498690	-5.794850	-4.095920	-2.795100	-6.171000	0.375570	-3.893360	5.581900	0.316500
H	1.991360	2.052930	1.887190	1.995790	2.052440	1.869040	1.998370	2.053630	1.869280	-4.656080	3.170320	-4.335030	6.738500	0.623410	0.086520	6.781100	0.568800	-0.105780
H	-2.767570	0.693950	1.809440	-2.777890	0.698440	1.812080	-2.781410	0.699570	1.822590	-3.209750	3.665300	-5.252010	3.518100	2.131200	-5.299400	-3.642190	2.162990	-5.169990
H	4.972500	-2.160270	1.182430	4.966170	-2.161760	1.130670	-4.339380	-3.252440	1.083890	-5.956390	-2.251210	-0.480150	-3.991700	5.351900	0.549170	-0.179690	-4.142430	-5.226940
H	-4.321370	-3.320460	1.136730	-4.330520	-3.283260	1.112670	4.984390	-2.130900	1.074180	1.150710	6.269690	-0.454720	-0.051780	-4.224700	-5.190700	-2.632790	-6.102510	0.475290
H	-0.641510	5.402590	1.118660	-0.632900	5.391720	1.079330	-0.635610	5.387190	1.073350	4.838690	-4.110610	-0.436990	-3.710200	2.181600	-5.120700	3.285750	2.113590	-5.368610
H	3.242540	0.625740	0.837100	3.239670	0.623970	0.813170	3.244430	0.631500	0.808260	3.838580	2.139730	-5.094480	-1.435000	5.061400	-3.701400	-3.771260	-3.669760	-3.704920
H	-1.031900	-3.137640	0.793120	-1.041890	-3.123130	0.775720	-1.053490	-3.113480	0.761840	-0.028520	-4.365020	-5.069350	-3.680500	-3.636300	-3.804900	1.140960	6.258530	-0.475510
H	-2.156010	2.466440	0.736390	-2.152990	2.466470	0.712690	-2.154430	2.466060	0.717810	-3.712210	1.952720	-5.252270	4.845100	-4.123900	-0.510610	4.636860	-1.365040	-4.148970
H	-2.668950	-6.183180	0.611970	-2.701650	-6.160720	0.582710	-2.678900	-6.142190	0.579130	5.004670	-1.369720	-3.674930	-5.936900	-2.227100	-0.557620	-1.187970	4.967790	-3.805380
H	6.705230	0.709660	0.528740	6.727620	0.654270	0.467270	6.735820	0.656410	0.387720	-3.672970	-3.788390	-3.687130	1.082600	6.245100	-0.557410	-5.969730	-2.097680	-0.550680
H	-3.993040	5.442360	0.149400	-3.946330	5.502970	0.131600	-3.920890	5.533320	0.156450	-4.319670	-3.290590	1.112130	4.668800	-1.438700	-3.932500	4.888400	-3.944420	-0.786880
H	-5.012700	-6.027350	-0.218920	-5.048750	-5.992620	-0.236160	-5.032040	-5.980450	-0.223950	-0.641130	5.393670	1.067270	2.775700	-4.484400	-1.843600	2.441430	4.648890	-1.861080
H	7.618680	-1.468460	-0.264230	7.633090	-1.520460	-0.343730	7.662070	-1.500080	-0.448210	4.954410	-2.172040	1.152270	2.366700	4.630600	-1.943800	-5.200130	-0.159650	-1.908170
H	4.874870	-4.105970	-0.398330	1.153120	6.271990	-0.447150	1.142980	6.265190	-0.463380	-1.128090	4.699880	-3.898820	-5.186500	-0.285220	-1.924000	-0.625520	5.386410	1.079640
H	1.139550	6.294790	-0.406170	4.851530	-4.099390	-0.459170	-5.956700	-2.201620	-0.521030	-4.096650	3.349100	-1.084280	-4.335700	-3.266800	1.071000	2.793270	-4.271330	-2.094020
H	-5.964750	-2.309570	-0.466070	-5.963380	-2.246220	-0.484820	4.875090	-4.050270	-0.538190	-0.853250	-5.175680	-0.737740	4.985600	-2.147600	1.028800	-4.365090	-3.201640	1.032010
H	-2.450170	7.227660	-0.650270	-2.410240	7.287470	-0.682490	-2.403940	7.331480	-0.663450	2.507330	4.667940	-1.788080	-0.636540	5.384200	1.054800	5.014930	-2.067980	0.873630
H	-0.812300	-5.213340	-0.702470	-0.848500	-5.187490	-0.733240	-0.837330	-5.165550	-0.749980	4.971550	1.832930	-0.793420	4.928400	1.809900	-1.114600	-4.007740	3.445080	-0.925420
H	4.973480	1.889650	-0.787480	4.983640	1.840170	-0.827120	4.958020	1.824290	-0.876490	-5.239050	-0.320000	-1.872600	-0.912070	-5.182200	-0.888550	4.902290	1.757640	-1.193850
H	-4.159950	3.296730	-1.075970	-4.108140	3.348650	-1.077970	-4.074990	3.381420	-1.057140	2.797140	-4.420580	-1.825120	0.901200	-4.482400	-2.727300	3.234550	3.038070	-2.897100
H	2.490070	4.710070	-1.762280	2.499950	4.676620	-1.794110	2.485480	4.665590	-1.811650	3.469440	3.050250	-2.648650	3.293900	3.018200	-2.824700	-4.291680	1.525850	-2.649740
H	2.843850	-4.437120	-1.794260	2.806980	-4.419520	-1.839130	2.817280	-4.377180	-1.899160	0.049680	-2.669020	3.526860	-4.359700	1.470100	-2.580200	0.836200	-4.414980	-2.730610
H	-5.267970	-0.381840	-1.871020	-5.244810	-0.318430	-1.879330	-5.216990	-0.276380	-1.907740	0.881260	-4.557050	-2.515130	-4.043200	3.266900	-0.776910	-0.837620	-5.074700	-0.877360
H	-5.483760	-4.844220	-2.362970	-5.526230	-4.794320	-2.370410	-5.526640	-4.785910	-2.356450	-4.324230	1.290500	-2.790340	2.873400	0.286530	-3.752000	-1.715100	2.514510	-3.628600
H	6.743040	-2.479320	-2.368780	6.737520	-2.521910	-2.444440	6.753680	-2.501780	-2.543470	2.254000	1.439140	3.522860	-1.808300	2.541600	-3.560400	-1.398870	-2.719700	-3.591330
H	0.934030	-4.597190	-2.479970	0.889640	-4.567060	-2.515190	0.888670	-4.542520	-2.547170	-2.387400	1.288470	3.436680	-1.300500	-2.778400	-3.599800	2.763510	0.296390	-3.755920
H	3.456450	3.115320	-2.633870	3.465780	3.076420	-2.652670	-1.001590	6.933820	-2.686560	2.304200	-1.553490	3.371740	0.107170	-2.664200	3.510100	-2.348350	1.270700	3.465910
H	-1.036690	6.824460	-2.664220	-0.997670	6.874330	-2.695270	3.426580	3.061110	-2.697870	-2.543750	-1.219000	3.264000	-2.151000	-3.117400	2.244300	2.280360	1.394640	3.451830
H	-4.367840	1.220430	-2.809280	-4.335950	1.291140	-2.790300	-4.318810	1.357890	-2.760490	0.169150	2.820030	3.263800	-2.339000	1.299600	3.491000	-1.667770	3.399640	2.165190
H	-1.256230	-2.956600	-3.538130	-1.298230	-2.905450	-3.546460	-1.310960	-2.882630	-3.556170	1.030140	-0.530090	4.007530	-1.658200	3.407900	2.176700	0.083460	-2.693720	3.426890
H	3.153820	0.385950	-3.600290	3.133190	0.350650	-3.624380	3.074930	0.323950	-3.632040	-1.045630	-0.628450	3.957650	2.313600	1.415500	3.415600	3.778030	-0.295340	2.140920
H	-3.623580	-3.856940	-3.673610	-3.669430	-3.802770	-3.682500	-3.681300	-3.790840	-3.681780	-0.103570	1.231440	3.952930	3.782700	-0.256260	2.127300	-2.119420	-3.134210	2.142660
H	4.991740	-1.305350	-3.677600	4.974470	-1.341790	-3.731690	-1.765560	2.366980	-3.738630	-2.091280	-3.161490	2.208600	-2.509900	-1.208200	3.334800	-2.507660	-1.240620	3.260780
H	-1.841680	2.286730	-3.760400	-1.788810	2.317380	-3.747720	4.957220	-1.339950	-3.800180	3.772900	-0.304350	2.257240	0.221300	2.811600	3.246800	0.193280	2.793170	3.252270
H	-1.189000	4.665790	-3.878710	-1.143970	4.706610	-3.893770	-1.139630	4.768150	-3.889500	-1.682870	3.403690	2.144910	2.350600	-1.555500	3.248000	2.338460	-1.581930	3.224110
H	-0.434470	-5.878010	-4.032190	-0.491000	-5.824730	-4.076000	-0.501780	-5.798480	-4.101430	3.132080	0.305270	-3.566730	-0.987660	-0.624710	3.980900	1.086160	-0.567930	3.915870
H	5.339940	2.500570	-4.056070	5.321570	2.457000	-4.106750	5.241920	2.429980	-4.204020	-1.301140	-2.879830	-3.535720	1.110700	-0.522700	3.932700	-0.060930	1.193420	3.920810
H	-4.748210	3.140360	-4.292770	-4.685510	3.182330	-4.314220	-4.663400	3.228880	-4.303670	-1.766380	2.304990	-3.734540	-0.021370	1.217200	3.935100	-0.993240	-0.653980	3.920780
H	-1.674380	-4.986120	-4.950620	-1.731420	-4.917930	-4.978760	-1.750360	-4.891060	-4.992270	0.794960	-2.761110	1.920980	-2.781700	0.702180	1.881100	-2.795320	0.704250	1.845850
H	5.147930	0.992300	-4.986090	5.110980	0.950640	-5.035820	-0.044010	-4.373620	-5.088310	-2.783150	0.700040	1.811550	0.773190	-2.762400	1.868800	2.004430	2.058330	1.830350
H	0.031960	-4.466060	-5.033550	-0.023400	-4.404160	-5.064420	5.006900	0.911820	-5.108150	1.998350	2.052120	1.877580	-1.080900	-3.129400	0.816970	0.783850	-2.761340	1.798790
H	3.886850	2.252820	-5.076780	3.853870	2.216130	-5.108160	3.744910	2.173190	-5.157430	3.239640	0.617310	0.825830	2.002800	2.057600	1.792000	3.237320	0.651010	0.728900
H	-3.322800	3.660310	-5.228830	-3.248830	3.686010	-5.241670	-3.228060	3.736900	-5.230730	-1.030130	-3.119650	0.773920	-2.168900	2.468900	0.747310	-2.163540	2.480170	0.718620
H	-3.813410	1.944430	-5.247290	-3.748810	1.972740	-5.249340	-3.724840	2.022520	-5.240980	-2.153580	2.464040	0.704350	3.211300	0.623670	0.685240	-1.076220	-3.089810	0.694240
C	1.375290	-1.036190	3.099310	1.379210	-1.035690	3.081760	1.382470	-1.040840	3.065930	-4.236380	-5.554960	-0.827700	-4.302700	-5.484000	-1.009500	6.787510	-1.060610	-1.522470
C	0.190090	1.744940	3.053920	0.190610	1.742640	3.030430	0.193190	1.737130	3.029290	6.872350	-0.993110	-0.849060	-2.703500	6.396900	-0.833960	-2.494570	6.494270	-1.052880
C	-1.618000	-0.680600	3.032700	-1.614550	-0.675540	3.026020	-1.611160	-0.677390	3.026020	-2.469440	6.338760	-1.228520	6.746500	-1.067600	-1.256700	-4.217440	-5.489330	-0.858020
C	0.355170	-2.074090	2.650500	0.355030	-2.071890	2.638780	0.354850	-2.073890	2.623410	6.382250	-1.565460	-2.024960	-4.546200	-4.765800	-2.182400	6.177470	-1.602770	-2.655860
C	1.606810	1.358600	2.646150	1.608050	1.358060	2.625990	1.610230	1.354810	2.621740	-4.502790	-4.881040	-2.021660	-1.982200	6.306900	-2.026700	-1.732120	6.314200	-2.208910
C	-1.987320	0.726950	2.581570	-1.987730	0.730450	2.573710	-1.986820	0.729380	2.579760	-1.675930	6.103650	-2.353250	6.157500	-1.645200	-2.383400	-4.531320	-4.799410	-2.031290
C	3.000670	-0.229400	1.489810	2.997000	-0.231160	1.465650	2.999130	-0.228100	1.453930	-3.327090	5.339500	-0.769910	-0.839640	-4.656200	-4.557100	-3.591130	3.065620	-4.544760
C	-1.671270	-2.519030	1.444740	-1.675260	-2.503220	1.432070	-1.682440	-2.490900	1.419750	-2.923570	-5.646250	-0.367740	-3.699000	3.062000	-4.463000	-0.931560	-4.590430	-4.562100
C	-1.315690	2.711280	1.406480	-1.311140	2.705130	1.382920	-1.310360	2.701830	1.386740	6.351590	0.222110	-0.406380	4.281300	1.628200	-4.688700	4.096650	1.628000	-4.807190
C	3.001840	-1.472500	0.638660	2.989510	-1.472040	0.612320	2.992240	-1.461230	0.589890	4.574290	1.654570	-4.437460	-2.995400	-5.618800	-0.544480	-3.299950	5.454100	-0.590800
C	-2.762530	-1.932650	0.589470	-2.762020	-1.899950	0.583330	-2.761320	-1.874810	0.570390	-0.805350	-4.787190	-4.416440	6.290400	0.167780	-0.798460	6.316130	0.141010	-0.995910
C	-0.234560	3.353310	0.577810	-0.223850	3.338610	0.556280	-0.223420	3.332870	0.558150	-3.643920	2.863590	-4.640530	-3.432300	5.296100	-0.386650	-2.888810	-5.574050	-0.445010
C	4.093050	-2.339750	0.564490	4.080050	-2.338480	0.521540	-0.022580	4.711620	0.477240	5.387460	-0.918430	-2.755780	-3.486500	-4.198600	-2.887800	-3.520560	-4.210060	-2.788290
C	-0.030410	4.732520	0.514290	-4.050520	-2.429660	0.496250	4.092810	-2.312390	0.474430	-3.460250	-4.315100	-2.753140	-2.001700	5.127600	-2.768900	-1.785360	5.105290	-2.900410
C	-4.048020	-2.471380	0.511140	-0.019630	4.717130	0.482300	-4.051850	-2.397220	0.473220	-1.750430	4.881120	-3.018680	5.127600	-0.984190	-3.050700	5.112510	-0.938830	-3.261800

C	4.034190	-3.417010	-0.311910	-2.919820	-5.648510	-0.356320	-2.904840	-5.631370	-0.358830	-3.410060	4.118400	-1.444080	-1.932300	-5.057200	-1.257000	-3.360840	4.245690	-1.290170
C	-2.884160	-5.678150	-0.331640	4.011930	-3.410810	-0.360140	0.963830	5.193190	-0.376000	-1.877450	-5.086460	-1.106200	5.265600	0.835390	-1.474300	5.252950	0.810160	-1.608230
C	0.958530	5.222110	-0.331890	0.971410	5.199990	-0.365070	-4.943820	-1.811370	-0.417310	5.361340	0.875310	-1.145030	-3.459100	4.116900	-1.136200	-1.874710	-4.990840	-1.209610
C	-4.955340	-1.906750	-0.377900	-4.951460	-1.851230	-0.390260	4.027840	-3.374240	-0.419760	-4.944990	-1.854900	-0.385230	-2.168200	-4.351300	-2.440000	-2.610200	4.064920	-2.455590
C	6.336240	0.264690	-0.397280	6.349600	0.213290	-0.457000	6.352100	0.215290	-0.534130	0.970620	5.197720	-0.368260	-2.751000	4.025100	-2.337900	4.650180	0.281180	-2.752780
C	-3.378310	5.278800	-0.737660	-3.331790	5.334980	-0.754740	-3.310830	5.372140	-0.734280	4.001170	-3.419100	-0.340520	4.682500	0.268590	-2.611500	-2.180620	-4.311150	-2.392010
C	-4.195710	-5.590990	-0.796000	-4.233260	-5.554520	-0.814000	-4.221520	-5.540960	-0.807700	4.878090	0.315050	-2.330790	4.005500	-3.435000	-0.413020	0.956030	5.187450	-0.388600
C	6.848300	-0.953870	-0.841040	6.857170	-1.003450	-0.910820	1.468530	2.937500	-0.971060	-2.135900	-4.424250	-2.309940	-4.931200	-1.824900	-0.431850	-4.952560	-1.721190	-0.438130
C	1.838130	-2.715790	-0.929380	1.810860	-2.704240	-0.952590	1.811850	-2.686920	-0.977420	-2.629050	3.883390	-2.579420	0.908740	5.174000	-0.449820	4.031060	-3.292100	-0.618620
C	1.462590	2.972920	-0.951560	1.474430	2.945750	-0.968030	6.871120	-0.991260	-1.001740	-4.042170	-2.434040	0.498660	-1.041300	-3.806100	-3.306900	-2.725000	2.813300	-3.314420
C	-3.274900	-0.330960	-1.000790	-3.256820	-0.284520	-0.997770	-3.237380	-0.250680	-1.008290	-0.023570	4.717180	0.476810	-2.827100	2.799400	-3.239400	-1.105290	-3.740180	-3.307980
C	-1.835740	-5.127770	-1.073900	-1.873260	-5.095930	-1.099550	-1.864710	-5.076930	-1.109680	4.069490	-2.346750	0.540790	3.647300	1.005900	-3.448800	3.559150	1.017300	-3.517490
C	2.891150	-3.609740	-1.087540	1.732120	4.304450	-1.117020	1.722140	4.295730	-1.128260	3.881110	1.035550	-3.228080	2.842800	-3.642200	-1.156000	1.690960	4.286280	-1.159600
C	1.720260	4.332800	-1.090210	2.861470	-3.597690	-1.126470	2.870570	-3.565230	-1.175090	-1.023660	-3.889430	-3.202760	4.087900	-2.341800	0.442250	-0.021710	4.709110	0.476280
C	5.356370	0.929330	-1.139500	-4.550660	-0.764440	-1.168060	-4.531800	-0.724690	-1.189320	-2.770150	2.619250	-3.414680	-4.048000	-2.403200	0.471670	-4.525970	-0.626160	-1.190520
C	-4.566100	-0.821070	-1.163010	5.362540	0.881130	-1.186690	-2.462470	6.379190	-1.193200	1.736390	4.299610	-1.112310	1.635700	4.267600	-1.222300	-4.067830	-2.336300	0.440410
C	-2.515570	6.278750	-1.185260	-2.472800	6.334460	-1.210460	5.345750	0.872910	-1.246640	-4.545260	-0.766400	-1.161200	-4.516000	-0.729410	-1.189500	2.853610	-3.484120	-1.343460
C	-3.470060	4.067090	-1.427350	-3.420190	4.117890	-1.435410	-3.394350	4.155910	-1.417110	2.852620	-3.600360	-1.110730	-0.044250	4.702400	0.445390	4.104930	-2.255340	0.303810
C	2.171530	1.862900	-1.678040	2.172780	1.831530	-1.697730	2.158650	1.821480	-1.703480	1.375050	-1.030900	3.094180	-1.587900	-0.670320	3.063300	-1.591280	-0.687940	3.001650
C	0.540490	-2.768260	-1.687430	0.510100	-2.743820	-1.704520	0.507140	-2.727440	-1.720770	-1.616810	-0.675600	3.021980	1.412300	-1.031300	3.008400	0.204730	1.722050	2.996950
C	-2.671130	0.817520	-1.759630	-2.637110	0.852940	-1.759600	-2.608120	0.882480	-1.768890	0.184020	1.744750	3.026540	0.227490	1.737900	3.002000	1.402750	-1.053490	2.984260
C	-4.458640	-4.930200	-1.998040	-4.499780	-4.885160	-2.010500	-4.497590	-4.873710	-2.003270	0.352990	-2.068930	2.650200	1.793700	-2.746100	-0.984550	1.432920	2.930320	-0.996610
C	6.359010	-1.518620	-2.020890	6.356770	-1.562870	-2.088550	6.363640	-1.550690	-2.176480	1.604420	1.358500	2.632450	1.392300	2.911700	-1.035500	-0.226490	3.331080	0.559810
C	-2.090700	-4.479280	-2.285660	-2.132000	-4.438050	-2.305520	-2.132970	-4.420630	-2.314340	-1.989350	0.731200	2.569740	-2.765000	-1.866900	0.595770	-3.226390	-0.171700	-0.997240
C	-1.725620	6.053460	-2.314500	-1.683400	6.103530	-2.338930	-1.678870	6.156900	-2.327410	-1.665170	-2.503320	1.432420	-3.230600	-0.244570	-0.981700	-2.771360	-1.831820	0.546020
C	4.874450	0.376750	-2.329400	4.869660	0.334060	-2.374770	4.845650	0.326090	-2.431740	2.992740	-0.235050	1.480260	2.993200	-1.481500	0.535340	1.785910	-2.634560	-1.083810
C	-2.692370	3.842220	-2.566900	-2.642880	3.887080	-2.574160	-2.623010	3.933660	-2.561760	-1.314200	2.701780	1.378100	-0.241960	3.324900	0.548630	2.988870	-1.435480	0.484440
C	-3.413820	-4.373400	-2.733270	-3.456790	-4.326110	-2.746620	-3.460950	-4.312850	-2.746930	-2.754880	-1.901890	0.586480	0.367680	-2.068300	2.616800	-1.979260	0.723690	2.579970
C	5.373770	-0.860610	-2.754960	5.365030	-0.901290	-2.810600	5.353450	-0.899100	-2.881700	-0.225680	3.338680	0.555900	-1.966900	0.736220	2.616700	1.617650	1.345190	2.569530
C	-1.808640	4.839990	-2.995250	-1.763010	4.884810	-3.010700	-1.753810	4.939220	-3.001660	2.981580	-1.476940	0.628220	-1.699700	-2.483600	1.462400	0.365490	-2.080910	2.552360
C	-0.975580	-3.957510	-3.182380	-1.019800	-3.911230	-3.202930	-1.028070	-3.889090	-3.218120	1.479930	2.941950	-0.956050	1.630700	1.354900	2.549600	-1.315040	2.701830	1.387180
C	3.892950	1.111740	-3.231620	3.879770	1.073160	-3.264480	3.829540	1.052560	-3.302230	-3.252550	-0.285070	-0.989490	-1.313100	2.701500	1.402900	2.996760	-0.216060	1.367290
C	-2.841560	2.589380	-3.417260	-2.789900	2.628240	-3.416300	-2.766830	2.676310	-3.406950	1.804650	-2.703710	-0.938680	2.992200	-0.221240	1.359100	-1.689680	-2.472850	1.371760
C	-0.745430	-4.879270	-4.375670	-0.799350	-4.821040	-4.407130	-0.814450	-4.794290	-4.426950	2.178720	1.819810	-1.672280	0.476510	-2.774000	-1.707800	2.066370	1.811220	-1.769740
C	4.609600	1.757950	-4.412670	4.583510	1.717720	-4.454320	4.495630	1.684840	-4.520040	-2.629490	0.849410	-1.753090	2.042600	1.789400	-1.795600	-2.570310	0.959120	-1.737470
C	-3.740000	2.845930	-4.622360	-3.675970	2.879330	-4.631830	-3.653370	2.928290	-4.622170	0.507730	-2.734480	-1.698410	-2.605900	0.897290	-1.731500	0.465680	-2.650410	-1.798190

Table S5. Total DFT hyperfine tensors of HoL^2 in A^{-3} ppm units.

Label	Axx	Axy	Axz	Ayx	Ayy	Ayz	Azx	Azy	Azz	Atom
	199753	-594	605	-594	198582	3897	605	3897	-345161	Ho
	1093	-1524	2098	-1524	-1420	-941	2098	-941	-590	P
	-2093	-354	-244	-354	1794	2293	-244	2293	-565	P
	515	1864	-1855	1864	-820	-1361	-1855	-1361	-586	P
	518	-925	596	-925	-116	-412	596	-412	-430	O
	-752	177	55	177	1134	723	55	723	-416	O
	850	755	-652	755	-432	-315	-652	-315	-444	O
	-2369	-5675	6318	-5675	-2960	-5328	6318	-5328	-1819	O
	-7595	2536	1445	2536	2410	8008	1445	8008	-1837	O
	2041	3147	-7759	3147	-7380	-2886	-7759	-2886	-1827	O
	-614	15	5414	15	-4955	-2	5414	-2	1758	N
	-3815	1894	-2762	1894	-1709	-4656	-2762	-4656	1790	N
	-3774	-1886	-2653	-1886	-1585	4647	-2653	4647	1666	N
	-4547	2510	-63	2510	6336	70	-63	70	-5124	N
	1384	-6060	70	-6060	377	40	70	40	-5226	N
	5882	3381	-35	3381	-4108	-91	-35	-91	-5170	N
mPh	-153	-31	-46	-31	-15	217	-46	217	167	H
mPh	-70	76	-169	76	-93	-146	-169	-146	163	H
mPh	-19	-45	212	-45	-144	-68	212	-68	163	H
pPh	-156	23	-64	23	-108	-157	-64	-157	265	H
pPh	-140	-32	-109	-32	-129	130	-109	130	269	H
pPh	-103	11	168	11	-166	28	168	28	268	H
py4	242	-426	-27	-426	47	21	-27	21	-292	H
py4	-274	122	-5	122	560	-40	-5	-40	-290	H
py4	465	295	33	295	-177	14	33	14	-291	H
oPh	-311	-38	-33	-38	218	465	-33	465	92	H
oPh	123	-210	416	-210	-210	-201	416	-201	86	H
oPh	64	249	-388	249	-149	-255	-388	-255	85	H
mPh	-347	-42	116	-42	-238	-340	116	-340	585	H
mPh	-233	-21	-363	-21	-366	57	-363	57	598	H
mPh	-315	67	232	67	-290	280	232	280	605	H
py5	-64	-554	-201	-554	393	298	-201	298	-326	H
py5	-206	468	-158	468	532	-328	-158	-328	-322	H
py5	757	75	358	75	-429	23	358	23	-325	H
py3	661	-447	271	-447	-277	-110	271	-110	-390	H
py3	-423	-189	-41	-189	808	278	-41	278	-391	H
py3	348	627	-228	627	37	-177	-228	-177	-389	H
ceqp	-911	-27	36	-27	73	-1304	36	-1304	825	H
ceqp	-143	-414	-1140	-414	-681	618	-1140	618	809	H
aeq	-198	444	1107	444	-634	691	1107	691	820	H
ceqp	-511	-792	-537	-792	683	1078	-537	1078	-181	H
aeq	1074	-123	1221	-123	-908	-75	1221	-75	-174	H
aeq	-298	922	-679	922	462	-1015	-679	-1015	-174	H
ceq	-163	-540	1169	-540	-602	-784	1169	-784	729	H
ceq	-955	82	96	82	214	1402	96	1402	707	H
ceq	-15	455	-1263	455	-742	-610	-1263	-610	722	H
cax	-894	118	-748	118	-1008	-473	-748	-473	1889	H
cax	-877	-105	789	-105	-1031	-397	789	-397	1895	H
cax	-1078	-14	-51	-14	-808	898	-51	898	1870	H
oPh	-1603	-65	126	-65	-560	-1977	126	-1977	2156	H
oPh	-802	-412	-1842	-412	-1472	872	-1842	872	2268	H
oPh	-966	476	1695	476	-1374	1123	1695	1123	2332	H

caxp	1823	-968	-2609	-968	-1694	663	-2609	663	-143	H
caxp	-1675	-1055	747	-1055	1788	-2634	747	-2634	-128	H
caxp	3	2024	1883	2024	128	1952	1883	1952	-146	H
aax	413	-2765	-925	-2765	1209	1062	-925	1062	-1640	H
aax	3458	1056	1413	1056	-1813	276	1413	276	-1664	H
aax	-1394	1778	-477	1778	3039	-1369	-477	-1369	-1662	H
	-225	-57	-94	-57	-49	315	-94	315	271	C
	-134	107	-230	107	-131	-234	-230	-234	265	C
	-40	-49	320	-49	-228	-76	320	-76	266	C
	-211	-58	-156	-58	-162	233	-156	233	373	C
	-219	53	-131	53	-147	-247	-131	-247	366	C
	-122	7	281	7	-249	15	281	15	371	C
	-362	-93	-108	-93	91	557	-108	557	278	C
	-91	245	-432	245	-171	-367	-432	-367	268	C
	63	-152	536	-152	-327	-184	536	-184	270	C
	-415	28	-69	28	-241	-437	-69	-437	651	C
	-312	-88	-356	-88	-361	270	-356	270	668	C
	-272	62	414	62	-403	165	414	165	670	C
	419	-733	-54	-733	106	22	-54	22	-488	C
	-450	220	6	220	973	-66	6	-66	-483	C
	820	497	47	497	-295	36	47	36	-485	C
	70	-963	-245	-963	438	310	-245	310	-648	C
	-490	628	-145	628	998	-373	-145	-373	-638	C
	1181	314	390	314	-671	56	390	56	-645	C
	-719	-68	-17	-68	1335	263	-17	263	-692	C
	876	-870	250	-870	-257	-125	250	-125	-696	C
	782	919	-229	919	-165	-151	-229	-151	-694	C
	-750	-289	-360	-289	62	1154	-360	1154	621	C
	-372	499	-819	499	-294	-874	-819	-874	591	C
	116	-216	1177	-216	-792	-275	1177	-275	607	C
	-820	171	-344	171	-359	-1032	-344	-1032	1180	C
	-637	-285	-744	-285	-588	812	-744	812	1220	C
	-352	112	1081	112	-878	220	1081	220	1228	C
	-955	-616	1838	-616	-1350	-1327	1838	-1327	2282	C
	-697	472	-2074	472	-1588	-905	-2074	-905	2261	C
	-1774	137	228	137	-485	2263	228	2263	2240	C
	-187	-2397	-708	-2397	1569	995	-708	995	-1538	C
	-958	1932	-500	1932	2334	-1107	-500	-1107	-1527	C
	3201	413	1202	413	-1821	108	1202	108	-1536	C
	-1876	-393	-51	-393	3481	1085	-51	1085	-1676	C
	2501	-2167	994	-2167	-869	-518	994	-518	-1690	C
	1861	2519	-942	2519	-242	-596	-942	-596	-1682	C
	-1976	-385	494	-385	231	-2942	494	-2942	1784	C
	35	-768	-2768	-768	-1731	1041	-2768	1041	1737	C
	-655	1158	2285	1158	-1061	1914	2285	1914	1760	C
	-1074	-1944	-1078	-1944	1960	2208	-1078	2208	-805	C
	2911	-348	2505	-348	-2028	-175	2505	-175	-798	C
	-467	2318	-1414	2318	1342	-2071	-1414	-2071	-794	C

Table S6. YbL[1] DFT computed harmonic frequencies and corresponding IR intensities.

harmonic frequency (cm^{-1})	IR intensity
37	9
42	7
46	2
51	11
54	2
55	8
96	9
105	3
125	4
142	13
149	3
156	12
158	7
165	36
168	18
180	6
184	8
195	15
197	44
211	21
215	29
226	49
235	43
253	16
267	39
271	1
273	10
279	6
285	11
310	5
310	4
320	2
341	25
352	6
357	6
395	7
406	19
413	9

429	15
441	7
442	5
450	1
458	17
459	8
460	15
478	16
481	16
510	5
513	5
518	4
536	28
553	9
557	5
561	5
604	8
611	7
621	13
642	12
644	13
650	10
690	31
693	52
694	47
751	9
752	10
753	23
789	34
791	29
793	76
800	17
802	17
822	118
824	124
825	91
846	18
871	7
873	2
874	12
878	10
920	9
921	10
953	2
957	2
959	1
977	28
979	14
981	17
1013	25
1018	27
1020	26
1042	3
1042	22
1042	7
1044	6
1045	33
1047	53
1048	28
1052	60
1052	47
1074	41
1077	25
1078	8
1092	22
1095	23
1097	29
1137	63
1148	8
1149	9
1150	10
1160	113
1161	103
1179	1
1203	1
1205	3
1215	2
1217	8
1217	11
1245	12
1246	14
1246	15
1265	11
1267	12
1273	7
1291	32
1295	35
1315	68

1317	79
1321	49
1323	57
1333	36
1333	44
1337	29
1370	2
1378	24
1379	30
1382	69
1401	41
1402	53
1420	30
1423	51
1425	83
1433	419
1435	542
1437	48
1440	331
1441	207
1444	81
1460	26
1464	42
1471	7
1472	12
1475	4
1491	119
1493	120
1496	16
1514	70
1519	93
1520	98
1520	14
1669	86
1670	82
1671	100
1688	430
1689	394
1691	207
1730	797
1731	735
1737	953
3032	60
3034	64
3036	38
3039	60
3047	44
3051	34
3075	23
3075	25
3080	53
3091	25
3105	15
3106	20
3128	4
3129	1
3137	9
3144	31
3148	26
3157	64
3223	4
3223	3
3224	3
3238	1
3238	1
3238	1
3250	1
3252	1
3253	0