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Supporting Information

Role of the Templating Heteroatom on Both Structural and Magnetic Properties of POM-Based SIM Lanthanoid Complexes

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Table S1. SHAPE Calculations for Dy^{III} complexes

Dysprosium (III)														
Coordination Number	CCDC/ICSD	HP-7	HPY-7	PBPY-7	COC-7	CTPR-7	JPBPY-7							
7	DAQJOW	34.407	20.283	5.737	0.799	1.223	9.416							
7	ZIXCER	32.561	20.717	6.159	1.433	0.446	9.113							
7	ZIXCAN	32.216	20.899	6.146	1.215	0.393	9.640							
Coordination Number	CCDC/ICSD	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
8	1908052	30.077	23.943	17.668	11.310	1.236	2.734	16.567	29.582	1.816	0.760	5.135	12.079	25.483
8	VUBLEM	30.687	22.526	14.960	8.251	0.858	1.531	15.602	28.463	2.190	1.832	4.675	9.006	23.629
8	ZIXCIV	32.807	23.444	15.016	10.874	2.695	2.516	13.288	27.921	1.656	0.989	4.497	11.497	22.958
8	KAMQAT	28.753	23.529	17.011	9.760	0.231	2.228	16.643	28.209	2.628	1.814	5.221	10.561	23.751
8	KAMPUM	30.074	23.492	14.112	6.315	0.768	1.967	15.959	29.058	3.420	2.842	5.433	7.083	24.166
8	WACJOC	29.917	22.002	16.572	10.801	0.727	2.030	15.306	28.576	1.876	1.150	4.346	11.426	23.779
8	MUJNOW	27.321	20.273	16.546	16.900	6.524	5.571	12.485	25.498	4.109	2.744	6.438	16.935	21.418
8	ZOFKOW	32.639	22.010	13.414	8.464	1.924	2.051	13.941	26.610	2.631	1.804	4.970	9.231	22.069
8	1964368	27.176	22.946	15.871	8.606	0.262	2.255	15.576	27.890	2.885	2.379	5.121	9.402	23.037
8	MERCOE	31.965	22.014	14.602	8.534	1.422	2.509	15.227	28.333	3.172	2.069	5.991	9.233	23.287
8	DEGCID	32.575	21.781	14.44	8.863	1.499	2.246	15.026	27.832	2.807	1.926	5.328	9.720	23.231
8	AWEPUP	29.737	23.288	14.471	6.92	0.723	2.187	15.479	28.474	3.306	2.83	5.434	7.721	23.388

Table S2. SHAPE Calculations for Er^{III} complexes.

Erbium (III)														
Coordination Number	CCDC/ICSD	HP-7	HPY-7	PBPY-7	COC-7	CTPR-7	JPBPY-7							
7	DAQKAJ	34.074	20.693	5.409	0.854	1.177	9.014							
Coordination Number	CCDC/ICSD	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
8	419267	27.803	23.367	17.257	9.851	0.167	2.526	16.208	27.702	2.83	2.323	5.217	10.649	23.062
8	1908053	32.155	23.754	17.681	11.208	1.619	3.131	15.990	28.523	1.311	1.320	4.597	11.327	25.483
8	VUBLIQ	30.595	22.711	15.711	8.499	0.824	1.703	15.719	27.826	2.197	1.885	4.763	9.224	23.179
8	MECMEP	30.122	23.042	16.457	9.993	0.462	2.270	15.936	28.258	2.000	1.463	4.68	10.657	24.102
8	OGUSUF	32.862	21.521	14.551	8.867	1.540	2.326	15.006	28.165	2.872	2.023	5.519	9.684	23.509
8	WACJUI	29.704	22.081	16.558	10.575	0.613	2.048	15.597	28.640	1.962	1.211	4.631	11.296	23.914
8	ZOFKUC	32.487	21.863	13.574	8.8585	1.853	2.052	13.982	26.612	2.594	1.765	4.968	9.349	22.1
8	1964360	26.745	23.582	16.97	9.642	0.092	2.512	16.606	28.186	2.872	2.26	5.298	10.457	23.278
8	ELIHEN	31.929	22.393	13.971	8.67	1.83	2.233	13.89	26.507	2.558	1.662	5.169	9.45	21.758
8	EYOZUP	31.406	22.069	15.49	9.259	1.111	2.768	15.754	28.059	3.12	2.091	5.934	10	23.309
8	MERCIY	31.776	22.034	14.806	8.735	1.212	2.542	15.434	28.295	3.223	2.131	6.057	9.357	23.356
8	FARDOT	29.76	22.827	14.414	6.964	0.682	2.078	15.188	28.606	3.332	2.827	5.485	7.708	22.933
8	AWEQAW	30.02	23.113	14.048	6.841	0.668	2.096	15.217	28.756	3.416	2.817	5.656	7.654	23.207

Table S3. SHAPE Calculations for Yb^{III} complexes.

Ytterbium (III)														
Coordination Number	CCDC/ICSD	HP-7	HPY-7	PBPY-7	COC-7	CTPR-7	JPBPY-7							
7	RERTEO	31.292	21.666	6.877	1.854	0.492	10.139							
Coordination Number	CCDC/ICSD	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
8	MECMOZ	20.702	23.26	16.098	9.550	0.407	2.229	15.667	28.179	2.098	1.630	4.732	10.239	23.387
8	WACKAP	29.476	21.97	16.327	10.511	0.612	2.115	15.032	28.622	1.728	1.206	4.378	11.141	24.166
8	ELIJIT	31.286	22.441	14.576	9.413	1.737	2.429	13.959	26.24	2.321	1.399	5.08	10.136	21.762
8	ARICAF	32.398	22.436	14.06	8.97	1.842	2.251	13.823	26.671	2.35	1.564	5.017	9.693	22.102
8	249433	28.361	23.109	16.603	9.312	0.174	2.45	16.286	28.689	2.836	2.343	5.28	10,076	23.627
8	RERTEO	32.455	23.169	16.38	11.705	2.61	2.188	13.095	27.188	0.999	1.409	3.406	11.858	24.831
8	AWEQIE	29.94	23.219	14.346	7.03	0.592	2.088	15.403	28.989	3.304	2.766	5.429	7.775	23.477