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Supplementary Materials: Low-Coordinate Dinuclear Dysprosium(III) Single Molecule Magnets Utilizing LiCl as Bridging Moieties and tris(amido)amine as Blocking Ligands

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Table S1. Description and contractions of the basis sets (two models: **S** - smaller, **L** - larger) employed in *ab initio* calculations of the Dy^{III} crystal field.

Basis set "S"	Basis set "L"
Dy.ANO-RCC-VDZP 7S6P4D2F1G	Dy.ANO-RCC-VTZP 8S7P5D3F2G1H
N.ANO-RCC-VDZ 3S2P	N.ANO-RCC-VDZP 3S2P1D (first coordination sphere) N.ANO-RCC-VDZ 3S2P (others)
O.ANO-RCC-VDZ 3S2P	O.ANO-RCC-VDZP 3S2P1D (first coordination sphere) O.ANO-RCC-VDZ 3S2P (others)
C.ANO-RCC-VDZ 3S2P	C.ANO-RCC-VDZ 3S2P
H.ANO-RCC-VDZ 2S	H.ANO-RCC-VDZ 2S
Li.ANO-RCC-VDZ 3S2P	Li.ANO-RCC-VDZ 3S2P
Si.ANO-RCC-VDZ 4S3P	Si.ANO-RCC-VDZ 4S3P
Cl.ANO-RCC-VDZ 4S3P	Cl.ANO-RCC-VDZP 4S3P1D (first coordination sphere) Cl.ANO-RCC-VDZ 4S3P (others)
Y.ANO-RCC-VDZ 6S5P3D	Y.ANO-RCC-VDZ 6S5P3D

Table S2. Summary of the energy splitting of the $^6H_{15/2}$ multiplet of the Dy1A in models: **L**, **S** with pseudo-*g*-tensors of each Kramers doublet and composition in the $|m_J\rangle$ basis of ground state.

Dy1A							
S				L			
Energy and Pseudo-*g*-tensor components (g_x, g_y, g_z) of 8 ground Kramers doublets							
Energy / cm^{-1}	Pseudo-*g*-tensor components			Energy / cm^{-1}	Pseudo-*g*-tensor components		
	g_x	g_y	g_z		g_x	g_y	g_z
0.000	0.0356	0.0767	19.0362	0.000	0.0282	0.0585	19.1373
124.009	0.3035	0.3625	15.8555	134.526	0.2553	0.3123	15.9039
253.409	1.4756	1.7296	13.2025	265.345	1.2463	1.4956	13.3187
357.379	3.2102	4.5264	10.2251	364.811	2.8686	4.0283	10.7887

451.222	3.2026	4.1248	10.9229	451.974	3.5257	4.4375	10.7066
566.117	1.2060	1.4777	13.9296	562.193	1.4393	1.6907	13.9177
698.965	0.3354	0.3998	16.3988	697.537	0.2709	0.4738	16.0279
788.316	0.0794	0.1930	19.1586	771.161	0.1225	0.3402	18.778
Composition of the ground Kramers doublet in the $\|m_J\rangle$ basis on the quantization axis within J = 15/2 manifold (only contributions above 0.1%)							
	82.7% $\|+\mathbf{15/2}\rangle$ 11.8% $\|+\mathbf{11/2}\rangle$ 3.2 % $\|-\mathbf{15/2}\rangle$ 1.0% $\|+\mathbf{7/2}\rangle$ 0.5% $\|-\mathbf{11/2}\rangle$ 0.3% $\|+\mathbf{9/2}\rangle$ 0.3% $\|+\mathbf{13/2}\rangle$				87.4% $\|+\mathbf{15/2}\rangle$ 11.1% $\|+\mathbf{11/2}\rangle$ 0.8% $\|+\mathbf{7/2}\rangle$ 0.3% $\|+\mathbf{9/2}\rangle$ 0.2% $\|+\mathbf{13/2}\rangle$		

Table S3. Summary of the energy splitting of the $^6H_{15/2}$ multiplet of the Dy1B in models: **L**, **S** with pseudo-*g*-tensors of each Kramers doublet and composition in the $|m_J\rangle$ basis of ground state.

Dy1B							
S				**L**			
Energy and Pseudo-*g*-tensor components (g_x, g_y, g_z) of 8 ground Kramers doublets							
Energy / cm^{-1}	**Pseudo-*g*-tensor components**			**Energy / cm^{-1}**	**Pseudo-*g*-tensor components**		
	g_x	g_y	g_z		g_x	g_y	g_z
0.000	0.0356	0.0762	19.0682	0.000	0.0279	0.0573	19.1709
121.383	0.3313	0.3984	16.0509	133.544	0.2873	0.3620	16.0444
242.221	1.5270	1.7894	13.1814	255.379	1.3586	1.6178	13.2410
342.243	3.0786	4.5987	10.3340	350.990	2.8127	4.2071	10.8107
429.902	3.0786	4.1894	11.0697	432.177	3.3182	4.3954	10.9957
536.231	1.2583	1.6053	13.7579	535.078	1.4303	1.7630	13.8052
654.832	0.4063	0.4660	16.7362	658.831	0.3844	0.4847	16.2977
757.531	0.0604	0.1354	19.3847	738.753	0.1045	0.2723	19.0061
Composition of the ground Kramers doublet in the $\|m_J\rangle$ basis on the quantization axis within J = 15/2 manifold (only contributions above 0.1%)							
	74.1% $\|+\mathbf{15/2}\rangle$ 12.7% $\|-\mathbf{15/2}\rangle$ 9.3% $\|+\mathbf{11/2}\rangle$ 1.6% $\|-\mathbf{11/2}\rangle$ 0.9% $\|+\mathbf{7/2}\rangle$ 0.5% $\|+\mathbf{9/2}\rangle$ 0.3% $\|+\mathbf{13/2}\rangle$ 0.2% $\|-\mathbf{7/2}\rangle$				76.8% $\|+\mathbf{15/2}\rangle$ 11.5% $\|-\mathbf{15/2}\rangle$ 8.5% $\|+\mathbf{11/2}\rangle$ 1.3% $\|-\mathbf{11/2}\rangle$ 0.8% $\|+\mathbf{7/2}\rangle$ 0.5% $\|+\mathbf{9/2}\rangle$ 0.3% $\|+\mathbf{13/2}\rangle$		