Supplementary Materials

Lanthanide-Radical Magnetic Coupling in $[LnPc_2]^0$: Competing Exchange Mechanisms Captured via Ab Initio Multi-Reference Calculations

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GEOMETRY OF $[LNPZ_2]^0$ MOLECULES

Table S1. Cartesian coordinates (Å) of the D_{4d} symmetry unique atoms in $[LnPz_2]^0$.

D_{4d}-$[LnPz_2]^0$	X	Y	Z
Ln	0.00000	0.00000	0.00000
N	1.96363	0.00000	1.39550
N	2.39530	2.39530	1.56000
C	2.77855	1.10129	1.53290
C	4.17999	0.70300	1.66060
H	4.99972	1.32549	1.73529

CASSCF/RASSI–SO ENERGIES OF $[LNPZ_2]^0$

Table S2. CASSCF/RASSI–SO energy levels (cm^{-1}) of $[LnPz_2]^0$.

	$[TbPz_2]^0$	$[DyPz_2]^0$	$[HoPz_2]^0$	$[ErPz_2]^0$
	0.00	0.00	0.00	0.00
	0.00	0.00	0.00	0.98
	6.09	3.88	3.33	0.98
	6.09	3.88	3.33	2.20
	325.82	86.40	24.99	62.09
	325.82	86.40	24.99	62.09
	330.53	91.27	26.95	62.48
	330.53	91.27	26.95	62.48
	554.47	110.01	48.31	161.59
	554.47	110.01	48.31	161.59
	558.03	113.27	50.94	162.38
	558.03	113.27	50.94	162.38
	...	...	...	...
	g-factors of the two lowest doublets			
	0.00	0.00	0.00	
1	0.00	0.00	0.00	-
	20.00	19.36	21.97	
	0.00	0.00	0.00	
2	0.00	0.00	0.00	-
	16.00	15.35	17.97	