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Supporting Information

Physical Stimuli and Chemical Modulations for Bistable Molecular Magnetic Materials

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1. Hysteresis Loop Measurement information of the aforementioned SMMs

Table S1 Hysteresis Loop Measurement information of the aforementioned SMMs.

Name[b]	Hysteresis T_{hy} [K]	Sweep Rate [mT s^{-1}]	Reference
$[Zn_2Dy(TTTT^{Br})_2(MeOH)]^+$	11	20	1
$[Zn_2Dy(TTTT^{Cl})_2(Me_2CO)](NO_3)$	14	20	2
$[Zn_2Dy(TTTT^{Cl})_2(MeOH)](CF_3SO_3)$	12	20	2
$[Zn_2Dy(TTTT^{Cl})_2(Me_2CO)](BPh_4)$	23	20	2
$[Zn_2Dy(TTTT^{Cl})_2(DMF)](BPh_4)$	22	20	2
$[Zn_2Dy(TTTT^{Cl})_2(NMP)](BPh_4)$	24	20	2
$[Dy(Cy_3PO)_2(H_2O)_5]Cl_3$	11	20	3
$[Dy(Cy_3PO)_2(H_2O)_5]Br_3$	20	20	3
$[Dy(^tBuPO(NH^iPr)_2)_2(H_2O)_5][I_3]$	12	1.8	4
$[Dy(HMPA)_2(H_2O)_5]Cl_3$	9 (diluted sample)	4	5
$[Dy(HMPA)_2(H_2O)_5]I_3$	9 (diluted sample)	4	5
$[Dy(Cy_3PO)_2(H_2O)_5](CF_3SO_3)_3$	2 (butterfly shaped)	1.8	6
$[Dy(O^tBu)_2(py)_5]^+$	8.8 (butterfly shaped)	1.2	7
$[Dy(L^a)_2(py)_5]^+$	22	1	8
[Dy(bbpen)Cl]	8	20	9
[Dy(bbpen)Br]	14	20	9
[Dy(bbpen-CH_3)Cl]	6	20	10
[Dy(bbpen-CH_3)Br]	15	20	10
$[Dy(bbpen)(tpo)_2]^+$	6	20	11
$[Dy_2(bbpen)_2\{Fe(CN)_6\}]^-$	2 (butterfly shaped)	20	12
$[Dy_2(bbpen)_2\{Co(CN)_6\}]^-$	15	20	12
$[(Cp^{ttt})_2Dy]^+$	60	3.9 (Ref. 13); 2.2(9) (Ref. 14)	13, 14

$[(Cp^{ipr4})_2Dy]^+$	32	3.1	15
$[(Cp^{ipr4Me})_2Dy]^+$	72	3.1	15
$[(Cp^{ipr4Et})_2Dy]^+$	66	3.1	15
$[(Cp^{ipr5})_2Dy]^+$	66	3.1	15
$[(Cp^{iPr5})Dy(Cp^*)]$	80	2.5	16

Abbreviations: H_3TTTT^{Br} = 2,2',2''-(((nitrilotris(ethane-2,1-diyl))tris(azanediyl))tris (methylene)) tris-(4-bromophenol); H_3TTTT^{Cl} = 2,2',2''-(((nitrilotris(ethane-2,1-diyl))tris(azanediyl))tris (methylene))tris(4-chlorophenol); DMF = N,N-Dimethylformamide; NMP = 1-Methyl-2-pyrrolidinone; Cy_3PO = tricyclohexylpho-sphine oxide; HMPA = hexamethylphosphoramide; HL^a = (S)-(-)-1-phenylethanol; H_2bbpen = N,N'-bis(2-hydroxybenzyl)-N,N'-bis(2-methylpyridyl)ethylenediamine); tpo = triphenyl phosphine oxide; Cp^{ttt} = 1,2,4-tri(tertbutyl)cyclopentadienide; Cp^{iPr5} = pentaisopropylcyclopentadienyl; Cp* = pentamethylcyclopentadienyl. [b] Lattice solvent/uncoordinated molecules and counterions are not listed whenever it would not cause misunderstanding.

2. Spin transition temperatures (K), hysteresis widths ΔT (K) for selected SCO materials

Table S2 Spin transition temperatures (K), hysteresis widths *Δ*T (K) for selected SCO materials.

Name	$T_{1/2}\downarrow$ [K]	$T_{1/2}\uparrow$ [K]	*Δ*T [K]	Reference
$[Fe^{II}(MebptH)_2(AgCN)_2]$	232	235	3	17
$[Fe^{II}(bpztH)_2(AgCN)_2]$	286	292	6	17
$[Fe(3\text{-}NH_2py)_2Ni(CN)_4]$	148	173	25	18
$[Fe(3\text{-}NH_2py)_2Pd(CN)_4]$	169	206	37	18
$[Fe(3\text{-}NH_2py)_2Pt(CN)_4]$	183	213	30	18
$\{Fe(3\text{-}Fpy)_2[Ni(CN)_4]\}$	206.5	233.0	26.5	19
$\{Fe(3\text{-}Fpy)_2[Pd(CN)_4]\}$	216.5	243.3	26.8	19
$\{Fe(3\text{-}Fpy)_2[Pt(CN)_4]\}$	212.2	239.3	27.1	19
$\{Fe(3\text{-}Clpy)_2[Pt(CN)_4]\}$	141.7	161.0	19.3	19
$[Fe(bipydz)(Au(CN)_2)_2]$` (**2**` in the paper)	273	277	4	20
$[Fe^{II}(bztrz)_2(Pd^{II}(CN)_4)]\cdot(H_2O,EtOH)$	135	154	19	21
$[Fe^{II}(bztrz)_2(Pd^{II}(CN)_4)]\cdot(3H_2O)$	118; 148	140; 166	22; 18	21
$[Fe(dpb)\{Au(CN)_2\}_2]\cdot(1.5)C_6H_{12}$	136	142	6	22
$[Fe(dpb)\{Au(CN)_2\}_2]$ (Desolvated Sample)	110	119	9	22
$[Fe(dpb)\{Au(CN)_2\}_2]\cdot(0.9)$Benzene	139; 207	144; 221	5; 14	22
$[Fe(dpb)\{Au(CN)_2\}_2]\cdot(0.7)$Naphthalene	141	214	73	22
$[Fe(dpb)\{Au(CN)_2\}_2]\cdot(0.3)$Anthracene	131	151	20	22
$[Fe(dpb)\{Au(CN)_2\}_2]\cdot(0.4)$Ferrocene	129	166	37	22
$[Fe(dpb)\{Au(CN)_2\}_2]\cdot(1.4)CS_2$	167	190	23	22
$[Fe(dpoda)\{Ag(CN)_2\}_2]\cdot(1.5)$naph	181; 190; 228	187; 194; 232	5; 4; 3	23

Abbreviations: MebptH = 3-(3-methyl-2-pyridyl)-5-(2-pyridyl)-1,2,4-triazole; bpztH = 3,5-bis(pyrazin-2-yl)-1,2,4-triazole; 3-NH_2py = 3-aminopyridine; bipydz = 3,6-bis(4-pyridyl)-1,2,4,5-

tetrazine; bztrz = (E)-1-phenyl-N-(1,2,4-triazol-4-yl)-methanimine; dpb = 1,4-di(pyridin-4-yl)benzene; dpoda = 2,5-di-(pyridyl)-1,3,4-oxadiazole.

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