

## The role of coordinated solvent on Co(II) ions in tuning the single molecule magnet properties in a $\{\text{Co}^{\text{II}}_2\text{Dy}^{\text{III}}_2\}$ system

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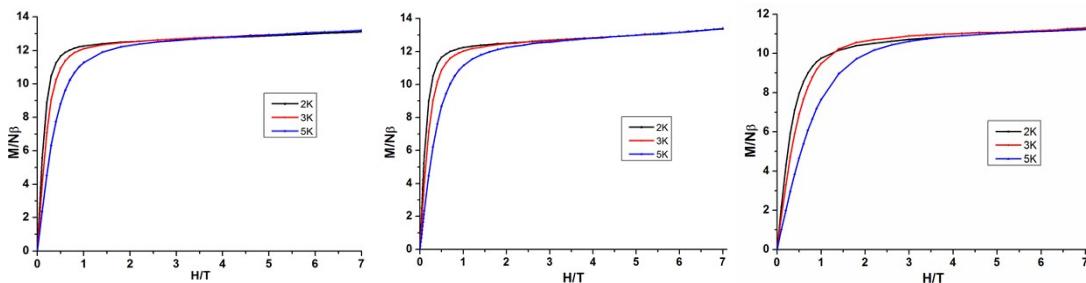
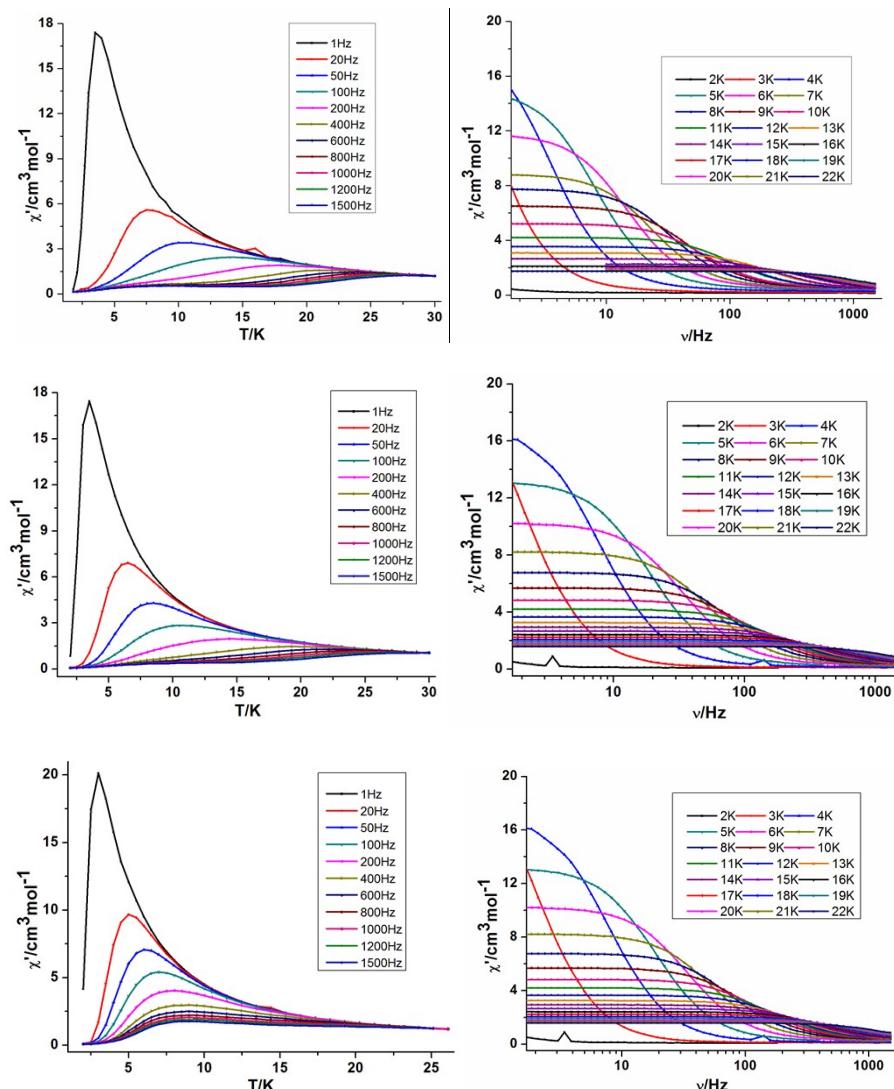
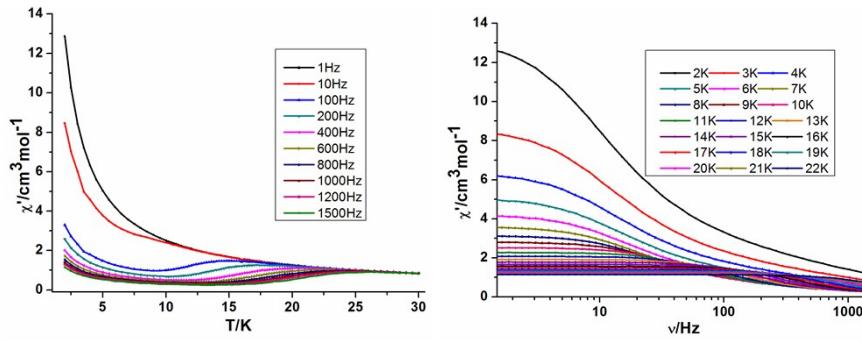
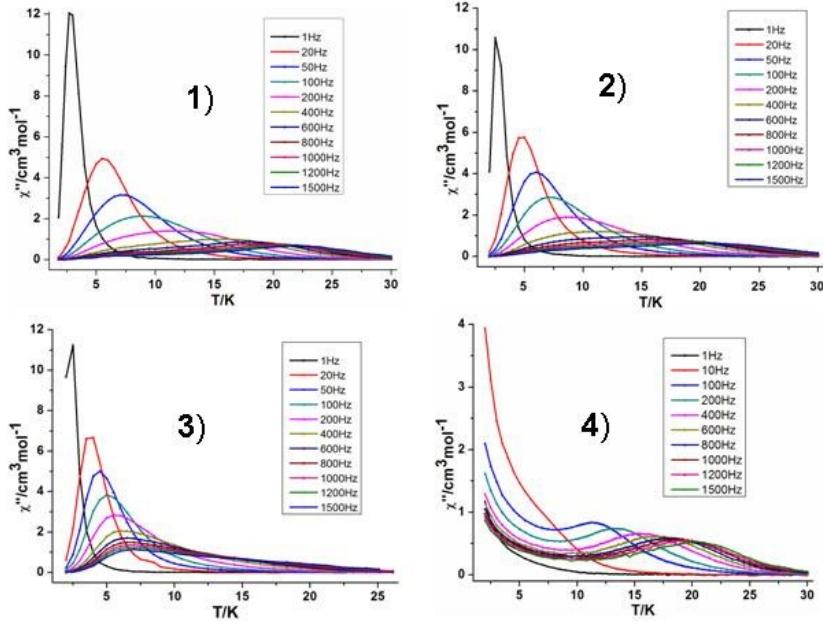


Fig S1 Plots of  $M$  vs  $H$  of 2-4 (left to right)

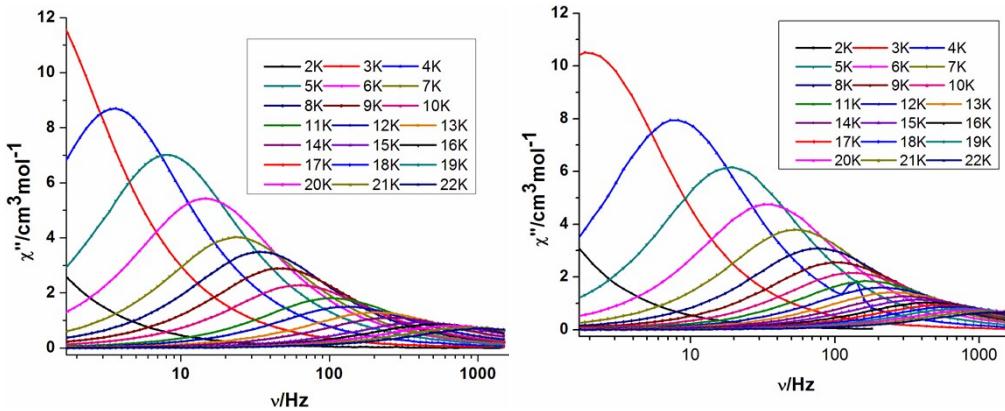


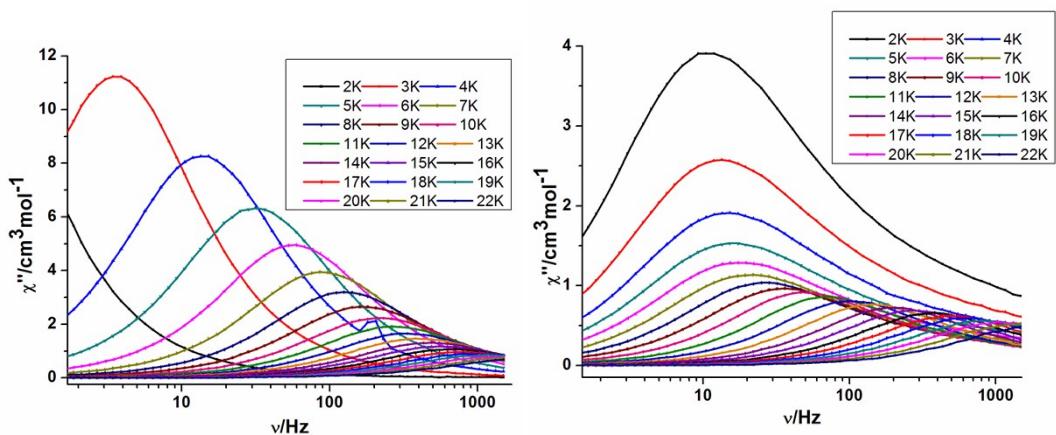


**Fig S2** Plots of  $\chi'$  vs  $T$  (left) and frequency (right) of 1-4 (up to down).

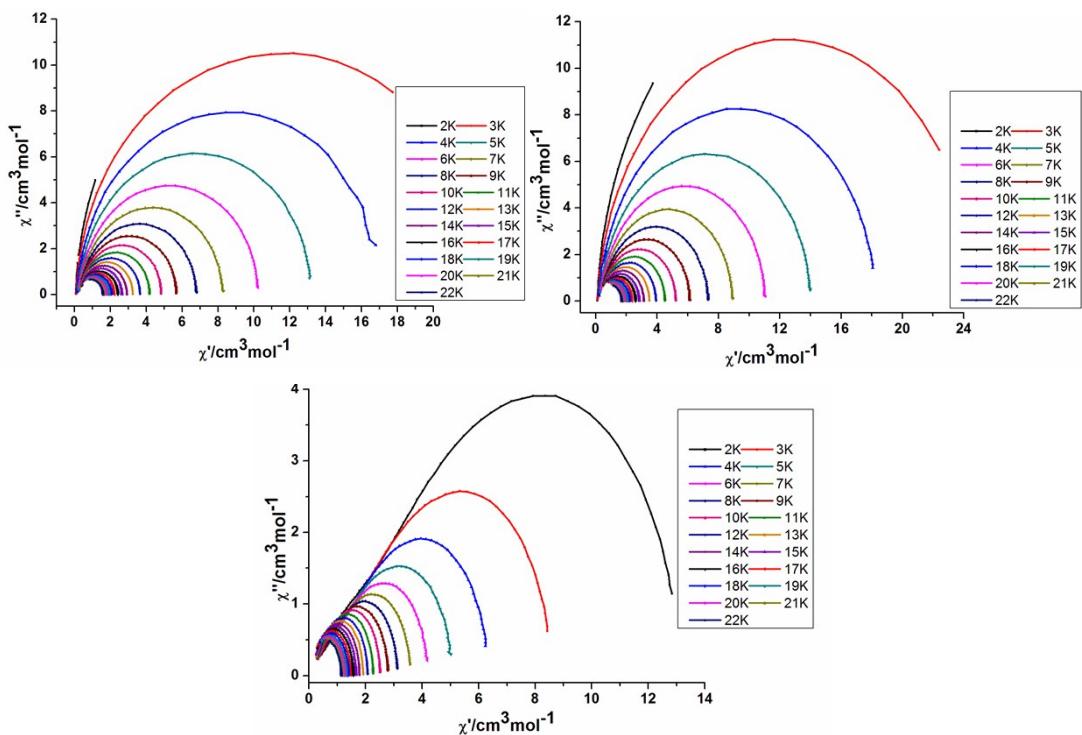


**Fig S3** Plots of  $\chi''$  vs  $T$  at indicated frequencies for complexes 1-4





**Fig S4** Plots of  $\chi''$  vs frequencies at indicated temperatures of compounds **1** (upper left), **2** (upper right), **3** (lower left) and **4** (lower right)



**Fig S5** Cole-Cole plots of **2** (upper left), **3** (upper right) and **4** (lower) from 2-22K

**Table S1** Analysis of Cole-Cole plots of complexes **2** and **3**

	T(K)	$\chi_0$ (cm <sup>3</sup> /mol)	$\chi_{\text{inf}}$ (cm <sup>3</sup> /mol)	$\alpha$	R <sup>2</sup>
<b>2</b>	5	13.2341(4)	0.02351(4)	0.0358(1)	0.98994
	6	10.2565(1)	0.2656(6)	0.03146(2)	0.99871
	7	8.2504(8)	0.2990(9)	0.02834(2)	0.99703
	8	6.7893(9)	0.3516(9)	0.02243(3)	0.99583
	9	5.6942(1)	0.3469(1)	0.02587(4)	0.99590
	10	4.8444(5)	0.3577(8)	0.02042(4)	0.99383
	12	3.6603(3)	0.3547(1)	0.01902(1)	0.99870
	13	3.2585(1)	0.3470(4)	0.01469(2)	0.99878
	15	2.6544(5)	0.3140(6)	0.01961(2)	0.99832
	16	2.4215(5)	0.3212(9)	0.01071(1)	0.99522
	18	0.3091(2)	2.0600(3)	0.0033(4)	0.99628
<b>3</b>	5	14.0491(1)	0.2495(7)	0.05252(1)	0.99856
	6	11.0703(3)	0.3074(8)	0.05085(3)	0.99712
	7	8.9275(5)	0.3500(1)	0.05214 (4)	0.99478
	8	7.3391(2)	0.38473(3)	0.04808(3)	0.99697
	9	6.1290(9)	0.4199(6)	0.03563(6)	0.99035
	10	5.2294(1)	0.4172(4)	0.03948(2)	0.99824
	12	3.9351(6)	0.4160(2)	0.03177(2)	0.99807
	13	3.5021(1)	0.3942(8)	0.03298(3)	0.99815
	15	2.8438(3)	0.3869(5)	0.02356(4)	0.99743
	16	2.5902(4)	0.3756(1)	0.01681(4)	0.99657
	18	2.1979(1)	0.3433(5)	0.01696(4)	0.99667

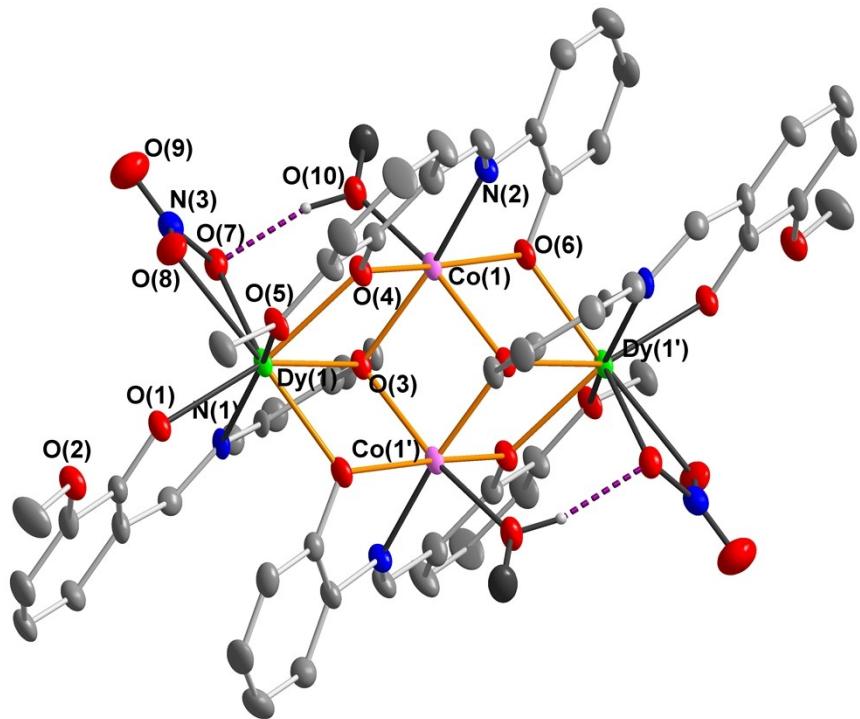
**Table S2** Continuous Shape Measurement calculation for metal ions in complexes **1-4**

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>
Co <sup>II</sup> (OC)	1.60	1.78	2.04	1.86
Co <sup>II</sup> (TPR)	10.46	9.79	8.92	9.64
OP	32.21	33.07	31.86	32.86
HPY	20.44	22.40	20.10	23.03
HBPY	14.90	15.64	15.64	15.44
CU	11.24	11.28	13.64	11.50
SAPR	3.82	2.94	4.90	3.04
TDD	2.87	2.90	2.85	2.40
JGBF	13.17	13.31	12.38	12.54
JETBPY	25.32	26.26	25.00	28.02
JBTPR	3.52	2.98	4.03	2.73
BTPR	3.25	2.60	3.83	2.31
JSD	3.96	4.36	3.96	3.59
TT	11.86	11.96	14.17	12.11

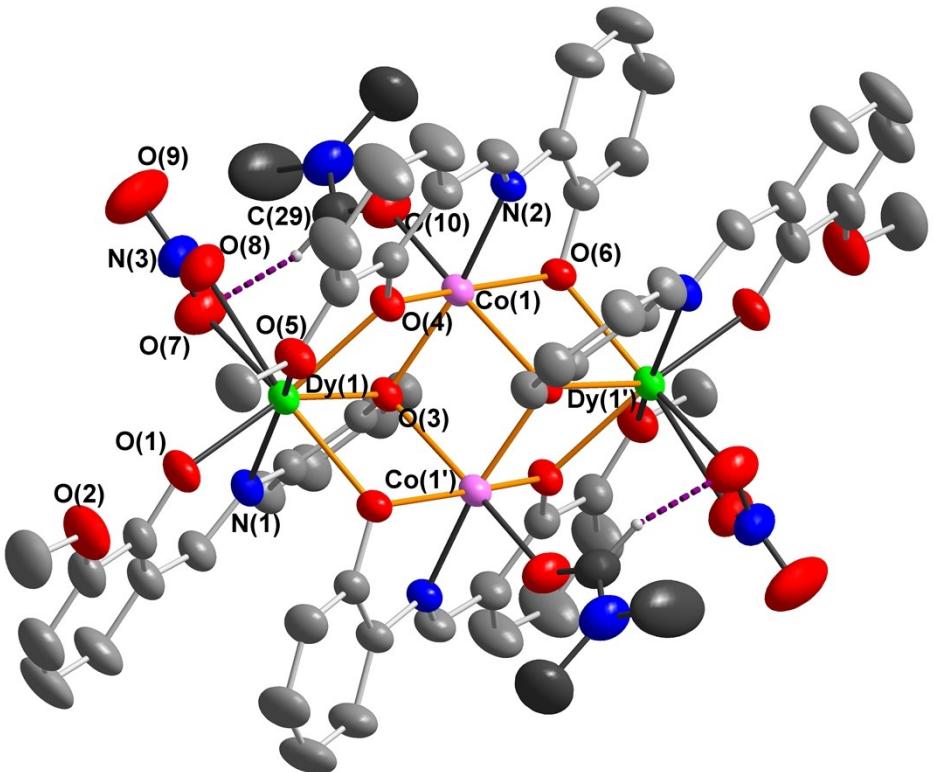
ETBPY	22.44	23.52	21.41	24.23
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Ideal structures, ML6: OC, Oh, Octahedron; TPR, D3h, Trigonal prism.

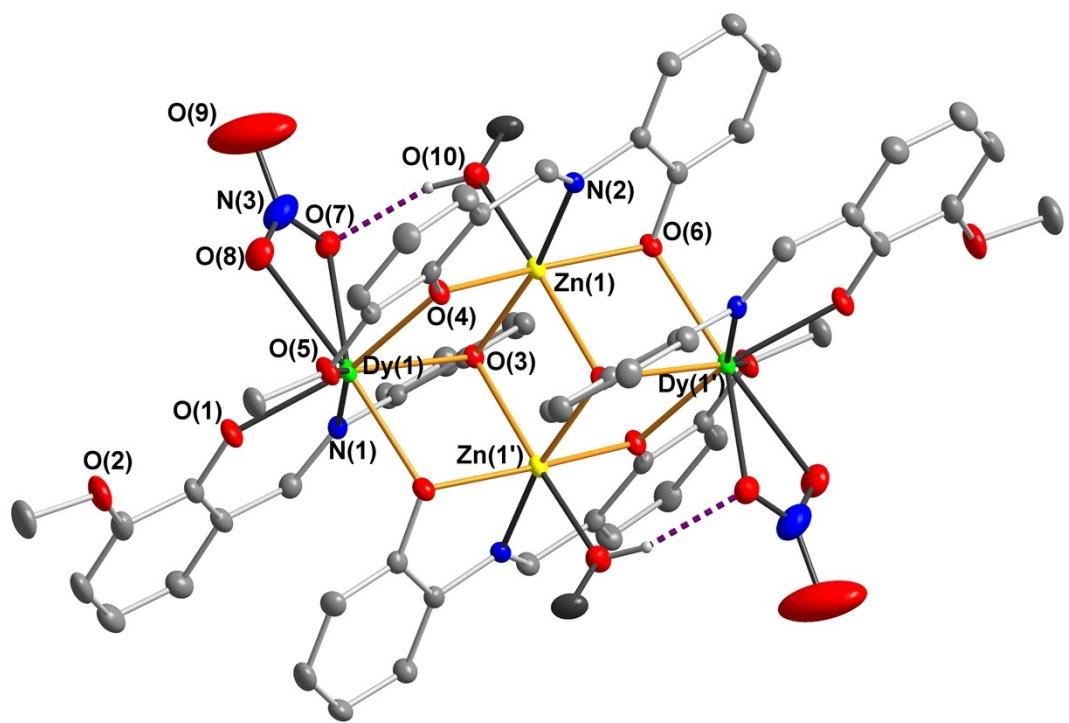
Ideal structures, ML8: OP, D8h, Octagon; HPY, C7v, Heptagonal pyramid ;HBPY, D6h, Hexagonal bipyramid; CU, Oh, Cube; SAPR, D4d, Square antiprism; TDD,D2d, Triangular dodecahedron; JGBF, D2d, Johnson gyrobifastigium J26; JETBPY, D3h, Johnson elongated triangular bipyramid J14; JBTPR, C2v, Biaugmented trigonal prism J50;BTPR, C2v, Biaugmented trigonal prism; JSD, D2d, Snub diphenoид J84; TT, Td, Triakis tetrahedron; ETBPY, D3h, Elongated trigonal bipyramid



**Fig S7** 50% thermal ellipsoid plot of the  $[Co_2Dy_2(L)_4(No_3)_2(MeOH)_2]$  cluster in 2



**Fig S8** 50% thermal ellipsoid plot of the  $[Co_2Dy_2(L)_4(No_3)_2(DMF)_2]$  cluster in 3



**Fig S9** 50% thermal ellipsoid plot of the  $[\text{Zn}_2\text{Dy}_2(\text{L})_4(\text{NO}_3)_2(\text{MeOH})_2]$  cluster in 4