

## Supplementary Materials

for

### A Mixed Valence $\text{Co}^{\text{II}}\text{Co}^{\text{III}}_2$ Field Supported Single Molecule Magnet: Solvent Dependent Structural Variation

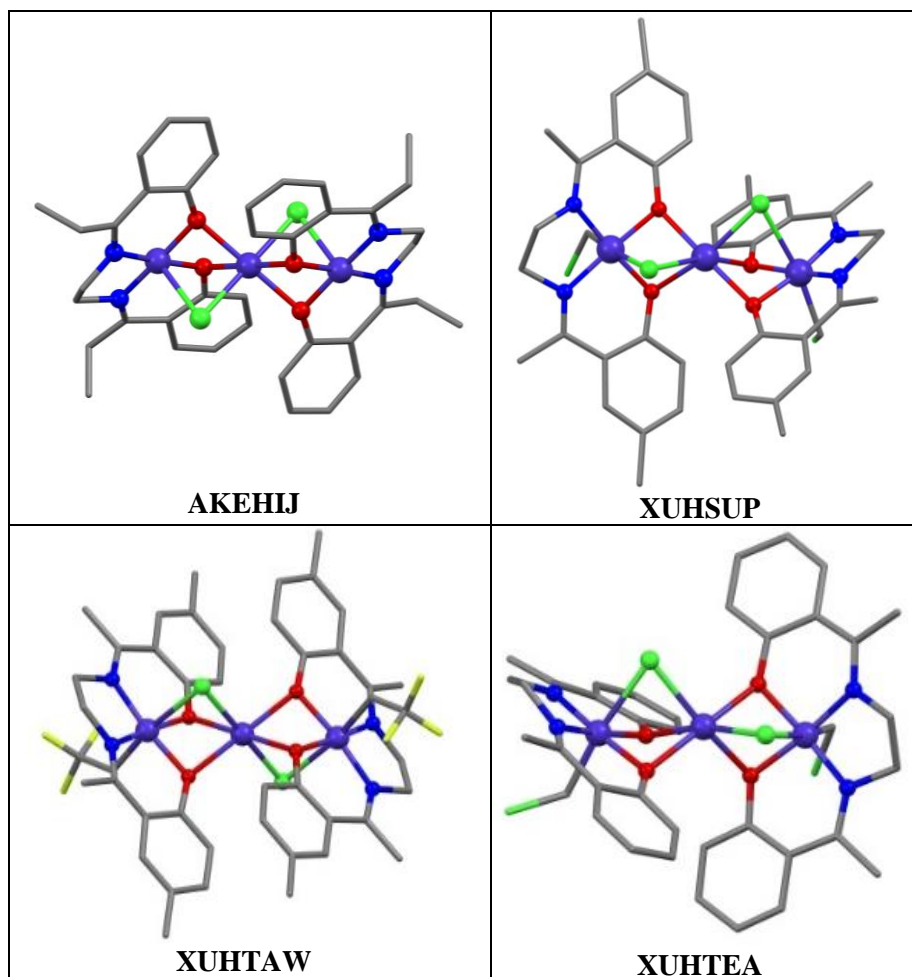
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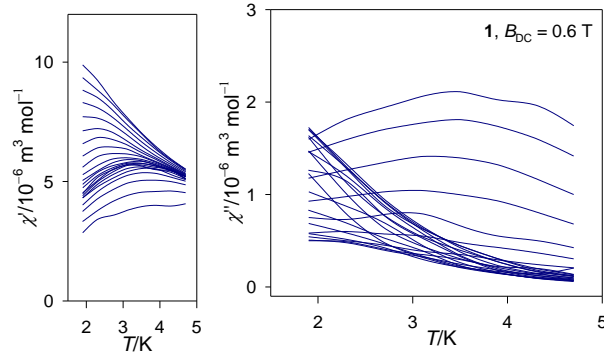
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**Figure S1.** Trinuclear cobalt compounds containing compartmental salen type Schiff base ligands [57-59]. Compounds are presented with their corresponding CCDC reference codes.

The real and imaginary components of the AC susceptibility in terms of the extended two-set Debye model

$$\begin{aligned}\chi'(\omega) &= \chi_s + (\chi_{T1} - \chi_s) \frac{1 + (\omega\tau_1)^{1-\alpha_1} \sin(\pi\alpha_1/2)}{1 + 2(\omega\tau_1)^{1-\alpha_1} \sin(\pi\alpha_1/2) + (\omega\tau_1)^{2-2\alpha_1}} \\ &\quad + (\chi_{T2} - \chi_{T1}) \frac{1 + (\omega\tau_2)^{1-\alpha_2} \sin(\pi\alpha_2/2)}{1 + 2(\omega\tau_2)^{1-\alpha_2} \sin(\pi\alpha_2/2) + (\omega\tau_2)^{2-2\alpha_2}} + \dots \\ \chi''(\omega) &= (\chi_{T1} - \chi_s) \frac{(\omega\tau_1)^{1-\alpha_1} \cos(\pi\alpha_1/2)}{1 + 2(\omega\tau_1)^{1-\alpha_1} \sin(\pi\alpha_1/2) + (\omega\tau_1)^{2-2\alpha_1}} \\ &\quad + (\chi_{T2} - \chi_{T1}) \frac{(\omega\tau_2)^{1-\alpha_2} \cos(\pi\alpha_2/2)}{1 + 2(\omega\tau_2)^{1-\alpha_2} \sin(\pi\alpha_2/2) + (\omega\tau_2)^{2-2\alpha_2}} + \dots\end{aligned}$$



**Figure S2.** Temperature dependence of the AC susceptibility components of **1** for frequencies  $f = 0.1 - 1500$  Hz at  $B_{DC} = 0.6$  T.

**Table S1.** Crystallographic data of **1** at 150 and 298 K.

<i>T</i> /K	150(2)	298(2)
Formula	C <sub>47</sub> H <sub>46</sub> Cl <sub>2</sub> Co <sub>3</sub> N <sub>4</sub> O <sub>6</sub>	C <sub>47</sub> H <sub>46</sub> Cl <sub>2</sub> Co <sub>3</sub> N <sub>4</sub> O <sub>6</sub>
FW	1010.57	1010.57
Crystal system	Orthorhombic	Orthorhombic
Space group	<i>Pbca</i>	<i>Pbca</i>
<i>a</i> /Å	13.4175(13)	13.4805(11)
<i>b</i> /Å	23.569(2)	23.6077(19)
<i>c</i> /Å	27.469(3)	27.937(2)
$\alpha / \beta / \gamma / ^\circ$	90.00	90.00
<i>V</i> /Å <sup>3</sup>	8686.8(15)	8890.9(13)
<i>Z</i>	8	8
$\theta / ^\circ$	2.277 – 27.192	2.259 – 25.731
$\mu$ (Mo K $\alpha$ )/mm <sup>−1</sup>	1.310	1.280
$\rho_{\text{calcd}}$ /g cm <sup>−3</sup>	1.545	1.510
<i>F</i> (000)	4152	4152
Index ranges	−16 < <i>h</i> < 17	−16 < <i>h</i> < 16
	−30 < <i>k</i> < 30	−28 < <i>k</i> < 25
	−35 < <i>l</i> < 35	−34 < <i>l</i> < 34
Rfs. collected	160792	103125
Rfs. unique/observed	9648 / 7976	8440 / 6608
<i>R</i> <sub>int</sub>	0.0561	0.0948
<i>R</i> <sub>1</sub> <sup>a</sup> / <i>wR</i> <sub>2</sub> <sup>b</sup> [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )]	0.0334 / 0.0789	0.0559 / 0.1076
<i>R</i> <sub>1</sub> <sup>a</sup> / <i>wR</i> <sub>2</sub> <sup>b</sup> [for all <i>F</i> <sub>o</sub> <sup>2</sup> ]	0.0480 / 0.0894	0.0781 / 0.1147
GOF on <i>F</i> <sup>2</sup>	1.096	1.124