

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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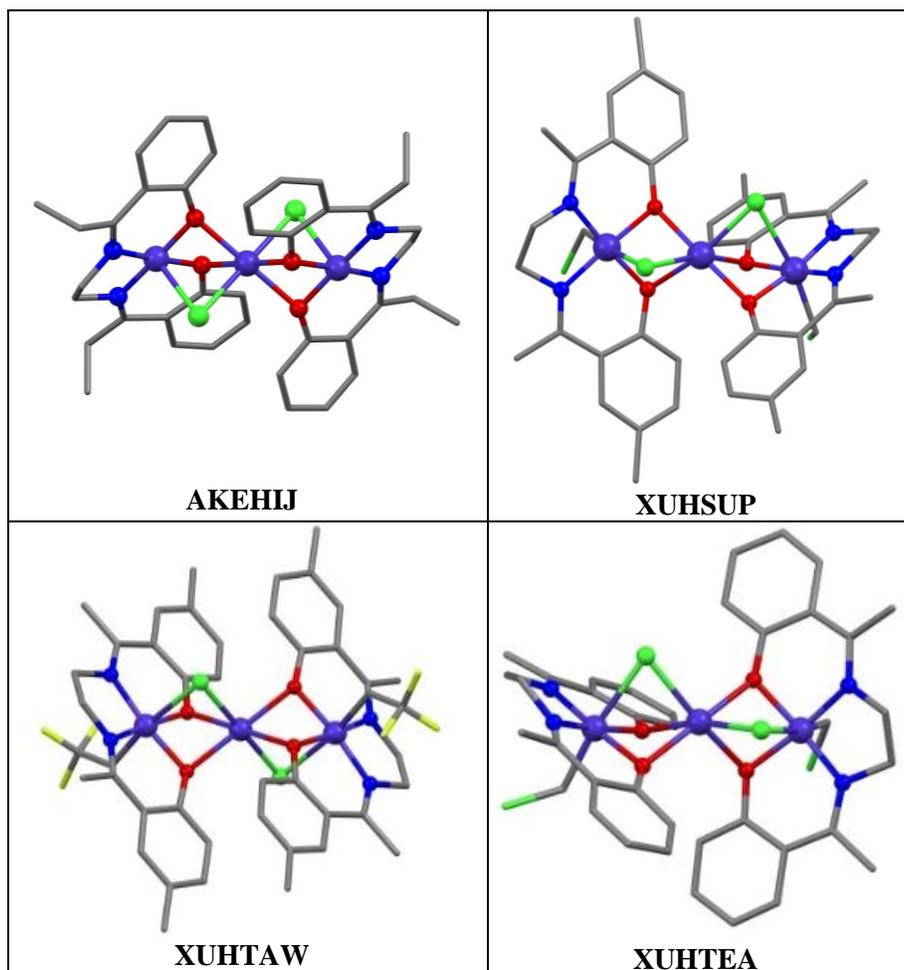


Figure S1. Trinuclear cobalt compounds containing compartmental salen type Schiff base ligands [57-59]. Compounds are presented with their corresponding CCDC reference codes.

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

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

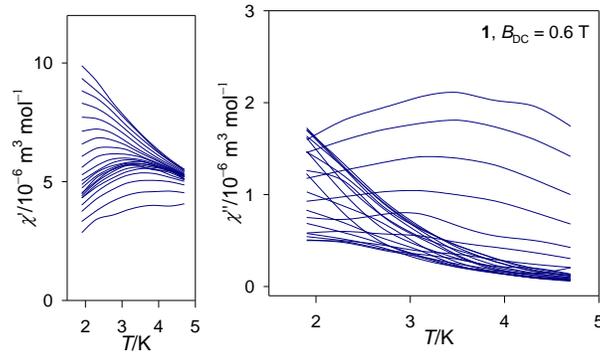


Figure S2. Temperature dependence of the AC susceptibility components of **1** for frequencies $f = 0.1 - 1500$ Hz at $B_{DC} = 0.6$ T.

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

<i>T</i> /K	150(2)	298(2)
Formula	C ₄₇ H ₄₆ Cl ₂ Co ₃ N ₄ O ₆	C ₄₇ H ₄₆ Cl ₂ Co ₃ N ₄ O ₆
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 ³	8686.8(15)	8890.9(13)
<i>Z</i>	8	8
$\theta / ^\circ$	2.277 – 27.192	2.259 – 25.731
μ (Mo K α)/mm ⁻¹	1.310	1.280
ρ_{calcd} /g cm ⁻³	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> _{int}	0.0561	0.0948
<i>R</i> ₁ ^a / <i>wR</i> ₂ ^b [<i>I</i> > 2 σ (<i>I</i>)]	0.0334 / 0.0789	0.0559 / 0.1076
<i>R</i> ₁ ^a / <i>wR</i> ₂ ^b [for all <i>F</i> _o ²]	0.0480 / 0.0894	0.0781 / 0.1147
GOF on <i>F</i> ²	1.096	1.124