

Supporting information

Synthesis, structural characterization and electrochemical and magnetic studies of $M(\text{hfac})_2$ ($M = \text{Cu}^{\text{II}}, \text{Co}^{\text{II}}$) and $\text{Nd}(\text{hfac})_3$ complexes of 4-amino-TEMPO

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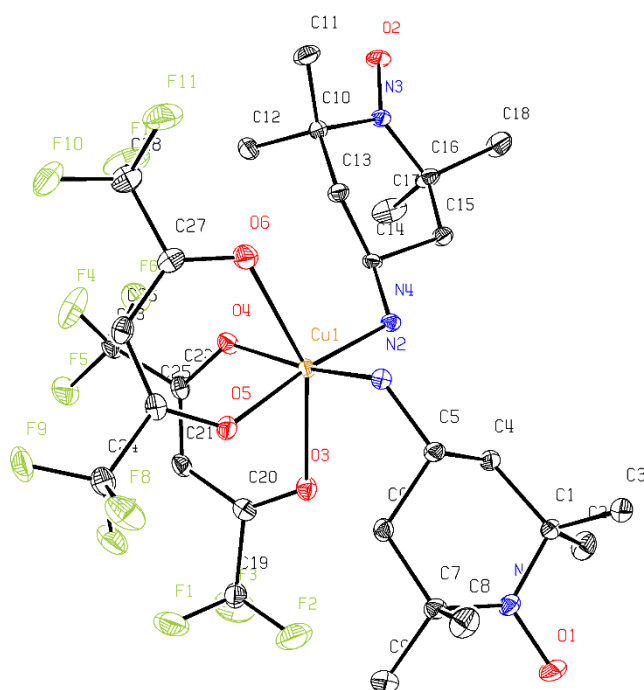


Figure S1. Asymmetric unit of **11** (thermal ellipsoids shown at 50% probability) including atomic numbering. Hydrogen atoms have been omitted for clarity.

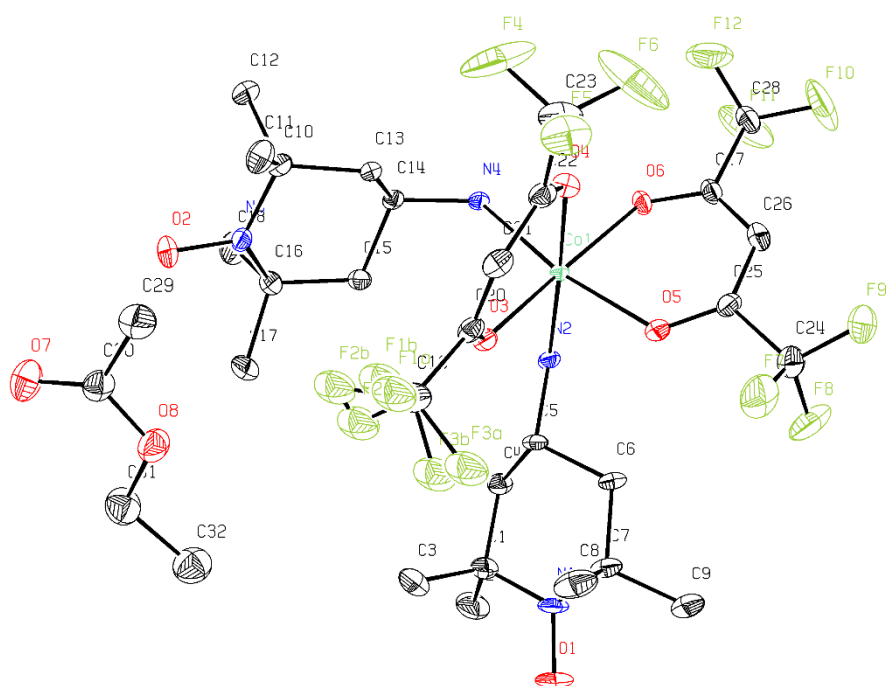


Figure S2. Asymmetric unit of **12** (thermal ellipsoids shown at 50% probability) including atomic numbering. Hydrogen atoms have been omitted for clarity.

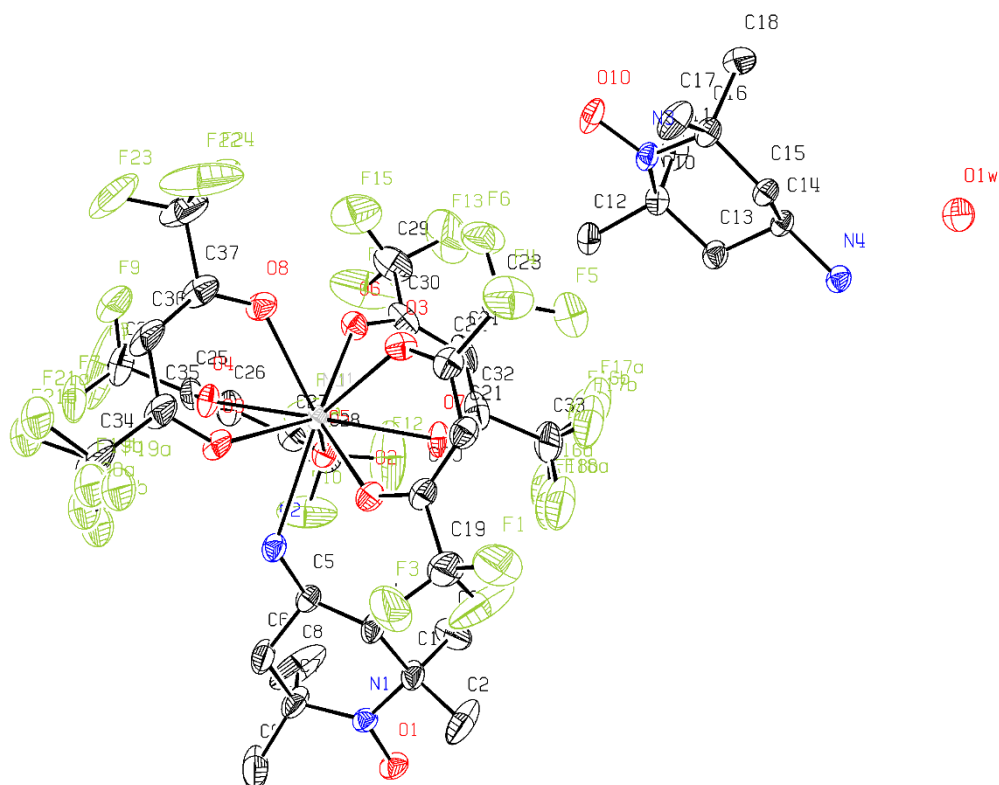


Figure S3. Asymmetric unit of **13** (thermal ellipsoids shown at 50% probability) including atomic numbering. Hydrogen atoms have been omitted for clarity.

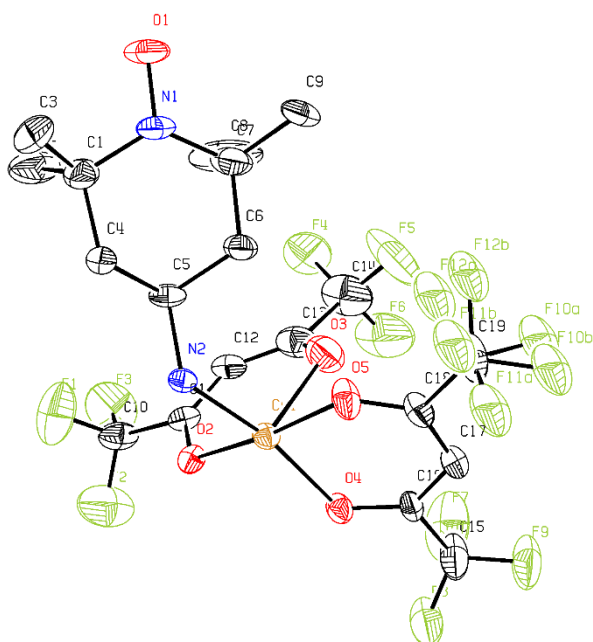


Figure S4. Asymmetric unit of **14** (thermal ellipsoids shown at 30% probability) including atomic numbering. Hydrogen atoms have been omitted for clarity.

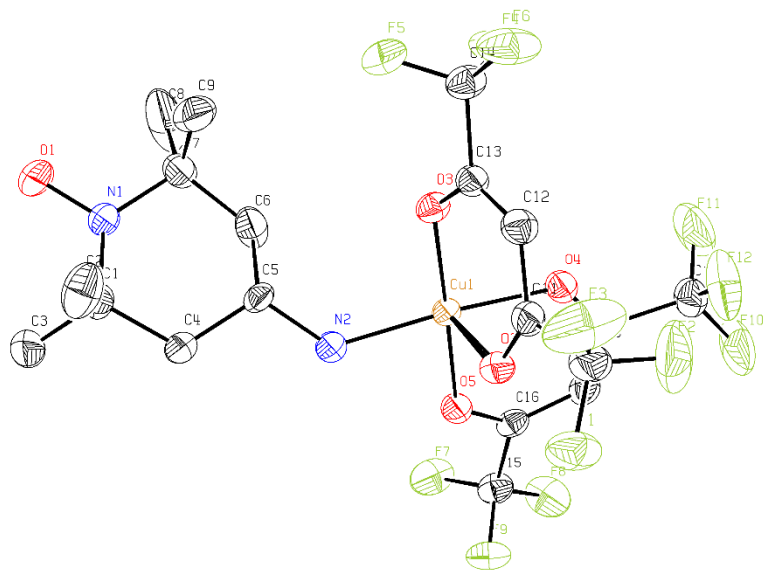


Figure S5. Asymmetric unit of **15** (thermal ellipsoids shown at 50% probability) including atomic numbering. Hydrogen atoms have been omitted for clarity.

Table S1. Hydrogen-bond geometry in **11-15** (values in Å and deg).

<i>Compound</i>	<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i><D—H···A</i>
11	N4—H4a···O2 ⁱ	0.91	2.19	3.045 (3)	157
	N4—H4b···O1 ⁱⁱ	0.91	2.20	3.042 (3)	153
	N2—H2a···O2 ⁱ	0.91	2.07	2.961 (3)	168
	C6—H6a···O3	0.99	2.45	3.373 (3)	154
	C9—H9b···F2	0.98	2.55	3.488 (4)	161
	C15—H15a···O1 ⁱⁱ	0.99	2.32	3.168 (4)	144
12	N2—H2a···O7 ⁱ	0.91	2.33	3.087 (4)	140
	N2—H2b···O2 ⁱ	0.91	2.21	3.017 (3)	148
	N4—H4a···O1 ⁱⁱ	0.91	2.12	2.939 (3)	149
	N4—H4b···O7 ⁱ	0.91	2.09	2.981 (4)	164
	C5—H5···O3	1.00	2.42	3.085 (4)	123
	C6—H6a···O5	0.99	2.30	3.173 (4)	146
	C13—H13a···O1 ⁱⁱ	0.99	2.39	3.157 (4)	134
	C15—H15a···O3	0.99	2.53	3.392 (4)	146
13	C5—H5···O5	1.00	2.41	3.099 (6)	126
	C3—H3b···F18b	0.98	2.49	3.386 (11)	152
	C9—H9a···F19a ⁱ	0.98	2.51	3.217 (11)	128
	C14—H14···F19b ⁱⁱ	1.00	2.54	3.238 (9)	127
	N4—H4c···O1 ⁱⁱⁱ	0.91	1.88	2.772 (5)	164
	N4—H4d···O10 ^{iv}	0.91	1.89	2.782 (5)	168
	N4—H4e···O1w	0.91	1.80	2.696 (5)	167
	C15—H15b···O10 ^{iv}	0.99	2.60	3.348 (5)	133
	C11—H11c···F21a ⁱⁱ	0.98	2.45	3.130 (8)	126
	O1w—H1wa···O8 ^{iv}	0.87	2.43	2.954 (5)	119
	O1w—H1wa···F24 ^{iv}	0.87	2.34	3.083 (6)	144
	O1w—H1wb···F6 ^{iv}	0.87	2.37	2.836 (5)	114
	O1w—H1wb···O3 ^{iv}	0.87	2.09	2.954 (5)	174
14	N2—H2A···F1 ⁱ	0.91	2.53	3.370 (4)	154
	N2—H2B···O2 ⁱ	0.91	2.47	3.045 (4)	121
	C5—H5···F9 ⁱ	1.00	2.52	3.354 (4)	141
15	N2—H2A···O4 ⁱ	0.89	2.44	3.293 (6)	161
	N2—H2B···O1 ⁱⁱ	0.89	2.06	2.887 (7)	154
	C6—H6A···O5	0.97	2.62	3.136 (9)	113
	C6—H6A···O3	0.97	2.41	3.307 (9)	153
	C4—H4A···F8 ⁱ	0.97	2.44	3.402 (9)	169
	C4—H4B···O1 ⁱⁱ	0.97	2.55	3.289 (9)	133
	C9—H9B···F11B ⁱⁱⁱ	0.96	2.53	3.053 (15)	114
	C9—H9C···F2 ^{iv}	0.96	2.63	3.223 (15)	120

Symmetry codes: For **11**: (i) $-x+1, y+1/2, -z+2$; (ii) $-x+1, y-1/2, -z+1$; For **12**: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $x+1/2, -y+3/2, z+1/2$; For **13**: (i) $-x+1, -y+1, -z$; (ii) $x-1, y, z$; (iii) $-x, -y+1, -z$; (iv) $-x, y+1/2, -z+1/2$; For **14**: (i) $-x+1, -y, -z$; For **15**: (i) $-x+3/2, -y+1/2, -z$; (ii) $x, -y+1, z-1/2$; (iii) $x, -y+1, z+1/2$; (iv) $-x+3/2, y+1/2, -z+1/2$.

Table S2. Temperature dependence of the conductivity of **15**.

Temperature (K)	Conductivity (S cm ⁻¹)
368	1.06 10 ⁻¹⁰
378	1.77 10 ⁻⁸
388	2.65 10 ⁻⁷
398	2.50 10 ⁻⁶
408	2.09 10 ⁻⁵

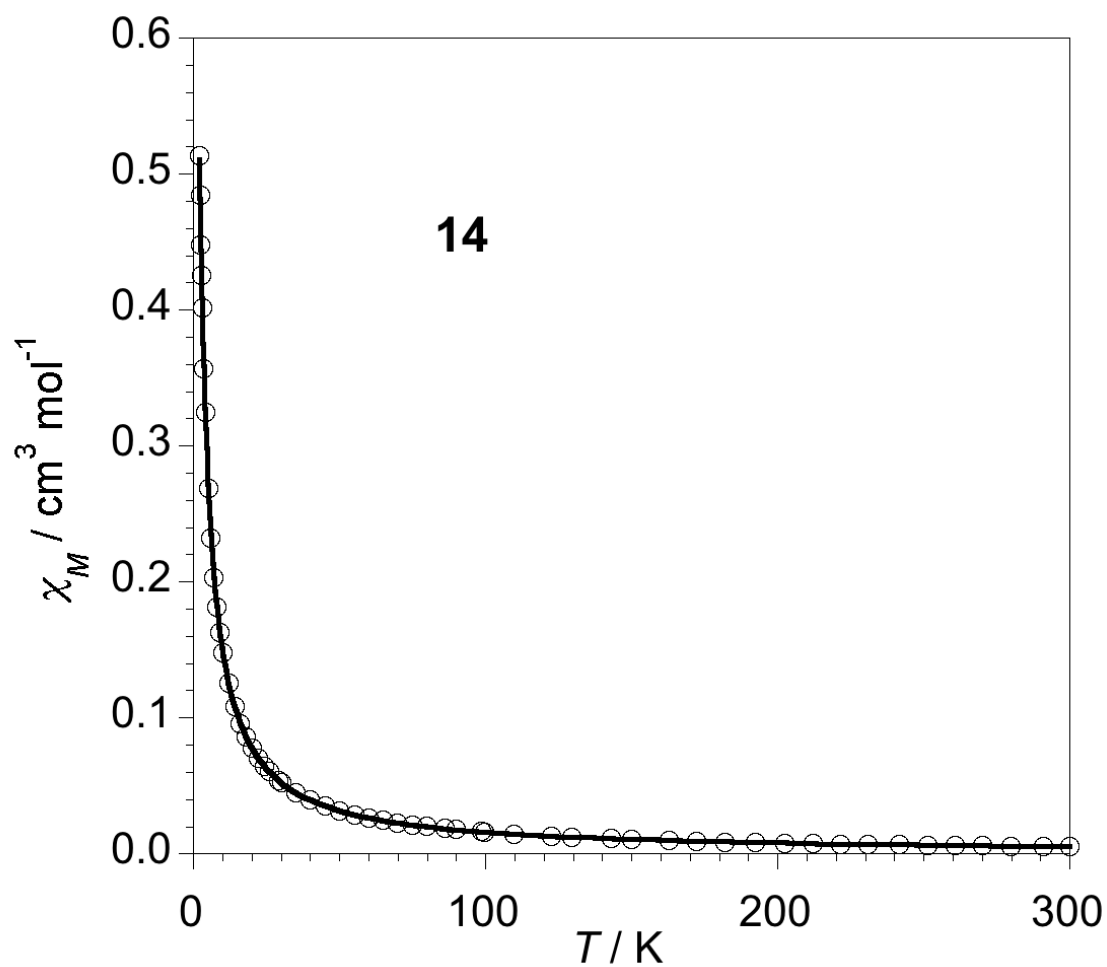


Figure S6. χ_M vs T plot of complex **14**. The circles represent the experimental results and the solid line represents the best-fit curve through equation (5).

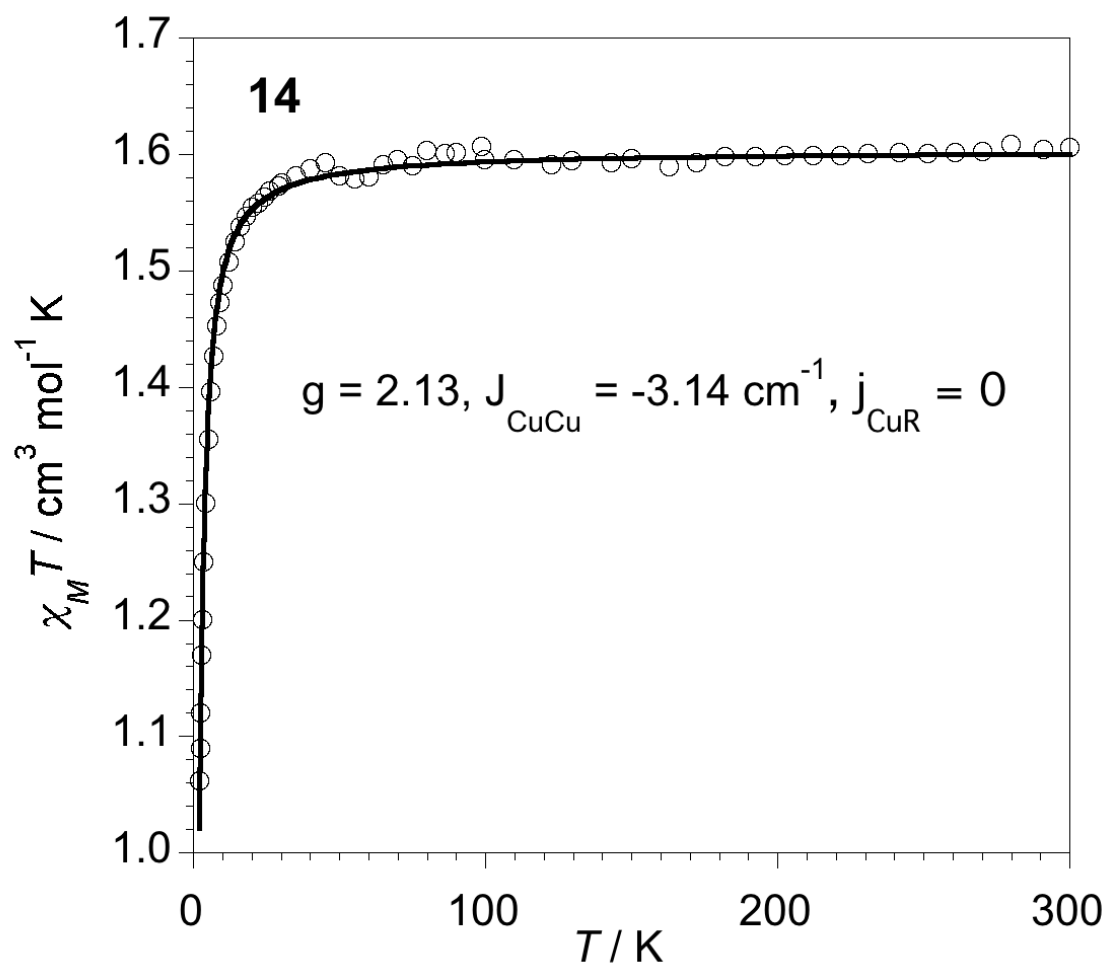


Figure S7. $\chi_M T$ vs T plot of complex **14**. The circles represent the experimental results and the solid line represents the best-fit curve through equation (5) but keeping constant $j = 0$.