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## Structure and properties of bivalent nickel and copper complexes with pyrazine-amide-thioether coordination: Stabilization of trivalent nickel

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### Electronic Supporting Information (ESI)

**Fig. S1.** UV/VIS spectrum (in CH<sub>2</sub>Cl<sub>2</sub>) of [Cu<sup>II</sup>(bpzctb)] (2).

**Fig. S2.** Reciprocal molar susceptibility vs temperature plots for

(a) [Ni<sup>II</sup>(bpzctb)] (1) and (b) [Cu<sup>II</sup>(bpzctb)] (2).

**Fig. S3.** EPR spectrum of a polycrystalline sample of [Cu<sup>II</sup>(bpzctb)] (2) at 300 K.

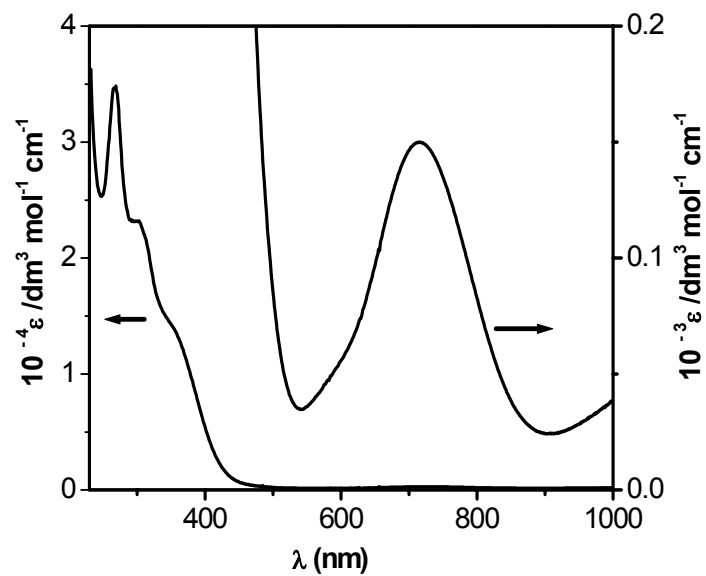
**Fig. S4.** EPR spectrum of [Ni<sup>III</sup>(bpzctb)]<sup>+</sup> (coulometrically generated in CH<sub>2</sub>Cl<sub>2</sub>) at 120 K.

**Fig. S5.** UV/VIS spectrum of [Ni<sup>III</sup>(bpctb)]<sup>+</sup> (coulometrically generated in CH<sub>2</sub>Cl<sub>2</sub>).

**Fig. S6.** EPR spectrum of [Ni<sup>III</sup>(bpctb)]<sup>+</sup> (coulometrically generated in CH<sub>2</sub>Cl<sub>2</sub>) at 300 K.

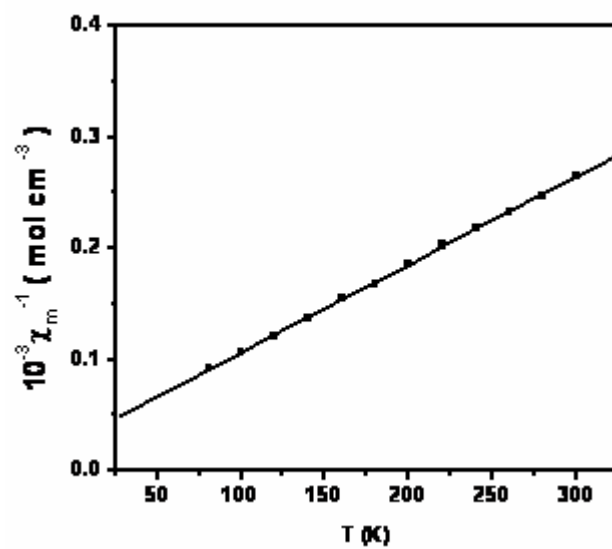
**Fig. S7.** EPR spectrum of [Ni<sup>III</sup>(bpctb)]<sup>+</sup> (coulometrically generated in CH<sub>2</sub>Cl<sub>2</sub>) at 120 K.

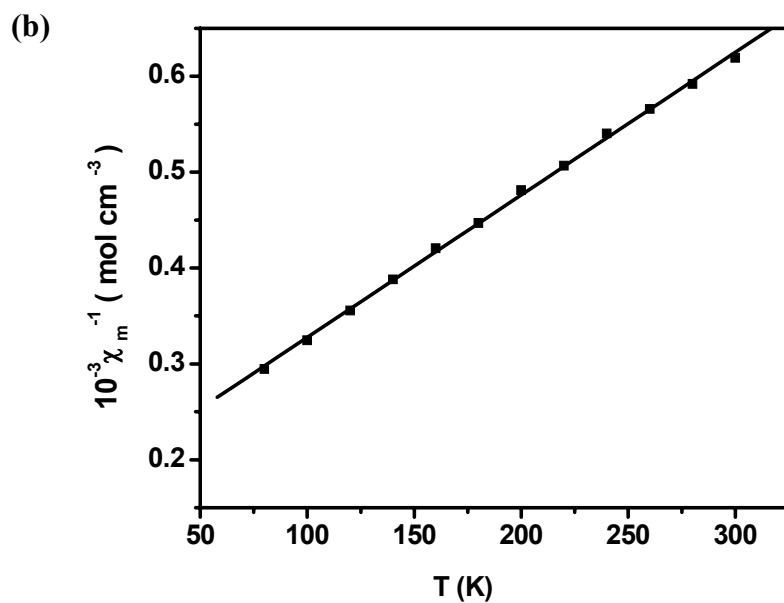
**Fig. S1.** UV/VIS spectrum (in CH<sub>2</sub>Cl<sub>2</sub>) of [Cu<sup>II</sup>(bpzctb)] (2).



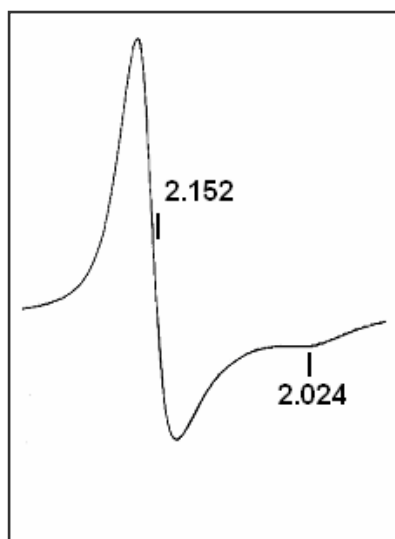
**Fig. S2.** Reciprocal molar susceptibility vs. temperature plots for (a) [Ni<sup>II</sup>(bpzctb)] (1) and (b) [Cu<sup>II</sup>(bpzctb)] (2).

(a)

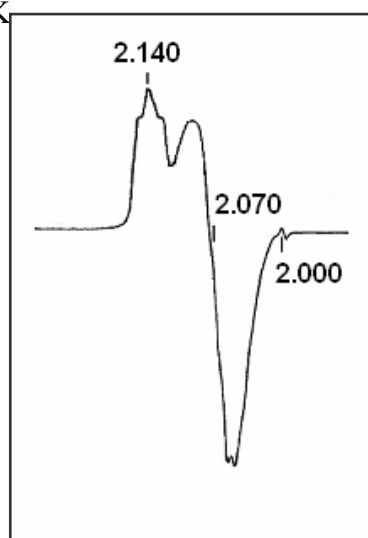




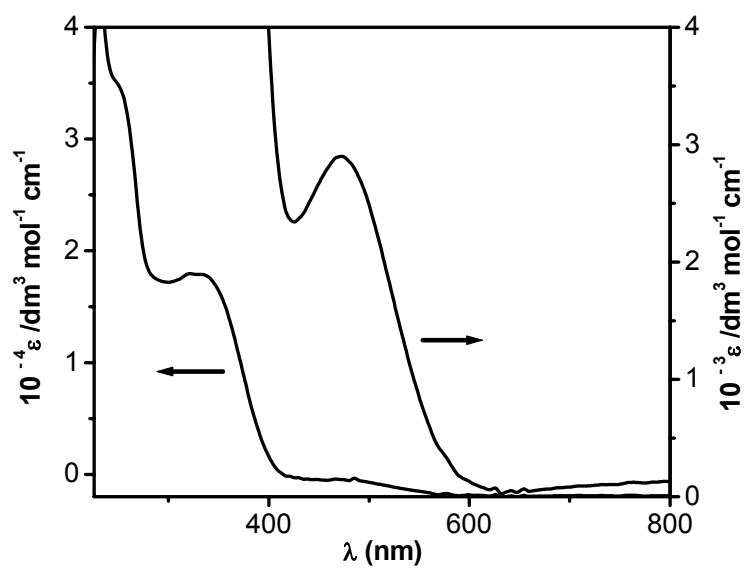
**Fig. S3.** EPR spectrum of a polycrystalline sample of  $[\text{Cu}^{\text{II}}(\text{bpzctb})]$  (2) at 300 K.



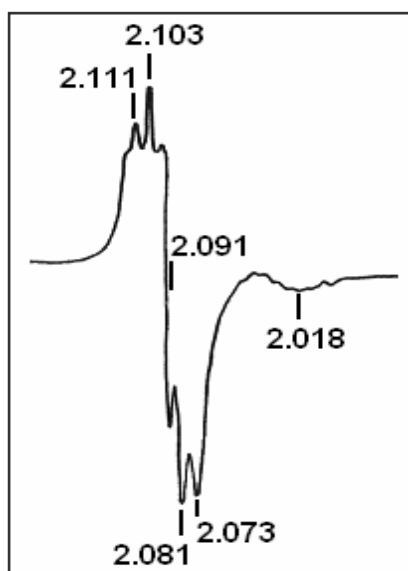
**Fig. S4.** EPR spectrum of  $[\text{Ni}^{\text{III}}(\text{bpzctb})]^+$  (coulometrically generated in  $\text{CH}_2\text{Cl}_2$ ) at 120 K.



**Fig. S5.** UV-vis spectrum of  $[\text{Ni}^{\text{III}}(\text{bpctb})]^+$  (coulometrically generated in  $\text{CH}_2\text{Cl}_2$ ).



**Fig. S6.** EPR spectrum of  $[\text{Ni}^{\text{III}}(\text{bpctb})]^+$  (coulometrically generated in  $\text{CH}_2\text{Cl}_2$ ) at 300 K.



**Fig. S7.** EPR spectrum of  $[\text{Ni}^{\text{III}}(\text{bpctb})]^+$  (coulometrically generated in  $\text{CH}_2\text{Cl}_2$ ) at 120 K.

