

Supplementary Information

Preparation and Structural Characterization of A Novel Dicopper(II) Complex with a Terminal Hydroxide. Structural Model of an Active Site in Phosphohydrolases

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Fig. S4 The spectral change of **1** (0.50 mM) from pH 3.9 to 9.6 in MeCN/H₂O (with a 1/1 ratio) solution at the range of 300-600 nm.

Scheme 1. HTNPDO.

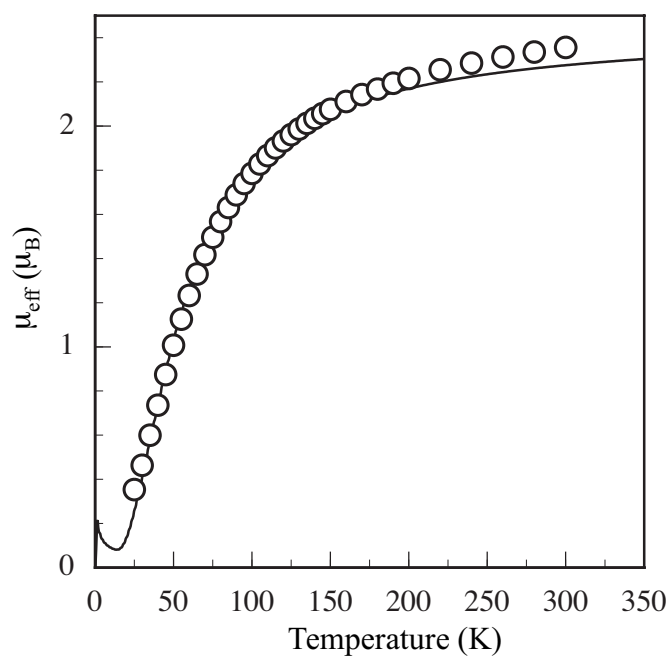


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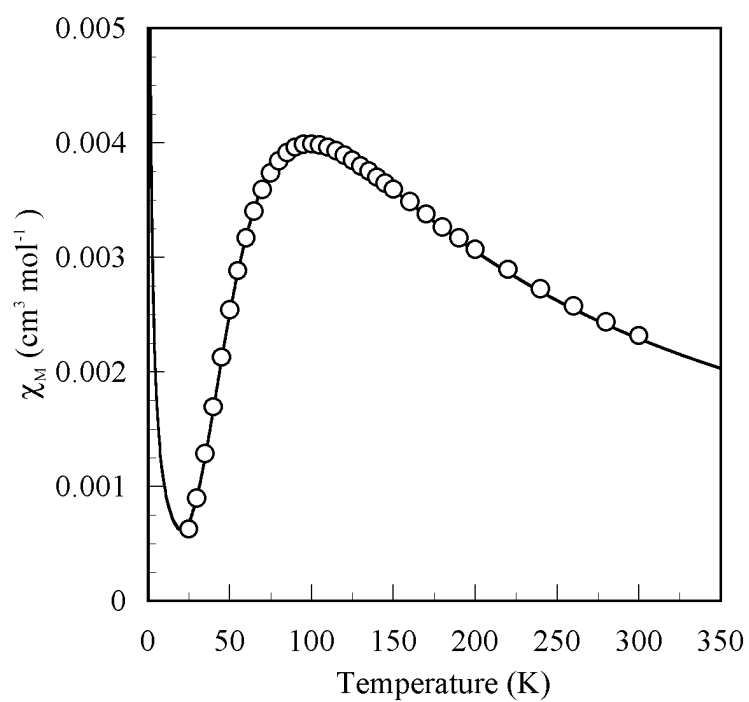


Fig. S2 The molar magnetic susceptibilities of **1** depended on temperature from 300 K to 20 K fitted using the modified Bleaney-Bowers equation.

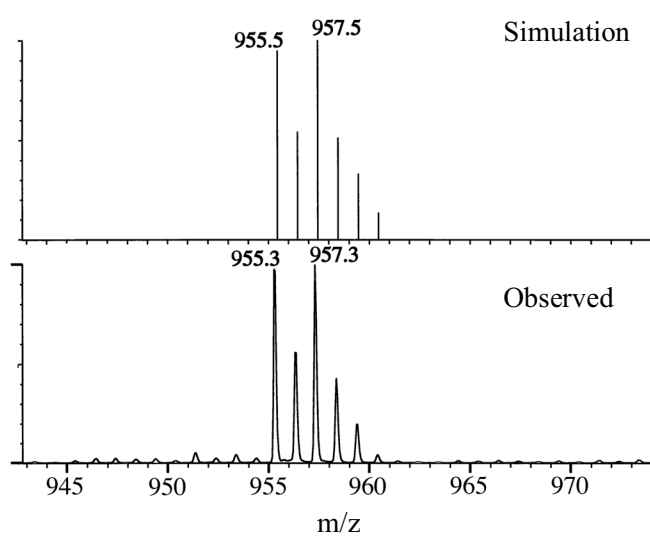


Fig. S3 Positive ion electrospray ionization mass spectrum of $[\text{Cu}^{\text{II}}_2(\text{TNPDO})(\text{OH})(\text{F})]^+$.

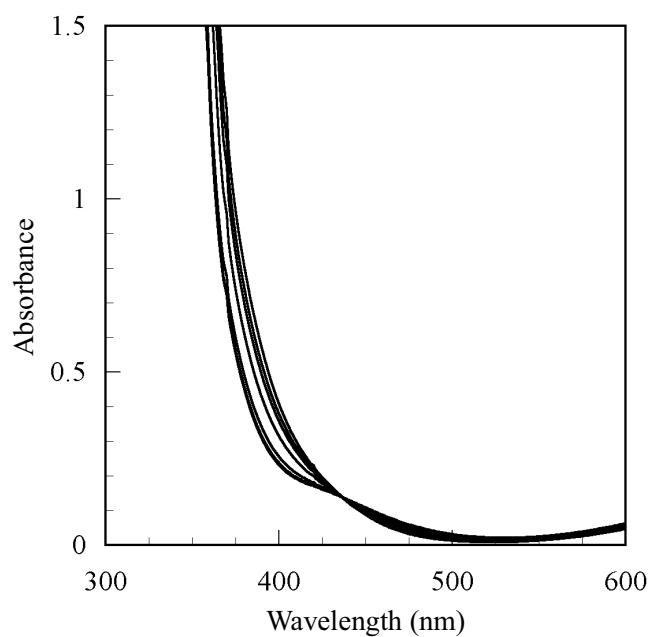
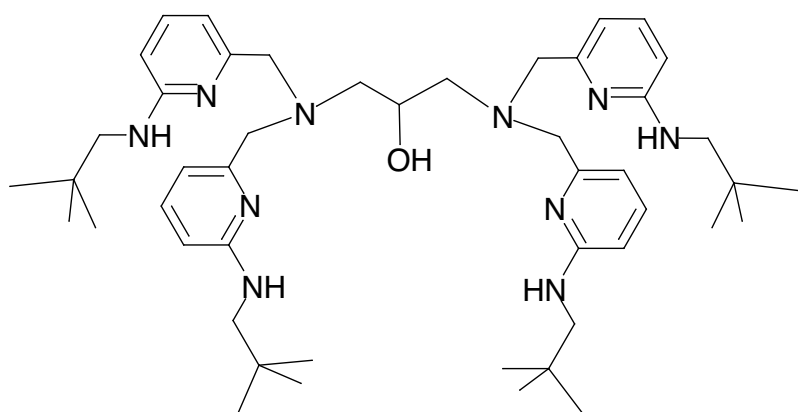


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