

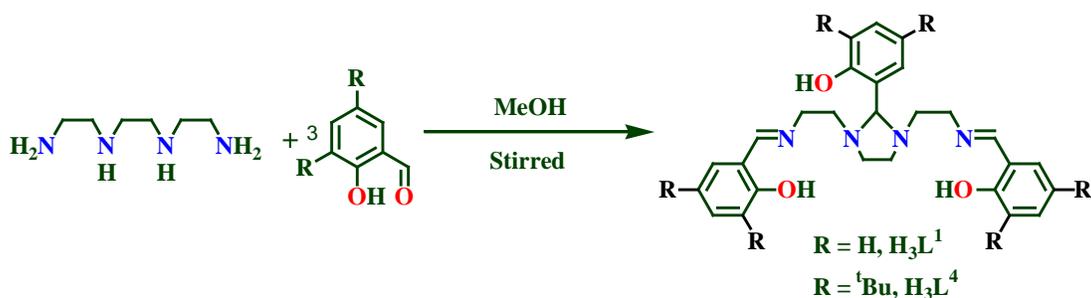
Electronic Supporting Information

Ligand Dependent Self-Assembly of Hydroxido-Bridged Dicopper Units Templated by Sodium Ion

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Synthesis

2-(2'-hydroxyphenyl)-1,3-bis[4-(2-hydroxyphenyl)-3-azabut-3-enyl]-1,3-imidazolidine (**H₃L¹**), 2-(3,5-di-*tert*-butyl-2-hydroxyphenyl)-1,3-bis[4-(3,5-di-*tert*-butyl-2-hydroxyphenyl)-3-azabut-3-enyl]-1,3-imidazolidine (**H₃L²**): These were prepared from single-step Schiff base condensation reactions of salicylaldehyde (1.59 mL, 15 mmol) and 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (3.51 g, 15 mmol), respectively with triethylenetetramine (0.75 mL, 5 mmol) in MeOH (30 mL) for 2 h. Light yellow solid products were collected by filtration, washed with a minimum volume of methanol, and dried in vacuo over P₄O₁₀.



Scheme S1 Synthesis of ligands.

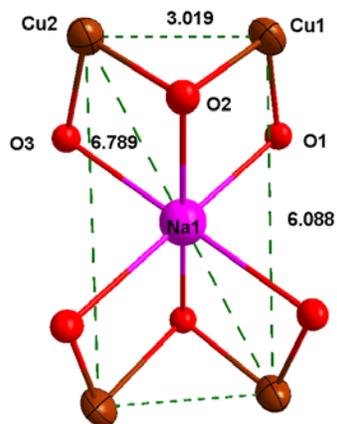


Figure S1 Rectangular geometry of [NaCu₄] complex with short and long Cu...Cu distances at 3.019 and 6.088Å and the longest diagonal of 6.789Å.

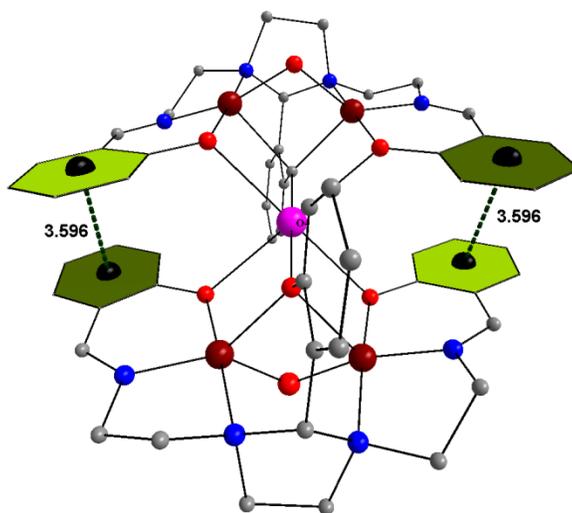


Figure S2 π-π interactions between terminal phenyl rings in complex 1.

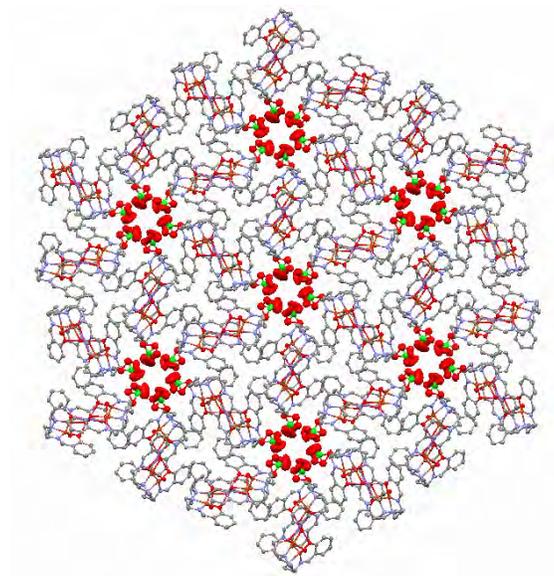


Figure S3 The particular face-to-face orientation of the [Cu₂] units along with perchlorate anions showing the cavities.

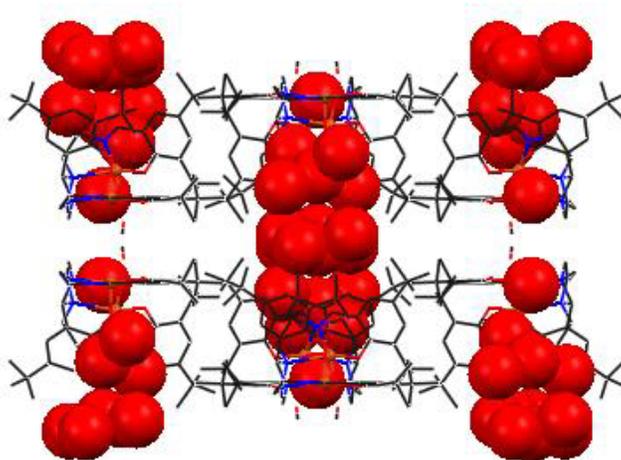


Figure S4 Generation of the cavity during crystal packing along crystallographic 'b' axis in which Na⁺ ions are fitting satisfactorily.