

Supporting Information

A Mixed Valent Heterometallic Cu^{II}/Na^I Coordination Polymer with Sodium-Phenyl Bonds

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Table S1. Hydrogen Bond Geometry

Donor	Hydrogen	Acceptor	D-H (Å)	H-A (Å)	D-A (Å)	DHA (°)
O(5)	H(10)	O(19)	0.84	1.86	2.662(4)	160.5
O(10)	H(20)	O(12)	0.84	1.99	2.793(4)	159.0
O(10)	H(20)	O(13)	0.84	2.61	3.309(5)	141.2
O(10)	H(20)	Cl(1)	0.84	2.81	3.634(3)	166.8
O(19)	H(30)	O(14) ⁱ	0.887(10)	1.958(16)	2.807(6)	160(4)
O(19)	H(40)	O(17) ⁱⁱ	0.883(10)	1.922(16)	2.785(5)	166(3)
O(19)	H(40)	Cl(2) ⁱⁱ	0.883(10)	2.66(3)	3.329(3)	134(3)

Symmetry Operators

ⁱ x+1, y, z+1 ⁱⁱ -x-1, y+1/2, -z-1
Table S2. EPR parameters of the polycrystalline powder of **1**.^[a]

Temperature / K	g_x	g_y	g_z
298	2.047	2.047	2.185
77	2.048	2.048	2.181

^[a] For Ref^[SI 1], $g_z = 2.182$, $g_x = g_y = 2.053$ at RT, and $g_z = 2.187$, $g_x = g_y = 2.054$ at 77 K.

Table S3. EPR parameters of **1** and Ref^[SI 1] in organic solvents.

Species	Solvent	g_x	$A_x / 10^{-4} \text{ cm}^{-1}$	g_y	$A_y / 10^{-4} \text{ cm}^{-1}$	g_z	$A_z / 10^{-4} \text{ cm}^{-1}$
1	DMSO	2.038	11	2.069	13	2.243	187
1	DMF	2.038	11	2.069	13	2.243	187
1	CH ₃ CN	2.039	12	2.070	14	2.243	188
Ref SI 1	DMSO	2.037	11	2.069	13	2.243	187
Ref SI 1	DMF	2.037	11	2.070	12	2.243	187

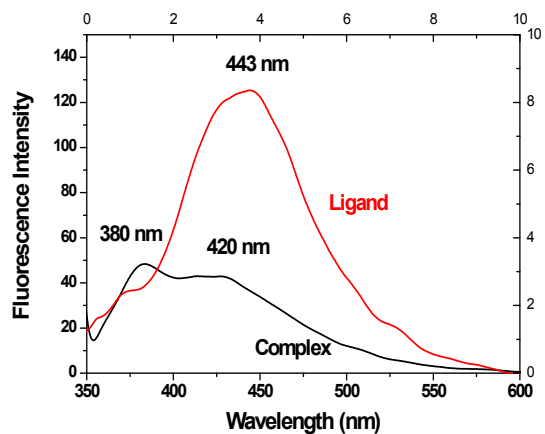


Fig. S11 Emission spectra of the ligand and complex 1 (in MeOH). λ_{ex} 330 nm (ligand); λ_{ex} 360 nm (complex). Fluorescence intensity is given in arbitrary units.

References

[SI 1] K. Das, A. Datta, J.K. Clegg, E. Garribba, S. Roy, C. Sinha, submitted to Polyhedron.