Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

A New Copper Species Based on An Azo-compound Utilized as A Homogeneous Catalyst for Water Oxidation

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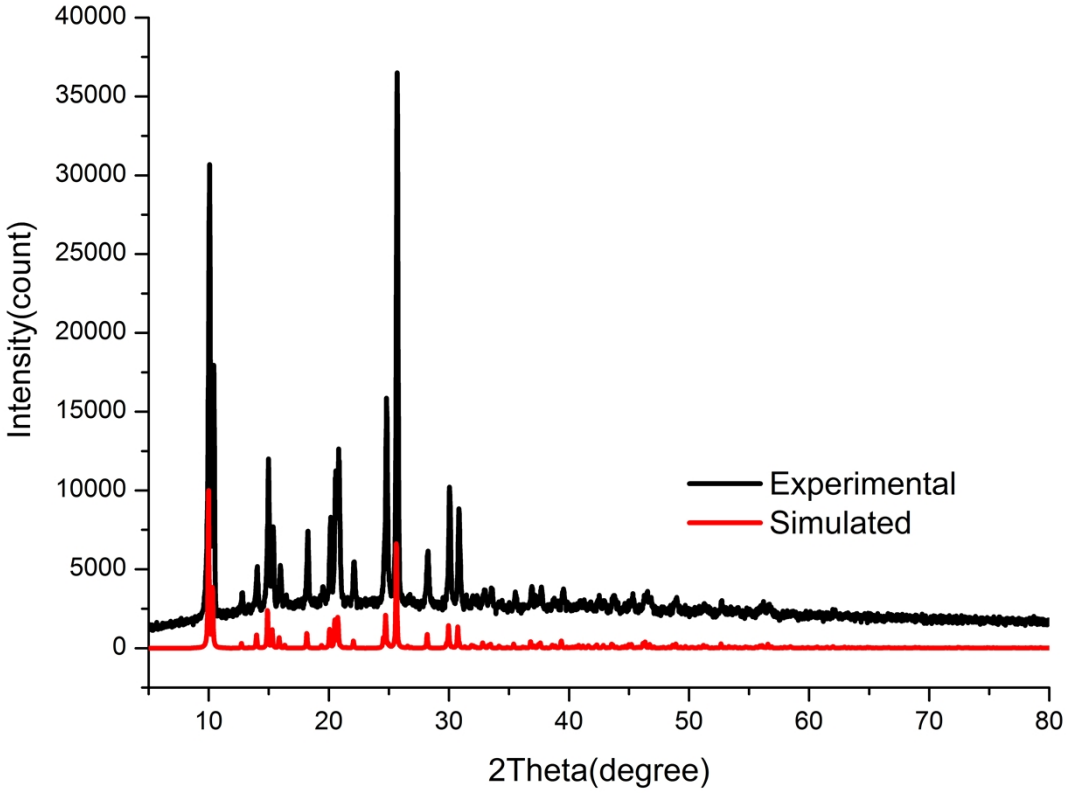

Figure s1. The PXRD patterns of **1**.

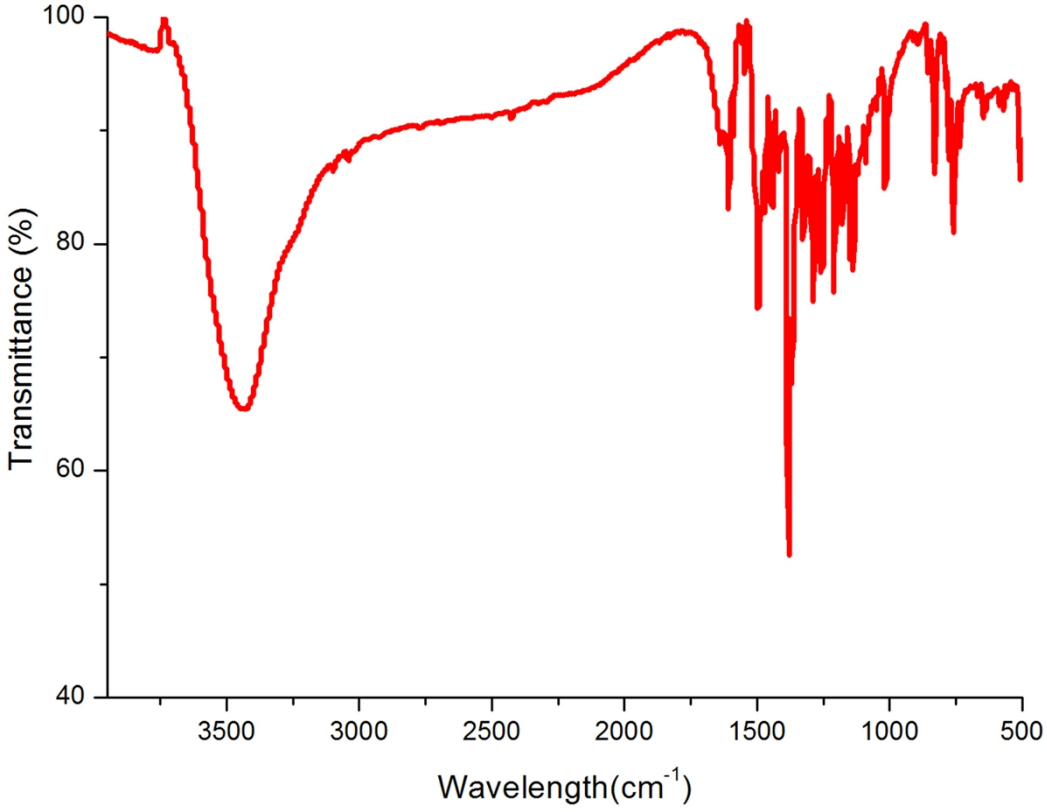

Figure s3. IR spectra of **1**.

Empirical formula	C_{15} H_{10} Cu N_4 O_4
Formula weight	373.81
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 9.046(3) A alpha = 90 deg. b = 11.876(4) A beta = 108.792(4) deg. c = 14.006(5) A gamma = 90 deg.
Volume	1424.5(8) A^3
Z, Calculated density	4, 1.743 Mg/m^3
Absorption coefficient	1.563 mm^-1
F(000)	756
Crystal size	0.21 x 0.17 x 0.15 mm
Theta range for data collection	2.93 to 27.59 deg.
Limiting indices	-11<=h<=11, -15<=k<=7, -17<=l<=18
Reflections collected / unique	8608 / 3289 [R(int) = 0.0580]
Completeness to theta = 27.71	99.5 %
Max. and min. transmission	0.7993 and 0.7349
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3289 / 0 / 217
Goodness-of-fit on F^2	0.922
Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1410
R indices (all data)	R1 = 0.1065, wR2 = 0.1754
Largest diff. peak and hole	0.428 and -0.646 e.A^-3

Table s1. Crystal data and structure refinement for **1**.