Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

A rare doubly nitrato and phenoxido bridged trimetallic Cu^{II} complex: EPR, antiferromagnetic coupling and theoretical rationalization

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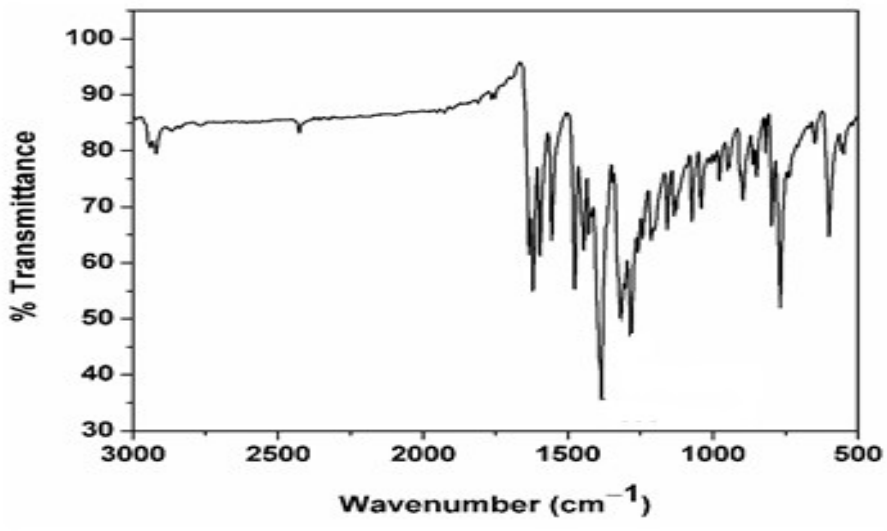
Figure S1. IR spectrum of complex **1**.



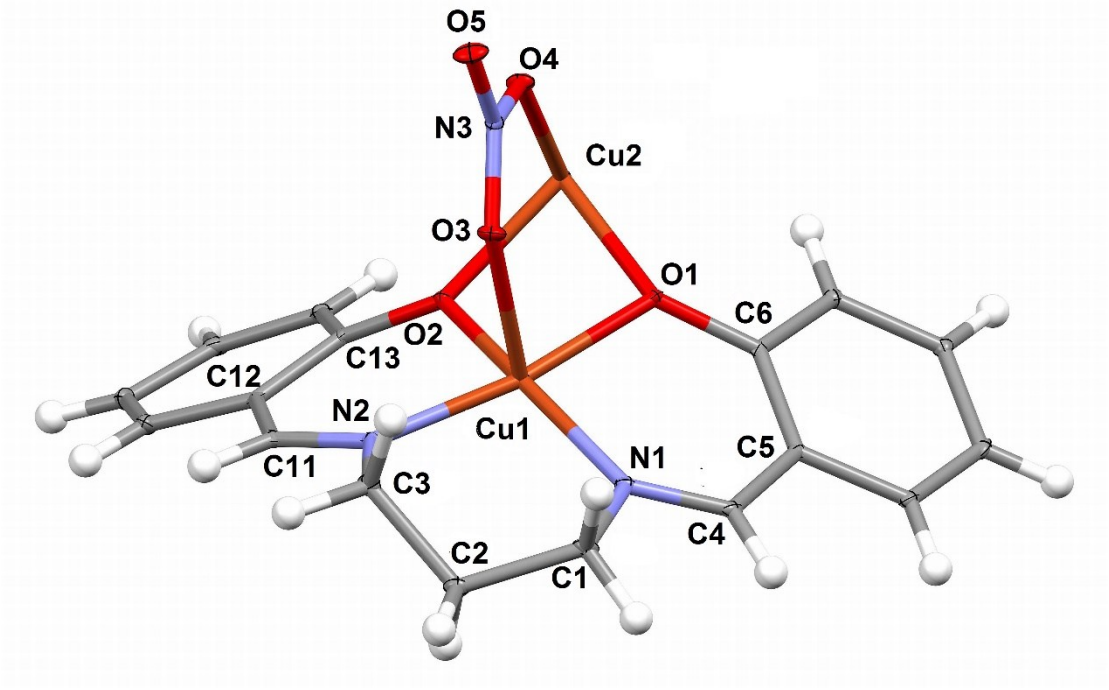


Figure S2. Ortep view (20% ellipsoid probability) of the asymmetric unit of complex **1**.

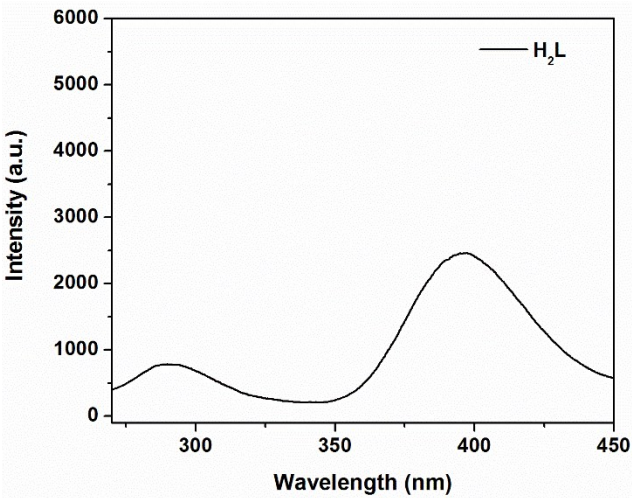


Figure S3. Solid state emission spectra of H_2L ligand, measured at room temperature upon excitation at 250 nm.

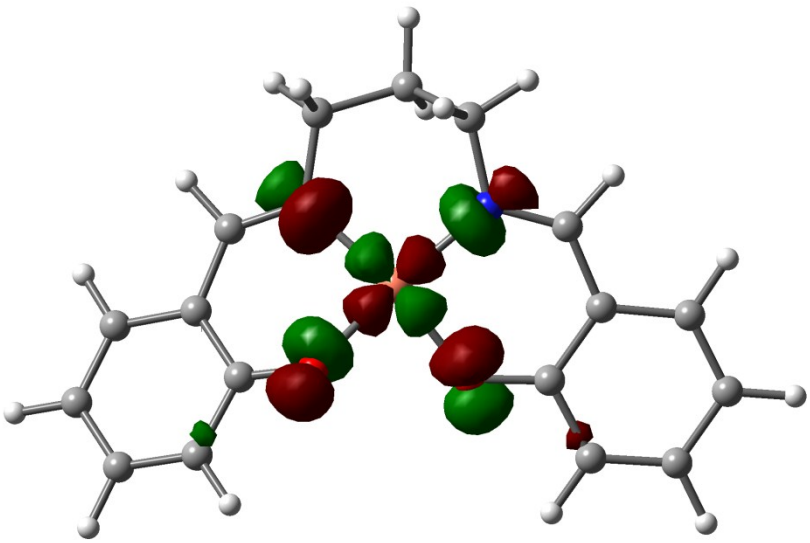


Figure S4. SOMO of the mononuclear complex CuL

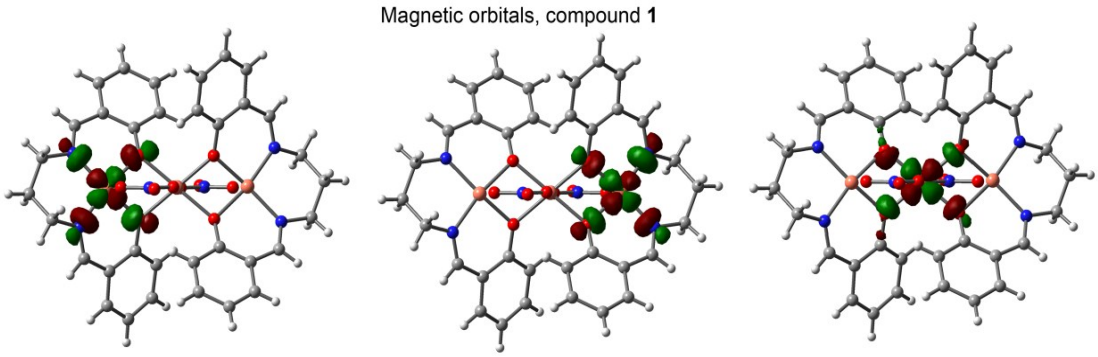


Figure S5. Magnetic orbitals of complex **1**.

Table S1. Relative energies (Hartrees and cm^{-1}) of the different spin states of compound 1.

Spin state $\|S = S_1 + S_2 + S_3, S' = S_1 + S_3\rangle$	Relative Energy (Hartrees)	Relative energy (cm^{-1})
$\|3/2, 1\rangle$, ααα; quartet[a]	0.0024372	534.9 = $-3J/2$
$\|-1/2,0\rangle$ ββα; doublet	0.0016239	356.4 = $-J$
$\|1/2,0\rangle$ ααβ; doublet	0.0016239	356.4 = $-J$
$\|1/2,1\rangle$ αβα; doublet	0.0000000	0

[a]Absolute energy: -7316.2895841 Hartries

Table S2. Mulliken spin population computed for the high spin (HS) and low spin ground state (LS) configuration of compound **1**. See **Figure 1** for numbering scheme.

Atom Label	Spin density (HS)	Spin density (LS)
Cu1/Cu1’	0.62	0.60
Cu2	0.72	-0.73
O1	0.14	0.02
O1’	0.14	-0.02
O2	0.13	0.02
O2’	0.13	-0.02
N1	0.10	0.10
N2	0.11	0.11
O3/O3’ (nitrate)	0.00	0.00
O4/O4’ (nitrate)	0.00	0.00