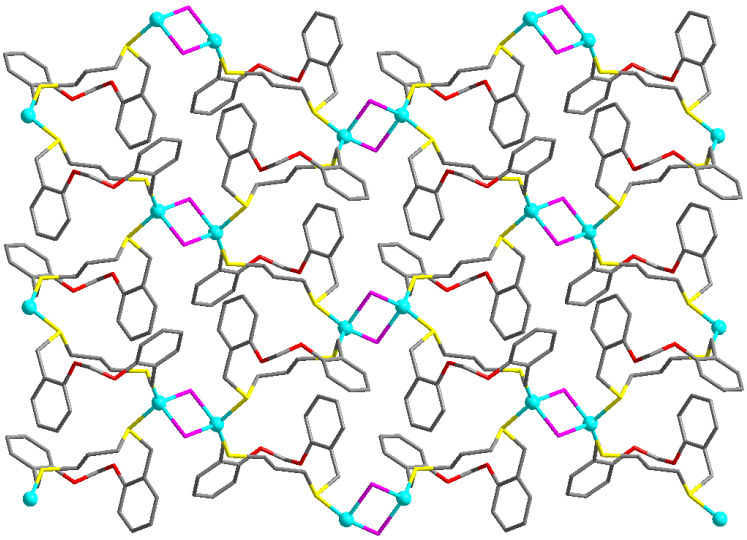
Electronic Supplementary Information

For

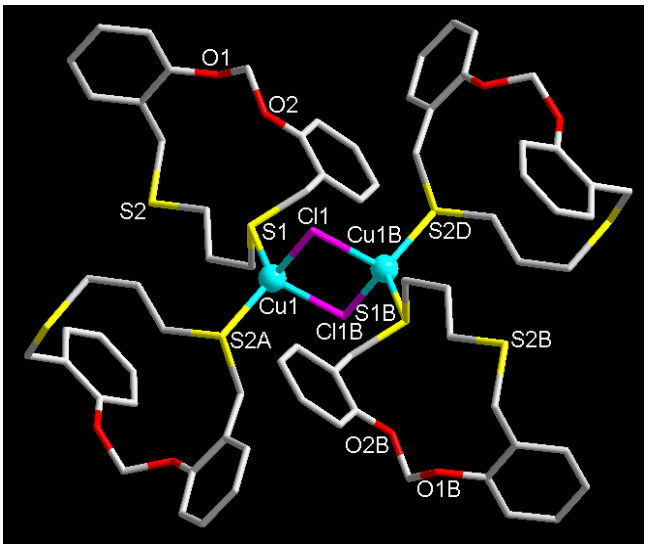
Exocyclic coordination chemistry of an O_2S_2-macrocycle with copper(I), mercury(II) and palladium(II) ions

Seulgi Kim, Eunji Lee, Ki-Min Park and Shim Sung Lee*

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 660-701, S. Korea

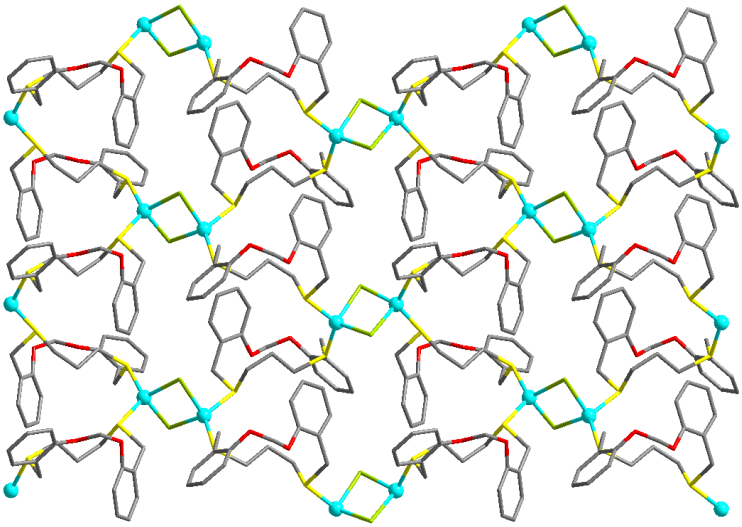


(a)

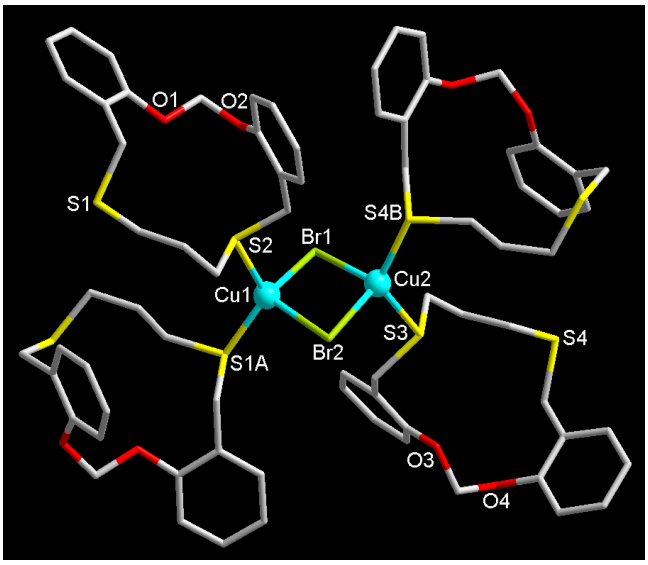


(b)

Fig. S1 2-D polymeric structure of **1**, $[(Cu_2Cl_2)\mathbf{L}]_n$: (a) fishnet-type network and (b) basic coordination unit.



(a)



(b)

Fig. S2 2-D polymeric structure of **2**, $[(Cu_2Br_2)\mathbf{L}]_n$: (a) fishnet-type network and (b) basic coordination unit.

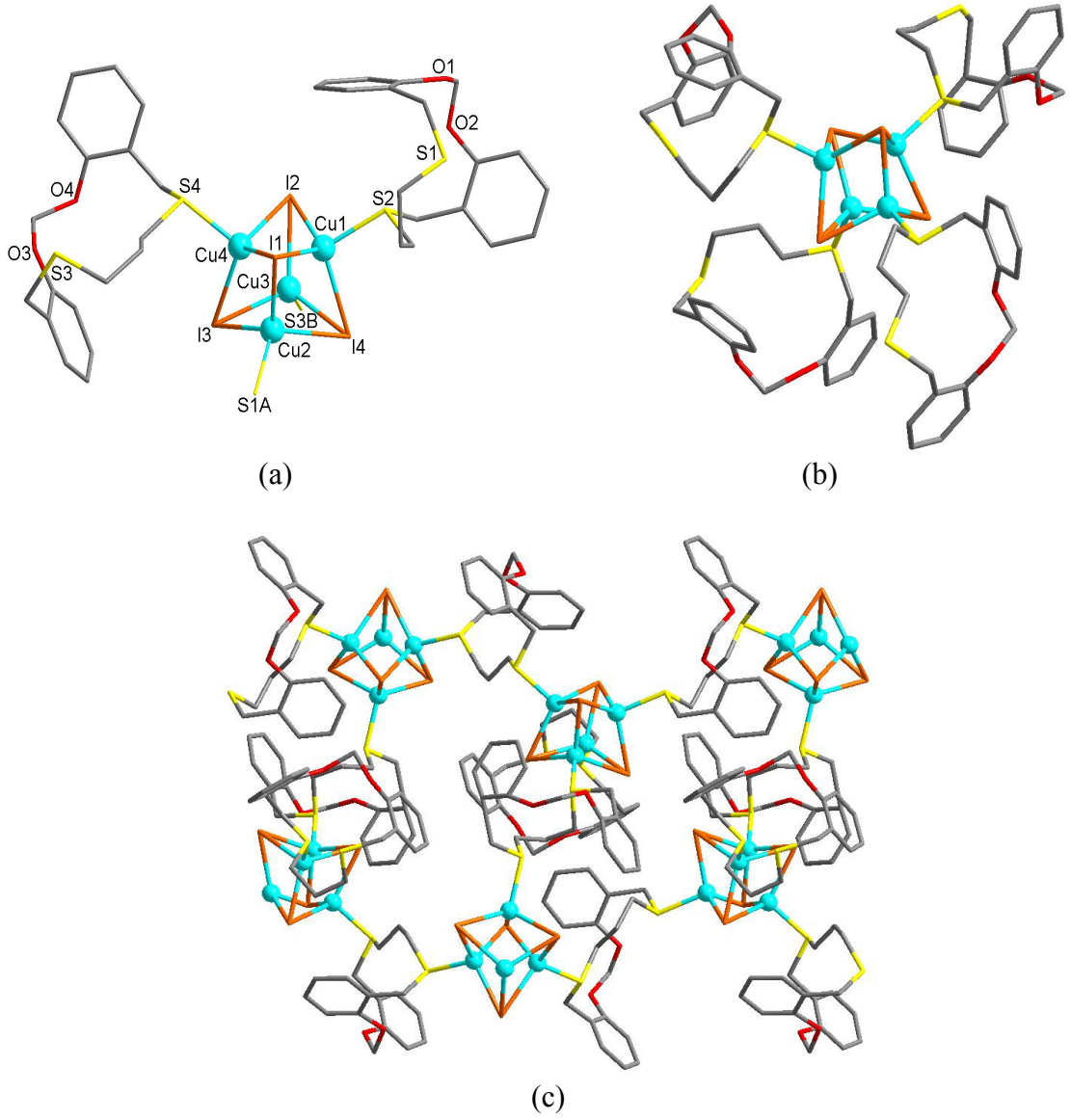


Fig. S3 A preliminary crystal structure of **3**, $\{[(Cu_4I_4)\mathbf{L}](H_2O)_{2.5}\}_n$: (a) the basic coordination unit, (b) the coordination environment of the Cu_4I_4-cubane core and (c) the 2-D network.

*Note for the crystal structure of **3***: since the structural refinement in the X-ray analysis was not completed (e.g. NPD) because of the poor crystallity and the slow decomposition in the air, it shows large *R*-values (see Table S2).

Table S1 Selected bond lengths (Å) and bond angles (°) for **3**

Cu1-S2	2.290(1)	Cu1-I2	2.704(1)
Cu1-I1	2.636(1)	Cu1-I4	2.730(1)
Cu2-S1A	2.363(1)	Cu2-I3	2.659(1)
Cu2-I4	2.652(1)	Cu2-I1	2.731(1)
Cu3-S3B	2.285(1)	Cu3-I3	2.657(1)
Cu3-I2	2.645(1)	Cu3-I4	2.719(1)
Cu4-S4	2.283(1)	Cu4-I3	2.703(1)
Cu4-I1	2.688(1)	Cu4-I2	2.734(1)
S2-Cu1-I1	114.4(1)	S2-Cu1-I4	102.8(1)
S2-Cu1-I2	101.8(1)	I1-Cu1-I4	107.0(1)
I1-Cu1-I2	115.3(1)	Cu3-Cu1-I4	60.7(1)
Cu3-Cu1-I2	59.2(1)	Cu4-Cu1-I4	106.5(1)
Cu4-Cu1-I2	61.3(1)	I2-Cu1-I4	115.0(1)
S1A-Cu2-I4	113.0(1)	S1A-Cu2-I1	100.5(1)
S1A-Cu2-I3	107.5(1)	I4-Cu2-I1	106.5(1)
I4-Cu2-I3	111.9(1)	I3-Cu2-I1	117.0(1)
S3B-Cu3-I2	106.3(1)	S3B-Cu3-I4	104.4(1)
S3B-Cu3-I3	104.7(1)	I2-Cu3-I4	117.4(1)
I2-Cu3-I3	113.0(1)	I3-Cu3-I4	109.9(1)
S4-Cu4-I1	105.8(1)	S4-Cu4-I2	104.4(1)
S4-Cu4-I3	107.3(1)	I1-Cu4-I2	112.6(1)
I1-Cu4-I3	117.0(1)	I3-Cu4-I2	108.8(1)

Symmetry operations: (A)-x+3/2,y-1/2,-z+3/2 (B)x,-y+1,z-1/2 (C) -x+3/2,y+1/2,-z+3/2 (D) x,-y+1,z+1/2

Table S2 Crystal and experimental data of **3**

	3
Formula	$C_{36}H_{45}Cu_4I_4O_{6.50}S_4$
Formula weight	1471.72
Temperature (K)	173(2)
Crystal system	Monoclinic
Space group	*C*2/*c*
Z	8
a (Å)	37.428(3)
b (Å)	17.7996(16)
c (Å)	18.6435(16)
α (°)	90
β (°)	118.5550(10)
γ (°)	90
V (Å^3)	10909.5(16)
D_{calc} (g/cm^3)	1.792
$2\theta_{max}$ (°)	52
R_1, wR_2 [$I > 2\sigma(I)$]	0.1323, 0.3239
R_1, wR_2 [all data]	0.1835, 0.3696
No. of reflection used [>2σ(*I*)]	10717 [R_{int} = 0.1403]