Electronic Supplementary Information

for

Endo- and/or exocyclic silver(I) and mercury(II) complexes of an NO_2S_2-macrocycle: effect of ligand ratio and anion

Hyun Jee Kim,[a] Kaniz Fatima Sultana,[a] Jai Young Lee[a,b] and Shim Sung Lee*[a]

[a] *Department of Chemistry and Research Institute of Natural Science, Gyeongsang National University, Jinju 660-701, S. Korea. E-mail: sslee@gnu.ac.kr*

[b] *Department of Chemistry, Konyang University, Nonsan 320-711, S. Korea.*

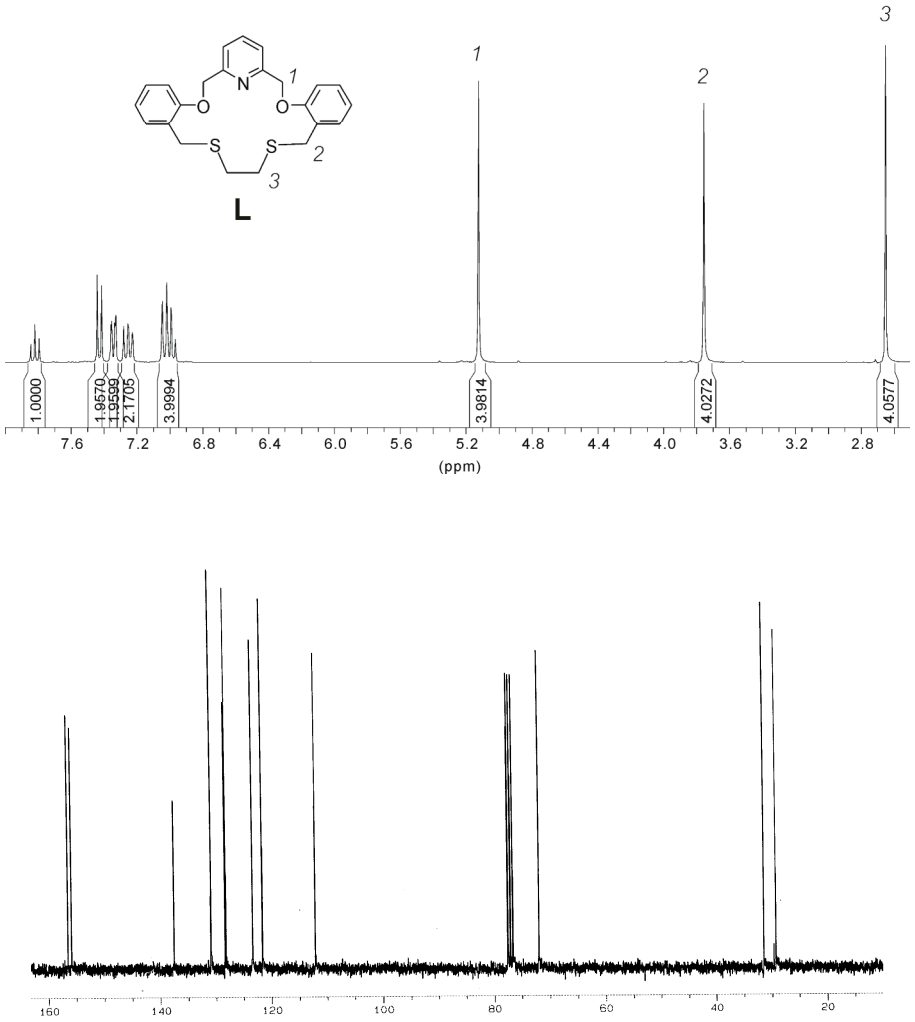

Fig. S1 ^{1}H and ^{13}C NMR spectra of **L**.

Crystallographic structure determinations

All data were collected on a Bruker Smart diffractometer equipped with a graphite monochromated Mo Kα (λ = 0.71073 Å) radiation source and a CCD detector. The 45 frames of two dimensional diffraction images were collected and processed to obtain the cell parameters and orientation matrix. The first 50 frames were retaken after complete data collection. The crystal showed no significant decay. The frame data were processed to give structure factors using the SAINT.[S1] The structure was solved by direct methods and refined by full matrix least squares methods on F^2 for all data using SHELXTL software.[S2] The non-hydrogen atoms were refined anisotropically. Thermal ellipsoids are drawn at the 30% probability level. In the structure **L** (Fig. 1), the ethylene unit

between S1 and S2 is disordered over two positions with occupancies of 0.77 and 0.23. In **4** (Fig. 6), the ethylene unit between S1 and S2 is also disordered over two positions with occupancies of 0.67 and 0.33

References

S1. Bruker, SMART and SAINT: *Area Detector Control and Integration Software Ver. 5.0*; Bruker Analytical X-ray Instruments: Madison, Wisconsin, 1998.

S2. Bruker, SHELXTL: *Structure Determination Programs Ver. 5.16*; Bruker Analytical X-ray Instruments: Madison, Wisconsin, 1998.

Table S1. Selected interatomic distances and torsion angles for **L**

O1···O2	5.023(3)	S1···S2	4.431(1)
O1-C1-C23-N1	72.5(3)	O2-C18-C19-N1	65.8(3)
S1-C9-C10-S2	172.8(2)	S1-C9'-C10'-S2	-170.6(7)

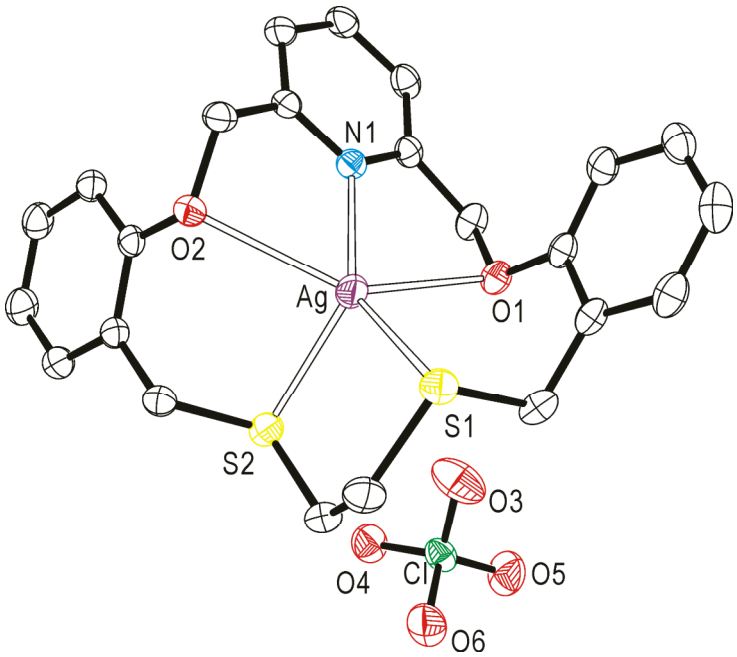

Fig. S2 Molecular structure of **1b**, [Ag(**L**)]ClO_4. Hydrogen atoms are omitted.

Table S2. Selected bond lengths, bond angles and torsion angle for **1b**, [Ag(**L**)]ClO_4

Ag-N1	2.213(2)	Ag-S1	2.485(1)
Ag-S2	2.522(1)	Ag-O1	2.585(2)
Ag-O2	2.650(2)		
S1-Ag-S2	89.5(3)	O1-Ag-O2	142.1(1)
O1-Ag-S1	89.0(1)	O1-Ag-S2	111.7(1)
N1-Ag-S1	143.3(1)	N1-Ag-S2	126.2(1)
N1-Ag-O1	71.3(1)	N1-Ag-O2	71.0(1)
O2-Ag-S2	87.0(1)		
S1-C9-C10-S2	49.2(4)		

Table S3. Comparison of Ag-X (X = N, S or O) bond lengths in **1a** and **2**

	1a	**2**
Ag-N1	2.250(6)	2.435(3)
Ag-S1	2.554(2)	2.603(1)
Ag-S2	2.557(2)	3.009(1)
Ag-S3		2.828(1)
Ag-S4		2.689(1)
Ag-O1	2.712(5)	2.890(2)
Ag-O2	2.665(5)	

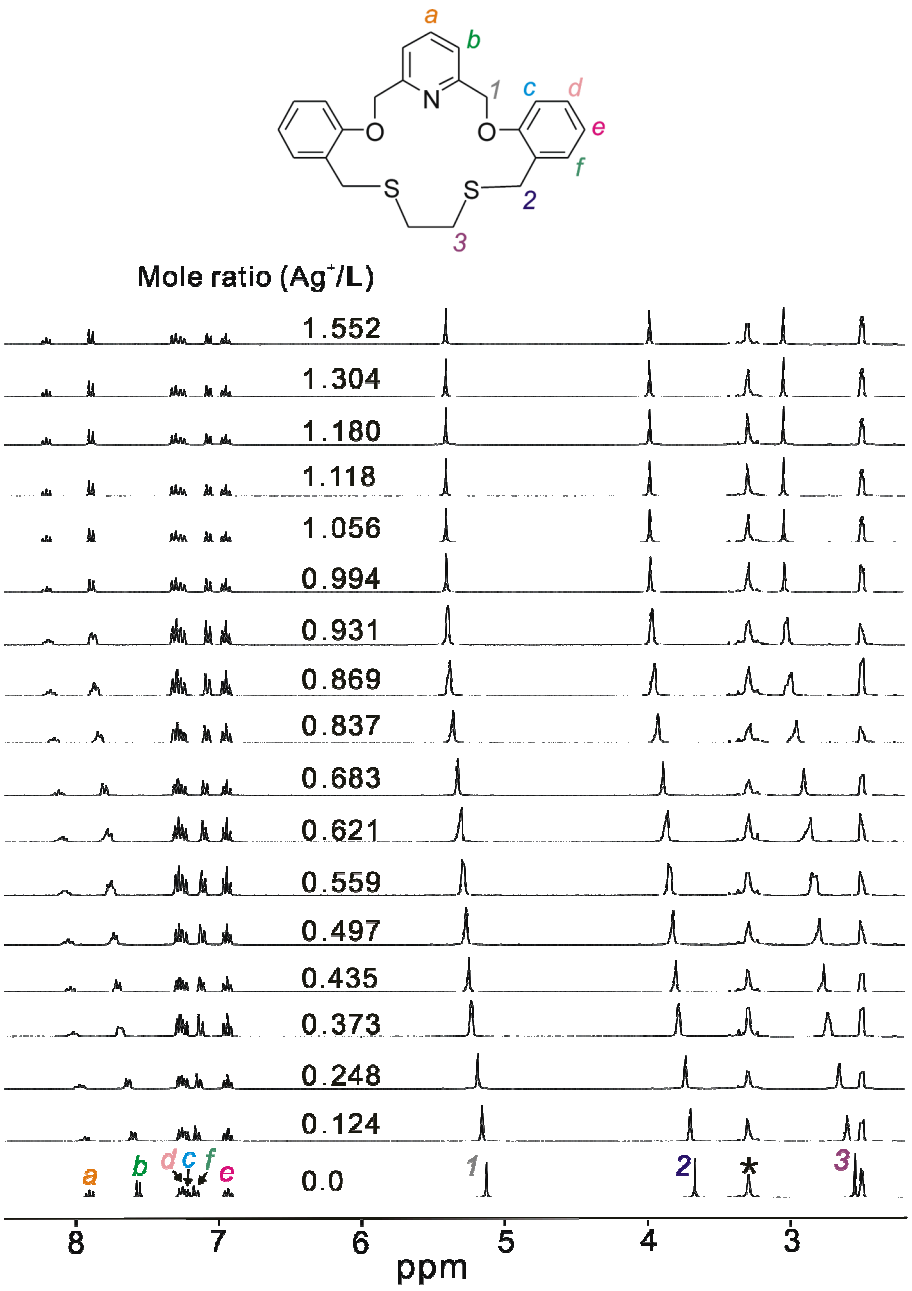

Fig. S3 ^{1}H NMR spectra of **L** by stepwise addition of $AgPF_6$ in DMSO-d_6.