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Supplementary Material

Endocyclic and Endo/Exocyclic Silver(I) Complexes of Thiaoxaaza-Macrocycles: Crystallographic and NMR Studies

Yunji Kang,[A] *Hyeong-Hwan Lee,*[A] *Huiyeong Ju,*[A] *Eunji Lee,*[A] *Seulgi Kim,*[A] *Joon-Hwa Lee,*[A] *In-Hyeok Park,*[A,B] *and Shim Sung Lee*[A,B]

[A]Department of Chemistry and Research Institute of Natural Science, Gyeongsang National University, Jinju 52828, South Korea
[B]Corresponding authors. Email: pihghost@nate.com; sslee@gnu.ac.kr

Table S1. Crystallographic data and refinement parameters

	L[1]	**L[2]**	**1**	**2**
formula	$C_{29}H_{27}NO_2S_2$	$C_{25}H_{27}NO_2S_3$	$C_{29}H_{27}AgN_2O_6S_2$	$C_{27}H_{30}Ag_2N_4O_8S_3$
formula weight	485.64	469.66	671.51	850.47
crystal system	Monoclinic	Triclinic	Monoclinic	Triclinic
space group	$P2_1/n$	P-1	$P2_1/n$	P-1
a (Å)	15.5129(5)	8.1248(2)	13.620(3)	8.0112(3)
b (Å)	9.4321(3)	8.5333(2)	14.598(3)	14.1442(5)
c (Å)	17.0231(5)	18.2789(5)	14.730(3)	14.5990(6)
α (°)	90	101.403(2)	90	111.102(2)
β (°)	96.581(2)	91.947(2)	109.446(11)	90.420(2)
γ (°)	90	113.320(2)	90	94.912(2)
V (Å^3)	2474.39(13)	1131.90(5)	2761.6(10)	1536.35(10)
Z	4	2	4	2
D_{calc}(g/cm^3)	1.304	1.378	1.615	1.838
μ (mm^{-1})	0.242	0.351	0.928	1.534
$2\theta_{max}$ (°)	52.00	52.00	52.00	52.00
reflections collected	34005	17939	41930	24334
independent reflections	4856 [R_{int} = 0.0411]	4441 [R_{int} = 0.0308]	5426 [R_{int} = 0.0403]	6024 [R_{int} = 0.0462]
goodness-of-fit on F^2	1.050	1.083	1.036	1.039
R_1, wR_2 [$I > 2\sigma(I)$]	0.0319, 0.0806	0.0308, 0.0791	0.0363, 0.1031	0.0290, 0.0766
R_1, wR_2 (all data)	0.0388, 0.0849	0.0362, 0.0880	0.0521, 0.1144	0.0336, 0.0793

Table S2. Selected bond distances (Å) and bond angles (°) for **1**

Ag1-S1	2.5046(10)	Ag1-S2	2.4698(9)
Ag1-O1	2.724(3)	Ag1-O2	2.748(2)
Ag1-N1	2.280(3)		
S1-Ag1-S2	115.22(3)	S1-Ag1-O1	79.04(5)
S1-Ag1-O2	125.49(5)	S1-Ag1-N1	121.18(7)
S2-Ag1-O1	121.28(5)	S2-Ag1-O2	85.24(5)
S2-Ag1-N1	123.39(7)	O1-Ag1-O2	134.44(7)
O1-Ag1-N1	67.69(9)	O2-Ag1-N1	66.76(9)

Table S3. Selected bond distances (Å) and bond angles (°) for **2**[a]

Ag1-S1	2.8121(7)	Ag1-S2	2.7271(7)
Ag1-S3	2.5777(7)	Ag1-O1	2.8547(18)
Ag1-N1	2.277(2)	Ag2-S1	2.5304(7)
Ag2-S2A	2.5406(7)	Ag2-O3	2.501(3)
Ag2-O4	2.767(3)	Ag2-O6	2.500(2)
S1-Ag1-S2	77.239(19)	S1-Ag1-S3	92.20(2)
S1-Ag1-N1	127.75(5)	S2-Ag1-S3	81.50(2)
S2-Ag1-N1	132.66(6)	S3-Ag1-N1	128.32(6)
S1-Ag2-O3	107.28(8)	S1-Ag2-O6	93.80(5)
S1-Ag2-S2A	143.63(2)	O3-Ag2-O6	89.58(8)
O6-Ag2-S2A	109.80(5)	O3-Ag2-S2A	100.37(8)

[a]symmetry operation A: x-1, y, z.