Electronic Supplementary Material for CrystEngComm

Supplementary Information

Tubular Architectures Formed by Acyclic Diamido-Metal-N-Hetreocyclic Carbenes with Skewed Conformation

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Experimental procedure

1: [*L1*H]Br: A mixture of 1-(2-pyrazinyl)- imidazole (30 mmol) and acetamide bromide (30 mmol) were refluxed in dry acetonitrile overnight. After cooling, the acetonitrile solution was removed by a rotary evaporator and the crude product was recrystallized from methanol to give a white product with a yield of 75%. The PF_6^- salt was obtained from the bromide salt by a simple metathesis reaction with an equivalence of NH_4PF_6. **1**: $Hg(OAc)_2$ (0.09 g, 0.285 mmol) was added to a solution of [*L1*H]PF_6 (0.20 g, 0.57 mmol) in dry acetonitrile (100 mL). After stirring for 16 hrs, the acetonitrile solution was filtered and dried by a rotary evaporator. The solid was washed with methanol and ether with a yield of 77%. Single crystals suitable for X-ray diffraction were obtained by recrystallization from acetonitrile. Calcd. for $HgC_{20}H_{21}N_{11}O_2P_2F_{12}$: C, 25.61; H, 2.26; N, 16.43. Found: C, 25.31; H,2.44; N, 16.89 %.

2: Compound **2** was obtained by the method similar to that of **1** with [*L2*H]PF_6 in place of [*L1*H]PF_6 (yield : 82%). Calcd. for $HgC_{18}H_{18}N_{10}O_2P_2F_{12}$: C, 24.10; H, 2.02; N, 15.62. Found: C, 24.23; H,1.94; N, 15.50 %.

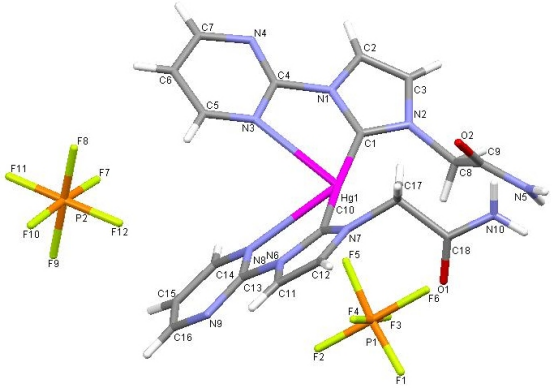
3: Compound **3** was obtained by the method similar to that of **2** with [*L2*H]BF_4 in place of [*L2*H]PF_6 (yield : 80%). Calcd. for $C_{18}H_{18}B_2F_8HgN_{10}O_2$: C, 27.70; H, 2.32; N, 17.94. Found: C, 27.43; H, 2.36; N, 17.85 %.

4: Ag_2O (0.166 g, 7.16 mmole) was added to a solution of [*L2*H]PF_6 (0.50 g,

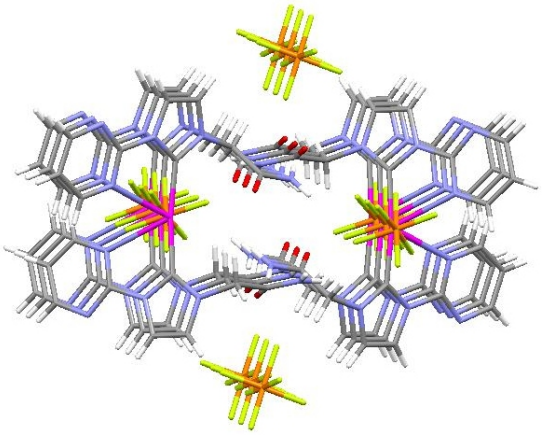
1.43 mmole) in dry acetonitrile (25 mL). After stirring for 72 hrs, the acetonitrile solution was filtered and dried by a rotary evaporator. The solid was washed with methanol and ether (yield : 85%). Single crystals suitable for X-ray diffraction were obtained by recrystallization from DMSO. Calcd. for $C_{22}H_{34}AgF_6N_{10}O_4PS_2$: C, 32.24; H, 4.18; N, 17.09. Found: C, 32.11; H,4.17; N, 17.01 %.

Crystal Structures

(a)



(b)



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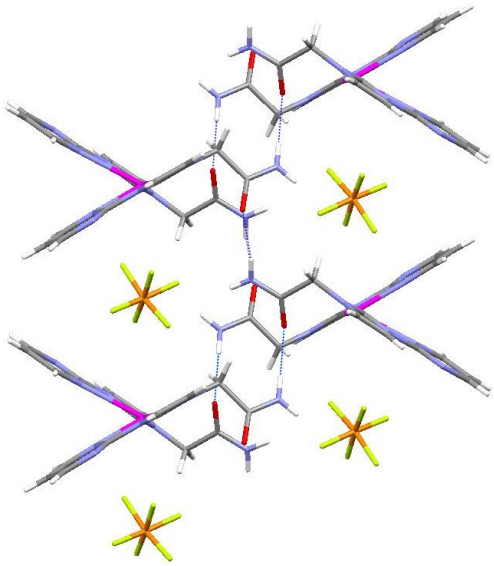
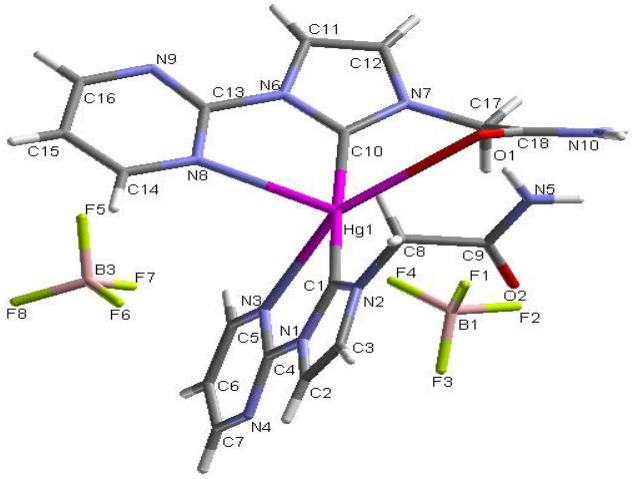


Figure 1. a) Crystal structure of complex **2**; b) Top view and c) Side view of the rectangular tube of **2**. The bond distances and angle of N-H---O hydrogen bond: (N)H---O: 2.05Å, N---O: 2.900(15)Å, N-H---O: 168°.

(a)



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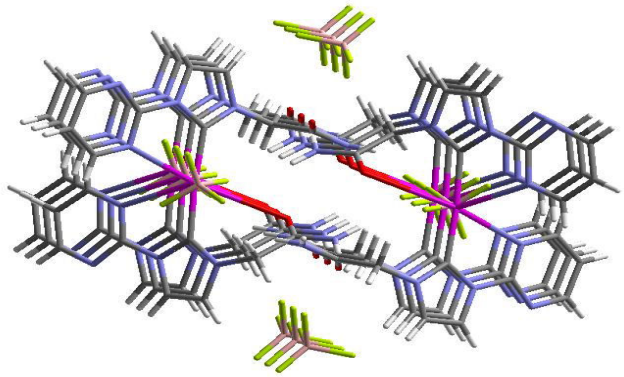


(c)

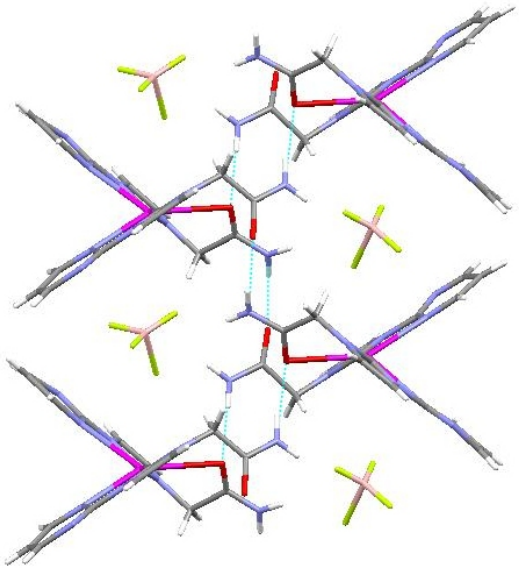
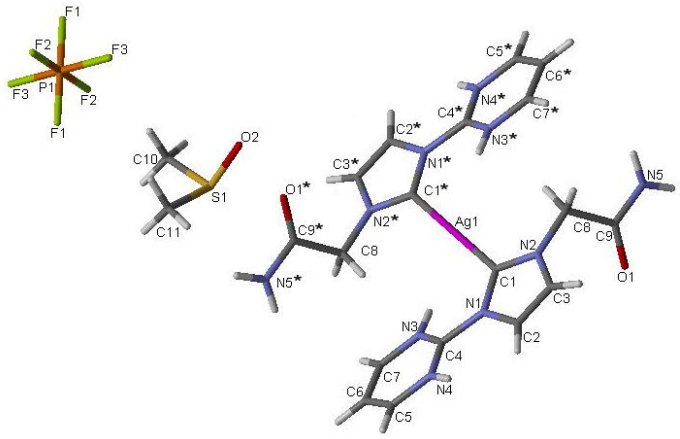


Figure 2. a) Crystal structure of complex **3**; b) Top view and c) Side view of the rectangular tube of **3**. The bond distances and angle of N-H---O hydrogen bond: (N)H---O: 1.99Å, N---O: 2.813(5)Å, N-H---O: 161°.

(a)



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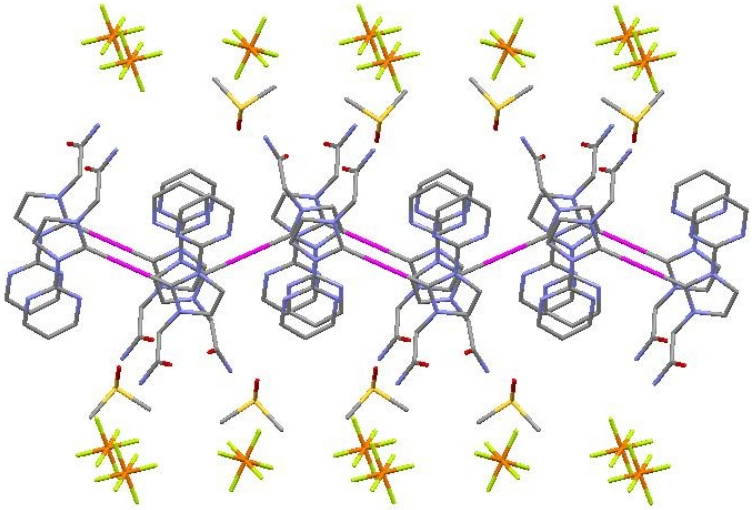

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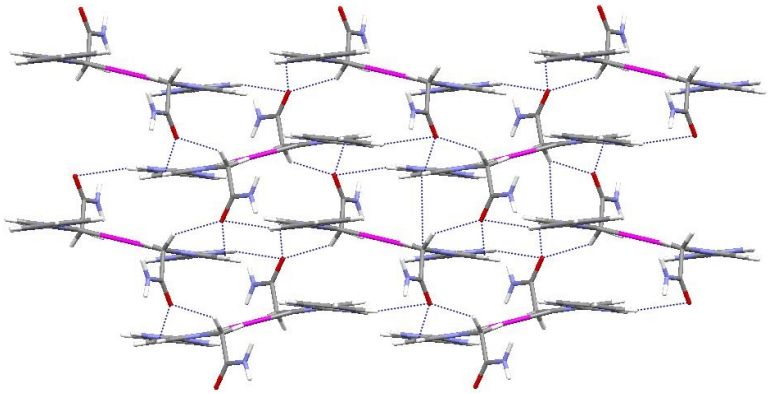

Figure 3. a) Crystal structure of complex **4**; b) two-dimensional layered structure and c) C-H---O hydrogen bonding framework. The Ag atoms are located on inversion centers. Atoms flagged with an asterisk (*) are at equivalent position (1-x,-y,-z)