Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Planar trinuclear complexes with linear arrays of metal ions

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Synthesis of precursor of ligand

1,6-di(ß-pyridyl)-1,3,4,6-hexanetetrone: A solution of sodium ethoxide (prepared from sodium (5.00 g, 217 mmol)), 2-acetylpyridine (26.3 g, 217 mmol), and ethyl oxalate (14.6 g, 100 mmol) in 120 mL of toluene was refluxed for 2 h under a nitrogen atmosphere. The solvent was removed by filtration, and aqueous acetic acid (15%) was added to the residue. The resulting yellow solid (2.4 g) was filtered, and used for the following ring-closure reaction without purification.

Synthesis of ligand

5,5'- pyridyl-3,3'-bi-1H-pyrazolyl (H_2L)

Hydrazine monohydrate (1.35 g, 27.0 mmol) was added to a chloroform solution (100 mL) of crude product of 1,6-di(ß-pyridyl)-1,3,4,6-hexanetetrone (2.0 g, 6.75 mmol), and the mixture was refluxed for 2 h. After cooling the mixed solution, the resulting colorless powder was filtered, and recrystallized from methanol to yield colorless microcrystals (0.72 g, 37 %). ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.6 (s, 2H, pz), 8.64 (d, 2H, py), 7.98-7.87 (m, 4H, py), 7.36 (m, 2H, py), 7.23 (s, 2H, pz). Selected IR (KBr): 3128(w), 1593(s), 1567(s), 1460(s), 1402(s), 1353(s), 1195(s), 1058(s), 994(s), 786(s) cm^{-1}. Anal. Calcd. (found) for $C_{16}H_{13}N_6O_{0.5}$ ($H_2L{\cdot}0.5H_2O$): C, 64.63 (64.76); H, 4.41 (4.36); N, 28.27 (28.11).

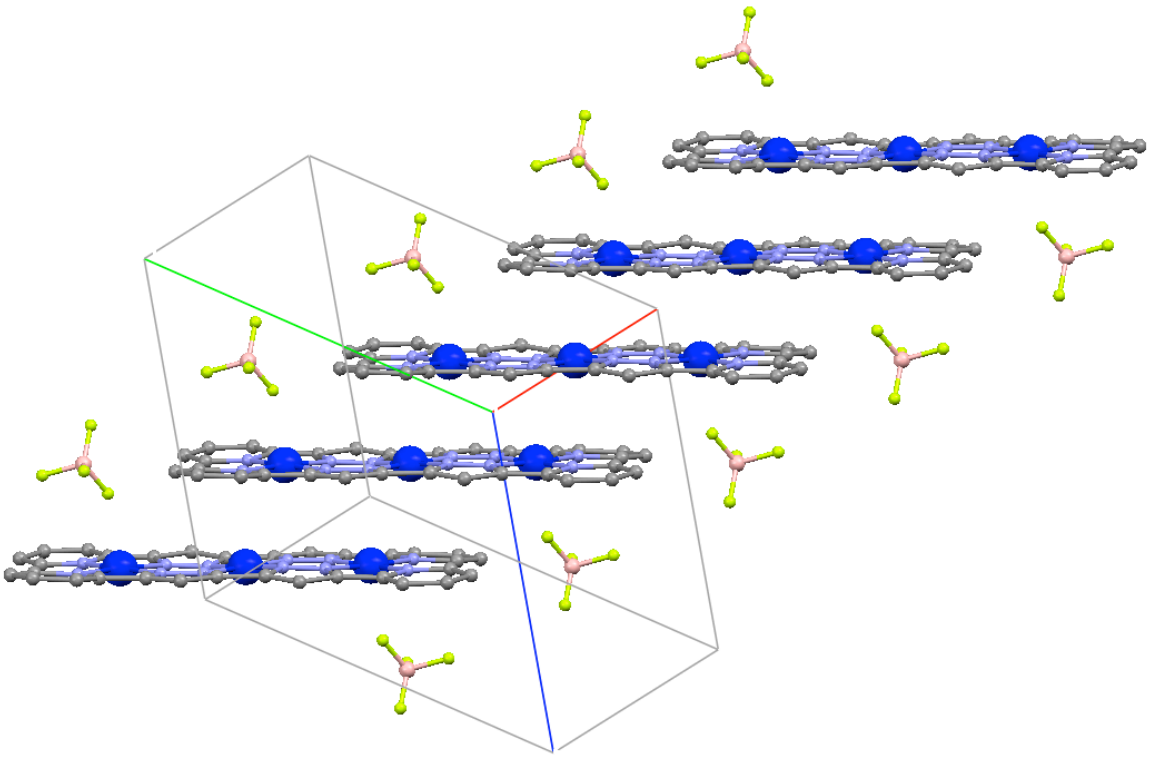

Figure S1. Packing structure of **1**.