Electronic Supplementary Material (ESI) for CrystEngComm

C-H…π synthon repetitivity in coordination compounds, established from single-crystal and powder diffraction

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Experimental

Chemicals and instrumentation

All chemicals were purchased from Aldrich or Merck and used without further purification. The synthesis and recrystallization of **L** and compounds **1**-**3** were carried out in air. Infrared spectra (4000–250 cm^{-1}) of solid sample were taken as 1% dispersion in CsI pellets using a BOMEM - MB102 spectrometer. Elemental analysis was performed using a Heraeus CHN-O Rapid analyzer. ^{1}H NMR spectrum was recorded on a Bruker AC-300 MHz spectrometer at ambient temperature in CD_3OD. All chemical shifts are quoted in part per million (ppm) relative to tetramethylsilane. Melting point was obtained by a Bamstead Electrothermal type 9200 melting point apparatus and corrected.

Synthesis of N-(2-pyrazine)-thiophene-3-acetamide, L.

A solution of 4 mmol 2-aminopyrazine (0.380 g) in 10 mL pyridine was added to a solution of 4 mmol thiophene-3-acetic acid (0.569 g) in 10 mL pyridine. The resulting solution was stirred at 313 K for 20 min, then 4 mmol triphenyl phosphate (1.04 mL) was added dropwise, and the reaction mixture was stirred at 373 K for 5 h and at ambient temperature for 24 h. A brown resulted solution was added to distilled water. A dark solid resulted with a yield of 75%, mp 166˚C. X-ray quality crystals were obtained by slow solvent evaporation in pure methanol at room temperature. ^{1}H NMR (CD_3OD, δ from TMS): 9.39(s, 1H-thiophene), 8.38(s, 1H-thiophene), 8.32(s, 1H-thiophene), 7.41-7.15(m, 3H-pyrazine) and 3.34(s, 2H-CH_2).

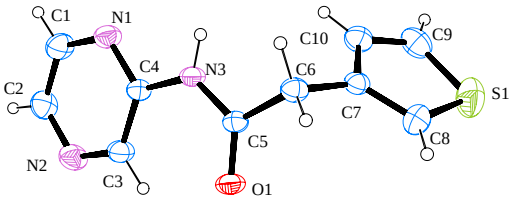

Figure S1. Molecular structure of **L** with the thermal ellipsoids at 30% probability level. H atoms are of arbitrary size.

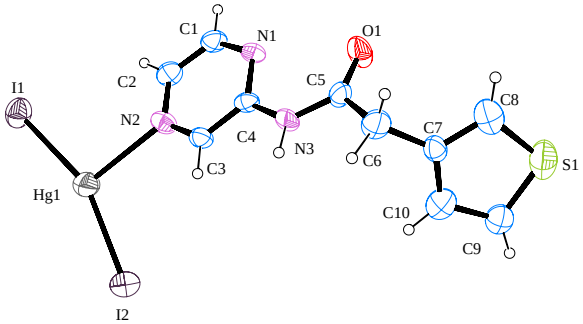

Figure S2. Molecular structure of **3** with the thermal ellipsoids at 30% probability level. H atoms are of arbitrary size.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for **L** and **1**-**3**.

	L	X = Cl	X = Br	X = I
C4-N3	1.399(2)	1.391(8)	1.364(1)	1.369(1)
C14-N6	-	1.378(8)	1.408(1)	-
C5-N3	1.357(2)	1.368(9)	1.370(1)	1.366(2)
C15-N6	-	1.360(8)	1.343(1)	-
C5-O1	1.231(2)	1.205(9)	1.229(1)	1.220(1)
C15-O2	-	1.222(7)	1.204(1)	-
C6-C7	1.494(3)	1.485(1)	1.497(1)	1.505(2)
C16-C17	-	1.501(1)	1.484(1)	-
C4-N3-C5	128.2(1)	126.5(6)	129.2(3)	130.3(8)
C14-N6-C15	-	128.4(5)	126.4(1)	-
N3-C5-O1	123.0(2)	122.2(6)	121.2(2)	123.5(11)
N6-C15-O2	-	122.1(6)	121.7(1)	-
N3-C5-C6	115.0(1)	114.6(6)	115.0(3)	116.2(9)
N6-C15-C16	-	115.0(5)	115.0(2)	-
C5-C6-C7	110.8(1)	114.0(6)	111.9(1)	111.2(10)
C15-C16-C17	-	112.0(6)	114.6(2)	-
C6-C7-C8	124.9(2)	123.2(8)	122.2(1)	123.0(11)
C16-C17-C18	-	123.7(1)	124.1(2)	-
O1-C5-C6-C7	82.9(2)	-0.4(1)	24.3(3)	-62.3(16)
O2-C15-C16-C17	-	87.6(8)	72.8(2)	-
C3-C4-N3-C5	-3.1(3)	-14.7(1)	-41.9(3)	174.9(11)
C13-C14-N6-C15	-	-13.8(1)	6.1(3)	-
C5-C6-C7-C8	-111.8(2)	-108.3(9)	-61.6(2)	93.8(15)
C15-C16-C17-C18	-	140.2(9)	117.0(3)	-
Hg-X1	-	2.324(2)	2.266(1)	2.614 (1)
Hg-X2	-	2.342(2)	2.332(1)	2.607(1)
Hg-N2	-	2.491(5)	2.499(2)	2.476(9)
Hg-N5	-	2.463(6)	2.571(1)	-
X1-Hg-X2	-	158.9(1)	159.7(1)	155.8(4)
X1-Hg-N2	-	99.3(1)	91.9(3)	100.2(2)
N2-Hg1-N5	-	108.1(2)	101.2(3)	-
X1-Hg1-N5	-	98.6(1)	97.2(2)	-
X2-Hg1-N2	-	93.0(1)	99.7(3)	103.7(2)
X2-Hg1-N5	-	93.7(2)	96.8(3)	-