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μ-2,3,5,6-Tetra-2-pyridylpyrazine-bis[dichloromercury(II)]

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.008 Å
R factor = 0.026
wR factor = 0.065
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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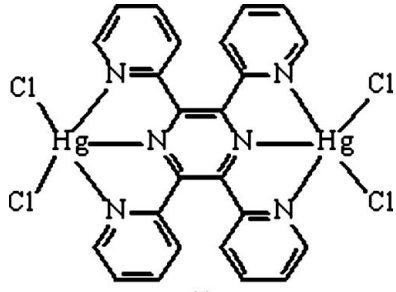
The title complex, μ-2,3,5,6-tetra-2-pyridylpyrazine-$\kappa^4N^2,N^6:N^3,N^5$-bis[dichloromercury(II)], $[Hg_2Cl_4(C_{24}H_{16}N_6)]$, displays a centrosymmetric dinuclear structure, in which the 2,3,5,6-tetra-2-pyridylpyrazine ligand coordinates in a bis-tridentate bridging manner to link two Hg ions that adopt a distorted octahedral coordination geometry including weak intermolecular Hg···Cl coordination.

Comment

Since the synthesis of 2,3,5,6-tetra(2-pyridinyl)pyrazine (tppz) was reported by Goodwin & Lyons (1959), there have been a considerable number of investigations of transition metal complexes containing tppz, as these materials may possess desirable photophysical or magnetic properties. Hence, some mono- and dinuclear and oligomeric transition metal (*e.g.* Re, Ru, Ni, Cu, Zn and Pt) complexes with tppz have been structurally characterized (Graf & Stoeckli-Evans, 1994; Graf *et al.*, 1997; Koman *et al.*, 1998; Hartshorn *et al.*, 1999; Sakai & Kurashima, 2003; Hadadzadeh *et al.*, 2005). In addition, one-, two- and three-dimensional materials constructed from molybdophosphonate (Burkholder *et al.*, 2003) and/or polyoxomolybdate (Allis *et al.*, 2004) subunits linked by binuclear Cu-tppz ligands have also been reported. In these complexes, tppz shows a variety of coordination modes; conformations and binding modes of tppz have been investigated recently by computational analysis (Padgett *et al.*, 2005). Until now, no crystal structures of Hg^{II} complexes of tppz have been documented.



(I)

The title complex, $Hg_2(tppz)Cl_4$, (I), is a neutral and centrosymmetric dinuclear complex (Fig. 1) in which the tppz ligand functions in a bis-tridentate bridging manner to link two Hg ions that are separated by 7.772 (5) Å. Each Hg^{II} center is five-coordinated by three N donors of tppz in one plane and two Cl atoms normal to this plane; the Cl···Hg···Cl angle is 158.88 (5)° (Table 1). However, if one accepts weak intermolecular Hg···Cl($1-x$, $2-y$, $2-z$) interactions of

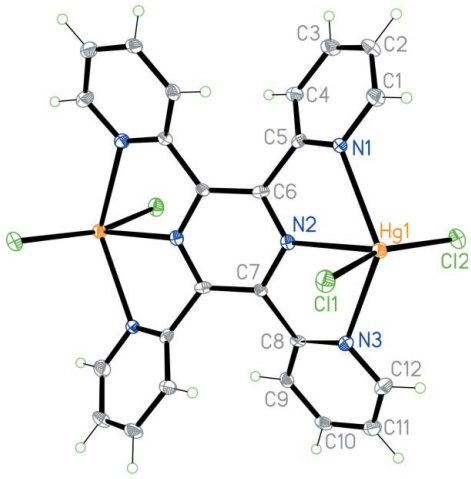


Figure 1
Structure of (I), showing displacement ellipsoids at the 50% probability level. Unlabeled atoms are related to labeled atoms by the symmetry code $(1-x, 1-y, 1-z)$.

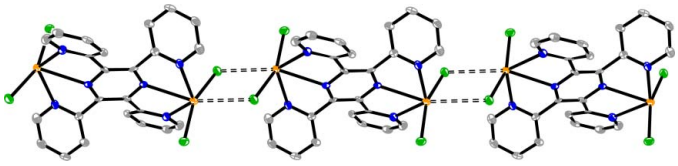


Figure 2
One-dimensional chain formed by weak Hg—Cl interactions (dashed lines); H atoms have been omitted for clarity.

3.265 (4) Å, the coordination geometry can be described as being based on an octahedron. The Hg···Cl weak coordination leads to the formation of a one-dimensional chain (Fig. 2). The two Hg^{II} ions are above and below the plane of the pyrazine ring of the tppz ligand, with the pyridine rings displaced out of the pyrazine plane; the dihedral angles between the pyrazine ring and each of the pyridyl rings are 42.9 (4)° (C1–C5/N1) and 24.3 (3)° (C8–C12/N3).

Experimental

In a test tube, an acetone (4 ml) solution of $HgCl_2$ (54 mg, 0.2 mmol) was carefully layered on top of a chloroform (4 ml) solution of 2,3,5,6-tetra(2-pyridyl)pyrazine (39 mg, 0.1 mmol) using ethylene glycol (2 ml) as an interlayer. After one week at room temperature, colorless block-shaped single crystals suitable for X-ray investigation appeared at the boundary, with a yield of 35%.

Crystal data

$[Hg_2Cl_4(C_{24}H_{16}N_6)]$
M_r = 931.41
Triclinic, $P\overline{1}$
a = 7.2045 (8) Å
b = 9.1939 (10) Å
c = 11.2326 (13) Å
α = 111.030 (2)°
β = 97.764 (2)°
γ = 106.370 (2)°
V = 642.71 (12) Å^3
Z = 1
D_x = 2.406 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3118 reflections
θ = 2.5–28.2°
μ = 12.37 mm^{-1}
T = 100 (2) K
Block, colorless
0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.076, T_{max} = 0.084
3571 measured reflections
2442 independent reflections
2341 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.0°
$h = -8 \rightarrow 6$
$k = -10 \rightarrow 11$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.065
S = 1.11
2442 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg1—Cl1	2.3569 (14)	Hg1—N2	2.610 (4)
Hg1—Cl2	2.3773 (14)	Hg1—N3	2.622 (4)
Hg1—N1	2.539 (4)		
Cl1—Hg1—Cl2	158.88 (5)	Cl2—Hg1—N2	102.98 (10)
Cl1—Hg1—N1	101.93 (11)	Cl2—Hg1—N3	89.52 (11)
Cl1—Hg1—N2	96.42 (10)	N1—Hg1—N2	64.68 (13)
Cl1—Hg1—N3	92.20 (11)	N1—Hg1—N3	126.19 (14)
Cl2—Hg1—N1	93.95 (11)	N2—Hg1—N3	62.25 (13)

H atoms were included in the riding-model approximation [C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The highest and lowest residual electron-density peaks are located 0.98 and 0.97 Å from atom Hg1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* and *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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