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#### Key indicators

Single-crystal X-ray study  
T = 120 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
R factor = 0.024  
wR factor = 0.062  
Data-to-parameter ratio = 16.3

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

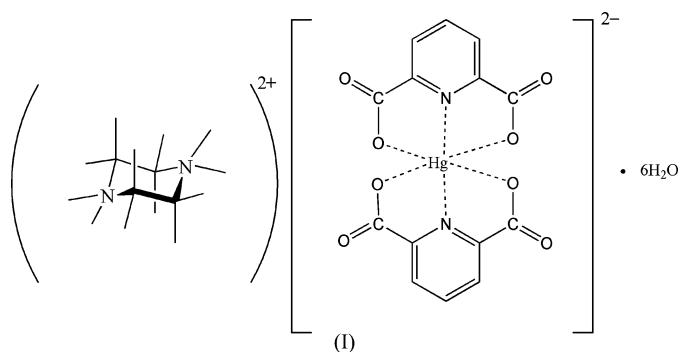
## Piperazinium bis(pyridine-2,6-dicarboxylato)-mercurate(II) hexahydrate

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The reaction of mercury(II) nitrate with the proton-transfer compound  $(\text{pipzH}_2)(\text{pydc})$ , where  $\text{pipz}$  is piperazine and  $\text{pydcH}_2$  is pyridine-2,6-dicarboxylic acid, in aqueous solution leads to the formation of the title compound,  $(\text{pipzH}_2)[\text{Hg}(\text{pydc})_2] \cdot 6\text{H}_2\text{O}$  or  $(\text{C}_4\text{H}_{12}\text{N}_2)[\text{Hg}(\text{C}_7\text{H}_3\text{NO}_4)_2] \cdot 6\text{H}_2\text{O}$ . The structure features six-coordinate  $\text{Hg}^{2+}$  (site symmetry 2) with a distorted octahedral geometry. Extensive intermolecular  $\text{O}-\text{H} \cdots \text{O}$ ,  $\text{N}-\text{H} \cdots \text{O}$  and  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonding involving the  $(\text{pydc})^{2-}$  ligand,  $(\text{pipzH}_2)^{2+}$  (site symmetry 2) as a counter-ion and uncoordinated water molecules forms a three-dimensional network.

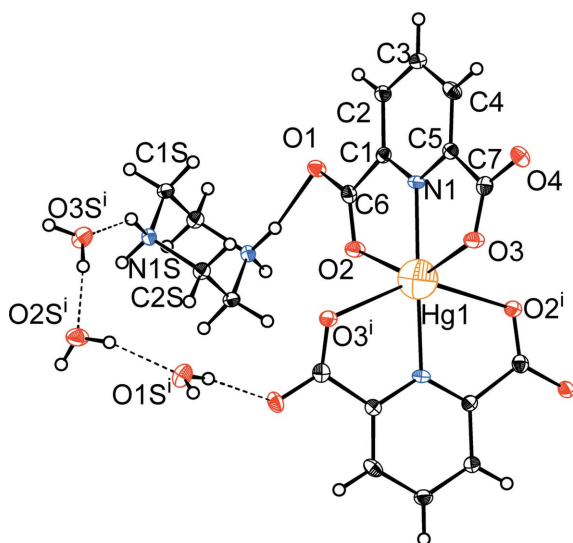
#### Comment

There are several studies on proton transfer between a carboxylic acid and a heterocyclic amine (Smith *et al.*, 2001, 2005; Lynch *et al.*, 1994). Continuing our research on proton-transfer systems, we have found a certain route to combine a carboxylic acid with an amine and produce some water-soluble self-associating ion pair systems, which can react with metal ions and result in different complexes (Aghabozorg, Ghadermazi & Ramezani-pour, 2006; Soleimannejad *et al.*, 2005; Moghimi, Aghabozorg *et al.*, 2005; Moghimi *et al.*, 2002, 2003; Aghabozorg, Akbari Saei & Ramezani-pour, 2005).



The resulting compounds with some remaining sites as electron donors can coordinate to many metallic ions (Aghabozorg, Nakhjavan *et al.*, 2006; Aghabozorg, Ghadermazi, Manteghi & Nakhjavan, 2006; Sheshmani *et al.*, 2006; Moghimi, Sheshmani *et al.*, 2005; Moghimi, Sharif *et al.*, 2005; Aghabozorg, Moghimi *et al.*, 2005; Aghabozorg, Dalir Kheir-ollahi *et al.*, 2005; Moghimi, Alizadeh *et al.*, 2005; Ramezani-pour *et al.*, 2005).

Here, we report the molecular structure of the title complex,  $(\text{pipzH}_2)[\text{Hg}(\text{pydc})_2] \cdot 6\text{H}_2\text{O}$ , (I) ( $\text{pipz}$  is piperazine and  $\text{pydcH}_2$  is pyridine-2,6-dicarboxylic acid). The structure of (I) is shown in Fig. 1; selected bond lengths are given in


**Figure 1**

The structure of (I), with displacement ellipsoids at the 50% probability level. [Symmetry code: (i)  $-x + 1, y, -z + \frac{1}{2}$ ] All unlabeled atoms of the complex and the cation are obtained by applying symmetry operation i.

Table 1. Hg<sup>2+</sup> (site symmetry 2) is six-coordinated by two (pydc)<sup>2-</sup> groups, *i.e.* each (pydc)<sup>2+</sup> coordinates through one N atom of the pyridine ring and two O atoms of (COO)<sup>-</sup> fragments. Atoms N1 and N1<sup>i</sup> of the two pydc fragments occupy the axial positions, and atoms O2, O2<sup>i</sup>, O3 and O3<sup>i</sup> form the equatorial plane. The Hg–N bond length is 2.198 (4) Å and the Hg–O distances are in the range 2.468 (3)–2.471 (3) Å, which are similar to those of the {[pyda-H][HgCl(pydc)·H<sub>2</sub>O]<sub>n</sub>} (pyda is pyridine-2,6-diamine) complex [Hg–N = 2.184 (6) Å] reported previously by our research team (Moghimi, Shokrollahi *et al.*, 2004). The N1–Hg–N1<sup>i</sup> angle deviates slightly from linearity [175.08 (16)°]. The coordination geometry about the central atom is thus distorted octahedral. The charge of the anionic complex is compensated by a piperazinium ion as counter-ion. A remarkable feature in the crystal structure of compound (I) is the presence of a large number of O–H···O and O–H···N hydrogen bonds (Table 2), with *D*···*A* distances ranging from 2.734 (4) to 2.839 (4) Å. A number of C–H···O interactions were also identified in PLATON (Spek, 2003) between CH groups of piperazinium ions and (COO)<sup>-</sup> groups of (pydc)<sup>2-</sup> fragments in addition to water molecules, although their chemical significance is uncertain. These interactions link the ions to form a three-dimensional network, as shown in Fig. 2. Dipole-dipole and van der Waals interactions help to stabilize the packing in the crystal structure.

## Experimental

The proton-transfer ion pair was prepared by a reaction between piperazine and pyridine-2,6-dicarboxylic acid. Starting with a 1:1 molar ratio of the reactants in THF, a puffy white precipitate was obtained. By recrystallization in an aqueous solution, pale-yellow crystals were obtained (Aghabozorg, Ghadermazi, Manteghi & Nakhjavan, 2006). Aqueous solutions of proton-transfer compound

(pipzH<sub>2</sub>)(pydc) (1 mmol, 0.253 g) and mercury(II) nitrate monohydrate (0.5 mmol, 0.171 g) were stirred at room temperature; the complexation reaction was complete after 30 minutes (opaque reaction mixture became transparent). Colorless crystals of compound (I) were obtained after four weeks at room temperature.

### Crystal data

(C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>)[Hg(C<sub>7</sub>H<sub>3</sub>NO<sub>4</sub>)<sub>2</sub>]·6H<sub>2</sub>O  
*M<sub>r</sub>* = 727.05  
 Orthorhombic, *Pbcn*  
*a* = 13.444 (7) Å  
*b* = 8.377 (4) Å  
*c* = 22.512 (13) Å  
*V* = 2535 (2) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.905 Mg m<sup>-3</sup>  
 Mo Kα radiation  
 $\mu$  = 6.15 mm<sup>-1</sup>  
*T* = 120 (2) K  
 Prism, colorless  
 0.19 × 0.16 × 0.14 mm

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1998)  
*T<sub>min</sub>* = 0.303, *T<sub>max</sub>* = 0.427

16680 measured reflections  
 2731 independent reflections  
 1739 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.045  
 $\theta_{\max}$  = 27.0°

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.024  
*wR* (*F*<sup>2</sup>) = 0.062  
*S* = 0.97  
 2731 reflections  
 168 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0328P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 2.66 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -1.19 \text{ e } \text{Å}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Hg1–N1	2.198 (4)	O2–C6	1.257 (5)
Hg1–O2	2.471 (3)	O3–C7	1.254 (5)
Hg1–O3	2.468 (3)	O4–C7	1.253 (4)
O1–C6	1.252 (4)		
N1–Hg1–N1 <sup>i</sup>	175.08 (16)	O2–Hg1–O2 <sup>i</sup>	104.86 (14)
N1–Hg1–O3	71.55 (10)	O1–C6–O2	124.9 (4)
N1 <sup>i</sup> –Hg1–O3	111.75 (10)	O1–C6–C1	116.8 (4)
O3 <sup>i</sup> –Hg1–O3	101.90 (14)	O2–C6–C1	118.3 (3)
N1–Hg1–O2	71.51 (10)	O4–C7–O3	126.2 (4)
N1 <sup>i</sup> –Hg1–O2	105.36 (10)	O4–C7–C5	115.8 (4)
O3–Hg1–O2	142.87 (9)	O3–C7–C5	118.0 (3)
O3–Hg1–O2 <sup>i</sup>	88.33 (10)		
N1–Hg1–O2–C6	–3.7 (3)	Hg1–O2–C6–O1	–176.1 (3)
N1–Hg1–O3–C7	–12.1 (3)	Hg1–O3–C7–O4	–167.1 (3)

Symmetry code: (i)  $-x + 1, y, -z + \frac{1}{2}$ .

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1S–H1SD···O1 <sup>ii</sup>	0.92	1.84	2.753 (4)	169
N1S–H1SD···O3S <sup>ci</sup>	0.92	1.99	2.765 (4)	141
O1S–H1SB···O4 <sup>iii</sup>	0.82	2.01	2.823 (4)	170
O1S–H1SA···O4	0.82	1.93	2.734 (4)	166
O2S–H2SB···O1S	0.82	1.95	2.756 (4)	165
O2S–H2SA···O1 <sup>iv</sup>	0.82	1.99	2.805 (4)	174
O3S–H3SB···O3 <sup>v</sup>	0.82	2.04	2.839 (4)	164
O3S–H3SA···O2S	0.82	1.97	2.792 (4)	174

Symmetry codes: (i)  $-x + 1, y, -z + \frac{1}{2}$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $-x + \frac{1}{2}, y + \frac{1}{2}, z$ ; (iv)  $-x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$ ; (v)  $-x + 1, -y + 2, -z$ .

The highest and deepest residual electron-density peaks in the difference Fourier synthesis is located 0.89 Å from Hg1; it is probably due to considerable absorption effects which could not be completely corrected.

The H atoms of the NH<sub>2</sub> groups and water molecules were found in difference Fourier syntheses (N–H = 0.92 Å and O–H = 0.82 Å). The H(C) atom positions were calculated (C–H = 0.95–0.99 Å). All H atoms were refined in isotropic approximation in a riding model with the  $U_{\text{iso}}(\text{H})$  parameters equal to  $1.2U_{\text{eq}}$  of the respective carrier atom.

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

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