

Dichloridobis(1,10-phenanthroline-5,6-dione- κ^2N,N')mercury(II)

Carlos A. L. Figueiras,^a João A. S. Bomfim,^a R. Alan Howie,^b Edward R. T. Tiekink^{c*} and James L. Wardell^{d‡}

^aDepartamento de Química Inorgânica, Instituto de Química, Universidade Federal do Rio de Janeiro, CP 68563, 21941-909 Rio de Janeiro, RJ, Brazil, ^bDepartment of Chemistry, University of Aberdeen, Old Aberdeen, AB15 5NY, Scotland, ^cDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and ^dDepartamento de Química, ICEx, Universidade Federal de Minas Gerais, 31270-901 Belo Horizonte, MG, Brazil

Correspondence e-mail: edward.tiekink@gmail.com

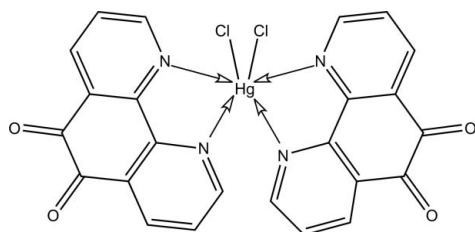
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.012$ Å; R factor = 0.037; wR factor = 0.094; data-to-parameter ratio = 15.6.

In the title compound, $[\text{HgCl}_2(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_2)_2]$, the Hg^{II} atom is located on a twofold rotation axis and exists within a distorted octahedral geometry defined by a *cis*- Cl_2N_4 donor set. Molecules are connected into layers in the *ac* plane via extensive $\text{C}-\text{H}\cdots\text{Cl}$ contacts as each Cl atom forms two such interactions. Contacts between the layers are of the type $\text{C}=\text{O}\cdots\pi$ [$\text{O}\cdots$ centroid distance = 3.110 (8) Å].

Related literature

For related main-group compounds of 1,10-phenanthroline-5,6-dione, see: de Alencastro *et al.* (2005). For the ligand synthesis, see: Yamada *et al.* (1992). For a related structure, see: Ramezanipour *et al.* (2005).



Experimental

Crystal data

$[\text{HgCl}_2(\text{C}_{12}\text{H}_6\text{N}_2\text{O}_2)_2]$	$V = 4427.12$ (19) Å ³
$M_r = 691.87$	$Z = 8$
Orthorhombic, <i>Fdd2</i>	Mo $K\alpha$ radiation
$a = 8.2261$ (2) Å	$\mu = 7.24$ mm ⁻¹
$b = 42.6761$ (11) Å	$T = 120$ K
$c = 12.6108$ (3) Å	$0.20 \times 0.10 \times 0.06$ mm

‡ Additional correspondence author, e-mail: j.wardell@abdn.ac.uk.

Data collection

Nonius KappaCCD diffractometer	10751 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	2487 independent reflections
$T_{\text{min}} = 0.204$, $T_{\text{max}} = 0.651$	2239 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.094$	$\Delta\rho_{\text{max}} = 2.27$ e Å ⁻³
$S = 1.05$	$\Delta\rho_{\text{min}} = -0.68$ e Å ⁻³
2487 reflections	Absolute structure: Flack (1983), 1163 Friedel pairs
159 parameters	Flack parameter: -0.012 (13)
1 restraint	

Table 1

Selected bond lengths (Å).

Hg—N1	2.439 (7)	Hg—Cl1	2.5270 (19)
Hg—N2	2.512 (6)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C2}-\text{H2}\cdots\text{Cl1}^i$	0.95	2.69	3.578 (8)	156
$\text{C9}-\text{H9}\cdots\text{Cl1}^{ii}$	0.95	2.78	3.701 (8)	164

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2254).

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supplementary materials

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Comment

In continuation of the previous studies of coordination compounds of 1,10-phenanthroline-5,6-dione (pdon) ligand (de Alencastro *et al.*, 2005), the title compound, $\text{HgCl}_2(\text{pdon})_2$, was investigated. The reaction of HgCl_2 with pdon (1:1 mol ratio) led to the isolation of a pure 1:1 complex, $\text{HgCl}_2(\text{pdon})$. However, as the product was unsuitable for X-ray crystallography, a further recrystallization from MeNO_2 solution was attempted, which led to the isolation of the title compound, a 1:2 complex. Of interest was that the 1:1 $\text{HgI}_2(\text{pdon})$ complex, prepared similarly to the chloride analogue, was recovered on recrystallization from MeNO_2 . Unfortunately this set of crystals also proved unsuitable for X-ray crystallography.

In the title compound, the Hg^{II} atom lies on a crystallographic twofold axis and exists within a *cis*- Cl_2N_4 donor set defined by two Cl atoms and four N atoms derived from two chelating pdon ligands (Fig. 1). There is a small disparity in the magnitude of the Hg—N bond distances, with Hg—N1 of 2.439 (7) Å being shorter than Hg—N2 of 2.512 (6) Å. Distortions from an ideal octahedral geometry are related in part to the acute chelate angle of 66.9 (2)°. The pdon ligand is essentially planar with a RMS of 0.226 Å for the N and C atoms, with O1 and O2 atoms lying, respectively, -0.079 (12) and 0.071 (13) Å out of the least-squares plane. The dihedral angle formed between the symmetry related 1,10-phenanthroline planes is 87.13 (11)°. The structural features described herein for the title compound resemble those found for $\text{HgCl}_2(1,10\text{-phenanthroline})_2$ (Ramezanipour *et al.*, 2005).

In the crystal structure, C—H \cdots Cl interactions are found so that each Cl atom is associated with two H atoms to form supramolecular arrays in the *ac* plane (Table 1 and Fig. 2). The most prominent interactions between the layers are of the type C=O $\cdots\pi$. The closest of these involves the carbonyl-O1 group and the centroid (*Cg*) of C4—C7, C11, C12 ring [O1 \cdots Cgⁱ = 3.110 (8) Å with the C5—O1 \cdots Cgⁱ angle being 133.1 (8)°, symmetry code: (i) -1/4+x, 1/4-y, -1/4+z] (Fig. 3).

Experimental

Solutions of HgCl_2 (0.272 mg, 1.0 mmol) in EtOH (5 ml) and of 1,10-phenanthroline-5,6-dione (Yamada *et al.*, 1992) (0.212 mg, 1.0 mmol) in EtOH (20 ml) were mixed and stirred at room temperature for 1 h. The precipitate was collected, washed with small portions of EtOH and petroleum ether and dried (yield 0.330 mg). Analysis, calculated for $\text{C}_{12}\text{H}_6\text{Cl}_2\text{HgN}_2\text{O}_2$ [$\text{HgCl}_2(\text{pdon})$]: C 29.9, H 1.3, N 5.8%; found: C 30.2, H 1.5, N 5.2%.

Recrystallization of $\text{HgCl}_2(\text{pdon})$ from MeNO_2 solution produced crystals of the title compound, $\text{HgCl}_2(\text{pdon})_2$.

Refinement

H atoms were geometrically placed with C—H = 0.95 Å, and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The maximum and minimum residual electron density peaks of 2.27 and 0.68 e Å⁻³ were located 0.91 and 0.82 Å from Hg atom, respectively.

Figures

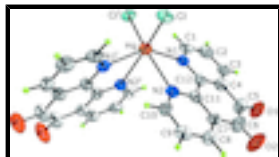


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x, -y, z$.]

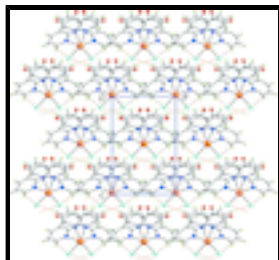


Fig. 2. Supramolecular array in the ac plane mediated by C—H \cdots Cl contacts (orange dashed lines). [Colour codes: Hg orange; Cl cyan; O red; N blue; C grey; H green.]

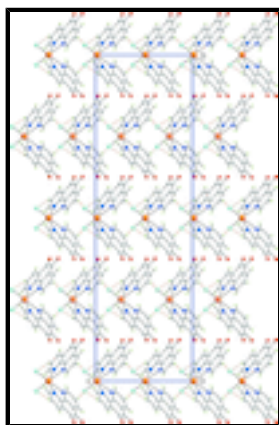


Fig. 3. Unit-cell contents viewed in projection down the a axis. The C—H \cdots Cl contacts are shown as orange dashed lines. [Colour codes: Hg orange; Cl cyan; O red; N blue; C grey; H green.]

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Crystal data

[HgCl₂(C₁₂H₆N₂O₂)₂]

M_r = 691.87

Orthorhombic, $Fdd2$

Hall symbol: $F\ 2\ -2d$

a = 8.2261 (2) Å

b = 42.6761 (11) Å

c = 12.6108 (3) Å

V = 4427.12 (19) Å³

Z = 8

F_{000} = 2640

D_x = 2.076 Mg m⁻³

Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 18660 reflections

θ = 2.9–27.5°

μ = 7.24 mm⁻¹

T = 120 K

Block, yellow

0.20 × 0.10 × 0.06 mm

Data collection

Nonius KappaCCD
diffractometer

Radiation source: Enraf Nonius FR591 rotating anode

2487 independent reflections

2239 reflections with $I > 2\sigma(I)$

Monochromator: 10 cm confocal mirrors $R_{\text{int}} = 0.075$
 Detector resolution: 9.091 pixels mm^{-1} $\theta_{\text{max}} = 27.5^\circ$
 $T = 120$ K $\theta_{\text{min}} = 3.0^\circ$
 φ and ω scans $h = -10 \rightarrow 8$
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $k = -55 \rightarrow 55$
 $T_{\text{min}} = 0.204$, $T_{\text{max}} = 0.651$ $l = -16 \rightarrow 16$
 10751 measured reflections

Refinement

Refinement on F^2 Hydrogen site location: inferred from neighbouring sites
 Least-squares matrix: full H-atom parameters constrained
 $R[F^2 > 2\sigma(F^2)] = 0.037$ $w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 3.1352P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.094$ $(\Delta/\sigma)_{\text{max}} < 0.001$
 $S = 1.05$ $\Delta\rho_{\text{max}} = 2.27 \text{ e } \text{\AA}^{-3}$
 2487 reflections $\Delta\rho_{\text{min}} = -0.68 \text{ e } \text{\AA}^{-3}$
 159 parameters Extinction correction: none
 1 restraint Absolute structure: Flack (1983), 1163 Friedel pairs
 Primary atom site location: structure-invariant direct methods Flack parameter: -0.012 (13)
 Secondary atom site location: difference Fourier map

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg	0.0000	0.0000	0.48512 (8)	0.04052 (12)
Cl1	0.1811 (2)	0.03035 (5)	0.61020 (15)	0.0486 (4)
O1	-0.3649 (8)	0.12440 (15)	0.2228 (6)	0.072 (2)
O2	-0.0592 (10)	0.12581 (18)	0.1361 (7)	0.081 (2)
N1	-0.2157 (8)	0.03565 (16)	0.4299 (5)	0.0406 (14)
N2	0.0815 (7)	0.03486 (14)	0.3337 (4)	0.0399 (13)
C1	-0.3618 (9)	0.03505 (19)	0.4754 (6)	0.0472 (16)
H1	-0.3840	0.0191	0.5258	0.057*
C2	-0.4837 (9)	0.0567 (2)	0.4528 (7)	0.050 (2)
H2	-0.5869	0.0554	0.4864	0.060*
C3	-0.4507 (11)	0.07993 (18)	0.3806 (6)	0.0459 (17)
H3	-0.5300	0.0955	0.3653	0.055*
C4	-0.3014 (10)	0.08061 (18)	0.3300 (6)	0.0435 (16)
C5	-0.2664 (10)	0.1051 (2)	0.2493 (14)	0.057 (3)
C6	-0.0923 (11)	0.1052 (2)	0.1979 (8)	0.059 (2)
C7	0.0217 (9)	0.0800 (2)	0.2297 (7)	0.0450 (17)
C8	0.1742 (11)	0.0790 (2)	0.1830 (6)	0.0482 (18)
H8	0.2071	0.0945	0.1335	0.058*
C9	0.2777 (9)	0.0545 (2)	0.2110 (6)	0.0453 (18)
H9	0.3818	0.0526	0.1792	0.054*

supplementary materials

C10	0.2257 (10)	0.03325 (19)	0.2861 (7)	0.0437 (17)
H10	0.2965	0.0166	0.3047	0.052*
C11	-0.0196 (9)	0.05763 (18)	0.3047 (6)	0.0409 (16)
C12	-0.1850 (9)	0.05809 (16)	0.3578 (7)	0.0413 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg	0.03662 (19)	0.04817 (18)	0.03677 (16)	0.00021 (19)	0.000	0.000
C11	0.0400 (9)	0.0635 (11)	0.0424 (9)	-0.0042 (8)	-0.0003 (8)	-0.0077 (8)
O1	0.062 (4)	0.064 (4)	0.091 (5)	0.015 (3)	0.005 (4)	0.029 (4)
O2	0.055 (4)	0.082 (5)	0.106 (6)	0.016 (4)	0.016 (4)	0.049 (4)
N1	0.042 (3)	0.046 (3)	0.034 (3)	-0.003 (3)	0.004 (2)	-0.003 (3)
N2	0.035 (3)	0.049 (3)	0.036 (3)	0.003 (3)	0.000 (2)	-0.001 (2)
C1	0.039 (4)	0.064 (4)	0.039 (3)	-0.007 (3)	-0.002 (3)	-0.005 (4)
C2	0.033 (4)	0.069 (5)	0.047 (4)	-0.006 (3)	0.001 (3)	-0.010 (3)
C3	0.044 (4)	0.047 (4)	0.047 (4)	0.006 (3)	-0.004 (3)	-0.011 (3)
C4	0.032 (3)	0.053 (4)	0.045 (4)	0.001 (3)	-0.006 (3)	-0.004 (3)
C5	0.048 (5)	0.055 (4)	0.067 (10)	0.002 (4)	-0.011 (5)	0.012 (5)
C6	0.052 (5)	0.059 (5)	0.067 (5)	0.000 (4)	-0.008 (4)	0.012 (4)
C7	0.044 (4)	0.048 (4)	0.043 (4)	-0.003 (3)	0.004 (3)	-0.001 (3)
C8	0.050 (5)	0.052 (4)	0.043 (4)	-0.004 (3)	-0.001 (3)	0.007 (3)
C9	0.037 (4)	0.062 (5)	0.038 (4)	-0.011 (3)	0.001 (3)	-0.007 (3)
C10	0.047 (5)	0.042 (4)	0.042 (4)	0.005 (3)	-0.007 (3)	-0.001 (3)
C11	0.043 (4)	0.042 (4)	0.038 (3)	0.000 (3)	-0.002 (3)	-0.009 (3)
C12	0.039 (4)	0.040 (3)	0.045 (3)	0.000 (3)	-0.009 (3)	-0.002 (3)

Geometric parameters (\AA , $^\circ$)

Hg—N1	2.439 (7)	C3—H3	0.9500
Hg—N2	2.512 (6)	C4—C12	1.401 (11)
Hg—C11	2.5270 (19)	C4—C5	1.487 (15)
O1—C5	1.203 (11)	C5—C6	1.572 (14)
O2—C6	1.206 (11)	C6—C7	1.483 (12)
N1—C1	1.332 (10)	C7—C11	1.386 (12)
N1—C12	1.344 (10)	C7—C8	1.387 (12)
N2—C11	1.330 (10)	C8—C9	1.392 (12)
N2—C10	1.331 (10)	C8—H8	0.9500
C1—C2	1.393 (12)	C9—C10	1.380 (11)
C1—H1	0.9500	C9—H9	0.9500
C2—C3	1.374 (13)	C10—H10	0.9500
C2—H2	0.9500	C11—C12	1.516 (11)
C3—C4	1.384 (11)		
N1—Hg—N1 ⁱ	146.8 (3)	C4—C3—H3	120.1
N1—Hg—N2 ⁱ	87.6 (2)	C3—C4—C12	118.4 (8)
N1 ⁱ —Hg—N2 ⁱ	66.9 (2)	C3—C4—C5	120.1 (7)
N1—Hg—N2	66.9 (2)	C12—C4—C5	121.4 (7)
N1 ⁱ —Hg—N2	87.6 (2)	O1—C5—C4	122.8 (9)

N2 ⁱ —Hg—N2	81.0 (3)	O1—C5—C6	119.8 (11)
N1—Hg—C11	106.71 (16)	C4—C5—C6	117.4 (8)
N1 ⁱ —Hg—C11	93.95 (16)	O2—C6—C7	124.1 (9)
N2 ⁱ —Hg—C11	159.31 (13)	O2—C6—C5	118.3 (9)
N2—Hg—C11	90.78 (14)	C7—C6—C5	117.5 (8)
N1—Hg—C11 ⁱ	93.95 (16)	C11—C7—C8	119.4 (8)
N1 ⁱ —Hg—C11 ⁱ	106.71 (16)	C11—C7—C6	122.0 (7)
N2 ⁱ —Hg—C11 ⁱ	90.78 (14)	C8—C7—C6	118.6 (8)
N2—Hg—C11 ⁱ	159.31 (13)	C7—C8—C9	117.9 (8)
C11—Hg—C11 ⁱ	102.75 (10)	C7—C8—H8	121.0
C1—N1—C12	118.3 (7)	C9—C8—H8	121.0
C1—N1—Hg	121.4 (5)	C10—C9—C8	118.6 (7)
C12—N1—Hg	120.0 (5)	C10—C9—H9	120.7
C11—N2—C10	118.1 (7)	C8—C9—H9	120.7
C11—N2—Hg	118.3 (5)	N2—C10—C9	123.5 (7)
C10—N2—Hg	123.4 (5)	N2—C10—H10	118.3
N1—C1—C2	123.3 (8)	C9—C10—H10	118.3
N1—C1—H1	118.4	N2—C11—C7	122.5 (7)
C2—C1—H1	118.4	N2—C11—C12	116.7 (7)
C3—C2—C1	118.2 (7)	C7—C11—C12	120.8 (7)
C3—C2—H2	120.9	N1—C12—C4	122.0 (8)
C1—C2—H2	120.9	N1—C12—C11	117.3 (7)
C2—C3—C4	119.8 (7)	C4—C12—C11	120.7 (7)
C2—C3—H3	120.1		
N1 ⁱ —Hg—N1—C1	135.2 (6)	C4—C5—C6—C7	2.9 (16)
N2 ⁱ —Hg—N1—C1	96.6 (6)	O2—C6—C7—C11	177.0 (10)
N2—Hg—N1—C1	177.8 (6)	C5—C6—C7—C11	-2.3 (14)
C11—Hg—N1—C1	-98.6 (6)	O2—C6—C7—C8	-2.6 (15)
C11 ⁱ —Hg—N1—C1	5.9 (6)	C5—C6—C7—C8	178.0 (9)
N1 ⁱ —Hg—N1—C12	-50.0 (5)	C11—C7—C8—C9	2.5 (12)
N2 ⁱ —Hg—N1—C12	-88.6 (6)	C6—C7—C8—C9	-177.8 (8)
N2—Hg—N1—C12	-7.4 (5)	C7—C8—C9—C10	-2.2 (12)
C11—Hg—N1—C12	76.2 (6)	C11—N2—C10—C9	2.3 (12)
C11 ⁱ —Hg—N1—C12	-179.2 (5)	Hg—N2—C10—C9	-172.5 (6)
N1—Hg—N2—C11	7.4 (5)	C8—C9—C10—N2	-0.2 (12)
N1 ⁱ —Hg—N2—C11	165.7 (5)	C10—N2—C11—C7	-1.9 (11)
N2 ⁱ —Hg—N2—C11	98.7 (5)	Hg—N2—C11—C7	173.2 (6)
C11—Hg—N2—C11	-100.4 (5)	C10—N2—C11—C12	177.9 (7)
C11 ⁱ —Hg—N2—C11	30.9 (8)	Hg—N2—C11—C12	-7.0 (8)
N1—Hg—N2—C10	-177.7 (6)	C8—C7—C11—N2	-0.5 (12)
N1 ⁱ —Hg—N2—C10	-19.5 (6)	C6—C7—C11—N2	179.8 (8)
N2 ⁱ —Hg—N2—C10	-86.5 (6)	C8—C7—C11—C12	179.7 (7)
C11—Hg—N2—C10	74.4 (6)	C6—C7—C11—C12	0.0 (12)
C11 ⁱ —Hg—N2—C10	-154.2 (5)	C1—N1—C12—C4	0.1 (11)
C12—N1—C1—C2	-0.6 (12)	Hg—N1—C12—C4	-174.9 (5)

supplementary materials

Hg—N1—C1—C2	174.3 (6)	C1—N1—C12—C11	-178.1 (6)
N1—C1—C2—C3	-0.5 (12)	Hg—N1—C12—C11	6.9 (9)
C1—C2—C3—C4	2.2 (12)	C3—C4—C12—N1	1.6 (11)
C2—C3—C4—C12	-2.7 (11)	C5—C4—C12—N1	-179.4 (9)
C2—C3—C4—C5	178.2 (9)	C3—C4—C12—C11	179.8 (7)
C3—C4—C5—O1	-2.1 (18)	C5—C4—C12—C11	-1.2 (13)
C12—C4—C5—O1	178.8 (11)	N2—C11—C12—N1	0.3 (10)
C3—C4—C5—C6	177.9 (9)	C7—C11—C12—N1	-179.9 (7)
C12—C4—C5—C6	-1.1 (16)	N2—C11—C12—C4	-178.0 (7)
O1—C5—C6—O2	3.5 (19)	C7—C11—C12—C4	1.9 (11)
C4—C5—C6—O2	-176.5 (10)	O1—C5—C6—O2	3.5 (19)
O1—C5—C6—C7	-177.1 (11)		

Symmetry codes: (i) $-x, -y, z$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots C11 ⁱⁱ	0.95	2.69	3.578 (8)	156
C9—H9 \cdots C11 ⁱⁱⁱ	0.95	2.78	3.701 (8)	164

Symmetry codes: (ii) $x-1, y, z$; (iii) $x+1/2, y, z-1/2$.

Fig. 1

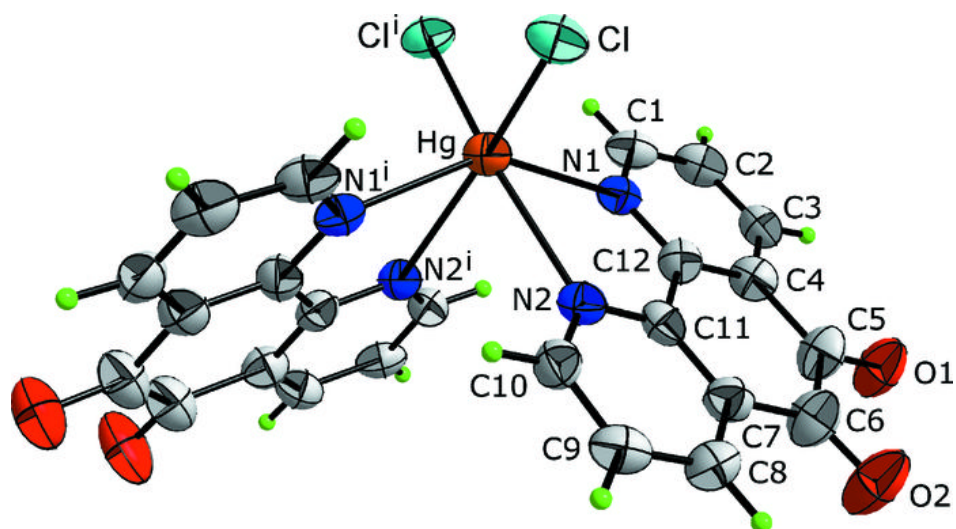


Fig. 2

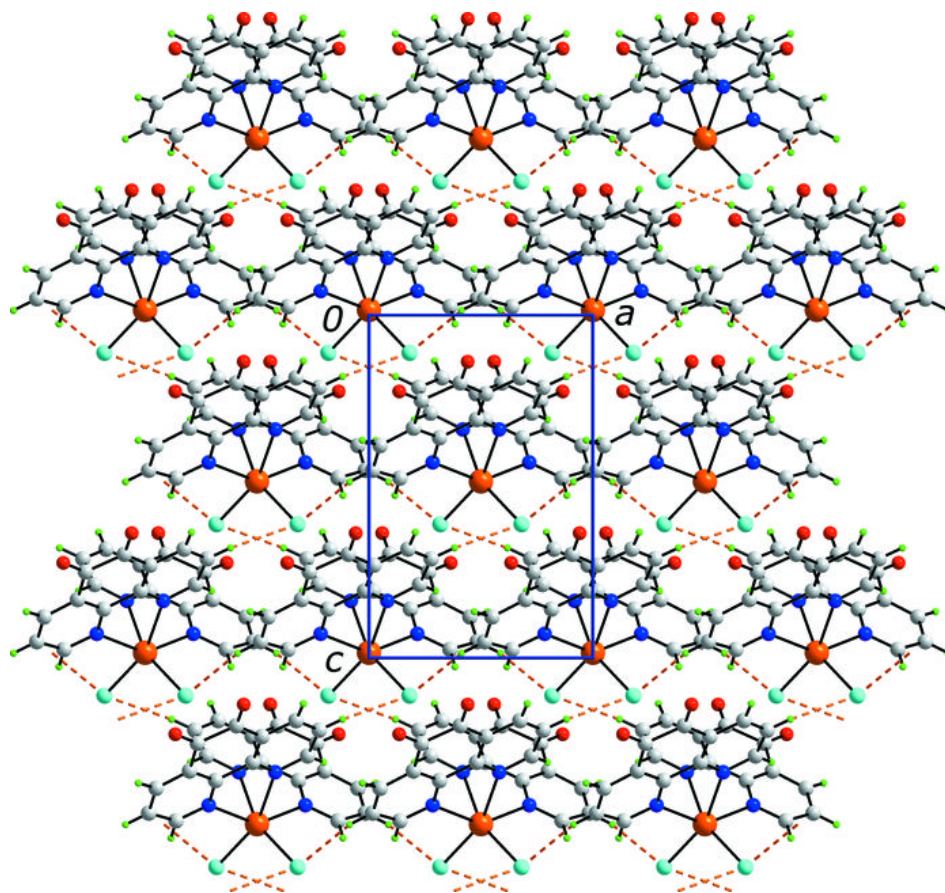


Fig. 3

