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Chloridо(2-formyl-6-hydroxyphenyl-κC^1)mercury(II)

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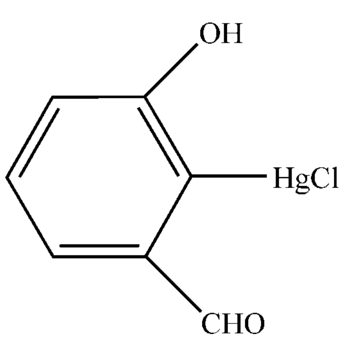
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.018 Å; R factor = 0.045; wR factor = 0.114; data-to-parameter ratio = 15.8.

In the planar [r.m.s. deviation 0.0265 Å] title compound, [Hg($C_7H_5O_2$)Cl], the Hg^{II} atom shows a typical linear coordination by a C atom of a benzene ring and a Cl atom. The benzene C atom and the aldehyde O atom chelate the Hg^{II} atom by assuming the Hg···O separation of 2.817 (9) Å as a weak intramolecular coordination bonding distance. The resulting five-membered metallacycle is nearly coplanar with the benzene ring dihedral angle 2.9 (1)°]. Intermolecular O—H···O hydrogen bonds are present in the crystal structure, resulting in a one-dimensional supramolecular architecture parallel to [201].

Related literature

For historical background and for properties of cyclometallated compounds, see: Dupont *et al.* (2005); Xu *et al.* (2009). For the properties of cyclomercurated compounds, see: Wu *et al.* (2001); Ryabov *et al.* (2003). For related structure, see: King *et al.* (2002); Zhou *et al.* (2005); Hao *et al.* (2007).



Experimental

Crystal data

[Hg($C_7H_5O_2$)Cl]
M_r = 357.15
Monoclinic, $P2_1/c$
a = 4.7200 (19) Å
b = 17.702 (7) Å
c = 10.506 (4) Å
β = 98.839 (5)°
V = 867.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 18.00 mm^{-1}
T = 296 K
0.08 × 0.01 × 0.01 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.327, T_{max} = 0.841
5002 measured reflections
1595 independent reflections
1130 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.114
S = 1.01
1595 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −2.32 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^i	0.82	1.93	2.730 (12)	165

Symmetry code: (i) $x-1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2180).

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Chlorido(2-formyl-6-hydroxyphenyl-κ*C*[1])mercury(II)

Chen Xu, Fei-Fei Cen, Zhi-Qiang Wang and Yu-Qing Zhang

S1. Comment

Cyclometallated compounds containing a metal-carbon bond stabilized by the intramolecular coordination of one or two neutral atoms have a very rich chemistry and are widely used in synthesis, catalysis and materials (Dupont *et al.*, 2005; Xu *et al.*, 2009). Among them, cyclomercurated compounds are easy to prepare through a C—H activation process and their ease in undergoing transmetallation for the synthesis of other organometallic compounds (Wu *et al.*, 2001; Ryabov *et al.*, 2003).

In the planar title compound (Fig. 1), the mercury(II) atom shows a typical linear coordination geometry with a carbon atom of the benzene ring and the chloride atom in *trans* position. O2—Hg1 distance (2.817 (9) Å) is shorter than the sum of van der Waals radii (3.29 Å)of Hg and O (King *et al.*, 2002), indicating the presence of the weak intramolecular coordination, while it is longer than those of the related Hg(II) complex (Zhou *et al.*, 2005). The C—Hg and Hg—Cl bond distances are within normal ranges. The C7—Hg1—Cl1 angle is 178.1 (3)°, slightly smaller than the ideal value of 180° in organic derivatives of mercury(Hao *et al.*, 2007). Intermolecular O—H···O hydrogen bonds are present in the crystal structure (Table 1), resulting in a one-dimensional supramolecular architecture (Fig.2).

S2. Experimental

The title compound was prepared from the *m*-hydroxybenzaldehyde with $Hg(OAc)_2$ and subsequent treatment with LiCl and recrystallized from dichloromethane-petroleum ether solution at room temperature to give the desired product as colorless crystals suitable for single-crystal X-ray diffraction (yield 82%; m.p 442–444 K). IR data (v_max/ cm^{-1}): 3408, 2926, 1651, 1567, 1445, 1291, 1199, 789. NMR δ(H) 7.18(1*H*,d), 7.45 (1*H*,t), 7.52(1*H*,d), 10.12(1*H*,s), 12.11(1*H*,m).

S3. Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with U_{iso}(H)=1.2U_{eq}(C).

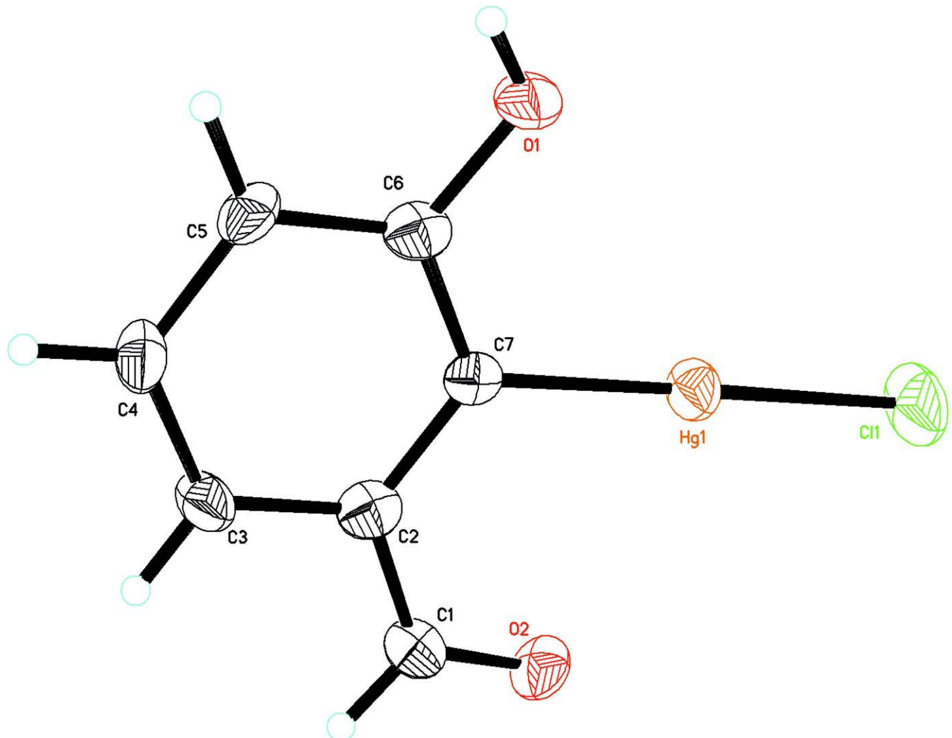

Figure 1

The molecular structure of the title compound with displacement ellipsoids at the 30% probability level.

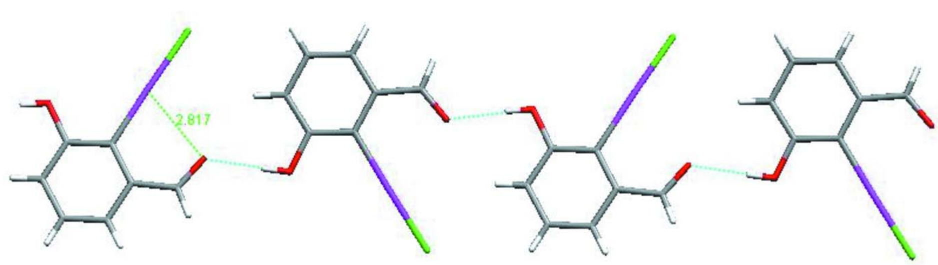

Figure 2

Partial view of the crystal packing showing the formation of the one-dimensional chain structure formed by the intermolecular O—H···O hydrogen bonds.

Chlorido(2-formyl-6-hydroxyphenyl-*κC*[1])mercury(II)

Crystal data

[Hg($C_7H_5O_2$)Cl]
M_r = 357.15
Monoclinic, $P2_1/c$
a = 4.7200 (19) Å
b = 17.702 (7) Å
c = 10.506 (4) Å
β = 98.839 (5)°
V = 867.4 (6) Å^3
Z = 4

F(000) = 640
D_x = 2.735 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1175 reflections
θ = 2.3–22.3°
μ = 18.00 mm^{-1}
T = 296 K
Block, colourless
0.08 × 0.01 × 0.01 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.327$, $T_{max} = 0.841$
5002 measured reflections
1595 independent reflections
1130 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.3°$
$h = -5 \rightarrow 5$
$k = -21 \rightarrow 21$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.114$
$S = 1.01$
1595 reflections
101 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 3.2348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -2.32$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Hg1	0.26063 (12)	0.66539 (3)	0.30597 (6)	0.0470 (2)
O1	−0.160 (2)	0.6917 (5)	0.5036 (10)	0.050 (2)
H1	−0.2948	0.6960	0.5439	0.074*
O2	0.468 (2)	0.7878 (5)	0.1758 (9)	0.052 (2)
Cl1	0.4684 (11)	0.5580 (2)	0.2416 (5)	0.0833 (14)
C1	0.345 (3)	0.8403 (7)	0.2208 (14)	0.043 (3)
H1A	0.3802	0.8888	0.1928	0.052*
C2	0.151 (3)	0.8330 (7)	0.3132 (13)	0.042 (3)
C3	0.039 (3)	0.8998 (7)	0.3574 (14)	0.051 (4)
H3	0.0837	0.9460	0.3235	0.061*
C4	−0.137 (3)	0.8974 (7)	0.4509 (13)	0.048 (4)
H4	−0.2123	0.9420	0.4788	0.058*

C5	−0.204 (3)	0.8276 (7)	0.5043 (13)	0.044 (3)
H5	−0.3193	0.8257	0.5683	0.053*
C6	−0.092 (3)	0.7611 (7)	0.4591 (12)	0.042 (3)
C7	0.087 (2)	0.7635 (7)	0.3644 (11)	0.032 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0477 (4)	0.0392 (3)	0.0583 (4)	0.0027 (3)	0.0213 (3)	−0.0048 (3)
O1	0.047 (6)	0.048 (5)	0.060 (6)	−0.006 (4)	0.027 (5)	0.003 (5)
O2	0.047 (6)	0.058 (6)	0.056 (6)	−0.003 (5)	0.028 (5)	−0.011 (5)
Cl1	0.098 (4)	0.044 (2)	0.117 (4)	0.016 (2)	0.045 (3)	−0.010 (2)
C1	0.033 (7)	0.043 (7)	0.054 (8)	−0.002 (6)	0.007 (6)	0.005 (7)
C2	0.029 (6)	0.053 (8)	0.043 (7)	−0.008 (6)	0.007 (6)	0.000 (6)
C3	0.058 (9)	0.034 (7)	0.070 (10)	0.012 (6)	0.038 (8)	0.012 (7)
C4	0.056 (9)	0.035 (7)	0.056 (9)	0.006 (6)	0.012 (7)	−0.010 (6)
C5	0.040 (8)	0.053 (8)	0.044 (8)	0.005 (7)	0.020 (6)	−0.007 (7)
C6	0.027 (7)	0.054 (8)	0.045 (8)	−0.012 (6)	0.007 (6)	0.000 (6)
C7	0.023 (6)	0.043 (7)	0.026 (6)	−0.004 (5)	−0.008 (5)	0.001 (5)

Geometric parameters (Å, º)

Hg1—C7	2.052 (12)	C2—C3	1.403 (17)
Hg1—Cl1	2.288 (4)	C3—C4	1.382 (17)
O1—C6	1.370 (14)	C3—H3	0.9300
O1—H1	0.8200	C4—C5	1.412 (18)
O2—C1	1.229 (14)	C4—H4	0.9300
C1—C2	1.440 (18)	C5—C6	1.402 (17)
C1—H1A	0.9300	C5—H5	0.9300
C2—C7	1.394 (16)	C6—C7	1.403 (16)
C7—Hg1—Cl1	178.1 (3)	C3—C4—H4	119.9
C6—O1—H1	109.5	C5—C4—H4	119.9
O2—C1—C2	125.4 (12)	C6—C5—C4	118.9 (11)
O2—C1—H1A	117.3	C6—C5—H5	120.6
C2—C1—H1A	117.3	C4—C5—H5	120.6
C7—C2—C1	122.4 (12)	O1—C6—C7	117.8 (11)
C7—C2—C3	120.1 (12)	O1—C6—C5	121.2 (11)
C1—C2—C3	117.3 (11)	C7—C6—C5	121.0 (12)
C4—C3—C2	120.6 (12)	C2—C7—C6	119.2 (11)
C4—C3—H3	119.7	C2—C7—Hg1	120.8 (9)
C2—C3—H3	119.7	C6—C7—Hg1	119.9 (9)
C3—C4—C5	120.2 (11)		
O2—C1—C2—C7	2 (2)	C3—C2—C7—C6	0.8 (19)
O2—C1—C2—C3	177.6 (14)	C1—C2—C7—Hg1	−1.9 (18)
C7—C2—C3—C4	−1 (2)	C3—C2—C7—Hg1	−177.8 (10)
C1—C2—C3—C4	−176.7 (14)	O1—C6—C7—C2	177.3 (12)

C2—C3—C4—C5	1 (2)	C5—C6—C7—C2	−1.1 (19)
C3—C4—C5—C6	−1 (2)	O1—C6—C7—Hg1	−4.2 (16)
C4—C5—C6—O1	−177.0 (12)	C5—C6—C7—Hg1	177.4 (10)
C4—C5—C6—C7	1 (2)	Cl1—Hg1—C7—C2	46 (10)
C1—C2—C7—C6	176.6 (12)	Cl1—Hg1—C7—C6	−132 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.93	2.730 (12)	165

Symmetry code: (i) $x-1$, $-y+3/2$, $z+1/2$.