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A synchrotron study of mercury(I) acetate

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Mercury(I) actetate, $[\mathrm{Hg(C_2H_3O_2)}]_n$, crystallizes as centrosymmetric dimers, $\mathrm{CH_3COO{-}Hg{-}Hg{-}OOCCH_3}$, with an Hg—Hg distance of 2.5202 (15) Å and an Hg—O distance of 2.152 (12) Å. The dimers are assembled into infinite ribbons by long, weaker Hg—O bonds [Hg—O = 2.6802 (12) Å]. There are no strong intermolecular forces between the ribbons.

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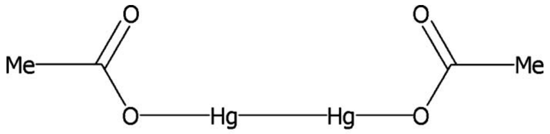
Key indicators

Single-crystal synchrotron study
T = 150 K
Mean σ(C–C) = 0.017 Å
Disorder in main residue
R factor = 0.043
wR factor = 0.109
Data-to-parameter ratio = 12.2

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

Comment

Full crystal structure data are known for very few simple mercury carboxylates (Sikirica & Grdenić, 1974; Allmann, 1973). Mercury(I) acetate, (I), crystallizes as extremely thin plates or needles which has prevented previous structure determination and, to date, only unit-cell information and possible space-group choices have been reported (Dorm & Lindh, 1967; Puff *et al.*, 1965). The crystal structure of (I) is reported for the first time here.



(I)

The unit-cell dimensions and systematic absences agree with previous reports. The structure is based on linear coordination of two monodentate acetate molecules to the Hg_2^{2+} ion (Fig. 1). The Hg—Hg and Hg—O distances [2.5202 (15) and 2.152 (12) Å, respectively] are similar to those reported for analogous compounds (Sikirica & Grdenić, 1974; Lindh, 1967). The carbonyl O atom of the acetate makes a weaker bond to one mercury of an adjacent Hg_2^{2+} unit [Hg—O = 2.6802 (12) Å]. These Hg—O contacts assemble the $\mathrm{Hg_2(OAc)_2}$ units into infinite ribbons which run parallel to a in the ac plane (Fig. 2). The relatively short distance between the methyl groups of adjacent ribbons in the ac plane [$\mathrm{C2}\cdots\mathrm{C2}^{\rm i}$ = 3.6387 (14) Å; symmetry code: (i) $1 - x$, $-y$, $1 - z$] may indicate a weak van der Waals attraction between them. Ribbons are stacked in an $ABAB$ fashion along b at a distance

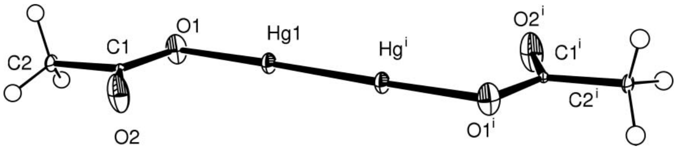


Figure 1
View of a single $\mathrm{Hg_2(OAc)_2}$ unit, shown with 50% probability displacement ellipsoids. Only one orientation of the disordered methyl group is shown for clarity. [Symmetry code: (i) $-x - 1$, $-y$, $-z$.]

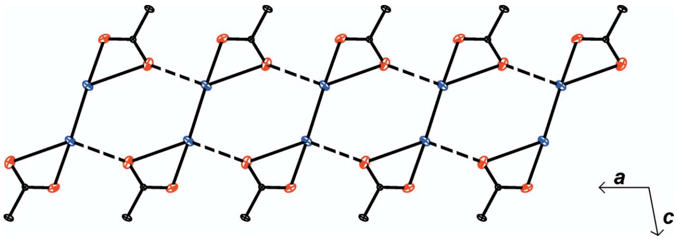


Figure 2
A single ribbon composed of $Hg_2(OAc)_2$ units, viewed down [010]. H atoms have been omitted for clarity. Inter-dimer bonds are drawn as dashed lines. Colour scheme: Hg blue, O red, and C black.

of 3.8974 (15) Å, and inter-ribbon Hg···Hg contacts [3.8974 (15) Å] may be significant in organizing the ribbons into stacks, but this distance somewhat exceeds the range suggested for mercurophilic interactions (Zamora *et al.*, 1997). The poor nature of X-ray diffraction images from all but the smallest crystals is understandable given the absence of strong intermolecular forces within the structure.

Experimental

$Hg(OOCH_3)_2$ (39.8 mg, 0.125 mmol) was dissolved in ethylene glycol (2.5 ml) and placed in a test tube. On to this was layered further pure ethylene glycol (10 ml). On to this methanol (2 ml) was layered and the tube sealed and left to stand in the dark. Large thin colourless hexagonal plates were obtained after about two weeks. All reagents were obtained from the Aldrich Chemical Company and used without further purification.

Crystal data

$[Hg(C_2H_3O_2)]$
$M_r = 259.63$
Monoclinic, $C2/m$
$a = 5.133$ (3) Å
$b = 5.866$ (3) Å
$c = 12.202$ (6) Å
$\beta = 99.779$ (7)°
$V = 362.1$ (3) Å^3
$Z = 4$
$D_x = 4.763$ Mg m^{-3}
Synchrotron radiation, $\lambda = 0.8464$ Å
Cell parameters from 1173 reflections
$\theta = 4.0$–32.4°
$\mu = 79.55$ mm^{-1}
$T = 150$ (2) K
Plate, colourless
0.02 × 0.02 × 0.01 mm

Data collection

Bruker APEXII diffractometer
Narrow-frame ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.204$, $T_{\max} = 0.672$
1173 measured reflections
404 independent reflections
395 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.046$
$\theta_{\max} = 32.4°$
$h = -6 \rightarrow 6$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.109$
$S = 1.10$
404 reflections
33 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 2.89$ e Å^{-3}
$\Delta\rho_{\min} = -5.57$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Hg1—O1	2.152 (12)	C1—O2	1.259 (15)
Hg1—Hg1$^{\rm i}$	2.5202 (15)	C1—C2	1.503 (16)
O1—C1	1.239 (15)		
O1—Hg1—Hg1$^{\rm i}$	178.0 (3)	O1—C1—C2	117.0 (11)
C1—O1—Hg1	108.2 (9)	O2—C1—C2	120.2 (9)
O1—C1—O2	122.9 (11)		

Symmetry code: (i) $-x-1, -y, -z$.

Although the large hexagonal plates (up to 1 mm in size) were found to scatter X-rays extremely well, the diffracted X-rays did not appear as isolated spots on the area detector but as ill-defined streaks. The plates were cut into much smaller pieces (*ca* 0.02 mm in size) and a large number were examined and displayed significant streaking. The diffraction patterns from one platelet were substantially better than from the others and a full sphere of data was collected from it. Data were collected on station 16.2 SMX at the Daresbury SRS, UK. The H atoms of the methyl group were geometrically positioned and refined as riding, with C—H = 0.98 Å and $U_{\rm iso}(H) = 1.5U_{\rm eq}(C)$. The methyl group is disordered about the mirror plane in two equally occupied orientations. The highest peak in the final difference Fourier map is located 0.97 Å from atom Hg1 and the deepest hole is located 0.77 Å from atom Hg1.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *APEXII*; data reduction: *APEXII*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *WinGX* (Version 1.164; Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

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