detailed analysis of hydrogen-bonding effects, water content, and bifluoride anion structure will have to await a neutron diffraction study.

In KCP(FHF), there are nine K^+ ion nearest neighbors with K—X distances ranging from 2·76 (1) to 3·32 (1) Å (see Table 2*c*). The O atom interactions are presented in Table 2(*d*) and range in distance from 2·76 (1) to 3·21 (3) Å.

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Mercury(II) Chromate

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Abstract. $HgCrO_4$, monoclinic, space group $P2_1/n$, a = 7·342 (1), b = 8·522 (1), c = 5·202 (1) Å, β = 94·00 (2)°, V = 343·4 Å^3, Z = 4, D_x = 6·12 g cm^{-3}. The structure was refined to a final R of 0·049 for 1163 counter reflections. Each Hg atom is almost linearly bonded to two O atoms [Hg—O 2·10 (1), 2·12 (1) Å] of different chromate tetrahedra forming endless zigzag chains. The Cr—O distances are 1·70 (bridging) and 1·61 Å (terminal).

Introduction. This investigation is part of a research project on inorganic Hg^{II} compounds. At least three different Hg^{II} chromates exist, $HgCrO_4$, $HgCrO_4 \cdot \frac{1}{2}H_2O$ and $Hg_3O_2CrO_4$ (Aurivillius & Malmros, 1961). Commercially available Hg^{II} chromates often consist of mixtures of these three phases. $HgCrO_4 \cdot \frac{1}{2}H_2O$ has been studied both by X-rays and neutrons (Aurivillius, 1972; Aurivillius & Stålhandske, 1975). $Hg_3O_2CrO_4$ (and $Hg_3O_2SeO_4$) are isotypic with $Hg_3O_2SO_4$ (Aurivillius & Malmros, 1961); the latter was studied by Nagorsen, Lyng, Weiss & Weiss (1962).

Cell dimensions for $HgCrO_4$, determined from powder photographs, are in good agreement with those given by Aurivillius & Malmros (1961). A single crystal, 0·12 × 0·14 × 0·25 mm, was picked out from a commercial product and used in the data collection. The intensities were measured on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromatized Mo $K\alpha$ radiation. The ω–2θ scan technique was used with a scan interval $\Delta\omega$ = (0·8 + 0·5 tan θ)° and a maximum time of 3·5 min for each reflexion. Of the 1508 reflexions with $\theta < 35°$ in one quadrant of reciprocal space, 1163 with $I > 3\sigma(I)$ were used in the structure analysis. Corrections were applied for Lorentz–polarization and absorption effects (μ = 487 cm^{-1}). The transmission factors, evaluated by numerical integration, varied from 0·009 to 0·056. The atomic positions were determined by Patterson and Fourier techniques. Full-matrix least-squares refinement was performed with anisotropic temperature factors for Hg and Cr and isotropic for O and with a parameter to correct for secondary extinction (Zachariasen, 1967). The form factors of Doyle & Turner (1968) were used with the anomalous dispersion

Table 1. *Fractional atomic coordinates* (×10^4) *with e.s.d.'s in parentheses*

	x	y	z
Hg	1583 (1)	366 (1)	2525 (1)
Cr	6637 (2)	1889 (2)	2766 (3)
O(1)	6055 (13)	3622 (11)	4078 (18)
O(2)	8471 (11)	1118 (11)	4388 (15)
O(3)	4934 (14)	711 (12)	2648 (20)
O(4)	7229 (12)	2215 (10)	37 (17)

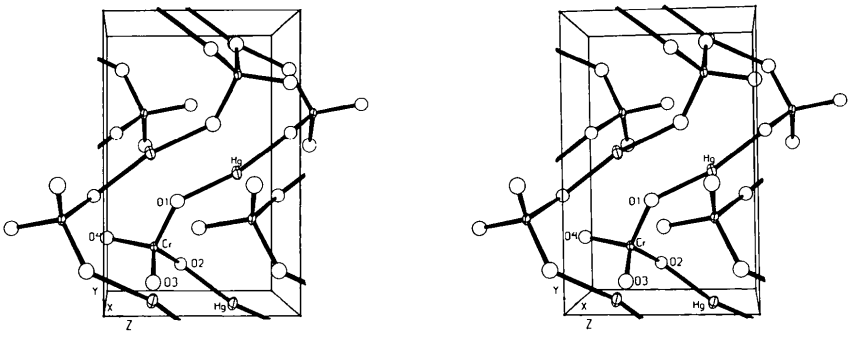


Fig. 1. A stereoview of the unit cell of $HgCrO_4$.

Table 2. *Bond lengths* (Å) *and angles* (°)

Hg–O(1)	2·097 (10)	O(1)–Hg–O(2)	163·3 (4)
–O(2)	2·121 (9)	Hg–O(1)–Cr	134·5 (5)
–O(3)	2·479 (10)	Hg–O(2)–Cr	126·5 (5)
–O(4)	2·510 (9)	O(1)–Cr–O(2)	109·0 (5)
–O(1)	2·554 (9)	O(1)–Cr–O(3)	109·9 (5)
–O(2)	2·651 (8)	O(1)–Cr–O(4)	109·6 (5)
–O(4)	2·787 (9)	O(2)–Cr–O(3)	111·6 (5)
Cr–O(3)	1·604 (11)	O(2)–Cr–O(4)	107·5 (4)
–O(4)	1·617 (9)	O(3)–Cr–O(4)	109·3 (5)
–O(2)	1·698 (9)		
–O(1)	1·712 (10)		

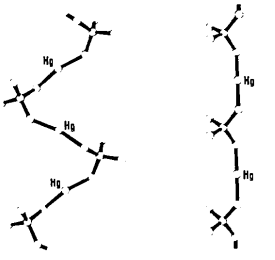
parameters for Hg and Cr of Cromer & Liberman (1970). The refinement converged to $R = 0{\cdot}049$ and $R_w = 0{\cdot}065$ with the isotropic extinction parameter $g = 0{\cdot}13\,(2)$. The function minimized was $\sum w_i(|F_o| - |F_c|)^2$, with $w_i^{-1} = \sigma^2(F_o) + (0{\cdot}025|F_o|)^2$. The final parameters are given in Table 1.*

Discussion. A stereoview of the unit cell is given in Fig. 1. The structure consists of infinite chains $(HgCrO_4)_n$, which also exist in $HgCrO_4.\frac{1}{2}H_2O$ (Fig. 2). The geometry is thus different from that of $HgSO_4$ (Kokkoros & Rentzeperis, 1963), which is described as built up of HgO_4 and SO_4 tetrahedra sharing corners.

In $HgCrO_4.\frac{1}{2}H_2O$ and $HgCrO_4$ each Hg atom is coordinated to two O atoms in an almost linear way with Hg–O 2·055 (2), 2·064 (2) Å, O–Hg–O 179·95 (5)° for $HgCrO_4.\frac{1}{2}H_2O$ and 2·097 (10), 2·121 (9) Å, 163·3 (4)° for $HgCrO_4$.

If the CrO_4 tetrahedra are assumed to be replaced by O atoms, the resulting $(Hg–O)_n$ chains of $HgCrO_4.\frac{1}{2}H_2O$ are endless linear chains (as expected, hitherto not observed) and those of $HgCrO_4$ are of the zigzag type, as are those in HgO(orth.) (Aurivillius, 1956).

In $HgCrO_4$ the chains are connected to form a three-dimensional network by five Hg–O contacts of 2·48–2·79 Å, all shorter than 2·90 Å, the sum of the van der Waals radii of Hg (1·50 Å, Grdenić, 1965) and O. In $HgCrO_4.\frac{1}{2}H_2O$ the endless chains are linked by weak hydrogen bonds and by five Hg–O contacts of 2·65–2·74 Å. In both compounds the polyhedron around Hg is a distorted pentagonal bipyramid.



(*a*) (*b*)

Fig. 2. Endless chains in (*a*) $HgCrO_4$ and (*b*) $HgCrO_4.\frac{1}{2}H_2O$.

A DTA analysis of $HgCrO_4.\frac{1}{2}H_2O$ shows complete dehydration in the temperature interval 185–205 °C.

The chromate tetrahedra in the two compounds are very similar with Cr–O distances of about 1·70 (bridging) and 1·60 Å (terminal) and O–Cr–O angles varying between 107 and 112°.

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33424 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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