The Mercury Vanadates with the Empirical Formulas $HgVO_3$ and Hg_2VO_4

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Needle-shaped crystals of $HgVO_3$ (orange) and Hg_2VO_4 (yellow) have been prepared by annealing mercury(II) oxide with an amorphous mercury vanadate of the approximate composition HgV_2O_6 in molar ratios varying between 1:1 and 4:1 in evacuated, sealed silica tubes at 400°C. The crystal structures of both compounds have been determined from four-circle diffractometer data. $HgVO_3$: $P\bar{1}$, $a = 359.2(1)$ pm, $b = 475.2(1)$ pm, $c = 858.8(1)$ pm, $\alpha = 88.32(1)°$, $\beta = 79.60(1)°$, $\gamma = 89.30(1)°$, $Z = 2$, $R = 0.034$ for 1763 structure factors and 32 variable parameters. Hg_2VO_4: $P2_1/n$, $a = 367.3(1)$ pm, $b = 1650.3(1)$ pm, $c = 1425.5(1)$ pm, $= 89.99(1)°$, $Z = 8$, $R = 0.038$ for 1668 F values and 91 variables. In both compounds the vanadium atoms are irregularly surrounded by five oxygen atoms. These coordination polyhedra share common edges, thus forming infinite $(VO_3^{1-})_n$ chains, which are aligned parallel to each other. In $HgVO_3$ these chains are linked by pairs of mercury(I) atoms, building two-dimensionally infinite layers of the composition $(Hg_2^{2+})_n(VO_3^{1-})_{2n}$. In contrast, in Hg_2VO_4 the $(VO_3^{1-})_n$ chains do not form any strong bonds to the mercury atoms. In that compound the mercury atoms occur in the oxidation states I and II, and together with some oxygen atoms they form infinite chains with the shape of condensed spirals surrounding the $(VO_3^{1-})_n$ chains and thus mimicking orthorhombic symmetry. This compound may be expressed by the formula $(Hg_2^{2+} \cdot 2HgO)_n(VO_3^{1-})_{2n}$. © 1996 Academic Press, Inc.

INTRODUCTION

Numerous oxovanadates of mercury have been reported in the past. In the 8th edition of Gmelin's Handbook (1) covering the literature up to 1966 some ten mercury vanadates are described with mercury : vanadium ratios varying between 3 : 1 and 1 : 2. The first compound reported with a crystal structure is the high temperature (β) modification of HgV_2O_6 (2). The low-temperature (α) modification of this compound has been suggested to be isotypic with ZnV_2O_6 and CdV_2O_6 (3). X-ray powder diagrams have been published by Angenault (4) for the tentative

compositions "HgV_2O_6," "$Hg_2V_2O_7$," "$Hg_4V_2O_9$," and "$Hg_6V_2O_{11}$." All of these four compounds have been assumed to crystallize dimorphic. Sleight (5) prepared a high pressure phase (II) of the vanadate $Hg_2V_2O_7$. This compound appears to crystallize with a pyrochlore-related structure, however, a full structure determination was not carried out. Structural data of the low temperature (α) modification of this compound have also been reported (6). Volkov *et al.* (7) investigated the $HgO-V_2O_3-V_2O_5$ system at high pressures (2.5 and 7.7 GPa) and observed several mercury vanadates to which they ascribed the formulas β-$Hg_xV_2O_5$ ($0.16 \leq x \leq 0.20$), $Hg_4V_{18}O_{39}$, α_p- and β_p-HgV_2O_4, HgV_2O_5, β-HgV_2O_6, β-$Hg_2V_2O_7$, and $Hg_3V_2O_8$. The powder patterns of the vanadates with the empirical formulas $HgVO_3$ and Hg_2VO_4, characterized in the present work, correspond to those of the compounds with the tentative formulas "β-$Hg_2V_2O_7$" and "β-$Hg_4V_2O_9$" assigned by Angenault (4). A preliminary account of this work has been given at a conference (8).

SAMPLE PREPARATION AND LATTICE CONSTANTS

We prepared $HgVO_3$ and Hg_2VO_4 by reaction of amorphous mercury vanadates with mercury(II) oxide. Starting materials were NH_4VO_3 (Merck, >99 %) and $Hg(NO_3)_2 \cdot H_2O$ (Fluka, >99 %). NH_4VO_3 was dissolved in a diluted solution of KOH. This solution was neutralized with HNO_3 and subsequently mixed with an aqueous solution of $Hg(NO_3)_2 \cdot H_2O$. The resulting yellow suspension was boiled for 30 min and the orange precipitate was separated by filtration, washed, and dried in a dessicator over calcium chloride for 2 days. The resulting amorphous products had colors varying between dark yellow and light brown. Their energy-dispersive X-ray fluorescence analyses showed mercury to vanadium ratios close to 1:2, suggesting the composition HgV_2O_6.

Red mercury(II) oxide (Merck >99 %) was then intimately mixed with this mercury vanadate in molar ratios varying between 1:1 and 4:1. Samples of 150–350 mg were sealed in evacuated silica tubes of 3–6 cm³, annealed for 1 week at 400°C and quenched in air. The Guinier powder

TABLE 1
Crystal Data of HgVO$_3$ and Hg$_2$VO$_4$

	HgVO$_3$	Hg$_2$VO$_4$[a]	
Space group	$P\bar{1}$	$P2_1/n$	$[P2_1/c]$
Lattice constants (Guinier powder)[b]			
a (pm)	359.2(1)	367.3(1)	[367.3(1)]
b (pm)	475.2(1)	1650.3(1)	[1650.3(1)]
c (pm)	858.8(1)	1425.5(1)	[1472.1(1)]
α (°)	88.32(1)		
β (°)	79.60(1)	89.99(1)	[104.46(1)]
γ (°)	89.30(1)		
V (nm^3)	0.1441	0.8641	[0.8641]
Lattice constants (CAD-4 diffr.)[b]			
a (pm)	358.8(1)	367.3(1)	
b (pm)	474.5(1)	1649.6(4)	
c (pm)	857.9(1)	1424.6(3)	
α (°)	88.33(1)	90.02(2)	
β (°)	79.59(1)	89.93(1)	
γ (°)	89.34(1)	89.95(1)	
V (nm^3)	0.1436	0.8632	
Formula weight	299.53	516.12	
Formula units/cell	$Z = 2$	$Z = 8$	
Calculated density (g/cm^3)	6.901	7.934	
Absorption coefficient $\mu_{MoK\alpha}$ (cm^{-1})	561	728	
Crystal dimensions (μm^3)	$110 \times 20 \times 10$	$300 \times 20 \times 20$	
Highest/lowest transmission	1.87	1.78	
$\theta/2\theta$ scans up to	$2\theta = 90°$	$2\theta = 78°$	
Range in h, k, l	±9, ±17, ±7	±5, ±21, ±24	
Total number of reflections	4710	12045	
Unique reflections	2355	3101	
Inner residual	$R_i = 0.025$	$R_i = 0.030$	
Reflections with $I_o > 1\ \sigma(I_o)$	1763	1668	
Number of variables	32	91	
Conventional residual	$R = 0.034$	$R = 0.038$	
Weighted residual	$R_w = 0.025$	$R_w = 0.037$	

[a] The structure of Hg$_2$VO$_4$ is pseudoorthorhombic. Therefore the nonstandard setting $P2_1/n$ of the space group $P2_1/c$ (No. 14) has been chosen for the description of this compound.

[b] The lattice constants obtained from single-crystal diffractometer data are usually affected by systematic errors due to absorption. Therefore the interatomic distances were calculated with the lattice constants from the powder data.

patterns of the reaction products usually showed mixtures of HgVO$_3$ and Hg$_2$VO$_4$. Almost single-phase HgVO$_3$ was obtained when the starting ratio was close to 1:1, while samples aiming for Hg$_2$VO$_4$ always contained various amounts of HgVO$_3$. Apparently some oxygen was liberated during these reactions, as was also suggested by the small amounts of elemental mercury frequently observed in the reaction products.

Usually the resulting mercury vanadates were well crystallized. Sometimes needle-shaped crystals of HgVO$_3$ (with orange color) or Hg$_2$VO$_4$ (yellow) were observed with up to 4 mm length.

The samples were characterized by their Guinier powder diagrams using CuKα_1 radiation with α-quartz ($a = 491.30$ pm, $c = 540.46$ pm) as an internal standard. The diagrams of HgVO$_3$ and Hg$_2$VO$_4$ were identical with those obtained by Angenault (4) for "β-Hg$_2$V$_2$O$_7$" and "β-Hg$_4$V$_2$O$_9$," respectively. The lattice constants (Table 1) were refined by least-squares fits. To ensure proper indexing, the observed powder patterns were compared with those calculated (9), using the positional parameters obtained during the structure determinations. In agreement with Angenault's results the lattice constants of Hg$_2$VO$_4$ are pseudoorthorhombic, however, the lower monoclinic symmetry has been clearly established by the structure refinement as discussed further below.

STRUCTURE DETERMINATIONS

Single crystals of Hg$_2$VO$_4$ were investigated in a Weissenberg camera with CuKα radiation. The films reflect the pseudoorthorhombic cell dimensions, however, the inten-
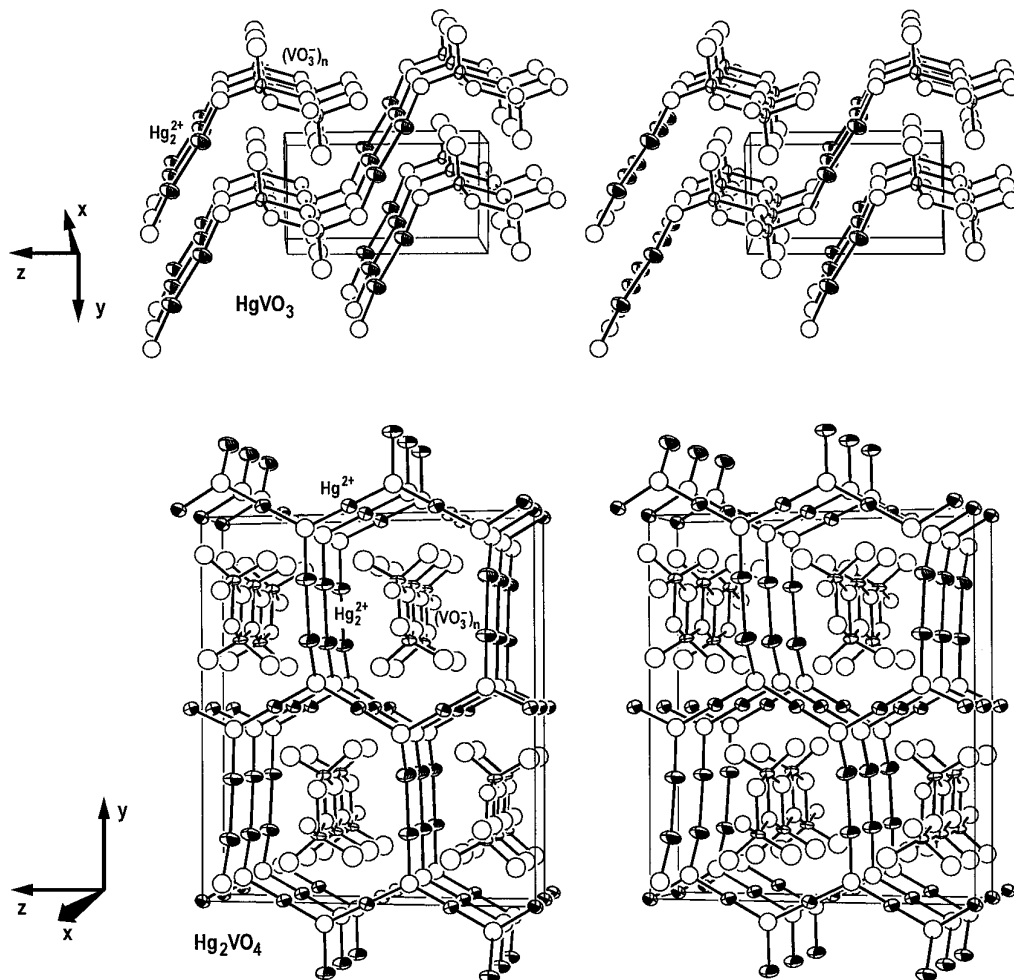
FIG. 1. Streoprojections of the $HgVO_3$ and Hg_2VO_4 structures. The metal atoms are shown with their thermal ellipsoids, the oxygen atoms with the isotropic B values, both at the 95% probability limits.

sity distribution, especially of the weak reflections, was that of a monoclinic lattice. The space group extinctions ($h0l$ observed only with $h + l = 2n$ and $0k0$ only with $k = 2n$) led to the space group $P2_1/n$, a nonstandard setting of $P2_1/c$ (No. 14). The setting $P2_1/n$ was retained because of its proximity to the orthorhombic cell, which is also reflected by the architecture of the cell content.

The intensity data for both structure determinations were collected on an automated four-circle diffractometer with graphite-monochromated $MoK\alpha$ radiation, a scintillation counter, and a pulse-height discriminator. The background was determined at both ends of each $\theta/2\theta$ scan. Empirical absorption corrections were applied from psi-scan data. Further details of the data collections are summarized in Table 1.

The structures were solved by interpretation of the Patterson maps, which led to the positions of all metal atoms in $HgVO_3$ and to the position of one mercury atom in Hg_2VO_4. The other atoms were located by difference Fou-
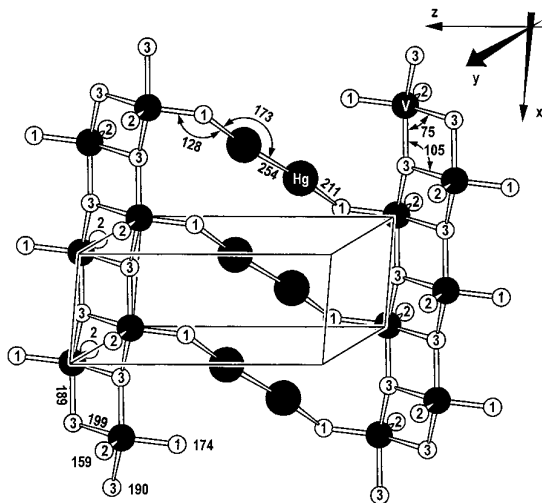

FIG. 2. A cutout from one two-dimensionally infinite net of the $HgVO_3$ structure. The oxygen atoms are shown as open circles. Single-digit numbers correspond to the atom designations. Some interatomic distances (pm) and angles (°) are also indicated.

TABLE 2
Atomic Parameters of HgVO$_3$ and Hg$_2$VO$_4$[a]

HgVO$_3$

Atom	$P\bar{1}$	x	y	z	B_{eq} or B
Hg	2i	0.28495(6)	0.18523(5)	0.57431(3)	1.409(3)
V	2i	0.1971(2)	0.3855(2)	0.13572(8)	0.77(1)
O1	2i	0.0980(11)	0.4968(8)	0.3303(4)	1.34(5)
O2	2i	0.1939(11)	0.0511(8)	0.1509(4)	1.68(6)
O3	2i	0.7138(10)	0.4830(7)	0.0906(4)	1.06(5)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg	162.5(7)	156.8(7)	206.9(7)	45.9(6)	−6.4(6)	−38.4(6)
V	86(3)	129(3)	73(2)	7(3)	−9(2)	9(2)

Hg$_2$VO$_4$

Atom	$P2_1/n$	x	y	z	B_{eq} or B
Hg1	4e	0.1238(3)	0.33090(5)	0.37609(7)	2.21(2)
Hg2	4e	0.9950(2)	0.99479(5)	0.24912(6)	1.00(1)
Hg3	4e	0.9985(3)	0.17978(5)	0.37438(6)	1.60(1)
Hg4	2a	0	0	0	0.92(2)
Hg5	2b	0	0	1/2	1.11(2)
V1	4e	0.5013(9)	0.1781(2)	0.6182(2)	0.82(5)
V2	4e	0.9991(9)	0.3279(2)	0.6301(2)	0.77(5)
O1	4e	0.509(4)	0.1260(11)	0.5180(11)	2.2(3)
O2	4e	0.014(4)	0.9369(10)	0.1239(12)	2.0(3)
O3	4e	0.000(4)	0.2063(9)	0.1242(11)	1.6(2)
O4	4e	0.486(4)	0.8905(10)	0.2931(10)	1.7(3)
O5	4e	0.963(4)	0.0468(10)	0.3742(12)	2.1(3)
O6	4e	0.502(4)	0.1024(9)	0.0438(9)	1.4(3)
O7	4e	0.499(4)	0.2880(9)	0.1231(10)	1.4(2)
O8	4e	0.497(4)	0.1206(10)	0.2296(10)	1.7(3)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg1	513(6)	99(3)	228(4)	−103(4)	−15(4)	8(4)
Hg2	152(3)	94(3)	134(3)	7(4)	5(3)	−14(3)
Hg3	301(4)	79(3)	227(3)	−33(4)	−1(3)	1(4)
Hg4	119(5)	97(5)	133(4)	8(5)	−7(4)	14(4)
Hg5	188(6)	101(5)	131(4)	1(5)	−8(4)	13(5)
V1	78(13)	67(13)	165(14)	5(16)	−4(12)	−2(16)
V2	80(13)	78(13)	134(13)	−6(18)	7(11)	−2(17)

[a] The isotropic thermal parameters B_{eq} and B are listed in units of 10^4 pm^2. The anisotropic thermal parameters U (pm^2) are defined by $\exp[-2\pi^2(h^2a^{*2}U_{11} + \cdots + 2klb^*c^*U_{23})]$.

rier syntheses. The structures were refined by full-matrix least-squares cycles using atomic scattering factors (10), corrected for anomalous dispersion (11). Parameters accounting for secondary isotropic extinction were optimized during the least-squares refinements. In the final least-squares cycles the metal atoms were refined with anisotropic and the oxygen atoms with isotropic thermal parameters. Stereoplots with the thermal ellipsoids of both structures are shown in Fig. 1. The atom parameters and interatomic distances are listed in Tables 2 and 3.

DISCUSSION

HgVO$_3$ and Hg$_2$VO$_4$ crystallize with new structure types, as is frequently the case for mercury compounds. Both compounds contain pentavalent vanadium with five oxygen neighbors. For simplicity we call this coordination a distorted trigonal bipyramid, although it could also be considered a distorted square pyramid. These trigonal bipyramidal VO$_5$ groups are linked via common edges, thus forming infinite (VO$_3^{1-}$)$_n$ chains, as can be seen from Figs. 2 and 3.

TABLE 3
Interatomic Distances of HgVO$_3$ and Hg$_2$VO$_4$[a]

HgVO$_3$

Hg:	Hg	254.3(1)	V:	O2	159.1(4)	O1:	V	174.1(4)	O2:	V	159.1(4)
	O1	211.2(4)		O1	174.1(4)		Hg	211.2(4)		Hg	286.6(4)
	O1	270.8(4)		O3	188.7(4)		Hg	270.8(4)	O3:	V	188.7(4)
	O2	286.6(4)		O3	189.6(4)		Hg	294.6(4)		V	189.6(4)
	O1	294.6(4)		O3	199.5(3)					V	199.5(3)

Hg$_2$VO$_4$

Hg1:	Hg3	253.6(1)	Hg4:	2O2	205(2)	O1:	V1	167(2)	O5:	Hg5	196(2)
	O2	220(2)		2O6	257(1)		Hg5	276(2)		Hg2	198(2)
	O4	264(1)		2O6	258(1)		Hg5	281(2)		Hg3	220(2)
	O6	267(1)	Hg5:	2O5	196(2)		Hg3	287(2)	O6:	V2	168(1)
	O2	292(2)		2O1	276(2)		Hg3	292(2)		Hg4	257(1)
Hg2:	O5	198(2)		2O1	281(2)	O2:	Hg2	203(2)		Hg4	258(1)
	O2	203(2)	V1:	O1	167(2)		Hg4	205(2)		Hg1	267(1)
	O4	257(1)		O4	170(2)		Hg1	220(2)	O7:	V1	191(1)
	O4	262(1)		O3	191(2)		Hg1	292(2)		V2	191(1)
	O8	278(2)		O7	191(1)	O3:	V1	191(2)		V1	193(1)
	O8	279(2)		O7	193(1)		V2	192(1)	O8:	V2	165(1)
Hg3:	Hg1	253.6(1)	V2:	O8	165(1)		V2	192(1)		Hg2	278(2)
	O5	220(2)		O6	168(1)	O4:	V1	170(2)		Hg2	279(2)
	O1	287(2)		O7	191(1)		Hg2	257(1)		Hg3	293(1)
	O1	292(2)		O3	192(1)		Hg2	262(1)		Hg3	293(1)
	O8	293(1)		O3	192(1)		Hg1	264(1)			
	O8	293(1)									

[a] All distances shorter than 345 (Hg–Hg, Hg–V, Hg–O), 305 (V–V, V–O), and 225 pm (O–O) are listed.
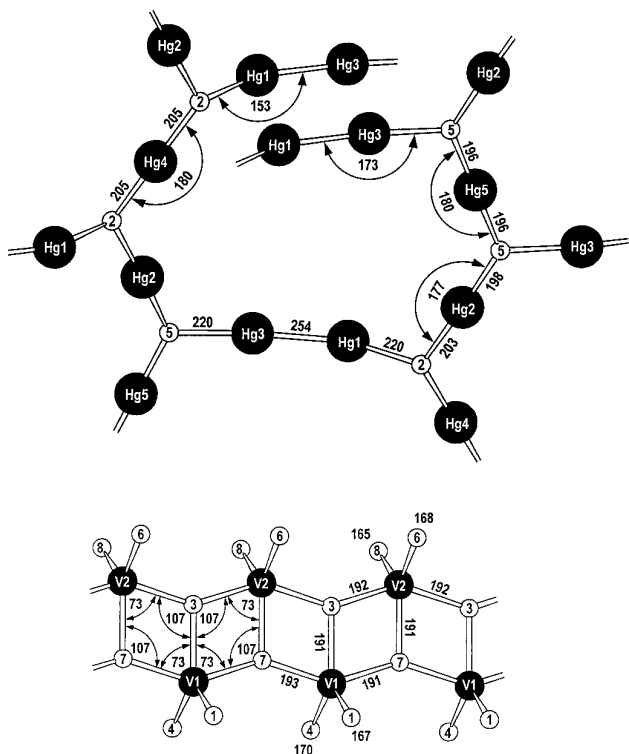

FIG. 3. Near-neighbor environments in the structure of Hg$_2$VO$_4$. Single-digit numbers correspond to the atom designations of the oxygen atoms. Selected interatomic distances and angles are given in pm units and degrees of arc.

Similar chains occur in the structures of other binary and ternary vanadium oxides, e.g., in ZnV$_2$O$_6$ (3, 4), NaVO$_3$ · 1.89H$_2$O (12), β-NaVO$_3$ (13), and V$_2$O$_5$ (14–17). To facilitate the comparison of the bond lengths and bond angles we label the oxygen atoms of these chains in the manner shown in Fig. 4. It can be seen from Table 4 that the V–O distances of the terminal O$_A$ and O$_B$ atoms are all rather short with average distances of 166.6, 168.5, and 166.5 pm for the vanadium atom in HgVO$_3$ and the two different
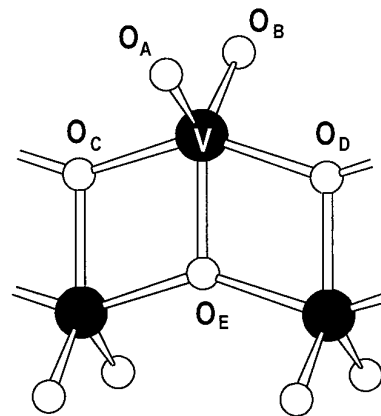

FIG. 4. A cutout of the infinite VO$_3$ chains occurring in various vanadates. The five oxygen atoms surrounding a central vanadium atom are labeled O$_A$–O$_E$ to facilitate the comparisons carried out in the Tables 4 and 5.

TABLE 4
Interatomic Distances (pm) within the Condensed Trigonal Bipyramidal VO_5 Groups of Compounds with VO_3 Chains[a]

	$HgVO_3$	Hg_2VO_4		ZnV_2O_6	$NaVO_3 \cdot 1.89H_2O$	β-$NaVO_3$	V_2O_5
V–O_A	159.1(4)	167(2)	165(1)	168	164.3(1)	163(2)	157.7(3)
V–O_B	174.1(4)	170(2)	168(1)	170	165.3(1)	170(3)	177.9(2)
V–O_C	188.7(4)	191(1)	192(1)	183	188.2(3)	192(1)	187.8(1)
V–O_D	189.6(4)	193(1)	192(1)	183	192.8(3)	192(1)	187.8(1)
V–O_E	199.5(3)	191(2)	191(1)	210	198.8(1)	199(2)	201.7(3)

[a] The oxygen atoms are labeled as shown in Fig. 4.

vanadium atoms in Hg_2VO_4, respectively. The O_C, O_D, and O_E atoms of these compounds all have three vanadium neighbors, and consequently their individual V–O bonds are weaker with an average distance of 192.6 pm for the vanadium atom in $HgVO_3$ and the same average distances of 191.7 pm for both vanadium atoms of Hg_2VO_4. It is remarkable that the O_E atoms have the greatest V–O distances in all compounds listed in Table 4 with Hg_2VO_4 as the only exception.

The angular distortions of the trigonal bipyramidal VO_5 groups are rather great (Table 5). The greatest deviation from an ideal bond angle occurs for the angle O_C–V–O_D, which is 180° for the ideal trigonal bipyramid and around 145° for the VO_5 groups in the two mercury vanadates. The O–V–O bond angles for the two vanadium atoms of Hg_2VO_4 are practically the same, and in general these trigonal bipyramidal VO_5 groups of Hg_2VO_4 are less distorted than the VO_5 group in $HgVO_3$.

In both structures the $(VO_3^{1-})_n$ chains are aligned parallel to each other. In $HgVO_3$ these chains are linked via pairs of mercury(I) atoms, thus forming two-dimensionally infinite,

TABLE 5
### Bond Angles (°) within the VO_5 Groups of $HgVO_3$ and Hg_2VO_4 as Compared to the Bond Angles of an Ideal Trigonal Bipyramid[a]

	Trigonal bipyramid	$HgVO_3$	Hg_2VO_4	
O_A–V–O_C	90	105.1	99.5	100.6
O_B–V–O_C	90	97.9	98.2	100.0
O_A–V–O_D	90	104.5	101.4	101.1
O_B–V–O_D	90	94.9	101.1	99.4
O_C–V–O_E	90	75.5	73.1	72.9
O_D–V–O_E	90	74.2	72.9	72.9
O_A–V–O_E	120	111.3	123.6	123.9
O_A–V–O_B	120	104.6	107.0	105.9
O_B–V–O_E	120	144.0	129.3	130.1
O_C–V–O_D	180	143.5	145.9	145.6

[a] The atom labels correspond to those of Fig. 4 and Table 4. The standard deviations are all equal or less than 0.2° in $HgVO_3$ and 0.8° in Hg_2VO_4.

puckered (almost folded) layers (Figs. 1 and 2). These layers are held together by weak mercury–oxygen interactions with Hg–O distances of 271, 287, and 295 pm. The shortest vanadium–oxygen distance between adjacent layers is 317 pm. The layered character of this structure is also apparent from the easy cleavage of the needle-like crystals.

In Hg_2VO_4 the $(VO_3^{1-})_n$ chains do not form any strong bonds to the mercury atoms (Figs. 1 and 5). The architecture of this structure is quite unusual. At the first sight the symmetry is orthorhombic, and this may be the reason why Angenault (4) was not successful in determining this structure. In fact, after having solved the structure in the monoclinic space group $P2_1/n$, and after studying various projections of the structure, we have in vain tried to find an orthorhombic setting. A ball-and-stick model of this compound, however, immediately revealed the lower symmetry. As can be seen from the parallel projection in the upper part of Fig. 5, the mercury and some oxygen atoms of this compound seem to form condensed 14-membered rings as they are known to occur in the structures of Hg_2OI (18), $Hg_4O_2(NO_3)_2$ (19, 20), and Hg_2ReO_5 (21). The corresponding perspective (central) projection in the lower part of Fig. 5, however, shows that there are no 14-membered rings. Instead, the mercury and oxygen atoms of these "rings" form spirals, and the arrangement of these spirals is incompatible with the mirror planes as suggested by the parallel projection to extend perpendicular to the z direction.

The mercury atoms of both compounds have the frequently occurring linear coordination (Figs. 2 and 3; all corresponding bond angles Hg–Hg–O and O–Hg–O deviate less than 8° from 180°; the only exception is the Hg3–Hg1–O2 angle of 153.2(4)° in Hg_2VO_4.). The mercury(I) atoms of $HgVO_3$ and Hg_2VO_4 form Hg–Hg bonds of 254.3 and 253.6 pm, respectively. These distances are quite close to the average Hg–Hg bond distance of 251.3 pm found for about 50 Hg–Hg bonds in some 30 mercury oxo-compounds (22). The average Hg(I)–O distance of these compounds is 217 pm, and considering the large standard deviations, this is compatible with the corresponding distances
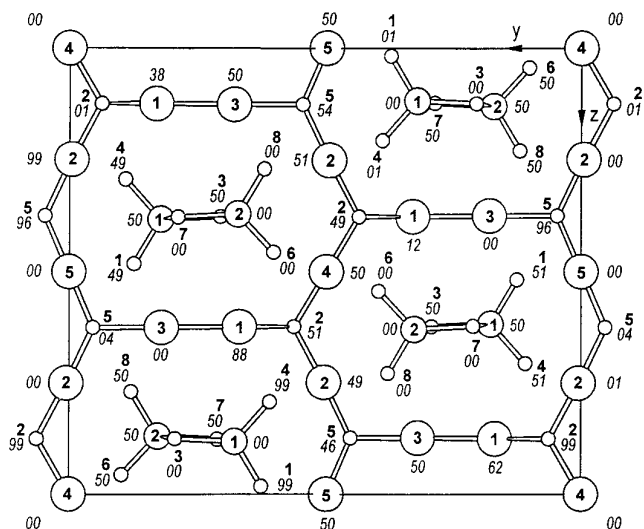
of 211.2(4) and 220(2) pm in $HgVO_3$ and Hg_2VO_4. The short Hg(II)–O bond distances of 196(2), 198(2), and 205(2) in Hg_2VO_4 are also quite close to the average Hg(II)–O bond distance of 206 pm found in a dozen other Hg(II) oxo-compounds with linear O–Hg(II)–O configuration (22).

ACKNOWLEDGMENTS

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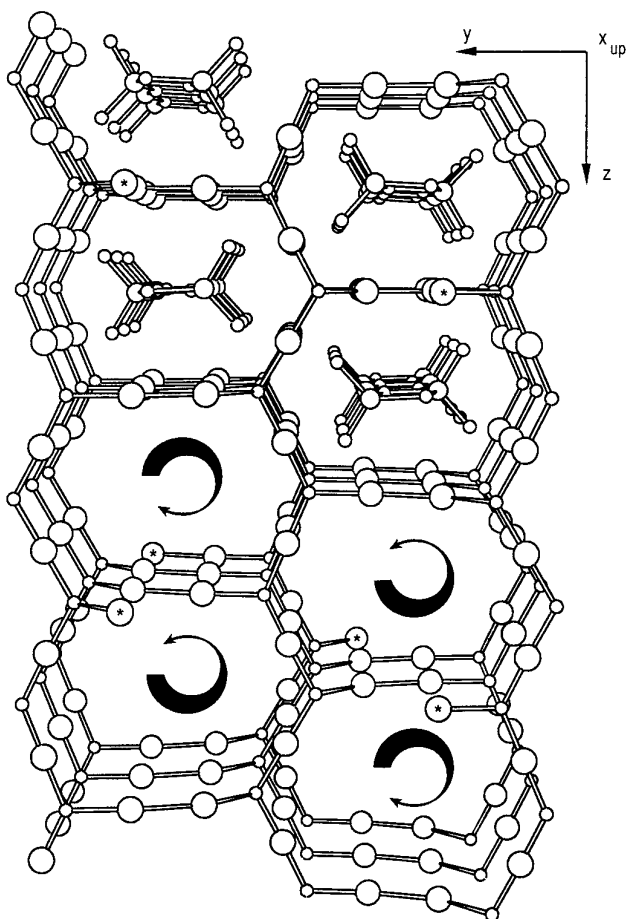
FIG. 5. Projections of the Hg_2VO_4 structure along the short translation period. Single-digit numbers in the parallel projection correspond to the atom designations. The heights of the atoms are indicated in hundredths. In the lower part of the perspective projection the vanadium–oxygen chain is omitted and the windings of the mercury–oxygen chains are indicated by arrows. Asterisks mark the atoms where these chains are broken.