Mercury(I) Molybdates and Tungstates: Hg_2WO_4 and Two Modifications of Hg_2MoO_4

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The high-temperature (β-) modification of Hg_2MoO_4 was prepared by solid-state reaction of HgO with MoO_2 at 400 °C. Well-crystallized samples of the low-temperature (α-) modification of Hg_2MoO_4 and isotypic Hg_2WO_4 were obtained by hydrothermal recrystallization of the microcrystalline powders at 180 °C. The crystal structures of these transparent yellow compounds were determined by single-crystal X-ray diffractometry. β-Hg_2MoO_4: $P2_1/c$, $Z = 4$, $a = 511.31(6)$ pm, $b = 901.83(7)$ pm, $c = 1086.0(1)$ pm, $\beta = 101.01(3)°$. α-Hg_2MoO_4 and Hg_2WO_4: $C2/c$, $Z = 4$, $a = 873.52(6)$ and 873.0(1) pm, $b = 1155.19(7)$ and 1147.6(3) pm, $c = 493.05(3)$ and 493.24(6) pm, $\beta = 115.196(5)°$ and 114.86(1)°, respectively. In β-Hg_2MoO_4 the molybdenum atoms are tetrahedrally coordinated by oxygen atoms and the MoO_4 tetrahedra are linked via Hg_2 dumb-bells, thus forming infinite zigzag chains. The low-temperature (α-)modification of Hg_2MoO_4 contains MoO_6 octahedra, which are linked via common edges to form zigzag chains, which are further linked via Hg_2 dumb-bells, resulting in puckered two-dimensionally infinite sheets. Bonding between adjacent sheets is achieved only via weak (secondary) Hg−O bonds of 254.8 pm, while the strong Hg−O bonds of the nearly linear O−Hg−Hg−O groups within the sheets have a length of 214.8 pm. The Hg−Hg bond lengths are practically the same in the three compounds with 252.3(1), 253.49(7), and 253.3(1) pm in β-Hg_2MoO_4, α-Hg_2MoO_4, and Hg_2WO_4, respectively. The average Mo−O distances within the MoO_4 tetrahedra and the MoO_6 octahedra are 176.2, and 196.5 pm, respectively. The structural chemistry of these compounds is discussed together with that of previously reported mercury I and II molybdates and tungstates.

Introduction

Only three mercury molybdates and one mercury tungstate are structurally well characterized. The structure of the mercury(II) molybdate(VI), $HgMoO_4$, and the isotypic mercury tungstate, $HgWO_4$, has been reported almost 30 years ago. It consists of distorted MoO_6 and WO_6 octahedra, respectively, that share common edges, thus forming infinite zigzag chains. These chains are oriented parallel to each other, and they are linked via Hg(II) atoms.[1,2]

More than 20 years later two other mercury molybdates $Hg_2Mo_2O_7$ and $Hg_2Mo_5O_{16}$ were characterized.[3,4] We now report the preparation and crystal structures of two modifications of Hg_2MoO_4. The low-temperature (α-) modification and the isotypic compound Hg_2WO_4 have already been characterized by their X-ray powder patterns, which could be indexed with *C*-centered monoclinic cells.[5] These are now confirmed by the structure determinations. Brief reports about the present work have been given at conferences.[6,7]

Experimental Section

Sample Preparation, Properties, and Lattice Constants. Single crystals of the high-temperature (β-) modification of Hg_2MoO_4 were prepared by solid-state reaction of yellow mercury oxide, HgO (Chempur, >99%), and MoO_2. The molybdenum dioxide was synthesized by chemical transport of elemental molybdenum and the trioxide, MoO_3, using iodine and water (from the silica tube) as transporting agent.[8] The transport was from 1000 to 800 °C. Powders of the oxides HgO and MoO_2 were mixed in the ideal ratio, annealed in evacuated silica tubes for 16 days at 400 °C, and quenched in air. The major product of this reaction was the mercury(II) molybdate $HgMoO_4$.[2] Other products were $Hg_2Mo_2O_7$,[3] MoO_3, and elemental mercury. Small single crystals of β-Hg_2MoO_4 were attached at the tube walls.

The isotypic compounds α-Hg_2MoO_4 and Hg_2WO_4 were prepared by hydrothermal recrystallization. Microcrystalline powders of α-Hg_2MoO_4 and Hg_2WO_4 were obtained by precipitation, reacting aqueous solutions of $Na_2MoO_4{\cdot}2H_2O$ and $Na_2WO_4{\cdot}2H_2O$ (both from Riedel de Haën, 99.5%), respectively, and $Hg_2(NO_3)_2{\cdot}2H_2O$ (Merck, p.a.). For the hydrothermal syntheses, 800 mg of α-Hg_2MoO_4 and Hg_2WO_4 were each sealed in evacuated silica tubes of about 12 cm^3 volume with 3.5 mL of water. The tubes were placed in a steel autoclave with 10 bar of nitrogen. After sealing, the autoclave was heated to 180 °C, held at that temperature for 60 h, and finally cooled to room temperature within 12 h.

The crystals of the high-temperature (β-) modification of Hg_2MoO_4 are needle-shaped with a dark-yellow, almost orange, color. The low-temperature (α-) modification and the corresponding tungstate also crystallize in the form of transparent needles. Their colors are of a lighter yellow. When ground to powders, α-Hg_2MoO_4 is lemon yellow, while Hg_2WO_4 is pale yellow. Energy-dispersive X-ray fluorescence analyses of the three compounds in a scanning electron microscope showed no impurity elements heavier than sodium.

The lattice constants of the three compounds were determined on the four-circle diffractometer. Those of α-Hg_2MoO_4 and Hg_2WO_4 were also determined by least-squares fits of the Guinier powder data using

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(1) Jeitschko, W.; Sleight, A. W. *Z. Naturforsch.* **1972**, *27b*, 203.
(2) Jeitschko, W.; Sleight, A. W. *Acta Crystallogr.* **1973**, *B29*, 869.
(3) Wessels, A. L.; Jeitschko, W. *Z. Naturforsch.* **1996**, *51b*, 37.
(4) Wessels, A. L.; Jeitschko, W. *J. Solid State Chem.* **1997**, *128*, 205.
(5) Wessels, A. L.; Czekalla, R.; Jeitschko, W. *Mater. Res. Bull.* **1998**, *33*, 95.
(6) Mormann, Th. J.; Jeitschko, W. *Z. Kristallogr. Suppl.* **1999**, *16*, 50.
(7) Mormann, Th. J.; Jeitschko, W. *Z. Kristallogr. Suppl.* **2000**, *17*, 133.
(8) Schäfer, H.; Grofe, Th.; Trenkel, M. *J. Solid State Chem.* **1973**, *8*, 14.

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Table 1. Crystal Data of β-Hg_2MoO_4, α-Hg_2MoO_4, and Hg_2WO_4[a]

empirical formula	β-Hg_2MoO_4	α-Hg_2MoO_4	Hg_2WO_4
space group	$P2_1/c$ (No. 14)	$C2/c$ (No. 15)	$C2/c$ (No. 15)
a (pm)	[511.31(6)]	873.52(6) [873.1(1)]	873.0(1) [872.9(1)]
b (pm)	[901.83(7)]	1155.19(7) [1154.7(3)]	1147.6(3) [1147.1(2)]
c (pm)	[1086.0(1)]	493.05(3) [492.75(7)]	493.24(6) [493.22(7)]
β (deg)	[101.01(3)]	115.196(5) [115.20(1)]	114.86(1) [114.87(1)]
V (nm^3)	[0.4916]	0.4502 [0.4495]	0.4484 [0.4480]
Z	4	4	4
fw	561.1	561.1	649.0
temp (°C)	21	21	21
λ (pm)	71.07	71.07	71.07
ρ_{calc} (g/cm^3)	7.58	8.28	9.61
μ (cm^{-1})	647	707	938
$R(F)^b$	0.035	0.024	0.033
$R_w(F^2)^b$	0.093	0.052	0.075

[a] The lattice constants were obtained from Guinier powder [single crystal] data. Standard deviations in the positions of the least significant digits are given in parentheses throughout the paper. [b] $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $R_w = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (VP)^2]$ where $P = (\max(F_o^2) + 2F_c^2)/3$ and $V = 0.0332$ for β-Hg_2MoO_4, $V = 0.0108$ for α-Hg_2MoO_4, and $V = 0.0144$ for Hg_2WO_4.

Cu Kα_1 radiation and α-quartz ($a = 491.30$ pm, $c = 540.46$ pm) as an internal standard (Table 1). They agree within three standard deviations with those reported earlier.[5]

Structure Determinations. Single crystals of all three compounds were selected for the structure determinations on the basis of Laue patterns. X-ray intensity data were collected at room temperature on an Enraf-Nonius CAD4 diffractometer with $\theta/2\theta$ scans using graphite-monochromated Mo Kα radiation, a scintillation counter with pulse-height discrimination, and background counts at both ends of each scan. Empirical absorption corrections were made from ψ scan data. The crystal data are listed in Table 1 and more detailed in the Supporting Information.

The structures were determined and refined with the program package SHELX-97.[9] The positions of the metal atoms were located by Patterson syntheses, and the oxygen sites were obtained through difference Fourier syntheses. For the refinements, a full-matrix least-squares program was used with atomic scattering factors, corrected for anomalous dispersion as provided by the program.[9] The weighting schemes reflected the counting statistics, and isotropic parameters correcting for secondary extinction were optimized as least-squares variables. In the final difference Fourier syntheses the highest and lowest values were 5.1 and −2.1 e/Å^3 for β-Hg_2MoO_4, 1.7 and −1.4 e/Å^3 for α-Hg_2MoO_4, and 3.6 and −3.4 e/Å^3 for Hg_2WO_4. The positional parameters of all three compounds were standardized using the program STRUCTURE TIDY.[10] The atomic parameters are listed in Table 2, and the anisotropic displacement parameters are given in a table of the Supporting Information.

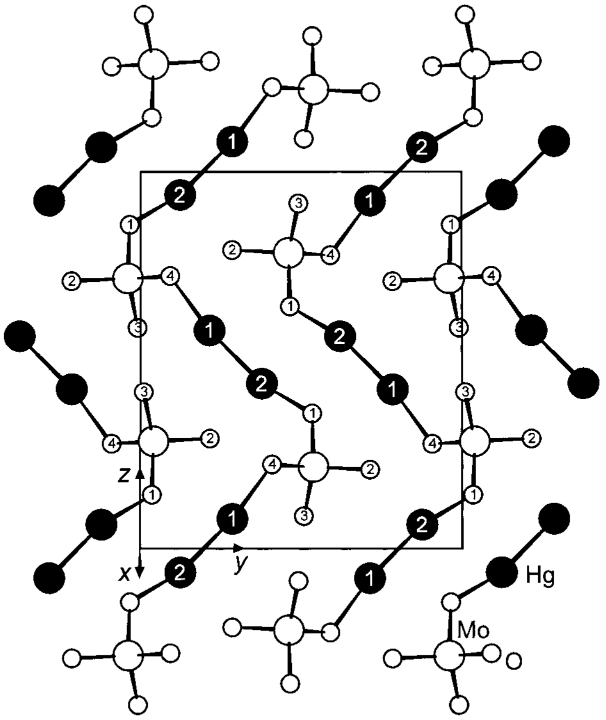

Figure 1. Projection of the monoclinic structure of the high-temperature (β-) modification of Hg_2MoO_4 along the (inclined) a axis.

Discussion

The structures of the high-temperature (β-) and low-temperature (α-) modifications of Hg_2MoO_4 differ essentially in the coordination of the molybdenum atoms. In β-Hg_2MoO_4 there are MoO_4 tetrahedra with no common oxygen atoms, while in α-Hg_2MoO_4 the molybdenum atoms have distorted octahedral coordination (Figures 1 and 2). The MoO_6 octahedra share edges, thus forming zigzag chains. The high-temperature modification was obtained by us only with a small yield at 400 °C. We have investigated a sample of the low-temperature modification on a high-temperature Simon−Guinier camera.[11] Up to 300 °C no phase transformation was observed. At higher temperature under normal pressure the compound decomposes. Nevertheless, the low-temperature modification may already be metastable at 300 °C, since the expected phase transition can be classified as reconstructive (as opposed to displacive) and therefore the transformation may require some time. Similar phase transitions between molybdates with high-temperature tetrahedral and low-temperature octahedral coordination of the molybdenum or tungsten atoms have been observed for the compounds $TMoO_4$ (T = Fe, Co, Ni)[12,13] and $SnWO_4$.[14,15]

Obviously, the tetrahedral coordination of the molybdenum atoms in β-Hg_2MoO_4 is favored at high temperature. Only two of the four oxygen atoms of each MoO_4 tetrahedron are tightly bound (to mercury atoms). This allows considerable thermal motion for the MoO_4 tetrahedra. Thus, a relatively large amount of thermal energy can be accommodated in the high-temperature modification, resulting in a large entropy term $T\Delta S$ in the Gibbs−Helmholtz equation. In the low-temperature modification

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(9) Sheldrick, G. M. *SHELX-97*: *A Program Package for the Solution and Refinement of Crystal Structures*; Universität Göttingen: Göttingen, Germany, 1997.
(10) Gelato, L. M.; Parthé, E. *J. Appl. Crystallogr.* **1987**, *20*, 139.
(11) Simon, A. *J. Appl. Crystallogr.* **1970**, *3*, 11.
(12) Trambouze, Y.; Colleuille, Y.; The, T. H. *C. R. Acad. Sci. Paris* **1956**, *242*, 497.
(13) Sleight, A. W.; Chamberland, B. L.; Weiher, J. F. *Inorg. Chem.* **1968**, *7*, 1093.
(14) Jeitschko, W.; Sleight, A. W. *Acta Crystallogr.* **1972**, *B28*, 3174.
(15) Jeitschko, W.; Sleight, A. W. *Acta Crystallogr.* **1974**, *B30*, 2088.

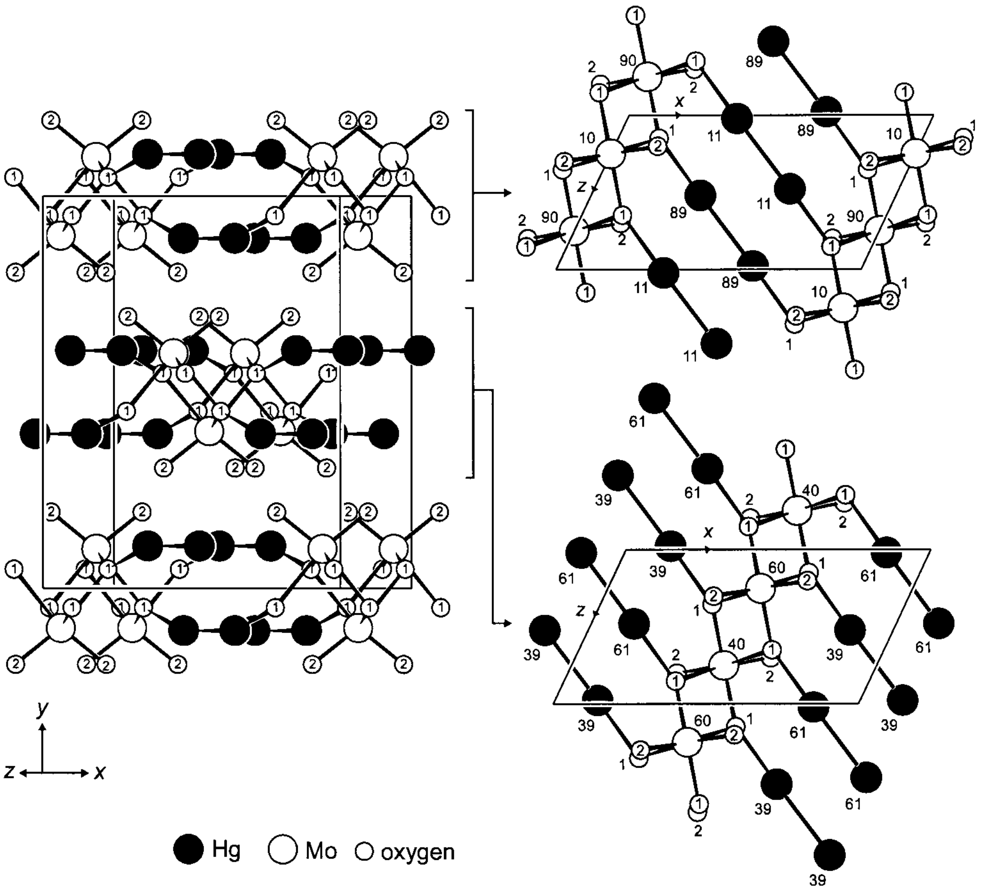

Figure 2. Crystal structure of α-Hg_2MoO_4. Strongly bonded atoms form layers that extend perpendicular to the *y* axis of the monoclinic cell. These layers are shown in projections along this axis at the right-hand side of the figure. Two-digit numbers correspond to the heights of the atoms in hundredths of the projection direction.

Table 2. Atomic Parameters of β-Hg_2MoO_4, α-Hg_2MoO_4, and Hg_2WO_4[a]

		x	*y*	*z*	B_{eq}
		β-Hg_2MoO_4 (Own Type, $P2_1/c$)			
Hg1	4e	0.44091(13)	0.28547(8)	0.07853(6)	1.87(2)
Hg2	4e	0.65470(14)	0.37735(8)	0.43669(6)	2.00(2)
Mo	4e	0.0307(2)	0.53982(14)	0.21623(11)	0.96 (2)
O1	4e	0.098(2)	0.0347(13)	0.1427(11)	2.0(2)
O2	4e	0.163(2)	0.7157(13)	0.2086(11)	2.1(2)
O3	4e	0.217(2)	0.0095(13)	0.4143(11)	2.0(2)
O4	4e	0.300(2)	0.4087(13)	0.2221(11)	2.1(2)
		α-Hg_2MoO_4 (Own Type, $C2/c$)			
Hg	8f	0.35870(5)	0.10714(3)	0.02189(8)	1.26(1)
Mo	4e	0	0.10025(10)	1/4	0.66(1)
O1	8f	0.1339(8)	0.0492(5)	0.6485(13)	0.88(9)
O2	8f	0.1416(8)	0.1938(6)	0.2010(15)	1.28(11)
		Hg_2WO_4 (α-Hg_2MoO_4 Type, $C2/c$)			
Hg	8f	0.35978(6)	0.10923(5)	0.02230(11)	1.24(1)
W	4e	0	0.09832(6)	1/4	0.59(1)
O1	8f	0.1339(10)	0.0502(8)	0.655(2)	0.79(13)
O2	8f	0.1424(11)	0.1940(8)	0.202(2)	1.23(14)

[a] The last column contains the equivalent isotropic values B_{eq} of the anisotropic displacement parameters ($\times 10^{-4}$, pm^2), as defined by $B_{eq} = 8\pi^2 U_{eq}$, where U_{eq} is one-third of the orthogonalized U_{ij} tensor.

the MoO_6 octahedra are more tightly bound because they have to share common oxygen atoms to result in the same composition, MoO_4. This is also apparent from the larger cell volume of the high-temperature modification: 0.1229 vs 0.1125 nm^3 per formula unit, a difference of almost 10%. It can be expected that the high-temperature form will also have larger thermal expansion. The fact that the high-temperature modification is less densely packed is also reflected by the thermal parameter values B_{eq}, which are all higher in the high-temperature modification when compared to those of the low-temperature form (Table 2), although both structures were determined from X-ray data collected at room temperature. Almost always the low- and the high-temperature modifications of dimorphic solid-state compounds differ in the number of variable positional atomic parameters, with the larger number of variable parameters occurring for the low-temperature form. Dimorphic Hg_2MoO_4 is one of the rare exceptions.

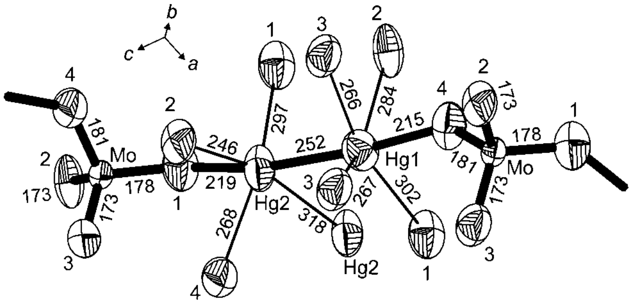

Figure 3. Near-neighbor environments of the metal atoms in β-Hg_2MoO_4. The thermal ellipsoids are drawn at the 95% probability limit. Single-digit numbers correspond to the designations of the oxygen atoms. The bond lengths (pm) are indicated by three-digit numbers.

The near-neighbor environments of the metal atoms in β-Hg_2MoO_4 are shown in Figure 3. The Mo−O distances in the tetrahedral MoO_4 groups range from 173.2 to 180.6 pm with an average of 176.2 pm. The average value compares well with the average distances found for other isolated tetrahedral MoO_4

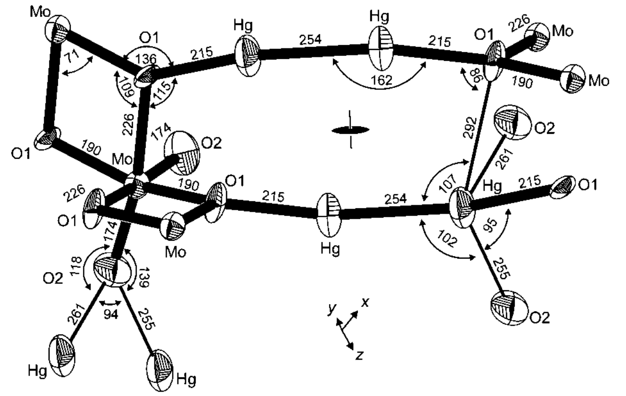

Figure 4. Atomic coordinations in low-temperature α-Hg_2MoO_4. Interatomic distances are in pm units, the angles in degrees of arc. The thermal ellipsoids are at the 95% probability limit.

groups, e.g., the five different MoO_4 tetrahedra in $La_2(MoO_4)_3$,[16] which have average Mo−O distances ranging between 177.1 and 178.1 pm or the five different isolated MoO_4 tetrahedra in $Ce_6(MoO_4)_8(Mo_2O_7)$[17] with average Mo−O distances between 175.3 and 177.5 pm.

The MoO_4 tetrahedra in β-Hg_2MoO_4 are linked via mercury(I) pairs, thus forming infinite zigzag chains −(MoO_4)−Hg−Hg−(MoO_4)−Hg−Hg− (Figure 1). The Hg−Hg distance of 252.3 pm compares well with the average of 251.3 pm found for about 50 Hg−Hg distances in some 30 mercury(I) oxocompounds.[18] This distance corresponds to a bond order of 1.[19] Together with the tightly bound oxygen neighbors O4 and O1 the mercury(I) atoms form nearly linear −O4−Hg1−Hg2−O1− groups with bond angles O4−Hg1−Hg2 and Hg1−Hg2−O1 of 171.4(3)° and 165.9(3)°, respectively. The short Hg−O distances of 214.8(11) and 218.6(11) pm compare well with the average of 217 pm found for other short Hg(I)−O distances.[18] In addition to these tightly bound oxygen atoms the Hg1 and Hg2 atoms have four and three other oxygen neighbors, respectively, with Hg−O distances between 245.9(11) and 302.5(12) pm. These interactions might be considered as weakly bonding. In addition to these weak Hg−O interactions the Hg2 atom has another Hg2 atom in its coordination shell at 318.1(1) pm. This distance is almost 30% greater than the short Hg1−Hg2 distance of 252.3(1) pm, and possibly this weak interaction is also (very weakly) bonding.

In Figure 4 we show the near-neighbor environments in α-Hg_2MoO_4. This compound has only one kind of mercury atom, and the short Hg−Hg and Hg−O distances of 253.5(1) pm and 214.8(6) pm, respectively, are comparable to the corresponding distances just discussed for the β-modification. The Hg−Hg−O1 angle of the ideally linear O1−Hg−Hg−O1 group is 161.8(2)°. The deviation from 180° is most likely due to packing effects.

The molybdenum atoms in the α-modification are situated in distorted oxygen octahedra. There are two short Mo−O distances of 173.5(6) pm, two medium-long Mo−O distances of 190.3(6) pm, and two long Mo−O distances of 225.8(6) pm. This environment with a very similar progression of Mo−O distances is found in many compounds with octahedral molybdate groups, e.g., $HgMoO_4$,[2] $Hg_2Mo_2O_7$,[3] and $Hg_2Mo_5O_{16}$.[4] In all of these compounds the oxygen atoms with the two short Mo−O bonds occupy an edge of their MoO_6 octahedra, and this is also the case for the oxygen atoms with the long Mo−O bonds, while the oxygen atoms of the medium-long Mo−O bonds occupy opposite corners of the MoO_6 octahedra. As could be expected, the oxygen atoms with the short Mo−O bonds of these compounds do not form any strong Hg−O bonds.

Table 3. Interatomic Distances in the Structures of β-Hg_2MoO_4 and α-Hg_2MoO_4/Hg_2WO_4[a]

				β-Hg_2MoO_4				
Hg1:	Hg2	252.3	Mo:	O3	173.2	O2:	Mo	173.2
	O4	214.8		O2	173.2		Hg2	245.9
	O3	266.4		O1	177.8		Hg1	283.9
	O3	267.1		O4	180.6	O3:	Mo	173.2
	O2	283.9	O1:	Mo	177.8		Hg1	266.4
	O1	302.5		Hg2	218.6		Hg1	267.1
Hg2:	Hg1	252.3		Hg2	297.2	O4:	Mo	180.6
	Hg2	318.1		Hg1	302.5		Hg1	214.8
	O1	218.6					Hg2	268.2
	O2	245.9						
	O4	268.2						
	O1	297.2						
				α-Hg_2MoO_4/Hg_2WO_4				
Hg:	Hg	253.5/253.3	Mo/W:	2O2	173.5/174.7	O2:	Mo/W	173.5/174.7
	O1	214.8/215.1		2O1	190.3/192.3		Hg	254.8/251.2
	O2	254.8/251.2		2O1	225.8/222.6		Hg	260.9/259.9
	O2	260.9/259.9	O1:	Mo/W	190.3/192.3			
	O1	292.4/295.8		Hg	214.8/215.1			
				Mo/W	225.8/222.6			
				Hg	292.4/295.8			

[a] For the calculation of these distances the lattice constants obtained from single-crystal data (β-Hg_2MoO_4) and the Guinier powder patterns (α-Hg_2MoO_4 and Hg_2WO_4) were used. All distances shorter than 330 pm (metal−metal) and 320 pm (metal−oxygen) are listed. The standard deviations are all equal to or less than 0.1 pm for the Hg−Hg distances and are 1 pm or less for the metal−oxygen distances.

The tungsten compound Hg_2WO_4 is isotypic with the low-temperature modification of Hg_2MoO_4. The positional and also the thermal parameters of the two compounds are very similar. As could be expected, the anisotropic thermal parameters of the heavy tungsten atom are all smaller than those of the molybdenum atom. The short Hg−Hg and Hg−O distances of both compounds are practically the same, while the short Mo−O distances are slightly shorter than the short W−O distances (Table 3). This difference corresponds to the difference reflected by the difference in the atomic radii listed for molybdenum and tungsten in the respective binary and ternary oxides by Shannon.[20] It can be expected that at high temperature the tungsten compound Hg_2WO_4 transforms to a modification with tetrahedral WO_4 groups in analogy to the phase transformation of Hg_2MoO_4. However, since these compounds have a tendency to decompose at higher temperature, considerable oxygen and mercury vapor pressure may be required to prevent such a decomposition.

The structure of α-Hg_2MoO_4 has some similarity with the structure of $HgMoO_4$.[2] In both compounds the MoO_6 octahedra share edges with two other MoO_6 octahedra, thus forming zigzag chains with the composition MoO_4. In α-Hg_2MoO_4 these chains are linked via Hg_2 dumb-bells, resulting in puckered two-dimensionally infinite sheets. Bonding between adjacent sheets occurs only via the weak (secondary) Hg−O bonds of 254.8(7) pm. In $HgMoO_4$ the zigzag chains of edge-sharing MoO_6 octahedra are linked by the Hg(II) atoms. Again, in this way two-dimensionally infinite sheets are formed. Both structures crystallize in the space group *C*2/*c*, and the mercury molybdate

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(16) Jeitschko, W. *Acta Crystallogr.* **1973**, *B29*, 2074.
(17) Gatehouse, B. M.; Same, R. *J. Solid State Chem.* **1978**, *25*, 115.
(18) Wessels, A. L. Darstellung und strukturelle Charakterisierung ternärer Quecksilberoxide. Doctoral Thesis, Universität Münster, Germany, 1996.
(19) Brown, I. D.; Gillespie, R. J.; Morgan, K. R.; Tun, Z.; Ummat, P. K. *Inorg. Chem.* **1984**, *23*, 4506.
(20) Shannon, R. D. *Acta Crystallogr.* **1976**, *A32*, 751.

sheets of both compounds extend perpendicular to the *y* direction. A major difference of the two structures lies in the arrangement of the sheets when viewed along the *y* direction. In $HgMoO_4$ these sheets are superimposed, while in α-Hg_2MoO_4 they are staggered (Figure 2). Thus, the *b* axis of the latter compound is twice as large as in $HgMoO_4$. Nevertheless, both compounds have $Z = 4$ formula units in the C-centered cell because the sheets of $HgMoO_4$ are puckered in a way that the *a* axis of the structure is doubled.

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Supporting Information Available: Listings of crystallographic data and anisotropic displacement parameters of β-Hg_2MoO_4, α-Hg_2MoO_4, and Hg_2WO_4. This material is available free of charge via the Internet at http://pubs.acs.org.

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