NOTIZEN

The Crystal Structures of $HgMoO_4$ and two Forms of $SnWO_4$

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Two forms of $SnWO_4$ have been prepared for the first time by reaction of SnO and WO_3 in evacuated silica capsules at temperatures between 600 and 900 °C. The two modifications transform into each other by a fast but diffusion-controlled phase transition at 670 °C. Single crystals of α-$SnWO_4$ were prepared by slow cooling from below the transition temperature. They are orthorhombic (Pnna) with $a=5.627$, $b=11.649$, $c=4.997$ Å, and $Z=4$. Metastable β-$SnWO_4$ can be obtained through rapid quenching from above 670 °C. It is cubic ($P2_13$) with $a=7.299$ Å, and $Z=4$. Single crystals of $HgMoO_4$ are monoclinic with $a=11.282$, $b=6.055$, $c=5.154$ Å, $\beta=112.27°$; the space group is C2/c and $Z=4$.

The structures have been solved and refined from single crystal x-ray data. Final conventional R-values are 0.032 (498 observed reflections) for α-$SnWO_4$, 0.034 (248 observed reflections) for β-$SnWO_4$, and 0.025 (853 reflections, including unobserved) for $HgMoO_4$. Positional parameters are as follows:

Atom	Position	x	y	z
α-$SnWO_4$	(Pnna-D_{2h}^6)			
Sn	4c	1/4	0	0.2196
W	4d	0.6677	1/4	1/4
O(1)	8e	0.377	0.299	0.999
O(2)	8e	0.102	0.396	0.604
β-$SnWO_4$	($P2_13$-T^4)			
Sn	4a	0.8416	0.8416	0.8416
W	4a	0.1644	0.1644	0.1644
O(1)	4a	0.304	0.304	0.304
O(2)	12b	0.864	0.773	0.547
$HgMoO_4$	(C2/c-C_{2h}^6)			
Hg	4c	1/4	1/4	0
Mo	4e	0	0.1880	1/4
O(1)	8f	0.0983	0.0906	0.0320
O(2)	8f	0.1139	0.3642	0.4684

The structures of the two $SnWO_4$ modifications are not related. Tungsten is tetrahedrally coordinated to oxygen in the β form, but the coordination is distorted octahedral in the α-form. The coordination around Sn^{2+} shows the "inert pair" effect in both structures. The metal atoms in $HgMoO_4$ are both in severely distorted octahedral coordination with Hg-O distances varying between 2.03 and 2.77 Å and Mo-O distances from 1.72 to 2.23 Å.

Detailed reports on these structures are in preparation.

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