Acta Cryst. (1964). 17, 618

Crystallographic data on UO₂WO₄ and UO₂MoO₄*. By E. F. JUENKE and S. F. BARTRAM, General Electric Company, Nuclear Materials and Propulsion Operation, Cincinnati, Ohio, U.S. A.

(Received 6 December 1963)

Double oxides of uranium with tungsten or molybdenum were prepared by co-calcining mixtures of their oxides in air at temperatures of 800–1000 °C. Only the compounds UO₂WO₄ and UO₂MoO₄ were formed; no other new phases were observed. Reduction of the starting materials or the calcined products at 1700 °C in hydrogen yielded tungsten or molybdenum metal and UO₂. These results are essentially in agreement with data reported on the U-W-O system by Trunov, Kovba & Spitsyn (1961). Although they show schematic line diagrams of X-ray patterns for the isostructural UO₂WO₄, UO₂MoO₄ and UO₂CrO₄ compounds, no crystallographic data were given.

Powder diffractometry and Weissenberg single-crystal photographs established the crystal symmetry as monoclinic with the following lattice constants:

	$\mathrm{UO_2WO_4}$	$\mathrm{UO_2MoO_4}$
\boldsymbol{a}	$7.205 \pm 0.003 \text{ Å}$	$7.200 \pm 0.003 \text{Å}$
\boldsymbol{b}	$5.482 \pm 0.002 \text{ Å}$	$5.480 \pm 0.002 \text{\AA}$
\boldsymbol{c}	$13.57 \pm 0.01 \text{ Å}$	$13.59 \pm 0.01 \text{ Å}$
β	104° 35′	104° 36′
Volume	$518.59 \ { m \AA}^3$	$518.96 \; { m \AA}^3$

Table 1. X-ray powder diffraction patterns

UO ₂ WO ₄			UO,	MoO ₄
d	Relative intensity	hkl	\overline{d}	Relative intensity
6.92	12	100	6.93	22
_		002	6.55	3
5.50	4	$\overline{1}02$	5.51	14
5.03	12	011	5.03	1
4.30	15	110, 111	4.30	19
4.19	100	$0\dot{1}2$	4.20	100
3.909	48	111	3.915	24
3.483	25	200	3.480	20
3.453	16	$\overline{2}02$	3.457	18
		013	3.423	4
3.363	12	112	3.367	11
3.333	18	Ī13	3.341	12
3.278	23	004	3.286	31
3.007	2	$\overline{2}11$	_	
2.940	14	210)	0.000	11
2.923	10	$\overline{2}12$	2.933	11
2.856	3	113 ´		_
2.827	3	$\overline{1}14$	2.833	5
2.816	3	014	2.820	4
2.802	8	202	2.801	5
2.757	8	$\overline{2}04$	2.762	7
_		020	2.739	2
2.720	4	104	2.721	5
2.678	2	021	2.683	4
2.546	28	$\overline{1}21,120$	2.548	10
2.495	2	212	_	
2.465	4	$\overline{2}14$	$2 \cdot 465$	3
$2 \cdot 452$	9	$\overline{1}22$	2.455	6
2.368	1	015		_
2.322	4	300	$2 \cdot 321$	5
2.304	7	122	$2 \cdot 305$	7

The space group was unambiguously determined from systematic absences to be $P2_1/c$ with 4 formula units in the unit cell. Calculated theoretical densities are 6.63 and 5.50 g.cm⁻³ for $\rm UO_2WO_4$ and $\rm UO_2MoO_4$ respectively. The measured value for the tungsten compound was 6.46 g.cm⁻³ by the displacement method.

Powder diffraction patterns of these compounds are shown in Table 1.

Table 1 (cont.)

UO	$_2\mathrm{WO}_{4}$	` ,	$\mathrm{UO_2MoO_4}$	
\overline{d}	Relative	hkl	d	Relative
$2 \cdot 257$	1	$\overline{1}06$	2.260	4
2.189	$\hat{3}$	$\overline{3}12$	2.188	$\bar{4}$
		$\overline{3}04$	2.172	ī
2.125	11	$\overline{3}13$	0.100	10
2.120	18	123	$2 \cdot 122$	10
2.103	5	024, 115	$2 \cdot 105$	4
2.085	4	ī16	2.089	3
2.039	7	311	0.000	8
2.034	7	302,016	2.036	
1.992	3	214	1.992	4
1.966	4	$\overline{2}16$	1.969	4
1.960	3	222	1.958	2
1.919	7	$\overline{1}25$	1.922	4
1.908	4	312	1.909	4
1.895	3	025	1.899	4
1.840	5	$\bar{3}06, 116$	1.841	6
1.825	6	223	1.823	4
1.808	5	031	1.809	4
1.803	12	$\overline{4}02$	1.800	6
1.783	2	215	_	
	3	(017	1.777	1
1.774		320	1.771	5
1.767	6	130, 313, 731	1.767	5
1.760	5	$\overline{2}17$		
1.742	2	$\overline{1}26$	1.743	4
1.737	7	131	1.736	5
1.715	2	321)	1 710	
1.711	2	026	1.712	1
1.697	2	ī08 ´	1.698	1
1.685	6	033	1.686	6

Formulae of these compounds have been written as uranyl orthotungstate or molybdate to conform to the original Russian nomenclature although no structural evidence is as yet available to confirm the existence of these groups of ions. The actual coordination of the metal atoms must be determined by rigorous structure analysis.

References

Trunov, V. K., Kovba, L. M. & Spitsyn, V. I. (1961). Doklady Akad. Nauk SSSR, No. 1, 114.

^{*} These data originated from work sponsored by the Fuels and Materials Development Branch, Division of Reactor Development, under Contract AT(40-1)-2847.