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On the Structure of the Series of Oxides $M^{II}UMo_4O_{16}$*

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A family of oxides $M^{II}UMo_4O_{16}$ (M^{II} = Mg, Mn, Cd, Ca, Hg, Sr, Pb) was recently described (*1*). Unit-cell dimensions were obtained from powder-diffraction photographs, and atom coordinates were derived from single-crystal intensity measurements on the calcium compound. The resulting structure type was described as triclinic, space group $P\bar{1}$. It is correctly described as monoclinic, space group $P2/n$.

The transformation $a' = a + b$, $b' = b$, $c' = c$ leads to the monoclinic cell dimensions listed in Table I. For none of the seven compounds do the angles α' or γ' differ significantly from 90°. (The angles α' are those given for α in Table I, Ref. (*1*), and are "90.00" in all seven cases. Only one of the derived values of γ' differs from 90.00° by more than 0.01°—that for the Mn compound, at 90.05°.)[1] The corresponding transformation $x' = x$, $y' = y - x$, $z' = z$, when applied to the coordinates in Table III, Ref. (*1*), lead to atom positions that are consistent with the symmetry of $P2/n$

TABLE I

COMPOUNDS $M^{II}UMo_4O_{16}$: REVISED CELL DIMENSIONS, SPACE GROUP $P2/n$

M	a (Å)	b (Å)	c (Å)	β (°)
Mg	11.393	6.505	7.920	89.80
Mn	11.415	6.557	8.010	89.93
Cd	11.432	6.625	8.150	90.37
Ca	11.447	6.651	8.236	90.44
Hg	11.431	6.645	8.248	90.50
Sr	11.476	6.762	8.474	90.85
Pb	11.454	6.811	8.554	90.85

TABLE II

COORDINATES OF THE CALCIUM COMPOUND, SPACE GROUP $P2/n$

Atom	N^a	x	y	z
U	2	0.25	0.7041	0.75
Ca	2	0.25	0.7039	0.25
Mo(1,2)		0.5962	−0.1702	0.7956
Mo(3,4)		0.0928	0.1687	0.7958
O(1,3)		0.933	0.151	0.246
O(2,16)		0.9372	0.147	0.749
O(4,13)		0.096	0.151	0.504
O(5,8)		0.128	0.418	0.758
O(6,7)		0.746	0.297	0.035
O(9,11)		0.097	0.156	0.005
O(10)	2	0.25	0.072	0.25
O(12,15)		0.125	0.419	0.263
O(14)	2	0.25	0.063	0.75

[a] Number in cell, if other than 4.

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[1] In Ref. (*1*), the cell dimensions for the Ca compound as given in the body of the text do not agree with those listed in the accompanying Table I and were apparently misprinted.

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within the reported errors. (The z coordinate of Mo(s), 0.7559, was obviously misprinted. I have assumed it to be 0.7959, which leads to correct Mo–O distances.)

Since neither the cell dimensions nor the atom coordinates need to be significantly changed to achieve the symmetry of $P2/n$, the bond lengths and general description of the structure remain unchanged. The n-glide plane of $P2/n$ requires the systematic absence of reflections $h0l$ with $(h + l)$ odd. A supplementary table of F's that would permit confirmation of these absences is apparently not available.

Reference

1. M. R. Lee and S. Jaulmes, *J. Solid State Chem.* **67**, 364 (1987).