Short Communications

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The symmetry of $Cu_3Mo_2O_9$.

By Lars Kihlborg and Rolf Norrestam, *Institute of Inorganic and Physical Chemistry, University of Stockholm, S*-104 05 *Stockholm, Sweden*

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The crystal structure of $Cu_3Mo_2O_9$ was recently described in the non-centrosymmetric space group $Pna2_1$. Further refinement indicates, however, that the structure is centrosymmetric, with space group *Pnam*. The interatomic distances and the description of the structure remain essentially unchanged.

The results of a crystal structure determination of the fully oxidized copper molybdate $Cu_3Mo_2O_9$ was recently published in this journal (Kihlborg, Norrestam & Olivecrona, 1971). The structure was solved by direct methods and described in the non-centrosymmetric space group $Pna2_1$, with the 14 atoms in fourfold general positions.

Dr David H. Templeton, University of California, Berkeley, California, has kindly pointed out to us that the parameters given are rather close to a centrosymmetric arrangement. Following his suggestion we have refined the structure in the space group *Pnam*. To conform with the usual description of this space group, the origin had to be shifted by $\Delta z \approx 0{\cdot}25$, placing Cu(1) at the origin and all other atoms, except two oxygen atoms, on the mirror planes at $z = \frac{1}{4}$ and $\frac{3}{4}$. The atom O(9) becomes symmetry-related to O(4), and the atom O(8) to O(5).

The result of this further refinement clearly indicates that there is no reason for treating the structure as acentric, and *Pnam* (No. 62) should be considered the proper space group. With the number of refinable parameters reduced from 56 in $Pna2_1$ to 37 in *Pnam* the *R* value increased only slightly, namely from 0·070 to 0·077. The standard deviations did not change significantly, except for the atoms which became symmetry-related, for which the standard deviations dropped to about one half their previous values. The new coordinates and isotropic temperature factors are given in Table 1. The coordinates have been shifted by an average of $1{\cdot}6\sigma$. The largest shift, 10σ, is in the *y* coordinate of Cu(1); the remaining shifts are all below 5σ. The temperature factors have improved and are less divergent, particularly those of the oxygen atoms. The interatomic distances, given in Table 2, have changed slightly, but the description and the discussion of the structure need no revision.

Table 1. *Space group, unit cell, fractional atomic coordinates and isotropic temperature factors*

Standard deviations are in parentheses.

Space group: *Pnam* (D_{2h}^{16}).
Unit-cell dimensions: $a = 7{\cdot}659$ (10), $b = 14{\cdot}613$ (15), $c = 6{\cdot}875$ (10) Å.

		x	*y*	*z*	*B*
Cu(1)	4(*a*)	0	0	0	0·60 (5)
Cu(2)	4(*c*)	0·1611 (4)	0·14030 (23)	$\frac{3}{4}$	0·65 (5)
Cu(3)	4(*c*)	0·2043 (4)	0·43607 (21)	$\frac{1}{4}$	0·65 (5)
Mo(1)	4(*c*)	0·26260 (27)	0·16603 (15)	$\frac{1}{4}$	0·51 (4)
Mo(2)	4(*c*)	0·15124 (30)	0·38535 (15)	$\frac{3}{4}$	0·50 (4)
O(1)	4(*c*)	0·0883 (25)	0·0149 (13)	$\frac{3}{4}$	0·98 (29)
O(2)	4(*c*)	0·1953 (30)	0·2684 (16)	$\frac{3}{4}$	1·86 (39)
O(3)	4(*c*)	0·4310 (34)	0·0945 (16)	$\frac{3}{4}$	2·14 (42)
O(4)	8(*d*)	0·2463 (19)	0·4353 (9)	0·9593 (24)	1·48 (23)
O(5)	8(*d*)	0·1389 (18)	0·1332 (9)	0·0382 (21)	1·30 (21)
O(6)	4(*c*)	0·2990 (27)	0·2809 (15)	$\frac{1}{4}$	1·43 (33)
O(7)	4(*c*)	0·4706 (29)	0·1075 (15)	$\frac{1}{4}$	1·62 (34)

Table 2. *Selected interatomic distances*

Cu(1)–2O(1)	1·860 (8) Å	Cu(3)–O(7)	1·900 (23) Å
Cu(1)–2O(4)	2·179 (15)	Cu(3)–O(1)	1·962 (19)
Cu(1)–2O(5)	2·234 (13)	Cu(3)–2O(4)	2·025 (17)
Cu(1)–2Cu(2)	2·946 (3)	Cu(3)–O(6)	2·381 (22)
Cu(1)–2Cu(3)	2·993 (4)	Cu(3)–O(3)	2·537 (24)
		Cu(3)–2Cu(1)	2·993 (4)
Cu(2)–O(2)	1·891 (23)	Cu(3)–Cu(2)	3·157 (5)
Cu(2)–O(1)	1·915 (19)		
Cu(2)–2O(5)	1·991 (15)	Mo(1)–O(6)	1·701 (22)
Cu(2)–O(3)	2·173 (26)	Mo(1)–2O(5)	1·802 (14)
Cu(2)–2Cu(1)	2·946 (3)	Mo(1)–O(7)	1·808 (22)
Cu(2)–Cu(3)	3·157 (5)		
		Mo(2)–O(3)	1·713 (26)
		Mo(2)–O(2)	1·741 (23)
		Mo(2)–2O(4)	1·770 (16)

Reference

Kihlborg, L., Norrestam, R. & Olivecrona, B. (1971). *Acta Cryst.* B**27**, 2066.