

The structure of $\text{Na}_2\text{Y}(\text{MoO}_4)(\text{PO}_4)$. Corrigendum. By RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA 91125, USA*

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Abstract

The structure of $\text{Na}_2\text{Y}(\text{MoO}_4)(\text{PO}_4)$ was described [Ben Amara & Dabbabi (1987). *Acta Cryst. C43*, 616–618] as monoclinic, space group $C2/c$, with $a = 13.928$ (11), $b = 18.016$ (10), $c = 6.847$ (6) Å, $\beta = 119.62$ (6)°, $Z = 8$. It should be described as orthorhombic, space group $Ibca$. The vectors (010), (101), (001) describe a body-centered cell with $a' = 18.016$, $b' = 12.108$, $c' = 6.847$ Å, $\alpha' = 89.83$, $\beta' = \gamma' = 90$ °, $Z = 8$; the corresponding coordinate transformations are $x' = y$, $y' = x$, $z' = x - z$.

The $Ibca$ coordinates, after appropriate averaging of equivalent atoms, are given in Table 1. None of the original $C2/c$ coordinates needs to be shifted by more than 2 e.s.d.'s to achieve the symmetry of $Ibca$; indeed, the r.m.s. value of the shift-to-sigma ratio is 0.8, somewhat below the expectation value of 1.0. On the other hand, the angle α' differs from its expectation value of 90° by nearly 3 e.s.d.'s (assuming that

the e.s.d. of 0.06° assigned to the original angle β would also apply to the new angle). It is by no means unusual that the e.s.d.'s assigned to unit-cell dimensions do not adequately represent the accuracies of these values; as normally derived, they are estimates of precision only.

Table 1. *Coordinates, space group Ibca.*

Numbers in parentheses are e.s.d.'s, estimated from the values in Table 1 of Ben Amara & Dabbabi (1987).

	x'	y'	z'
Na(1,2)	0.5974 (2)	0.1876 (3)	-0.2646 (5)
Y	0.75	0.07186 (4)	0.0
Mo(1,2)	0.42828 (4)	0.0	-0.25
P	0.25	0.1811 (1)	0.0
O(1,3)	0.3717 (2)	0.0239 (3)	-0.4596 (6)
O(2,4)	0.4818 (3)	0.1174 (4)	-0.2072 (7)
O(5,6)	0.1816 (2)	0.2564 (3)	0.0152 (5)
O(7,8)	0.2416 (2)	0.1020 (2)	-0.1752 (4)

Reference

BEN AMARA, M. & DABBABI, M. (1987). *Acta Cryst. C43*, 616–618.

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