SHORT COMMUNICATION

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Structure of $Na_3M_3(CO_3)_5$. Corrigendum.

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Abstract

The crystal structure of this burbankite-type mineral, where M represents a mixture of rare-earth metals, Ca,Na and Sr, was described as monoclinic, space group $P2_1$, with $a = 10{\cdot}412\,(4)$, $b = 10{\cdot}414\,(4)$, $c = 6{\cdot}291\,(3)$ Å, $\gamma = 119{\cdot}80\,(5)°$, $Z = 2$ [Ginderow (1989). *Acta Cryst.* C45, 185–187]. It should be described as orthorhombic, space group $Cmc2_1$ (a higher sub-group of $P6_3mc$), with $a = 10{\cdot}444$, $b = 18{\cdot}018$, $c = 6{\cdot}291$ Å, $Z = 4$. Revised coordinates are given.

The vectors defining the new cell edges are [110], [$\bar{1}$10] and [001]; the corresponding coordinate transformations are $x' = 1/2(x + y)$, $y' = 1/2(y - x)$, $z' = z$. After averaging the transformed coordinates over appropriate pairs of atoms, the $Cmc2_1$ coordinates in Table 1 result. Included in Table 1 are the e.s.d.'s in the *averaged* coordinates, as estimated from the values reported by Ginderow (1989; Table 2), and, in square brackets, the shifts in the coordinates of individual *unaveraged* atoms necessary to achieve the symmetry of $Cmc2_1$. These latter values are, on the average, slightly smaller than the individual-atom e.s.d.'s reported by Ginderow.

The revised structure requires that the sites $M(2)$ and $M(3)$ be equivalent. The population parameters of these two sites were refined separately by Ginderow, and the resulting values were 0·947 (3) and 0·962 (3) – a marginally significant difference. However, the B_{eq} value for $M(3)$ was slightly larger than for $M(2)$, 1·08 (2) *vs* 1·06 (2) Å^2, so the difference is presumably not real. The remaining metal site, $M(1)$, has an appreciably larger population parameter, 1·114 (3); as Ginderow pointed out, this site appears to be preferentially occupied by the heavier rare-earth atoms. [A population factor of 1·0 corresponds to a mixture of 10 metal atoms in the proportions found in burbankite (Ginderow, 1989).] Since the coordinate shifts necessary to achieve the higher symmetry are so small, there are no significant changes in the interatomic distances reported by Ginderow (1989). The metal site $M(1)$ and the Na(2) atom are now seen to lie on a mirror plane, and three of the CO_3 groups lie across a mirror plane.

The structure remains pseudo-hexagonal; however, it no longer seems 'probable that the majority of burbankite-type minerals crystallize in the monoclinic system' (Ginderow, 1989).

Table 1. *Coordinates* ($\times 10^4$) *space group* $Cmc2_1$

Numbers in parentheses are e.s.d.'s in the transformed (and, where appropriate, averaged) coordinates; numbers in square brackets are shifts in the individual (unaveraged) coordinates necessary to achieve the symmetry of $Cmc2_1$ (see text).

	x	y	z	B_{eq}
$M(1)$	0 (–)[0]	–1587 (1)[–]	0 (–)[–]	1·03 (2)
$M(2,3)$	2610 (1)[0]	5794 (1)[0]	18 (4)[1]	1·07 (1)[1]
Na(1,3)	2153 (4)[1]	2616 (3)[0]	1905 (7)[1]	1·6 (1)[0]
Na(2)	0 (–)[4]	4770 (3)[–]	1895 (10)[–]	1·5 (2)[–]
C(1)	0 (–)[2]	–2 (8)[–]	1666 (19)[–]	1·1 (2)[–]
O(1)	0 (–)[2]	706 (7)[–]	1671 (25)[–]	2·3 (4)[–]
O(2,3)	1042 (8)[13]	–358 (5)[11]	1597 (19)[10]	2·5 (3)[1]
C(2)	0 (–)[12]	6672 (7)[–]	258 (15)[–]	1·2 (3)[–]
O(4)	0 (–)[12]	5966 (7)[–]	263 (17)[–]	1·9 (3)[–]
O(5,6)	1050 (8)[4]	7034 (5)[9]	229 (13)[14]	2·0 (2)[0]
C(3,4)	2042 (8)[9]	4018 (5)[10]	–338 (10)[4]	0·9 (2)[2]
O(8,9)	1654 (7)[16]	3890 (4)[0]	1527 (13)[7]	1·5 (2)[0]
O(10,13)	2778 (7)[2]	3543 (4)[5]	–1298 (14)[18]	1·6 (2)[0]
O(12,14)	1692 (7)[2]	4606 (4)[4]	–1325 (13)[3]	1·6 (2)[0]
C(5)	0 (–)[17]	1968 (7)[–]	–353 (14)[–]	0·9 (3)[–]
O(7)	0 (–)[1]	2228 (6)[–]	1511 (10)[–]	1·4 (2)[–]
O(11,15)	1069 (7)[6]	1838 (4)[7]	–1302 (12)[8]	1·6 (2)[0]

Reference

GINDEROW, D. (1989). *Acta Cryst.* C45, 185–187.

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