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On the Structure of $Na_2Ti_4O_9$[1]

RICHARD E. MARSH

Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125

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The structure of the compound formulated as $Na_2Ti_4O_9$ was recently described (*1*) as triclinic; space group $P\bar{1}$, with a = 10.653(4), b = 11.647(3), c = 2.9392(6) Å; α = 97.25(3), β = 90.00(11), γ = 102.44(2)°; Z = 2. It is properly described as monoclinic, space group $C2/m$, with a = 23.108, b = 2.9392, c = 10.653 Å; β = 102.54°; Z = 4. Lattice vectors defining the monoclinic cell are [021], [001], and [100]; the corresponding coordinate transformations are $x' = y/2$, $y' = z - y/2$, $z' = x$. For all atoms the transformed coordinates y' are less than one e.s.d. from the values 0.0 or 0.5—mirror planes in $C2/m$; the transformed "temperature factor" coefficients also obey the symmetry of $C2/m$ within their e.s.d.'s, the values of β_{12} and β_{23} being insignificantly different from 0.0. The revised, $C2/m$ coordinates are in Table I.

There are no other significant changes in the description of the structure.

TABLE I

COORDINATES, SPACE GROUP $C2/m$[a]

Atom	x	y	z
Na(1)	0.1366(2)	0.0	0.5974(3)
Na(2)	0.0742(3)	0.0	0.3068(7)
Na(3)	0.1407(2)	0.5	0.1041(6)
Ti(1)	0.0	0.0	0.0
Ti(2)	0.2232(1)	0.5	0.3745(1)
Ti(3)	0.2151(1)	0.5	0.8791(1)
Ti(4)	0.0608(1)	0.5	0.8090(1)
Ti(5)	0.0	0.0	0.5
O(1)	0.0746(2)	0.0	0.9394(4)
O(2)	0.0230(2)	0.5	0.1233(4)
O(3)	0.0308(2)	0.0	0.6947(4)
O(4)	0.1721(2)	0.0	0.3186(4)
O(5)	0.2033(2)	0.0	0.9918(4)
O(6)	0.2418(2)	0.0	0.7812(4)
O(7)	0.0560(2)	0.5	0.4878(4)
O(8)	0.1369(2)	0.5	0.7829(4)
O(9)	0.2152(2)	0.5	0.5528(4)

Note. Occupancy factors (*1*): Na(1), 0.97(1); Na(2), 0.48(1); Na(3), 0.63(1).

[a] E.s.d.'s (in parentheses) are from Table II in Ref. (*1*).

Reference

1. J. AKIMOTO AND H. TAKEI, *J. Solid State Chem.* **83,** 132 (1989).

[1] This work is Contribution No. 8089 from the Arthur Amos Noyes Laboratory.

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