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Ferrobustamite: The crystal structures of two Ca, Fe bustamite-type pyroxenoids: correction

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Recently Prof. WERNER BAUR pointed out to me that the interatomic distances reported by RAPOPORT and BURNHAM (1973, Table 4) for natural ferrobustamite from Skye, with composition corresponding to $Wo_{79}Fs_{21}$, are inconsistent with the atomic coordinates given in Table 3 of that paper. Upon investigation, I find that the published distances were calculated from a set of atomic coordinates different

Table 1. $Wo_{79}Fs_{21}$ *atom coordinates, temperature factors, and metal site occupancies*

Atom	multiplicity	occupancy	x	y	z	B
M(1)	2	.99(4)Ca .01(4)Fe	.2000(6)	.4211(5)	.3774(3)	.61(7)Å^2
M(2)	2	.88(4)Ca .12(4)Fe	.1992(6)	.9291(5)	.3754(3)	.85(7)
M(3)	1	.41 Ca[1] .59 Fe	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	.49(8)
M(4)	1	.60(7)Ca[1] .40(7)Fe	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{1}{4}$	1.15(11)
Si(1)	2		.1870(8)	.3960(8)	.6343(4)	1.06(8)
Si(2)	2		.1897(9)	.9497(8)	.6342(4)	1.15(9)
Si(3)	2		.3966(7)	.7247(7)	.5231(4)	.78(7)

[1] Occupancy values for M(3) were dependent parameters, adjusted to give the correct total chemical constraint. Occupancy values of both M(3) and M(4) are almost certainly incorrect; see original text for discussion of this point.

Table 1. *(Continued)*

Atom	multi-plicity	occu-pancy	x	y	z	B
O(1)	2		.429(2)	.735(2)	.403(1)	1.1(2)
O(2)	2		.406(2)	.226(2)	.409(1)	1.1(2)
O(3)	2		.318(2)	.474(2)	.730(1)	1.5(2)
O(4)	2		.310(3)	.935(3)	.727(1)	1.9(3)
O(5)	2		.016(3)	.628(3)	.358(1)	1.9(3)
O(6)	2		.013(2)	.129(2)	.371(1)	1.1(2)
O(7)	2		.269(2)	.511(2)	.542(1)	1.3(2)
O(8)	2		.275(3)	.882(2)	.541(1)	2.1(3)
O(9)	2		.220(3)	.182(2)	.619(1)	2.2(3)

Table 2. *Interatomic distances for* $Wo_{79}Fs_{21}$[1]

Bond lengths		Bond lengths	
M(1)—O(1)	2.484 Å	M(4)—O(2) (× 2)	2.398 Å
O(2)	2.423	O(3) (× 2)	2.394
O(4)	2.335	O(4) (× 2)	2.419
O(5)	2.303	O(9) (× 2)	2.670
O(6)	2.270	Mean of six	2.404
O(7)	2.358	Mean of eight	2.470
Mean of six	2.362		
		Si(1)—O(3)	1.622
M(2)—O(1)	2.512	O(5)	1.574
O(2)	2.439	O(7)	1.631
O(3)	2.294	O(9)	1.642
O(5)	2.315	Mean	1.617
O(6)	2.279		
O(8)	2.372	Si(2)—O(4)	1.542
Mean of six	2.369	O(6)	1.551
		O(8)	1.638
M(3)—O(1) (× 2)	2.245	O(9)	1.656
O(3) (× 2)	2.169	Mean	1.597
O(4) (× 2)	2.223		
Mean of six	2.212	Si(3)—O(1)	1.599
		O(2)	1.591
		O(7)	1.674
		O(8)	1.676
		Mean	1.635

[1] These distances are only approximate due to twinning (see original text), thus no standard deviations are listed. The precision is probably no greater than about ± .03 to .05 Å.

from those in the paper, and, further, that the coordinates themselves are not the correct set.

Table 1 lists the correct atomic parameters resulting from least-squares refinement using all observed reflections for $Wo_{79}Fs_{21}$. Table 2 lists the interatomic distances calculated from the coordinates of Table 1. These distances are not precise because the data from this crystal were affected by complex twinning, and the cautionary footnotes from the original paper are repeated here.

This correction does not affect the conclusions drawn in the original paper in any substantial way. Changes made in mean polyhedral bond distances are in all cases less than our original estimates of the standard error of those means. I thank Prof. BAUR for pointing out this error and apologize to any reader who has attempted to use the incorrect values.

Reference

P. A. RAPOPORT and C. W. BURNHAM (1973), Ferrobustamite: The crystal structures of two Ca,Fe bustamite-type pyroxenoids. Z. Kristallogr. **138**, 419—438.