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Refinement of the Callaghanite Structure[1]

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Abstract

The crystal structure of callaghanite, $Cu_8Mg_8(CO_3)_4(OH)_{24}\cdot 8H_2O$, has been refined from 2860 three-dimensional MoKα data collected by means of a Picker four-circle goniostat; a_o = 10.0060(7)Å, b_o = 11.7520(8)Å, c_o = 8.2132(7)Å and $\cos\beta$ = −0.2987(1) (β = 107°23′). The six Mg-O distances range 2.060(1)-2.119(1)Å; the five Cu-O distances range 1.926(1)-2.483(1)Å and the C-O bond distances are 1.282(1) and 1.284(3)Å.

Callaghanite was first described and named by Beck and Burns (1954), and subsequently the structure was determined by Brunton, Steinfink, and Beck (1958). I have refined the structural parameters to illustrate how much better the cell and atomic parameters are as a result of 15 years of improvements in computer technology and automated data collection. The basic structural features of callaghanite are unchanged.

The single crystals of callaghanite are from the Washington A. Roebling collection, specimen No. R9406, of the Smithsonian Institution, Washington, D.C. A crystal fragment ground to ellipsoidal shape, 0.260 × 0.208 × 0.195 mm, was used as the source of data. The data collection and refinement techniques are the same as that of Brunton, Harris, and Kopp (1972). The cell parameters were refined by least-squares adjustment of 48 MoKα_1 (0.70926Å) reflections; a_0 = 10.0060(7)Å, b_0 = 11.7520(8)Å, c_0 = 8.2132(7)Å and $\cos\beta$ = −0.2987(1) (β = 107°23′).

The results of the refinement are listed in Tables 1[2] and 2. The discrepancy factor $R|F_0|^2 = \Sigma|F_0^2 - (sF_c)^2|/\Sigma|F_0^2| = 0.0386$ for all 2860 reflections and 0.0384 for 2690 reflections whose F_0^2 values are greater than sigma F_0^2.

TABLE 2. Interatomic Distances and Angles for Callaghanite

Cu-OH(2)	1.926(1)Å	Cu-OH(1)	1.934(1)Å	Cu-OH(2)	1.957(1)Å
Cu-OH(1)	1.959(1)	Cu-H_2O	2.483(1)	Cu-Cu	2.8899(4)
Mg-H_2O	2.060(1)	Mg-O(1)	2.061(1)	Mg-OH(1)	2.066(1)
Mg-OH(3)	2.084(1)	Mg-OH(1)	2.086(1)	Mg-OH(3)	2.119(1)
2[C-O(1)]	1.282(1)	C-O(2)	1.284(3)	O(1)-O(2)	2.215(2)
O(1)-O(1)	2.235(2)	O(1)-OH(2)	2.866(2)	O(1)-H_2O	2.925(2)
O(2)-H_2O	2.681(2)	OH(1)-OH(1)	2.606(2)	OH(1)-OH(3)	2.703(2)
OH(1)-OH(2)	2.935(2)	OH(2)-OH(2)	2.593(2)	OH(2)-H_2O	2.653(2)
OH(2)-OH(3)	2.755(2)	OH(3)-OH(3)	2.637(2)	OH(3)-H_2O	2.875(2)
O(1)-C-O(1)	121.3(2)°	2[O(1)-C-O(2)]	119.35(9)°		

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[2] A structure factor table can be obtained by ordering NAPS Document No. 02059 from Microfiche Publications, 305 East 46th Street, New York, N. Y. 10017; remitting in advance $1.50 for microfiche or $5.00 for photocopies, payable to Microfiche Publications. Please check the most recent issue of this journal for the current address and prices.