

SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.

Acta Cryst. (1978). B34, 2385–2386

The crystal structure of hopeite, $\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$: errata. By A. WHITAKER, *Department of Physics, Brunel University, Uxbridge, Middlesex, England*

(Received 10 March 1978; accepted 28 March 1978)

An error has been found in calculating the r.m.s. displacements and orientations of the vibration ellipsoids in hopeite [Whitaker, A. (1975). *Acta Cryst.* B31, 2026–2035]. This has been corrected. The correct r.m.s. displacements and orientations are included together with a new table of bond lengths corrected for thermal vibrations. The effect of the corrections on the latter is so small that the general conclusions of the original paper still hold.

Introduction

The crystal structure of hopeite, $\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$, has been reported (Whitaker, 1975). It has recently been pointed out that the anisotropic temperature factors and the r.m.s. displacements do not agree. This has been found to be due to a difference in defining the anisotropic temperature factors, B_{ij} ($i \neq j$), in the programs for least squares and calculation of thermal ellipsoids. This error has now been corrected.

Bond lengths corrected for thermal vibrations

Busing & Levy (1964) pointed out that one of the effects of thermal vibration is to alter the apparent bond lengths. These values have been recalculated and included in Table 2 for three of the cases they discuss; (a) the atoms are vibrating in phase, (b) the outer atoms are 'riding' on the inner ones and (c) the atoms are moving independently of each other.

Re-analysis of thermal ellipsoids

The r.m.s. displacements and the direction cosines of the thermal vibration ellipsoids are given in Table 1. The errors in the displacements were obtained by calculating the vibration ellipsoids for the values of anisotropic temperature factors plus the standard deviations and minus the standard deviations and averaging over similar atoms.

Comparison of the r.m.s. values in this table with those in the original table indicates that the differences between the two sets of results are in general small: most are less than the error and the largest, for O(7), corresponds to 1.4 times the error. However, there are considerable differences in some of the direction cosines and because of this the relationships between the axes of the vibration ellipsoids and the appropriate bond were recalculated.

Consider the O atoms about Zn(1) – O(1), O(2), O(3) and O(4); the shortest axes of vibration make angles of 4, 23, 41 and 51° with the respective bond while the largest axes make angles of 90, 90, 54 and 81° with the respective bond.

In the case of Zn(2), there are four oxygen neighbours O(5), O(6^{iv}), O(7) and O(7^{iv}); the longest axes of vibration are at angles of 88, 89, 90 and 88° to the respective Zn–O bond while the shortest ones are at angles of 52, 44, 41 and 15° respectively.

For P, the longest axes of vibration of O(4), O(5), O(6) and O(7) are at angles of 89, 87, 69 and 89° to the respective P–O bond, while the shortest ones are at angles of 82, 16, 24 and 60° respectively.

Table 1. *R.m.s. displacements and orientation with respect to crystallographic axes*

	R.m.s. displacement	Direction cosine with respect to		
		a	b	c
Zn(1)	0.157 (2)	0.000	1.000	0.000
	0.124 (2)	0.361	0.000	0.933
	0.109 (2)	0.933	0.000	−0.361
Zn(2)	0.110 (2)	0.000	0.995	−0.101
	0.071 (2)	0.046	0.101	0.994
	0.066 (2)	0.999	−0.004	−0.046
P	0.091 (4)	0.726	0.681	−0.096
	0.085 (4)	0.634	−0.607	0.480
	0.070 (4)	0.268	−0.409	−0.872
O(1)	0.180 (13)	0.000	−1.000	0.000
	0.125 (13)	0.797	0.000	−0.604
	0.080 (13)	0.604	0.000	0.797
O(2)	0.204 (13)	0.000	−1.000	0.000
	0.147 (13)	0.303	0.000	−0.953
	0.060 (13)	0.953	0.000	0.303
O(3)	0.183 (13)	−0.424	−0.695	−0.581
	0.146 (13)	−0.346	−0.468	0.813
	0.109 (13)	0.837	−0.546	0.042
O(4)	0.175 (13)	0.823	−0.333	0.461
	0.108 (13)	0.335	0.939	0.079
	0.089 (13)	−0.459	0.090	0.884
O(5)	0.230 (13)	0.925	0.356	−0.136
	0.114 (13)	0.363	−0.931	0.032
	0.050 (13)	0.116	0.079	0.990
O(6)	0.172 (13)	0.109	−0.341	−0.934
	0.106 (13)	0.085	−0.933	0.351
	0.052 (13)	0.990	0.118	0.072
O(7)	0.138 (13)	−0.410	−0.779	−0.474
	0.094 (13)	0.341	−0.613	0.713
	0.044 (13)	0.846	−0.130	−0.517

Table 2. *Bond lengths corrected for thermal vibrations*

	Uncorrected bond length	Corrected bond length			Standard deviation
		(a) (in phase)	(b) (riding)	(c) (independent)	
Zn(1)—O(1)	2.099 Å	2.099 Å	2.101 Å	2.119 Å	0.008 Å
Zn(1)—O(2)	2.116	2.117	2.122	2.139	0.009
Zn(1)—O(3)	2.159	2.159	2.162	2.177	0.007
Zn(1)—O(4)	2.048	2.048	2.050	2.066	0.006
Mean	2.099	2.099	2.102	2.119	0.003
Zn(2)—O(5)	1.912	1.916	1.924	1.931	0.006
Zn(2)—O(6 ^{iv})	1.930	1.932	1.936	1.943	0.005
Zn(2)—O(7)	1.996	1.996	1.998	2.006	0.005
Zn(2)—O(7 ^{iv})	1.999	2.000	2.002	2.010	0.005
Mean	1.963	1.965	1.968	1.976	0.003
P—O(4)	1.521	1.523	1.529	1.538	0.006
P—O(5)	1.515	1.521	1.532	1.542	0.006
P—O(6)	1.536	1.536	1.544	1.553	0.005
P—O(7)	1.564	1.565	1.567	1.576	0.005
Mean	1.537	1.539	1.545	1.555	0.003

These values are almost identical (maximum difference 0.002 Å) and the general conclusions are the same as for the previous paper.

The author would like to thank N. Armağan, A. Aydın Uraz and Y. Aka of Fen Fakültesi, Fizik Bölümü, Ankara

University, Turkey, for pointing out the discrepancy in the original paper.

References

- BUSING, W. R. & LEVY, H. A. (1964). *Acta Cryst.* **17**, 142–146.
 WHITAKER, A. (1975). *Acta Cryst.* **B31**, 2026–2035.