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ZUNYITE: A COMPARISON OF NEUTRON- AND X-RAY-DIFFRACTION STUDIES

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A least squares refinement of the structure of zunyite, using *3D* X–ray data, was recently reported by us (Louisnathan and Gibbs, 1972). Our study clarified the Al/Si distribution in the structure and confirmed Kamb's (1960) proposal that O(3) is a hydroxyl ion by locating the hydrogen atom at a distance of 0.73Å from O(3). A second H atom, proposed by Kamb to be in the vicinity of O(4), could not be precisely located using the X–ray data. A neutron diffraction study of zunyite by Bartl (1970) has since been brought to our attention. Bartl's study confirms Kamb's proposal that O(3) and O(4) are hydroxyl ions by locating H atoms at 0.990 and 0.989Å away from these oxygen atoms, respectively. The hydrogen–bonded distances, O(3)–H···Cl, O(4)–H···O(4′), and the tetrahedral Si–O and Al–O distances obtained in our study are statistically identical to those obtained by Bartl:

	Neutron diffraction Bartl (1970)	X-ray diffraction Louisnathan & Gibbs (1972)
O(3)–H ··· Cl	3.041(21)Å	3.052(7)Å
O(4)–H ··· O(4′)	2.791(20)	2.813(8)
Si(1)–O(2)	1.632(14)	1.628(10)
Si(2)–O(2)	1.616(20)	1.629(10)
Si(2)–O(5)	1.647(20)	1.632(5)
Al(t)–O(1)	1.798(14)	1.798(9)

The mean *T*–O bond length of 1.633Å within the Y_5O_{16} group and of 1.798Å in the XO_4 group indicates an ordered Al/Si distribution in agreement with the Pauling–Kamb (1933, 1960) model in contradiction to the proposals of Zagal'skaya and Belov (1964).

We are very grateful to Dr. H. Bartl for bringing his abstract on the neutron diffraction study of zunyite to our attention, and we regret having overlooked his important contribution to the understanding of the zunyite structure.

References

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