JOURNAL OF SOLID STATE CHEMISTRY 102, 281–282 (1993)

BRIEF COMMUNICATIONS

On the Structure of $Na_5V_2P_3O_{14} \cdot H_2O$

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Received March 18, 1992; in revised form May 26, 1992; accepted June 1, 1992

The recently published acentric $Na_5V_2P_3O_{14} \cdot H_2O$ structure (*1*) (space group *Cm* with $a = 6.3089(4)$ Å, $b = 20.1038(8)$ Å, $c = 5.1172(5)$ Å, $\beta = 91.134(6)°$, $Z = 2$) contained no mention of anomalous scattering (or absolute configuration), although a strong effect was expected from the use of the Cu$K\alpha$ radiation. It was long ago demonstrated that the neglect of anomalous scattering can lead to systematic errors in bond lengths (*2*). In the case of $Na_5V_2P_3O_{14} \cdot H_2O$, an abnormally short V–O(3) distance of 1.490(8) Å was indicative of a possible pitfall.

Testing the mirror image of the structural model given in Ref. (*1*), using the same data set with the SHELX76 program (*3*) on a VAX computer, led to the results gathered in Table I. Considerable improvement in R (0.025) was obtained (0.049 in Ref. (*1*)). Impressive modifications of bond lengths were observed: the greatest change concerning the V–O(3) distance (1.620(4) Å) being now more realistic from the crystal chemistry point of view. Refinements using Friedel pairs would have been better, unfortunately they were not measured, with the exception of the *hk*0 reflections.

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

References

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2. D. W. J. CRUICKSHANK AND W. S. MCDONALD, *Acta Crystallogr.* **23**, 9 (1967).
3. G. M. SHELDRICK, "SHELX76. Program for Crystal Structure Determination," Univ. of Cambridge, England (1976).

0022-4596/93 $5.00

TABLE I

ATOMIC COORDINATES AND THERMAL PARAMETERS FOR $Na_5V_2P_3O_{14} \cdot H_2O$ (U_{ij} ARE $\times 10^4$)

Atom	x	y	z	B_{eq}
V	$\frac{1}{2}$	0.84891(3)	$\frac{1}{2}$	0.71(3)
P1	0.0028(2)	0.81446(4)	0.5001(3)	0.72(3)
P2	0.3500(3)	0	0.4582(3)	0.77(5)
Na1	0.1687(5)	0.9142(1)	0.9905(5)	2.27(8)
Na2	0.7458(3)	0.7599(1)	0.0239(4)	1.57(8)
Na3	0.8213(5)	0	0.4045(8)	3.8(2)
O1	0.758(1)	0	0.904(2)	8.9(7)
O2	0.0147(5)	0.8112(1)	0.7948(7)	1.0(1)
O3	0.5003(6)	0.8456(2)	0.8164(7)	1.4(1)
O4	0.8049(5)	0.8524(1)	0.3985(7)	1.1(1)
O5	0.4977(5)	0.7565(2)	0.3750(6)	0.9(1)
O6	0.1961(5)	0.8504(1)	0.3887(7)	0.9(1)
O7	0.4979(5)	0.9404(1)	0.3882(7)	1.1(1)
O8	0.1531(7)	0	0.2846(9)	1.1(2)
O9	0.3044(9)	0	0.746(1)	1.7(2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
V	61(4)	88(3)	119(3)	0(3)	−8(2)	2(2)
P1	67(5)	102(4)	103(4)	2(4)	−1(3)	9(4)
P2	78(6)	98(6)	116(6)	0	−8(5)	0
Na1	497(14)	186(9)	182(9)	2(7)	19(9)	−63(8)
Na2	121(9)	311(12)	165(10)	7(7)	−16(7)	−25(7)
Na3	103(15)	928(32)	425(24)	0	73(15)	0
O1	147(32)	2899(182)	313(40)	0	−40(27)	0
O2	120(15)	179(14)	95(14)	8(11)	−10(11)	−1(10)
O3	176(18)	215(16)	160(16)	−3(12)	4(14)	30(12)
O4	82(17)	145(14)	190(18)	24(11)	−10(13)	−1(10)
O5	138(13)	97(12)	112(14)	10(11)	−13(10)	−23(11)
O6	83(16)	126(13)	148(16)	23(11)	−16(13)	−11(10)
O7	99(13)	99(12)	225(15)	33(12)	20(11)	11(10)
O8	43(17)	190(20)	164(21)	0	−47(16)	0
O9	286(26)	214(22)	153(21)	0	57(21)	0

Note. U_{ij} relate to the expression: $T = \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$.