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SCHNEIDERHÖHNITE, $Fe^{2+}Fe_3^{3+}As_5^{3+}O_{13}$, A DENSELY PACKED ARSENITE STRUCTURE

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ABSTRACT

The crystal structure of schneiderhöhnite, $Fe^{2+}Fe_3^{3+}As_5^{3+}O_{13}$, *a* 8.924(2), *b* 10.016(3), *c* 9.103(3) Å, α 59.91(2), β 112.41(2), γ 81.69(2)°, *V* 590.8(3) Å^3, space group P$\bar{1}$, has been solved by direct methods and refined to a residual R of 4.5% on 3184 unique observed [I>2.5σ(I)] reflections of graphite-monochromated Mo*K*α radiation. Five unique As positions, each with trigonal pyramidal co-ordination, form two (As_2O_5) dimers and one (AsO_3) monomer. In five unique Fe positions, each with distorted pseudo-octahedral co-ordination, the observed <Fe–O> distances show four of the octahedra to be occupied by Fe^{3+} and the fifth by Fe^{2+}. The octahedra polymerize by sharing edges and corners, which unite with the arsenite pyramids to form a complex, densely packed framework structure. A brief survey of recently refined arsenite minerals shows a fairly constant geometry for the arsenite group, with <As–O> = 1.776(12) Å and <O–As–O> = 97.2(2.0)°.

Keywords: crystal structure, arsenite, schneiderhöhnite, Tsumeb.

SOMMAIRE

La structure cristalline de la schneiderhöhnite, $Fe^{2+}Fe_3^{3+}As_5^{3+}O_{13}$, *a* 8.924(2), *b* 10.016(3), *c* 9.103(3) Å, α 59.91(2), β 112.41(2), γ 81.69(2)°, *V* 590.8(3) Å^3, groupe spatial P$\bar{1}$, a été résolue par méthodes directes et affinée jusqu'au résidu R= 4.5% sur 3184 réflexions observées uniques [I>2.5 σ (I)] en radiation Mo*K*α monochromatisée sur graphite. Cinq positions uniques d'As, chacune à coordination pyramidale trigonale, forment deux dimères As_2O_5 et un monomère AsO_3. Dans cinq positions uniques de Fe, chacune avec un octaèdre difforme comme polyèdre de coordination, les distances <Fe–O> observées indiquent que quatre des pseudo-octaèdres sont occupés par Fe^{3+} et le cinquième, par Fe^{2+}. Les octaèdres se polymérisent en mettant en commun arêtes et sommets, lesquels s'unissent aux pyramides trigonales pour former une structure complexe en charpente à empilement compact. Une brève revue des arsenites minéraux dont la structure a été affinée récemment montre que le groupe des arsenites est caractérisé par une géométrie assez constante, avec <As–O> = 1.776(12) Å et <O–As–O> = 97.2(2.0)°.

(Traduit par la Rédaction)

Mots-clés: structure cristalline, arsenite, schneiderhöhnite, Tsumeb.

INTRODUCTION

Schneiderhöhnite is an iron arsenite first reported by Ottemann *et al.* (1973). It occurs at Tsumeb, S.W. Africa, in a druse in the deep oxidation zone, associated with chalcocite and zincian stottite.

EXPERIMENTAL

The crystal used in this work is from the Tsumeb copper deposit, S.W. Africa, and was obtained from the Department of Mineralogy and Geology, Royal Ontario Museum, collection number M33238. The crystal was mounted on a Nicolet *R*3*m* automated four-circle diffractometer, and twenty-five intense reflections were centred using graphite-monochromated Mo*K*α X radiation. Least-squares refinement of the setting angles produced the cell dimensions given in Table 1, together with an orientation matrix relating the crystal axes to the diffractometer axes. A total of 3833 reflections was measured over one asymmetric unit out to a maximum 2θ of 60° according to the experimental procedure of Hawthorne (1985). An empirical absorption-correction (ψ-scan) was applied, together with corrections for Lorentz, polarization and background effects; of the 3469 unique reflections, 3187 were classed as observed [I>2.5σ(I)].

STRUCTURE SOLUTION AND REFINEMENT

Scattering curves for neutral atoms together with anomalous dispersion corrections were taken from Cromer & Mann (1968) and Cromer & Liberman (1970), respectively. *R* indices are of the form given in Table 1 and are expressed as percentages. The SHELXTL system of programs was used for the computational procedures.

The structure was solved by direct methods. The phase set with the maximum combined figure of merit gave a satisfactory solution, and all atomic positions were derived from the initial model and a difference-Fourier map calculated after the first few cycles of refinement. For an isotropic thermal model, refinement converged to an *R* index of 6.4%. Conversion to anisotropic temperature-factors and refinement of all variables converged to an *R* index of 4.9% (observed) and an R_w index of 6.1% (observed). Final positional parameters are given in Table 2, anisotropic temperature-factor coefficients in Table 3, selected interatomic distances and angles in Tables 4 and 5, and a bond-valence analysis is offered in Table 6. Observed and calculated structure-factors are available from the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2.

DISCUSSION

Description of the structure

There are five unique As sites with trigonal pyramidal co-ordination, this co-ordination resulting from the $4s^2$ stereoactive lone pair of electrons on each As^{3+} cation. The variation in both individual and mean bond-lengths in the $(As^{3+}O_3)$ groups lies within the normal range exhibited by natural and synthetic arsenites. There are five unique Fe sites, all with pseudo-octahedral co-ordination. The variation in mean octahedral bond-lengths is compatible with Fe(1) = Fe(2) = Fe(3) = Fe(4) = Fe^{3+} and Fe(5) = Fe^{2+}, as indicated by sum of the relevant ionic radii: Fe(1) = Fe(2) = Fe(3) = Fe^{3+} – ^{III}O =

TABLE 1. MISCELLANEOUS INFORMATION: SCHNEIDERHÖHNITE

a	8.924(2)Å	Crystal size (mm)	0.08x0.28x0.30
b	10.016(3)	Rad/Mono	Mo|Gr
c	9.103(3)	Total |Fo|	3673
α	59.91(2)°	|Fo| > 4 σ.	3184
β	112.41(2)	Final R(obs)	4.5%
γ	81.69(2)	Final R_w(obs)	4.9%
V	590.8(3)$Å^3$	μ (cm^{-1})	197

Space Group $P\bar{1}$

Unit cell contents: $2[Fe^{2+}Fe^{3+}_3As^{3+}_5O_{13}]$

$R = \Sigma(|Fo|-|Fc|)/\Sigma|Fo|$

$R_w = [\Sigma w(|Fo|-|Fc|)^2/\Sigma wFo^2]^{\frac{1}{2}}$, $w = 1$

TABLE 2. ATOMIC PARAMETERS FOR SCHNEIDERHÖHNITE

	x	y	z	$U^*_{equiv.}$
As(1)	0.8020(1)	0.3006(1)	0.9938(1)	0.48(3)
As(2)	0.6696(1)	0.1689(1)	0.4947(1)	0.45(3)
As(3)	0.8843(1)	0.9023(1)	0.1653(1)	0.41(3)
As(4)	0.7322(1)	0.7385(1)	0.8569(1)	0.43(3)
As(5)	0.7555(1)	0.5380(1)	0.5125(1)	0.62(3)
Fe(1)	0	0	1/2	0.42(6)
Fe(2)	1/2	1/2	0	0.43(6)
Fe(3)	0.8861(1)	0.3823(1)	0.3186(1)	0.33(5)
Fe(4)	0.4546(1)	0.1967(1)	-0.0798(1)	0.48(5)
Fe(5)	0.6363(1)	0.8945(1)	0.3863(1)	0.55(5)
0(1)	0.7959(6)	0.5808(6)	0.3174(7)	0.7(2)
0(2)	0.4326(6)	0.2002(6)	0.3831(7)	0.7(1)
0(3)	0.3994(6)	0.1247(6)	0.1315(7)	0.8(2)
0(4)	0.8763(7)	0.1068(6)	0.0244(7)	0.8(2)
0(5)	0.7526(6)	0.0298(6)	0.4512(7)	0.7(3)
0(6)	0.9205(6)	0.2214(6)	0.2470(7)	0.6(2)
0(7)	0.5559(6)	0.7309(6)	0.3323(7)	0.7(2)
0(8)	0.0046(6)	0.8515(6)	0.4090(7)	0.7(2)
0(9)	0.7131(6)	0.5508(6)	0.0133(7)	0.6(2)
0(10)	0.1213(6)	0.3717(6)	0.3916(7)	0.8(3)
0(11)	0.6498(6)	0.3551(6)	0.2939(7)	0.7(2)
0(12)	0.6656(6)	0.9617(6)	0.1256(7)	0.5(2)
0(13)	0.4059(6)	0.6856(6)	0.0210(7)	0.6(1)

$^*U_{equiv.} = U_{equiv.} x10^2$

TABLE 3. ANISOTROPIC TEMPERATURE-FACTOR COEFFICIENTS FOR SCHNEIDERHÖHNITE

	U^*_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
As(1)	34(3)	48(3)	45(3)	-17(3)	25(3)	-12(2)
As(2)	19(3)	53(3)	44(3)	-19(3)	19(3)	-12(2)
As(3)	11(3)	51(3)	55(3)	-31(3)	17(2)	-5(2)
As(4)	9(3)	50(3)	53(3)	-19(3)	20(2)	-11(2)
As(5)	50(3)	53(3)	61(3)	-26(3)	24(3)	-22(2)
Fe(1)	8(6)	36(5)	54(6)	-18(5)	11(5)	2(5)
Fe(2)	7(6)	42(5)	47(6)	-16(5)	6(5)	-4(5)
Fe(3)	1(4)	29(4)	36(4)	-10(3)	-0(3)	4(3)
Fe(4)	26(4)	53(4)	50(4)	-27(4)	15(4)	-14(3)
Fe(5)	49(4)	58(4)	67(4)	-39(4)	34(4)	55(5)
0(1)	68(22)	77(21)	60(22)	-42(19)	35(19)	-18(18)
0(2)†	1(15)	83(15)	41(13)	0(0)	0(0)	0(0)
0(3)	71(23)	63(21)	86(23)	-36(19)	49(20)	9(18)
0(4)	81(23)	43(20)	60(22)	-13(19)	40(19)	1(18)
0(5)	40(1)	73(21)	141(25)	-73(20)	62(20)	-38(18)
0(6)	45(21)	57(20)	50(21)	-28(18)	22(18)	-17(17)
0(7)	34(21)	81(21)	78(22)	-40(19)	34(19)	-33(18)
0(8)	44(22)	56(20)	37(21)	-16(18)	-20(18)	-4(17)
0(9)	24(21)	64(20)	75(23)	-31(19)	26(19)	-20(17)
0(10)	26(21)	112(22)	107(24)	-70(21)	25(19)	-33(18)
0(11)	41(21)	42(20)	67(22)	-6(18)	16(19)	-12(17)
0(12)	13(20)	66(20)	68(22)	-38(19)	20(18)	-17(17)
0(13)†	4(15)	37(13)	57(13)	0(0)	0(0)	0(0)

$^*U_{ij} = U_{ij}x10^4$; †non-positive definite

TABLE 4. SELECTED BOND-LENGTHS (Å) IN SCHNEIDERHÖHNITE

As(1)-0(4)a	1.797(7)	As(4)-0(2)e	1.805(5)
As(1)-0(6)a	1.768(6)	As(4)-D(3)e	1.744(7)
As(1)-0(13)e	1.788(6)	As(4)-0(9)a	1.784(5)
<As(1)-0>	1.784	<As(4)-0>	1.778
As(2)-0(2)	1.858(5)	As(5)-0(1)	1.799(7)
As(2)-0(5)	1.767(8)	As(5)-0(7)	1.787(4)
As(2)-0(11)	1.758(5)	As(5)-0(10)e	1.771(7)
<As(2)-0>	1.794	<As(5)-0>	1.786
As(3)-0(4)c	1.761(5)		
As(3)-0(8)d	1.796(6)		
As(3)-0(12)	1.790(6)		
<As(3)-0>	1.782		
Fe(1)-0(5)f,g	2.022(6) x2	Fe(4)-0(1)b	2.164(4)
Fe(1)-0(6)f,g	1.976(4) x2	Fe(4)-0(3)	1.974(7)
Fe(1)-0(8)h,i	2.036(7) x2	Fe(4)-0(7)b	1.991(7)
<Fe(1)-0>	2.011	Fe(4)-0(12)h	2.050(4)
		Fe(4)-0(12)b	2.157(6)
Fe(2)-0(9),b	2.014(6) x2	Fe(4)-0(13)b	1.943(6)
Fe(2)-0(11),b	1.967(5) x2	<Fe(4)-0>	2.047
Fe(2)-0(13),b	2.055(7) x2		
<Fe(2)-0>	2.012	Fe(5)-0(2)c	2.200(7)
		Fe(5)-0(3)c	2.158(4)
Fe(3)-0(1)	2.027(7)	Fe(5)-0(5)c	2.001(7)
Fe(3)-0(6)	2.044(7)	Fe(5)-0(7)	2.079(7)
Fe(3)-0(8)e	2.064(4)	Fe(5)-0(10)e	2.338(4)
Fe(3)-0(9)	2.056(4)	Fe(5)-0(12)	2.253(7)
Fe(3)-0(10)d	1.913(6)	<Fe(5)-0>	2.172
Fe(3)-0(11)	2.106(6)		
<Fe(3)-0>	2.035		

$1.36 + 0.645 = 2.005$ Å; Fe(4) = $\mathrm{Fe}^{3+} - {}^{\mathrm{III}}\mathrm{O}' = 1.367 + 0.645 = 2.012$ Å; Fe(5) = $\mathrm{Fe}^{2+} - {}^{\mathrm{III}}\mathrm{O} = 1.363 + 0.78 = 2.143$ Å. The differences between the observed and calculated values can be ascribed to the effects of polyhedron distortion (Brown 1981).

TABLE 5. POLYHEDRAL EDGE-LENGTHS (Å) AND ANGLES (°) IN SCHNEIDERHÖHNITE

0(4)a-0(6)a	2.727(10)	0(4)a-As(1)-0(6)a	99.8(2)
0(4)a-0(13)	2.769(9)	0(4)a-As(1)-0(13)	101.2(3)
0(6)a-0(13)	2.612(6)	0(6)a-As(1)-0(13)	94.6(3)
<0-0>As(1)	2.703	<0-As(1)-0>	98.5
0(2)-0(5)	2.763(8)	0(2)-As(2)-0(5)	99.2(3)
0(2)-0(11)	2.762(9)	0(2)-As(2)-0(11)	99.6(2)
0(5)-0(11)	2.639(8)	0(5)-As(2)-0(11)	96.9(3)
<0-0>As(2)	2.721	<0-As(2)-0>	98.6
0(4)c-0(8)d	2.688(7)	0(4)c-As(3)-0(8)d	98.2(3)
0(4)c-0(12)	2.696(9)	0(4)c-As(3)-0(12)	98.8(2)
0(8)d-0(12)	2.694(6)	0(8)d-As(3)-0(12)	97.3(3)
<0-0>As(3)	2.693	<0-As(3)-0>	98.1
0(2)e-0(3)e	2.682(11)	0(2)e-As(4)-0(3)e	98.1(3)
0(2)e-0(9)a	2.719(6)	0(2)e-As(4)-0(9)a	98.5(3)
0(3)e-0(9)a	2.657(8)	0(3)e-As(4)-0(9)a	97.7(3)
<0-0>As(4)	2.686	<0-As(4)-0>	98.1
0(1)-0(7)	2.522(10)	0(1)-As(5)-0(7)	89.3(3)
0(1)-0(10)e	2.769(11)	0(1)-As(5)-0(10)e	101.7(3)
0(7)-0(10)e	2.590(7)	0(7)-As(5)-0(10)e	93.4(3)
<0-0>As(5)	2.627	<0-As(5)-0>	94.8
0(5)f,g-0(6)f,g	2.953(5) x2	0(5)f,g-Fe(1)-0(6)f,g	95.2(2) x2
0(5)f,g-0(6)g,f	2.688(5) x2	0(5)f,g-Fe(1)-0(6)g,f	84.5(2) x2
0(5)f,g-0(8)h,i	2.930(10) x2	0(5)f,g-Fe(1)-0(8)h,i	92.4(3) x2
0(5)f,g-0(8)i,h	2.808(9) x2	0(5)f,g-Fe(1)-0(8)i,h	87.6(3) x2
0(6)f,g-0(8)h,i	3.055(10) x2	0(6)f,g-Fe(1)-0(8)h,i	99.2(2) x2
0(6)f,g-0(8)i,h	2.600(9) x2	0(6)f,g-Fe(1)-0(8)i,h	80.8(2) x2
<0-0>Fe(1)	2.839	<0-Fe(1)-0>	90.0
0(9),b-0(11),b	2.662(8) x2	0(9),b-Fe(2)-0(11),b	83.9(2) x2
0(9),b-0(11)b,	2.961(9) x2	0(9),b-Fe(2)-0(11)b,	96.1(2) x1
0(9),b-0(13),b	2.918(9) x2	0(9),b-Fe(2)-0(13),b	91.6(3) x2
0(9),b-0(13)b,	2.837(9) x2	0(9),b-Fe(2)-0(13)b,	88.4(3) x2
0(11),b-0(13),b	2.723(6) x2	0(11),b-Fe(2)-0(13),b	85.2(2) x2
0(11),b-0(13)b,	2.961(7) x2	0(11),b-Fe(2)-0(13)b,	94.8(2) x2
<0-0>Fe(2)	2.844	<0-Fe(2)-0>	90.0
0(1)-0(8)e	3.421(12)	0(1)-Fe(3)-0(8)e	113.5(3)
0(1)-0(9)	2.764(10)	0(1)-Fe(3)-0(9)	85.2(2)
0(1)-0(10)d	2.933(9)	0(1)-Fe(3)-0(10)d	96.2(3)
0(1)-0(11)	2.825(9)	0(1)-Fe(3)-0(11)	86.2(3)
0(6)-0(8)e	2.600(9)	0(6)-Fe(3)-0(8)e	78.5(2)
0(6)-0(9)	2.651(6)	0(6)-Fe(3)-0(9)	80.6(2)
0(6)-0(10)d	2.859(9)	0(6)-Fe(3)-0(10)d	92.4(3)
0(6)-0(11)	2.870(10)	0(6)-Fe(3)-0(11)	87.5(3)
0(8)e-0(10)d	2.787(8)	0(8)e-Fe(3)-0(10)d	88.9(2)
0(8)e-0(11)	2.701(5)	0(8)e-Fe(3)-0(11)	80.7(2)
0(9)-0(10)d	3.270(9)	0(9)-Fe(3)-0(10)d	110.9(2)
0(9)-0(11)	2.662(8)	0(9)-Fe(3)-0(11)	79.5(2)
<0-0>Fe(3)	2.862	<0-Fe(3)-0>	90.0
0(1)b-0(3)	3.071(9)	0(1)b-Fe(4)-0(3)	95.7(2)
0(1)b-0(7)b	2.522(10)	0(1)b-Fe(4)-0(7)b	74.6(2)
0(1)b-0(12)b	3.074(10)	0(1)b-Fe(4)-0(12)b	90.7(2)
0(1)b-0(13)b	3.072(9)	0(1)b-Fe(4)-0(13)b	96.7(2)
0(3)-0(12)h	2.717(9)	0(3)-Fe(4)-0(12)h	84.9(2)
0(3)-0(12)b	2.774(11)	0(3)-Fe(4)-0(12)b	84.3(3)
0(3)-0(13)b	2.950(11)	0(3)-Fe(4)-0(13)b	97.7(3)
0(7)b-0(12)h	3.138(10)	0(7)b-Fe(4)-0(12)h	101.9(2)
0(7)b-0(12)b	2.746(8)	0(7)b-Fe(4)-0(12)b	82.8(3)
0(7)b-0(13)b	2.932(10)	0(7)b-Fe(4)-0(13)b	96.4(3)
0(12)h-0(12)b	2.643(9)	0(12)h-Fe(4)-0(12)b	77.8(2)
0(12)h-0(13)b	2.940(8)	0(12)h-Fe(4)-0(13)b	94.8(2)
<0-0>Fe(4)	2.882	<0-Fe(4)-0>	89.9
0(2)c-0(3)c	3.389(12)	0(2)c-Fe(5)-0(3)c	102.1(2)
0(2)c-0(5)c	3.135(12)	0(2)c-Fe(5)-0(5)c	96.4(3)
0(2)c-0(7)	2.968(10)	0(2)c-Fe(5)-0(7)	87.8(3)
0(2)c-0(10)e	3.097(9)	0(2)c-Fe(5)-0(10)e	86.0(2)
0(3)c-0(5)c	2.946(8)	0(3)c-Fe(5)-0(5)c	90.1(2)
0(3)c-0(7)	3.176(10)	0(3)c-Fe(5)-0(7)	97.1(2)
0(3)c-0(12)	2.716(9)	0(3)c-Fe(5)-0(12)	76.0(2)
0(5)c-0(10)e	3.275(10)	0(5)c-Fe(5)-0(10)e	100.5(2)
0(5)c-0(12)	3.328(12)	0(5)c-Fe(5)-0(12)	97.6(3)
0(7)-0(10)e	2.590(7)	0(7)-Fe(5)-0(10)e	71.5(2)
0(7)-0(12)	2.746(8)	0(7)-Fe(5)-0(12)	78.6(2)
0(10)e-0(12)	3.339(10)	0(10)e-Fe(5)-0(12)	93.3(2)
<0-0>Fe(5)	3.059	<0-Fe(5)-0>	89.8

TABLE 6. EMPIRICAL BOND-VALENCE* TABLE FOR SCHNEIDERHÖHNITE

	As(1)	As(2)	As(3)	As(4)	As(5)	Fe(1)	Fe(2)	Fe(3)	Fe(4)	Fe(5)	Σ
0(1)					0.962			0.477	0.328		1.767
0(2)		0.818		0.946						0.297	2.061
0(3)				1.123					0.555	0.330	2.008
0(4)	0.967		1.070								2.037
0(5)		1.052				0.483x2↓				0.500	2.035
0(6)	1.049					0.551x2↓		0.455			2.055
0(7)					0.994				0.528	0.405	1.927
0(8)			0.970			0.465x2↓		0.430			1.865
0(9)				1.003			0.495x2↓	0.440			1.938
0(10)					1.040			0.663		0.223	1.926
0(11)		1.079					0.565x2↓	0.383			2.027
0(12)			0.986						0.447 0.335	0.260	2.028
0(13)	0.992						0.441x2↓		0.607		2.040
	3.008	2.949	3.026	3.072	2.996	2.998	3.002	2.848	2.800	2.015	

*bond-valences in v.u., calculated from the curves of Brown (1981).

The basic structural arrangement is shown in Figure 1. There are two dimeric $(\mathrm{As_2O_5})^{4-}$ groups and an isolated $(\mathrm{AsO_3})^{3-}$ group. These combine with the $(\mathrm{FeO_6})$ octahedra to form a dense compact framework. The octahedra polymerize by sharing polyhedron edges and corners, and the variation in the angular polyhedron distortions can be ascribed to cation–cation repulsion across shared elements. The variation in bond lengths can be interpreted in terms of the bond-valence requirements of the anions (Table 6), and several sites show a considerable variation in individual bond-lengths. The O(1) anion bond-valence sum of 1.767 v.u. shows significant deviation from the ideal value of 2 v.u.; small amounts of Ge could substitute for As at the As(5) site, but this would not significantly improve the situation; the origin of this discrepancy is thus not clear.

Geometry of the $(\mathrm{As^{3+}O_3})$ group

Several arsenite minerals have had their structures determined and refined to a fair degree of precision; data are summarized in Table 7, and give an indication of the kind of variations expected in arsenite-group minerals. The grand <As–O> is 1.776 Å, with a standard deviation of 0.012 Å, and the grand <O–As–O> is 97.2°, with a standard deviation of 2.0°. Several studies (Baur 1974, 1978, Shannon 1975, Hawthorne & Faggiani 1979) have shown that mean bond-lengths for specific cations can be affected by (are correlated with) other aspects of the structure. Such factors are given for the structures listed in Table 7. Stepwise multiple-regression analyses with both <As–O> and <O–As–O> as the independent variables show no significant correlation between the independent variables and any of the other parameters, and we are unable to ascribe the variations in <As–O> and <O–As–O> to these structural variations. Arsenite minerals are generally highly absorbing with regard to X radia-

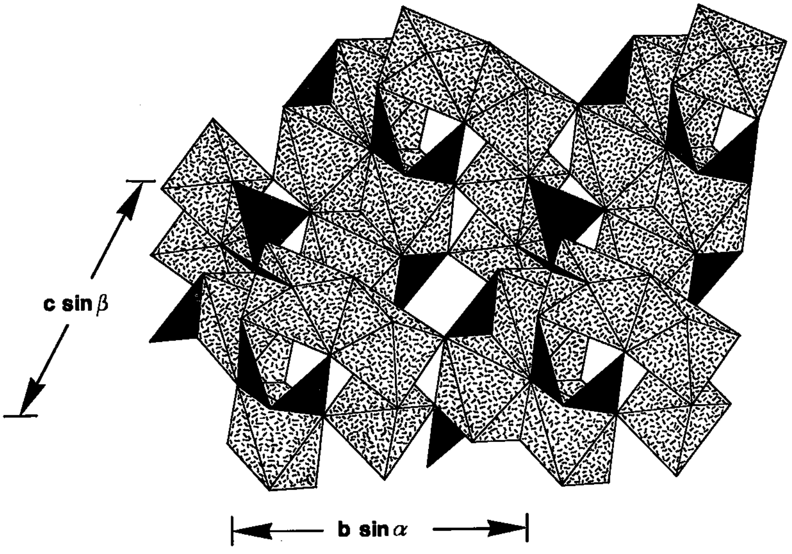

FIG. 1. The crystal structure of schneiderhöhnite, viewed down the X axis; Fe octahedra are hatched, AsO_3 groups are shown in black.

TABLE 7. BOND LENGTHS (Å) AND ANGLES (°), MEAN OXYGEN COORDINATION NUMBER (C.N.), BOND LENGTH (Δ) AND ANGLE (σ^2) DISTORTION PARAMETERS, AND MEAN CATION ELECTRONEGATIVITY (<x>) FOR ARSENITE GROUPS FROM PRECISELY REFINED MINERAL STRUCTURE

	As-O	As-O	As-O	<As-O>	O-As-O	O-As-O	O-As-O	<O-As-O>	<C.N.>	*Δ	*σ^2	<x>	Ref.
Reinerite	1.753(5)	1.772(3)	1.772(3)	1.766	97.6(1)	97.6(1)	100.0(1)	98.4	3.00	0.26	1.28	1.86	(1)
"	1.772(4)	1.771(3)	1.771(3)	1.771	95.2(1)	95.2(1)	100.0(1)	96.8	3.00	0.00	5.12	1.86	"
Cafarsite	1.78(2)	1.78(2)	1.78(2)	1.78	96.4(8)	96.4(8)	96.4(8)	96.4	4.00	0.00	0.00	1.75	(2)
"	1.74(1)	1.74(1)	1.79(1)	1.76	97.4(5)	93.8(5)	96.0(5)	95.7	4.33	1.83	2.20	1.75	"
"	1.73(1)	1.75(2)	1.80(1)	1.76	92.3(7)	101.2(5)	95.5(8)	96.3	3.67	2.80	13.55	1.75	"
Stenhuggarite	1.778(7)	1.775(7)	1.776(6)	1.776	99.6	99.0	91.3	96.6	3.30	0.01	14.28	1.85	(3)
"	1.736(7)	1.826(7)	1.801(6)	1.788	92.7	101.3	94.3	96.1	3.33	4.50	13.95	1.85	"
Claudetite	1.79(1)	1.81(1)	1.72(1)	1.77	98.9(6)	103.3(6)	93.7(6)	98.6	2.00	4.74	15.40	2.18	(4)
"	1.77(1)	1.79(1)	1.75(1)	1.77	94.9(6)	98.0(6)	89.7(6)	94.2	2.00	0.85	11.73	2.18	"
Asbecasite	1.787(7)	1.757(8)	1.846(7)	1.797	102.8(3)	94.9(3)	90.1(3)	95.9	3.33	4.23	27.42	1.62	(5)
Dixenite	1.779(5)	1.779(5)	1.779(5)	1.779	94.8(2)	94.8(2)	94.8(2)	94.8	3.00	0.00	0.00	1.76	(6)
"	1.755(5)	1.755(5)	1.755(5)	1.755	98.0(2)	98.0(2)	98.0(2)	98.0	4.00	0.00	0.00	1.76	"
"	1.721(5)	1.762(5)	1.779(5)	1.754	98.1(3)	103.8(2)	106.6(3)	102.8	3.67	1.93	12.51	1.76	"
Armangite	1.760(3)	1.782(3)	1.795(3)	1.779	91.7(2)	92.5(2)	103.3(2)	95.8	4.00	0.66	27.98	1.82	(7)
"	1.745(3)	1.772(3)	1.814(4)	1.777	92.3(2)	100.0(2)	106.0(2)	99.4	3.67	2.55	31.44	1.82	"
"	1.773(3)	1.776(4)	1.809(4)	1.786	93.6(2)	94.8(2)	100.6(2)	96.3	3.67	0.83	9.34	1.82	"
Paulmooreite	1.747(9)	1.750(9)	1.826(9)	1.774	95.7(4)	98.3(5)	99.9(4)	98.0	3.67	4.25	3.00	2.26	(8)
"	1.733(9)	1.772(8)	1.842(9)	1.782	95.4(4)	100.6(5)	98.7(4)	98.3	3.00	6.40	4.62	2.26	"
Hematolite	1.79(1)	1.79(1)	1.79(1)	1.79	94.2(5)	94.2(5)	94.2(5)	94.2	4.00	0.00	0.00	1.66	(9)
Magnussonite	1.750(6)	1.758(6)	1.779(6)	1.762	94.0(3)	94.0(3)	107.0(3)	98.3	4.00	0.48	37.56	1.70	(10)
Schneiderhohnite	1.797(7)	1.768(6)	1.788(6)	1.784	99.8(2)	101.2(3)	94.6(3)	98.5	2.67	0.46	8.06	2.02	(11)
"	1.852(5)	1.767(8)	1.758(5)	1.794	99.2(3)	99.6(2)	96.9(3)	98.6	3.00	5.58	1.42	2.02	"
"	1.761(5)	1.796(8)	1.790(5)	1.782	98.2(3)	98.8(2)	97.3(3)	98.1	3.00	0.74	0.11	2.02	"
"	1.805(5)	1.744(6)	1.784(5)	1.778	98.1(3)	98.5(3)	97.7(3)	98.1	3.00	2.03	0.11	2.02	"
"	1.799(7)	1.787(4)	1.771(7)	1.786	89.3(3)	101.7(3)	93.4(3)	94.8	3.00	0.41	26.61	2.02	"

References: (1) Ghose et al. (1977); (2) Edenharter et al. (1977); (3) Coda et al. (1977); (4) Pertlik (1978); (5) Cannillo et al. (1969); (6) Araki & Moore (1981); (7) Moore & Araki (1979a); (8) Araki et al. (1980); (9) Moore & Araki (1978); (10) Moore & Araki (1979b); (11) This study.

* $\Delta = \sum_{3}\{(l_i - \langle l_i \rangle)^2/\langle l_i \rangle^2\}/3$; $\sigma^2 = \sum_{3}\{(\text{O-As-O}) - \langle \text{O-As-O} \rangle\}^2/3$

tion; this often leads to a lower precision on the bond lengths. In addition, inadequacies in the absorption correction commonly give rise to inaccurate bond-lengths. Consequently, it is possible that some of the observed variations in Table 7 arise from experimental error, and obscure any structural effects that may affect the geometry of the arsenite group.

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