SHORT STRUCTURAL PAPERS

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Refinement of the Structure of Descloizite

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Abstract. $PbZnVO_4OH$, orthorhombic, *Pnma*, $Z = 4$, $D_c = 6{\cdot}202$ Mg m^{-3}; cell constants at 293 K: $a = 7{\cdot}593$ (2), $b = 6{\cdot}057$ (1), $c = 9{\cdot}416$ (2) Å; λ(Mo $K\alpha$) = 0·71069 Å. Examination of 41 (VO_4) tetrahedra in 31 crystal structures showed that the ⟨V–O⟩ bond length is significantly correlated with anion coordination number and the average electronegativity of the next-nearest neighbour cations, but not with tetrahedral distortion.

Introduction. Single-crystal precession photographs exhibited orthorhombic symmetry with systematic absences $hk0$, $h = 2n + 1$; $0kl$, $k + l = 2n + 1$, $h00$, $h = 2n + 1$; $0k0$, $k = 2n + 1$; $00l$, $l = 2n + 1$ consistent with the space group *Pnma* as assigned by Barnes & Qurashi (1952). This was confirmed by the diffractometer data; none of the $0kl$ reflexions listed by Qurashi & Barnes (1964) as observed were greater than 2σ above background. Perhaps these were due to Renninger effects in the earlier studies. Cell dimensions were determined by least-squares refinement of 15 reflexions automatically aligned on a four-circle diffractometer. Data collection and reduction procedures were as described by Hawthorne & Calvo (1977); the crystal used for the data collection was ground to a sphere 0·14 mm in diameter. A total of 511 unique reflections were collected, of which 405 were considered as observed [I(net) $\geq 3\sigma$]. Scattering factors for neutral atoms were taken from Cromer & Mann (1968) with anomalous-dispersion corrections from Cromer & Liberman (1970). Atomic parameters given by Qurashi & Barnes (1954) were used as input to the least-squares program *RFINE* (Finger, 1969), and with anisotropic thermal parameters of the form $\exp\left(-\sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_j \beta_{ij}\right)$, convergence occurred at R and R_w factors (unit weights) of 4·9 and 5·8% respectively (observed reflections). Final parameters are given in Table 1. Interatomic distances and angles were calculated with the program *ERRORS* (L. W. Finger, personal communication) and are given in Table 2.*

Table 1. *Atomic positions and equivalent isotropic temperature factors* (Å²)

	x	y	z	B_{eq}
Zn	$\frac{1}{2}$	0	0	1·21 (6)
Pb	0·1288 (2)	$\frac{1}{4}$	0·1759 (1)	1·31 (4)
V	0·8672 (8)	$\frac{3}{4}$	0·1882 (5)	0·86 (8)
O(1)	0·8720 (23)	0·5108 (22)	0·2900 (15)	1·3 (2)
O(2)	0·0430 (31)	$\frac{3}{4}$	0·0861 (27)	1·8 (4)
O(3)	0·6884 (28)	$\frac{3}{4}$	0·0692 (24)	1·1 (4)
OH	0·6457 (35)	$\frac{1}{4}$	0·0650 (24)	1·6 (4)

Discussion. It has been shown that mean interatomic distances in tetrahedral oxyanions are to some extent a function of the structure in which they occur. Shannon & Prewitt (1969) and Brown & Gibbs (1969) showed the effect of anion coordination number on ⟨Si–O⟩ distances, and Shannon (1971, 1975, 1976) and Shannon & Calvo (1973*a*) have shown the effect of both anion coordination number and average cation electronegativity on mean bond lengths in numerous tetrahedral oxyanions. Baur (1974) showed that ⟨P–O⟩ distances are significantly affected by both anion coordination and tetrahedral distortion, and Brown & Shannon (1973) have shown that distortion has a significant effect on mean bond lengths for octahedrally coordinated cations. One may thus conjecture

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34060 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 2. *Selected interatomic distances* (Å) *and angles* (°) *in descloizite*

V—O(1)	1·738 (14) ×2	Pb—O(1)^b	2·451 (17) ×2
V—O(2)^a	1·645 (24)	Pb—O(1)^d	2·730 (15) ×2
V—O(3)	1·760 (23)	Pb—O(2)^e	2·790 (25)
⟨V—O⟩	1·720	Pb—O(3)^f	2·693 (22)
		Pb—OH^g	2·443 (22)
Zn—O(1)^b	2·204 (14) ×2	⟨Pb—O⟩	2·613
Zn—O(3)^c	2·182 (16) ×2		
Zn—OH	1·973 (16) ×2		
⟨Zn—O⟩	2·120		
V tetrahedron			
O(1)—O(1)^h	2·90 (3)	O(1)—V(1)—O(1)^h	113·0 (9)
O(1)—O(2)^a	2·73 (3) ×2	O(1)—V(1)—O(2)^a	107·8 (7) ×2
O(1)—O(3)	2·89 (2) ×2	O(1)—V(1)—O(3)	111·6 (6) ×2
O(2)^a—O(3)	2·70 (3)	O(2)^a—V(1)—O(3)	104·7 (10)
⟨O—O⟩	2·81	⟨O—V—O⟩	109·4
Zn octahedron			
O(1)^b—O(3)^c	3·10 (3) ×2	O(1)^b—Zn—O(3)^c	90·0 (7) ×2
O(1)^b—O(3)^f	3·10 (2) ×2	O(1)^b—Zn—O(3)^f	90·0 (7) ×2
O(1)^b—OH	2·95 (3) ×2	O(1)^b—Zn—OH	89·5 (8) ×2
O(1)^b—OH^l	2·97 (2) ×2	O(1)^b—Zn—OH^l	90·5 (8) ×2
O(3)^c—OH	3·05 (3) ×2	O(3)^c—Zn—OH	94·2 (7) ×2
O(3)^c—OH^l	2·83 (3) ×2	O(3)^c—Zn—OH^l	85·8 (7) ×2
⟨O—O⟩	3·00	⟨O—Zn—O⟩	90·0
Pb polyhedron			
O(1)^b—O(1)^d	5·00 (2) ×2	O(1)^b—Pb—O(1)^d	149·3 (1) ×2
O(1)^b—O(1)^i	3·16 (3)	O(1)^b—Pb—O(1)^i	80·2 (7)
O(1)^b—O(1)^j	3·87 (2) ×2	O(1)^b—Pb—O(1)^j	96·5 (4) ×2
O(1)^b—O(2)^e	4·49 (2) ×2	O(1)^b—Pb—O(2)^e	117·9 (5) ×2
O(1)^b—O(3)^f	3·10 (3) ×2	O(1)^b—Pb—O(3)^f	74·0 (5) ×2
O(1)^b—OH^g	3·15 (2) ×2	O(1)^b—Pb—OH^g	80·2 (6) ×2
O(1)^d—O(1)^j	3·16 (3)	O(1)^d—Pb—O(1)^j	70·7 (7)
O(1)^d—O(2)^e	3·93 (3) ×2	O(1)^d—Pb—O(2)^e	90·8 (5) ×2
O(1)^d—O(3)^f	5·01 (3) ×2	O(1)^d—Pb—O(3)^f	134·9 (4) ×2
O(1)^d—OH^g	2·95 (3) ×2	O(1)^d—Pb—OH^g	69·2 (6) ×2
O(2)^e—O(3)^f	2·70 (3)	O(2)^e—Pb—O(3)^f	58·9 (6)
O(2)^e—OH^g	5·11 (3)	O(2)^e—Pb—OH^g	155·1 (8)
O(3)^f—OH^g	4·91 (3)	O(3)^f—Pb—OH^g	146·0 (8)

Symmetry code: $(a) = 1 + x, y, z$; $(b) = x - \frac{1}{2}, \frac{1}{2} - y, z$; $(c) = x, y - 1, z$; $(d) = x - 1, y, z$; $(e) = -x, 1 - y, \frac{1}{2}z$; $(f) = 1 - x, 1 - y, -z$; $(g) = x - \frac{1}{2}, y, \frac{1}{2} - z$; $(h) = x, 1\frac{1}{2} - y, z$; $(i) = x - \frac{1}{2}, y, z$; $(j) = x - 1, \frac{1}{2} - y, z$; $(k) = 1\frac{1}{2} - x, y - \frac{1}{2}, -z$; $(l) = 1 - x, -y, -z$.

that mean interatomic distances in tetrahedral oxyanions are a function of anion coordination number, average cation electronegativity and tetrahedral distortion. Baur (1978) has examined the effect of these three variables, together with several others, on ⟨Si—O⟩ bond lengths, and has shown that only anion coordination number, the number of bridging anions per tetrahedron and the mean value of the secant of the bridging angles Si—O—T contribute significantly to ⟨Si—O⟩ variations. Variation in bridging angles V—O—T was not considered in the present study as we are interested in the development of an equation for predictive purposes in the simulation of crystal structures.

A total of 41 ⟨V—O⟩ distances (Table 3) were used, data being included only if $\langle\sigma\rangle \leq 0.01$ Å. Data for $Ca_3V_2O_8$ (Gopal & Calvo, 1973*a*) were excluded because the presence of positional disorder has affected the observed V—O distances. Anion coordination numbers (CN) were evaluated individually, the parameter Δ (Brown & Shannon, 1973) was used as a measure of tetrahedral distortion and the tetrahedral angle variance λ (Robinson, Gibbs & Ribbe, 1971) was evaluated. The electronegativity was also evaluated individually, as the average electronegativity per cation—O bond $\{\bar{\chi} = [(\sum_{CN} \chi^{cat}) - \chi^{V}]/(CN - 1)\}$. The grand $\langle V—O\rangle^{IV}$ distance is 1·721 (8) Å. The tetrahedral angle variance and the number of bridging anions per tetrahedron did not show significant correlation with either ⟨V—O⟩ or the mean ionic radius of V^{5+} and are not considered further. A stepwise linear regression was performed on ⟨V—O⟩, Δ, CN and $\bar{\chi}$ with ⟨V—O⟩ as the dependent variable. The correlation with CN was not significant at the 0·01 level. Baur (1974) has argued that the variation in ionic radii for O^{2-} given by Shannon & Prewitt (1969) is a good measure of the variation in $\langle X—O\rangle$ bond lengths due to variation in anion coordination number. Accepting this, the effect of anion coordination number may be removed by using ionic radius instead of ⟨V—O⟩ distance. Stepwise linear regression was performed on r^V, Δ and $\bar{\chi}$ with r^V as the dependent variable; the correlation with Δ was not significant at the 0·01 level. Hence the ionic radius of V^{5+} in tetrahedral coordination appears to be solely a function of the electronegativity of the next-nearest neighbour cations:

$$r(V^{5+}) = 0{\cdot}325 + 0{\cdot}020(3)\bar{\chi}, \quad R = 0{\cdot}724.$$

This may be incorporated with the dependence of $r(O^{2-})$ on coordination number to give the equation

$$\langle V—O\rangle = 1{\cdot}649 + 0{\cdot}020\bar{\chi} + 0{\cdot}013CN.$$

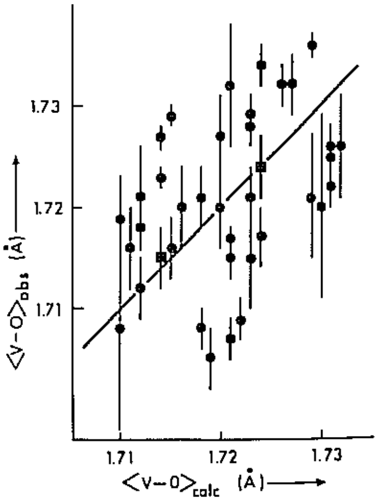

Fig. 1. Comparison of observed and calculated ⟨V—O⟩ distances.

Table 3. *Data for vanadate structures*

$\bar{\chi} = (\sum_{CN} \chi^{cat} - \chi^{V})/(CN - 1)$; $\Delta = \sum_{i=1}^{4} [(l_i - \langle l \rangle)/\langle l \rangle]^2 \times 10^3/4$.

	$\langle V{-}O \rangle_a$ (Å)	CN	r (Å)	$\bar{\chi}$	Δ
$Pb_2V_2O_7$[a]	1·721 (6)	3·25	0·355	1·90	1·04
	1·726 (5)	3·50	0·357	1·90	1·11
$LiVO_3$[b]	1·727 (1)	3·25	0·361	1·20	2·30
$Cu_5V_2O_{10}$[c]	1·722 (2)	3·25	0·356	2·00	0·54
	1·725 (2)	3·50	0·356	2·00	0·75
$Mg_3V_2O_8$[d]	1·729 (1)	3·25	0·363	1·20	0·78
$Cu_3V_2O_8$[e]	1·726 (2)	3·25	0·360	2·00	0·75
$Zn_3V_2O_8$[f]	1·715 (5)	3·25	0·349	1·60	0·84
$Ba_2V_2O_7$[g]	1·715 (3)	3·50	0·346	1·00	1·24
	1·721 (3)	3·74	0·348	0·99	1·25
	1·715 (3)	3·50	0·346	1·00	1·19
	1·724 (3)	3·50	0·355	1·00	1·35
$Zn_2V_2O_7$[h]	1·716 (3)	2·50	0·359	1·65	0·61
$Co_2V_2O_7$[i]	1·732 (2)	2·75	0·372	1·82	2·01
	1·734 (2)	3·00	0·371	1·82	1·31
$Ni_2V_2O_7$[i]	1·728 (2)	2·75	0·368	1·90	2·02
	1·732 (2)	3·00	0·369	1·90	1·29
Li_3VO_4[j]	1·717 (1)	4·00	0·341	1·00	0·00
$Co_3V_2O_8$[k]	1·732 (3)	3·25	0·366	1·80	0·68
$Ni_3V_2O_8$[k]	1·736 (1)	3·25	0·370	1·90	0·68
$NdVO_4$[l]	1·721 (5)	3·00	0·358	1·20	0·00
YVO_4[m]	1·718 (2)	3·00	0·355	1·20	0·00
$FeVO_4$[n]	1·720 (4)	2·50	0·363	1·90	1·40
	1·727 (4)	2·50	0·370	1·90	1·07
	1·720 (4)	2·25	0·367	1·90	0·91
Ca_2VO_4Cl[o]	1·707 (1)	4·00	0·331	1·00	0·01
$Cd_2V_2O_7$[p]	1·718 (10)	2·75	0·358	1·73	0·36
$Ca_5(VO_4)_3OH$[q]	1·707 (2)	4·00	0·331	1·00	0·06
$NaVO_3$[r]	1·723 (1)	3·25	0·357	1·12	2·20
KVO_3[s]	1·724 (2)	4·50	0·342	0·84	2·29
$RbVO_3$[s]	1·717 (3)	4·50	0·335	0·84	2·50
$CsVO_3$[s]	1·721 (3)	4·50	0·339	0·77	2·40
α-$Cu_2V_2O_7$[t]	1·709 (2)	2·50	0·352	1·99	0·48
β-$Cu_2V_2O_7$[u]	1·712 (3)	2·50	0·355	1·49	0·78
α-$Na_3Er(VO_4)_2$[v]	1·708 (2)	3·75	0·335	0·98	0·41
$Mg_2V_2O_7$[w]	1·715 (2)	2·75	0·355	1·82	1·53
	1·729 (2)	3·00	0·366	1·74	0·50
$K_2V_3O_8$[x]	1·705 (3)	4·00	0·329	0·90	1·20
$Ca_2V_2O_7.H_2O$[y]	1·719 (4)	3·00	0·356	1·12	0·77
	1·716 (4)	3·00	0·359	1·12	0·94
$PbZnVO_4OH$[z]	1·720 (9)	3·50	0·351	1·78	0·67

References: (*a*) Shannon & Calvo (1973*b*). (*b*) Shannon & Calvo (1973*c*). (*c*) Shannon & Calvo (1973*d*). (*d*) Krishnamachari & Calvo (1971). (*e*) Shannon & Calvo (1972). (*f*) Gopal & Calvo (1971). (*g*) Hawthorne & Calvo (1978). (*h*) Gopal & Calvo (1973*b*). (*i*) Sauerbrei, Faggiani & Calvo (1974). (*j*) Shannon & Calvo (1973*a*). (*k*) Sauerbrei, Faggiani & Calvo (1973). (*l*) Baglio & Sovers (1971). (*m*) Lohmüller, Schmidt, Deppisch, Gramlich & Scheringer (1973). (*n*) Robertson & Kostiner (1972). (*o*) Banks, Greenblatt & Post (1970). (*p*) Au & Calvo (1967). (*q*) Kutoglu (1974). (*r*) Marumo, Isobe & Iwai (1974). (*s*) Hawthorne & Calvo (1977). (*t*) Calvo & Faggiani (1975). (*u*) Mercurio-Lavaud & Frit (1973). (*v*) Salmon, Parent, Le Flem & Vlasse (1976). (*w*) Gopal & Calvo (1974). (*x*) Galy & Carpy (1975). (*y*) Konnert & Evans (1975). (*z*) This work.

A number of observed and calculated ⟨V–O⟩ distances using this equation are given in Fig. 1. These equations should be of use both for predictive purposes and as a check on observed $\langle V^{5+}{-}O \rangle^{IV}$ distances.

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References

Au, P. K. L. & Calvo, C. (1967). *Can. J. Chem.* **45**, 2297–2302.

Baglio, J. A. & Sovers, O. J. (1971). *J. Solid State Chem.* **3**, 458–465.

Banks, E., Greenblatt, M. & Post, B. (1970). *Inorg. Chem.* **9**, 2259–2267.

Barnes, W. H. & Qurashi, M. M. (1952). *Am. Mineral.* **37**, 407–422.

Baur, W. H. (1974). *Acta Cryst.* B**30**, 1195–1215.

Baur, W. H. (1978). *Acta Cryst.* B**34**, 1751–1756.

Brown, G. E. & Gibbs, G. V. (1969). *Am. Mineral.* **54**, 1528–1539.

Brown, I. D. & Shannon, R. D. (1973). *Acta Cryst.* A**29**, 266–282.

Calvo, C. & Faggiani, R. (1975). *Acta Cryst.* B**31**, 603–605.

Cromer, D. T. & Liberman, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

Finger, L. W. (1969). *RFINE. A Fortran* IV *Computer Program for Structure Factor Calculation and Least-squares Refinement of Crystal Structures.* Geophysics Laboratory, Carnegie Institute, Washington (unpublished).

Galy, J. & Carpy, A. (1975). *Acta Cryst.* B**31**, 1794–1797.

Gopal, R. & Calvo, C. (1971). *Can. J. Chem.* **49**, 3056–3059.

Gopal, R. & Calvo, C. (1973*a*). *Z. Kristallogr.* **137**, 67–85.

Gopal, R. & Calvo, C. (1973*b*). *Can. J. Chem.* **51**, 1004–1009.

Gopal, R. & Calvo, C. (1974). *Acta Cryst.* B**30**, 2491–2493.

Hawthorne, F. C. & Calvo, C. (1977). *J. Solid State Chem.* **22**, 157–170.

Hawthorne, F. C. & Calvo, C. (1978). *J. Solid State Chem.* **23**. In the press.

Konnert, J. A. & Evans, H. T. Jr (1975). *Acta Cryst.* B**31**, 2688–2689.

Krishnamachari, N. & Calvo, C. (1971). *Can. J. Chem.* **49**, 1629–1637.

Kutoglu, A. (1974). *Neues Jahrb. Mineral. Monatsh.* pp. 210–218.

Lohmüller, G., Schmidt, G., Deppisch, B., Gramlich, V. & Scheringer, C. (1973). *Acta Cryst.* B**29**, 141–142.

Marumo, F., Isobe, M. & Iwai, S. (1974). *Acta Cryst.* B**30**, 1628–1630.

Mercurio-Lavaud, D. & Frit, B. (1973). *C. R. Acad. Sci. Sér. C*, **277**, 1101–1104.

Qurashi, M. M. & Barnes, W. H. (1954). *Am. Mineral.* **39**, 416–435.

QURASHI, M. M. & BARNES, W. H. (1964). *Can. Mineral.* **8**, 23–39.

ROBERTSON, B. & KOSTINER, E. (1972). *J. Solid State Chem.* **4**, 29–37.

ROBINSON, K., GIBBS, G. V. & RIBBE, P. H. (1971). *Science*, **172**, 567–570.

SALMON, R., PARENT, C., LE FLEM, G. & VLASSE, M. (1976). *Acta Cryst.* B**32**, 2799–2802.

SAUERBREI, E. E., FAGGIANI, R. & CALVO, C. (1973). *Acta Cryst.* B**29**, 2304–2306.

SAUERBREI, E. E., FAGGIANI, R. & CALVO, C. (1974). *Acta Cryst.* B**30**, 2907–2909.

SHANNON, R. D. (1971). *Chem. Commun.* pp. 821–822.

SHANNON, R. D. (1975). Proc. NATO Conf. on Petrophysics, Newcastle-upon-Tyne.

SHANNON, R. D. (1976). *Acta Cryst.* A**32**, 751–767.

SHANNON, R. D. & CALVO, C. (1972). *Can. J. Chem.* **50**, 3944–3949.

SHANNON, R. D. & CALVO, C. (1973*a*). *J. Solid State Chem.* **6**, 538–549.

SHANNON, R. D. & CALVO, C. (1973*b*). *Can. J. Chem.* **51**, 70–76.

SHANNON, R. D. & CALVO, C. (1973*c*). *Can. J. Chem.* **51**, 265–273.

SHANNON, R. D. & CALVO, C. (1973*d*). *Acta Cryst.* B**29**, 1338–1345.

SHANNON, R. D. & PREWITT, C. T. (1969). *Acta Cryst.* B**25**, 925–946.

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Paradamite

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Abstract. Zn_2AsO_4OH, $P\bar{1}$, $Z = 2$, $D_c = 4{\cdot}595$ Mg m^{-3}; cell constants at 293 K: $a = 5{\cdot}638\,(3)$, $b = 5{\cdot}827\,(3)$, $c = 6{\cdot}692\,(2)$ Å, $\alpha = 103{\cdot}25\,(4)$, $\beta = 104{\cdot}37\,(3)$, $\gamma = 87{\cdot}72\,(4)°$; λ(Mo $K\alpha$) = 0·71069 Å. Paradamite is isostructural with tarbuttite, Zn_2PO_4OH.

Introduction. Paradamite is a dimorph of adamite and was first characterized by Switzer (1956). Finney (1966) derived the unit cell and proposed that paradamite is isostructural with tarbuttite, Zn_2PO_4OH, and Hawthorne (1976) has discussed the relationship between the adamite and tarbuttite structure types.

Single-crystal precession photographs of paradamite from Mapimi, Mexico, exhibit triclinic symmetry; the unit cell chosen is analogous to that used by Cocco, Fanfani & Zanazzi (1966) for tarbuttite. The unit-cell parameters were derived by least-squares refinement of 15 high-angle reflexions aligned automatically on a four-circle diffractometer. A full set of intensity data (1384 reflexions) was collected over one hemisphere out to a 2θ of 65° from an irregular equidimensional crystal of radius 0·09 mm, following the experimental procedure of Hawthorne & Ferguson (1975). Standard data-reduction procedures with a spherical absorption correction ($\mu = 20{\cdot}2$ mm^{-1}) resulted in 1202 unique reflexions of which 1132 were considered as observed ($I_{\rm net} > 3\sigma$). Structure refinement was carried out on an IBM 370/158 computer using the program *RFINE* (Finger, 1969). Scattering factors for neutral atoms were taken from Cromer & Mann (1968) with anomalous-dispersion corrections from Cromer & Liberman (1970). The atomic parameters given by Cocco *et al.* (1966) for tarbuttite, Zn_2PO_4OH, were assumed as the starting parameters for paradamite Several cycles of full-matrix least-squares refinement resulted in convergence (for isotropic temperature factors) at a conventional R of 6·2% (observed reflexions). Conversion to anisotropic temperature factors of the form $\exp(-\sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_j \beta_{ij})$ resulted in convergence (maximum shift/error <0·01) at an R of 4·8% and an R_w (unit weights) of 5·8%. Final atomic positions and equivalent isotropic temperature factors are given in Table 1. Interatomic distances and angles

Table 1. *Atomic positions and equivalent isotropic temperature factors* (Å^2)

	x	y	z	B_{eq}
Zn(1)	0·3928 (2)	0·2498 (2)	0·5008 (2)	0·86 (2
Zn(2)	0·0214 (2)	0·7355 (2)	0·1867 (1)	0·72 (2
As	0·8312 (2)	0·2476 (1)	0·2745 (1)	0·49 (2
O(1)	0·7627 (11)	0·9689 (10)	0·1391 (9)	0·79 (9
O(2)	0·9421 (12)	0·3885 (11)	0·1233 (9)	0·94 (9
O(3)	0·5779 (11)	0·3837 (11)	0·3342 (9)	0·85 (9
O(4)	0·9549 (11)	0·7478 (11)	0·4968 (9)	0·71 (8
OH	0·3519 (11)	0·8899 (12)	0·2997 (9)	0·89 (9

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