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The crystal structure of paulmooreite, $Pb_2[As_2O_5]$: dimeric arsenite groups

TAKAHARU ARAKI, PAUL B. MOORE

*Department of the Geophysical Sciences, The University of Chicago
Chicago, Illinois 60637*

AND GEORGE D. BRUNTON

*Division of Reactor Chemistry, Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830*

Abstract

Paulmooreite, $Pb_2[As_2O_5]$, was studied in detail by three-dimensional X-ray diffractometry on a Picker four-circle goniostat using Mo$K\alpha$ radiation. The new mineral is monoclinic, space group $P2_1$ or $P2_1/m$ including exceedingly weak reflections but refined in $P2_1/a$, $Z = 4$, $a = 13.584(4)$, $b = 5.650(2)$, $c = 8.551(3)$A, $\beta = 108.78(2)°$. $R = 0.064$ ($R_w = 0.057$) for 2709 independent reflections. The structure was solved by Patterson, Fourier and least-squares refinement techniques.

The structure is based on $[As_2O_5]^{4-}$ corner-linked dimers which link to distorted Pb–O polyhedra, leading to the weakest links across {001}, the plane of perfect cleavage. For $^{[4]}Pb^{[3]}As_2O_5$, bond distance averages are As(1)–O = 1.774, As(2)–O = 1.782, Pb(1)–O = 2.380, and Pb(2)–O = 2.436A. The $[AsO_3]^{3-}$ groups are trigonal pyramids, and PbO_4 groups are distorted tetragonal pyramids. For bonds < 3.8A, distorted $Pb(1)O_5$ and $Pb(2)O_6$ polyhedra occur. Due to lone-pair electrons about the cations, the coordination polyhedra are "one-sided," the electron pairs presumably residing around the empty vertices.

Introduction

About a decade ago, an unknown mineral from Långban, Sweden was investigated in a cursory fashion and subsequently reported as likely being a new species, corresponding to Flink unknown 49 (Moore *et al.*, 1971). Later study revealed the mineral to be the same as Flink unknown 305. A more detailed examination led to an electron microprobe study which revealed only lead and arsenic in the atomic ratio 1:1. Owing to the extreme rarity of the mineral we despaired of obtaining a more detailed wet-chemical analysis, especially for water and elements with atomic number less than 9, so we undertook a formal three-dimensional crystal structure analysis. Shortly after the structure was solved, the species was announced as the new mineral paulmooreite, $Pb_2As_2O_5$, by Dunn *et al.*, 1979. These authors also noted its occurrence on Flink unknown 305, a specimen from which our crystal was taken for structure analysis (Riksmuseet Stockholm No. 252356) before it was submitted to their study and recatalogued (NMNH # 142974). Thus, by a remarkable coincidence, the new species and the structure were determined independently almost simultaneously.

Experimental section

Single crystals of the type specimen were examined and a suitable fragment was ground into an ellipsoid which measured 0.059 × 0.13 × 0.10 mm along its principal axes. Least-squares refinement employing 20 high-angle Mo$K\alpha_1$ reflections from a Picker four-circle goniostat with a Kevex Si–Li solid-state detector led to determination of the cell parameters $a = 13.584(4)$, $b = 5.650(2)$ and $c = 8.551(3)$A, $\beta = 108.78(2)°$.

Three-dimensional data were collected with unfiltered Mo$K\alpha$ radiation, Mo$K\beta$ being eliminated by a 400V wide pulse-height analyzer window. Reflections were step-scanned in increments of 0.02° in 2θ over a range of $2\theta = (3.3 \times 114.6\ \Delta\lambda/\lambda)°$. Each step was counted for one second, and background was counted on each side of a reflection for fifteen seconds. The variance whose reciprocal was used in least-squares adjustment of structure parameters was

$\sigma^2(F_o^2) = [T + B + (0.03(T - B))^2]/A(Lp)^2$, where T = total counts, B = background counts, A = absorption correction, and L and p the Lorentz and polarization corrections.

These data were collected five years ago when the composition of paulmooreite was not precisely known. Semi-quantitative results indicated the presence of major Pb and As. The original linear absorption coefficient was $\mu_\alpha = 755$ cm^{-1} assuming an arsenate–carbonate composition. The correct $\mu_\alpha = 643$ cm^{-1} for $Pb_2[As_2O_5]$ differs significantly, but examination of the orientations of the thermal vibration ellipsoids suggests that errors in absorption corrections were minimal, and we therefore did not reprocess the raw data.

Solution and refinement of the structure

A three-dimensional Patterson synthesis, *P(uvw)*, formed the basis of the structure solution which was solved by applying the heavy-atom method. Pb is the major heavy atom, and the solution of the prominent vector densities should have been straightforward. Peaks of the Patterson synthesis implied the presence of two Pb atoms in the asymmetric unit, but their coordinate relations presented problems early on. The correct solution established the cause of this problem: vectors between the independent Pb positions led to many vector densities situated at (~0, ~0, ~$\frac{1}{2}$), *etc.*, which presented difficulties in the proper selection of the origin. When the correct solution was found, the As atoms were located employing an electron-density synthesis, and the oxygen positions were then easily obtained through further iteration. Since the formula was then unknown, difference syntheses were required to test for the possible presence of light atoms, such as C, B, Be, *etc.* The featureless character of the difference synthesis, after two cycles of coordinate refinement, led to a structure based on 2Pb, 2As and 5O in the asymmetric unit. Bond distance calculations led to the unambiguous assignment of atomic species and scattering curves.

Table 1. Paulmooreite. Atomic coordinate parameters†

Atom	x	y	z
Pb(1)	0.87944(3)	0.34777(9)	0.85850(5)
Pb(2)	0.19928(3)	0.65316(9)	0.65005(5)
As(1)	0.93649(9)	0.87122(23)	0.61423(14)
As(2)	0.12882(9)	0.12912(24)	0.88433(14)
O(1)	0.8488(6)	0.6698(17)	0.6518(12)
O(2)	0.8642(6)	0.1238(16)	0.6227(10)
O(3)	0.0316(7)	0.8904(19)	0.8209(11)
O(4)	0.2060(7)	0.0530(18)	0.7597(11)
O(5)	0.1999(7)	0.9990(20)	0.0698(10)

†Estimated standard errors refer to the last digit.

Table 2. Paulmooreite. Anisotropic thermal vibration parameters (×10^5)†

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Pb(1)	210(2)	1403(13)	522(5)	- 28(4)	68(2)	- 74(7)
Pb(2)	202(2)	1342(13)	609(6)	- 45(4)	102(3)	62(7)
As(1)	183(5)	1206(34)	520(13)	- 14(11)	119(7)	57(18)
As(2)	186(5)	1284(35)	550(14)	52(11)	123(7)	- 24(18)
O(1)	221(42)	1195(251)	885(126)	- 71(90)	155(59)	-120(155)
O(2)	206(41)	1297(264)	607(108)	91(82)	87(53)	- 99(138)
O(3)	193(42)	2612(380)	593(113)	-417(103)	22(56)	158(170)
O(4)	210(41)	1800(296)	801(124)	- 66(95)	289(59)	-115(163)
O(5)	295(48)	1989(325)	434(99)	-163(104)	14(55)	29(154)

†Coefficients in the expression $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}\ell^2 + 2\beta_{12}hk + 2\beta_{13}h\ell + 2\beta_{23}k\ell)]$. Estimated standard errors in parentheses refer to the last digit.

Scattering curves for Pb^{2+}, As^{3+}, and O^{1-} were obtained from Cromer and Mann (1968), and anomalous dispersion corrections, $\Delta f''$, for Pb and As from Cromer and Liberman (1970). Refined variables included the scale factor (1 parameter), atomic coordinate parameters (27), and anisotropic thermal vibration parameters (54), and with 2709 independent $|F_o|$ this leads to a data-to-variable parameter ratio of about 33:1. Convergence was assured at $R = 0.064$, and $R_\omega = 0.057$ for all 2709 reflections, where

$$R = \frac{\sum \| F_o| - |F_c \|}{\sum |F_o|} \quad \text{and} \quad R_w = \left[\frac{\sum_w(|F_o| - |F_c|)^2}{\sum_w |F_o|^2}\right]^{1/2}$$

with $w = \sigma^{-2}$ of F_o. The parameter $w(F_o - F_c)^2$ was minimized during the refinement.

Table 1 lists refined atomic coordinate parameters, Table 2 the anisotropic thermal vibration parameters, Table 3 the ellipsoids of vibration and their equivalent isotropic temperature factors, Table 4 the bond distances and angles, and Table 5 the electrostatic valence balances. Table 6 lists the observed and calculated structure factors.[1]

In this study we refined the structure based on the space group $P2_1/a$. As also noted by Dunn *et al.* (1979), we found extremely weak (*h0l*) reflections with *l* odd, which implied that the true space group is $P2_1/m$ or $P2_1$. However, these reflections were barely detectable above background in the course of the data collection. Selecting the acentric group would have forced a doubling of the number of atoms in the

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[1] To obtain a copy of Table 6, order Document AM-80-125 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D.C. 20009. Please remit $1.00 in advance for the microfiche.

Table 3. Paulmooreite. Parameters for the ellipsoids of vibration†

Atom	i	μ_i	θ_{ia}	θ_{ib}	θ_{ic}	Bequiv. Å^2
Pb(1)	1	0.1246(7)	59(2)	77(1)	52(2)	1.555(8)
	2	0.1427(6)	31(4)	100(3)	138(5)	
	3	0.1523(7)	92(3)	163(1)	74(3)	
Pb(2)	1	0.1279(7)	22(3)	70(2)	98(2)	1.561(8)
	2	0.1391(7)	92(3)	60(2)	144(3)	
	3	0.1536(7)	112(1)	37(1)	55(3)	
As(1)	1	0.119(2)	156(20)	104(5)	53(13)	1.35(2)
	2	0.131(2)	113(7)	71(8)	134(7)	
	3	0.142(2)	96(4)	24(6)	67(6)	
As(2)	1	0.118(2)	159(23)	72(4)	62(9)	1.42(2)
	2	0.136(2)	102(5)	92(7)	149(8)	
	3	0.147(2)	107(3)	161(10)	79(8)	
O(1)	1	0.128(15)	42(45)	51(36)	92(19)	1.76(13)
	2	0.143(14)	48(47)	137(53)	110(31)	
	3	0.174(12)	94(16)	104(18)	20(34)	
O(2)	1	0.123(14)	35(90)	125(31)	102(24)	1.56(13)
	2	0.136(13)	103(40)	115(38)	139(38)	
	3	0.161(13)	122(20)	134(21)	52(37)	
O(3)	1	0.095(17)	31(14)	65(8)	90(14)	2.14(17)
	2	0.140(14)	79(15)	73(9)	161(20)	
	3	0.230(15)	119(6)	31(8)	71(9)	
O(4)	1	0.094(15)	158(34)	92(9)	50(19)	1.78(14)
	2	0.162(14)	104(12)	136(40)	123(19)	
	3	0.180(14)	74(10)	134(40)	57(19)	
O(5)	1	0.115(14)	74(12)	86(13)	35(18)	1.98(15)
	2	0.156(14)	43(26)	50(18)	118(26)	
	3	0.194(14)	129(22)	40(17)	71(15)	

† i = ith principal axis; μ_i = rms amplitude, θ_{ia}, θ_{ib}, θ_{ic} = angles (deg.) between the ith principal axis and the cell axes a, b, and c. The equivalent isotropic thermal parameter, B, is also listed.

asymmetric unit with subsequent difficulties in parameter refinement owing to high coordinate correlations, and the centric $P2_1/m$ was clearly incorrect; we therefore refined the structure using space group $P2_1/a$. Convergence of the refinement with sensible bond distances and angles suggests that this model is basically correct.

Description of the structure

The crystal structure of paulmooreite is of interest because of the presence of [As$_2^{3+}$O$_5$]$^{4-}$ doublets (which, to our knowledge, is unique among minerals and related inorganic compounds) and because of 4s^2 lone electron pairs about As^{3+} and 6s^2 pairs about Pb^{2+}. The result is the appearance of trigonal pyramidal oxygen coordination about As^{3+} and a range of Pb^{2+}–O distances, from 2.25 to 3.06A for values accepted within 3.8A. We have chosen 4-coordination by oxygen for Pb(1) and Pb(2), with distances between 2.26 and 2.55A, defining distorted tetragonal pyramids. The distances Pb(1)–O(3) 2.94, and Pb(2)–O(2) 2.80 and Pb(2)–O(1) 3.06A are also included in Table 4, and appear as dashed bonds in Figures 1 and 2. Accepting 4-coordination, the averages are $^{[4]}$Pb(1)–O 2.38 and $^{[4]}$Pb(2)–O 2.44A respectively, to be compared with $^{[4]}$Pb(2)–O 2.36 and $^{[4]}$Pb(3)–O 2.42A in alamosite, Pb^{2+}SiO$_3$ (Boucher and Peacor, 1968). In larsenite, Pb^{2+}[ZnSiO$_4$], the $^{[4]}$Pb(2)–O 2.47A average is found (Prewitt *et al.*, 1967). As in paulmooreite, a break occurs between the inner distances and the longer distances: for example, in larsenite $^{[3]}$Pb(1)–O distances range from 2.26 to 2.43A but three additional distances occur between 2.88 and 3.18A, and two additional Pb(2)–O 2.85 and 3.15A distances also occur.

The $^{[3]}$As^{3+}–O 1.77 and 1.78A averages are close to 1.76A in magnussonite (Moore and Araki, 1979a), 1.78 and 1.79A in stenhuggarite (Coda *et al.*, 1977),

Table 4. Paulmooreite. Bond distances and angles†

As(1)	
As(1)-O(2)	1.747(9)
-O(1)	1.750(9)
-O(3)	1.826(9)
average	1.774

		O–As–O′ Angle (°)
O(1)-O(2)*	2.592(14)	95.7(4)
O(2)-O(3)	2.703(13)	98.3(5)
O(1)-O(3)	2.739(12)	99.9(4)
average	2.678	98.0

As(2)	
As(2)-O(5)	1.733(9)
-O(4)	1.772(8)
-O(3)	1.842(9)
average	1.782

		O–As–O′ Angle (°)
O(3)-O(5)**	2.645(11)	95.4(4)
O(4)-O(5)	2.696(12)	100.6(5)
O(3)-O(4)	2.743(12)	98.7(4)
average	2.695	98.3

Pb(1)		Pb(2)	
Pb(1)-O(4)$^{(2)}$	2.301(9)	Pb(2)-O(1)$^{(2)}$	2.260(9)
-O(2)	2.332(8)	-O(4)	2.437(10)
-O(5)$^{(1)}$	2.409(10)	-O(5)$^{(3)}$	2.502(9)
-O(1)	2.477(9)	-O(2)$^{(1)}$	2.545(9)
-O(3)$^{(1)}$	2.942(9)	-O(2)$^{(2)}$	2.803(9)
average (inner 4)	2.380	-O(1)$^{(1)}$	3.055(9)
grand average	2.492	average (inner 4)	2.436
		grand average	2.600

†Estimated standard errors refer to the last digit. Bond distances listed are those below 3.80A. The equivalent positions (referred to Table 1) in superscripts are (1) = -x, -y, -z; (2) = ½+x, ½-y, z; (3) = ½-x, ½+y, -z.

*O–O′ edge shared between As(1) and Pb(2).

**O–O′ edge shared between As(2) and Pb(1).

Table 5. Paulmooreite. Relations in bond strength–bond length*

	Coordinating Cations					Bond Length Deviations			
Anions	Pb(1)	Pb(2)	As(1)	As(2)	Δp_O	Pb(1)	Pb(2)	As(1)	As(2)
					A. With $^{[4]}$Pb(1) and $^{[4]}$Pb(2)				
O(1)	1	1	1	-	0.00	+0.097	-0.176	-0.024	------
O(2)	1	1	1	-	0.00	-0.048	+0.109	-0.027	------
O(3)	-	-	1	1	0.00	------	------	+0.052	+0.060
O(4)	1	1	-	1	0.00	-0.079	+0.001	------	-0.010
O(5)	1	1	-	1	0.00	+0.029	+0.066	------	-0.049
					B. With $^{[5]}$Pb(1) and $^{[6]}$Pb(2)				
O(1)	1	2	1	-	+0.067	-0.015	+0.455,-0.340	-0.024	------
O(2)	1	2	1	-	+0.067	-0.160	-0.005,+0.203	-0.027	------
O(3)	1	-	1	1	+0.400	+0.450	------	+0.052	+0.060
O(4)	1	1	-	1	-0.267	-0.191	-0.163	------	-0.010
O(5)	1	1	-	1	-0.267	-0.083	-0.098	------	-0.049

*Δp_O is the deviation of the bond strength sum from neutrality (p_O = 2.00). A bond length deviation is the polyhedral average subtracted from the individual bond distance. Results for both $^{[4]}$Pb(1) and $^{[4]}$Pb(2), and $^{[5]}$Pb(1) and $^{[6]}$Pb(2) are presented.

Table 7. Paulmooreite. Observed and calculated powder patterns*

Observed		Calculated		
I/Io	d(obs)	I/Io	d(calc)	hkℓ
30	6.45	21	6.430	200
30	6.12	16	6.078	$\bar{2}01$
50	4.26	27	4.244	210
40	4.06	17	4.066	$\bar{2}02$
		6	4.048	002
40	3.50	19	3.483	$\bar{3}11$
		8	3.468	211
50	3.42	25	3.409	$\bar{1}12$
100	3.30	100	3.291	012
20	3.22	14	3.215	400
		12	3.039	$\bar{4}02$
70	3.02	14	3.020	$\bar{3}12$
		31	3.005	112
80	2.905	50	2.904	$\bar{4}11$
		10	2.794	410
80	2.761	48	2.759	120
20	2.708	25	2.704	401
15	2.676	13	2.676	$\bar{4}12$
		8	2.661	212
1	2.565	2	2.562	$\bar{2}21$
		2	2.558	121
		1	2.534	$\bar{2}13$
15	2.506	15	2.501	$\bar{4}03$
20	2.453	14	2.448	$\bar{5}11$
15	2.360	4	2.359	320
		6	2.357	$\bar{1}22$
5	2.258	7	2.260	$\bar{6}01$
15	2.218	14	2.216	$\bar{3}22$
15	2.167	12	2.164	321
1	2.128	1	2.122	420
		3	2.047	412
		6	2.033	$\bar{4}04$
60	2.024	17	2.024	004
2	1.998	7	1.999	$\bar{2}14$
		3	1.978	$\bar{3}14$
10	1.954	9	1.956	$\bar{3}23$
		5	1.907	$\bar{6}13$
		5	1.897	322
2	1.867	1	1.863	130
		1	1.827	$\bar{7}11$
5b	1.818	2	1.822	611
70	1.766	7	1.765	$\bar{5}23$
		15	1.761	521
		5	1.733	$\bar{3}31$
60b	1.725	3	1.728	$\bar{7}13$
		6	1.724	330
		7	1.724	$\bar{1}32$
		8	1.716	413
15	1.691	6	1.691	$\bar{3}24$
		2	1.689	$\bar{1}24$
		4	1.684	$\bar{8}01$
20	1.666	3	1.666	$\bar{3}32$
		12	1.663	132
		5	1.631	$\bar{8}03$
10	1.612	4	1.614	$\bar{8}11$
		5	1.610	$\bar{4}15$
5	1.596	6	1.594	$\bar{7}21$
5	1.579	11	1.581	124
		4	1.567	$\bar{8}13$
		4	1.557	513
10	1.553	2	1.555	$\bar{6}05$
		6	1.548	$\bar{5}31$
5	1.526	5	1.527	$\bar{7}23$
2	1.502	1	1.502	224
2	1.488	1	1.488	801
2	1.439	4	1.439	811
		2	1.418	613
		1	1.416	215
5	1.415	1	1.415	$\bar{2}06$
		4	1.413	040
2	1.405	2	1.405	$\bar{3}34$
5	1.380	2	1.382	$\bar{3}16$
5	1.347	4	1.346	$\bar{8}15$
5	1.310	3	1.312	016
		2	1.307	$\bar{7}33$
1	1.290	1	1.289	405
2	1.267	2	1.266	116
		1	1.257	415
5	1.255	2	1.253	731
		2	1.252	441
5	1.229	2	1.230	$\bar{4}43$
		4	1.228	533
1	1.207	1	1.207	921
		1	1.205	723
1	1.198	1	1.196	541
5	1.160	2	1.160	$\bar{7}35$
2	1.139	2	1.136	$\bar{3}36$
2	1.130	1	1.130	$\overline{12}.02$
		1	1.129	605
		2	1.109	525
2	1.090	1	1.089	931
		2	1.074	$\bar{7}27$
5	1.072	2	1.072	$\bar{4}51$
		2	1.069	136

*The observed data were reported by Dunn *et al.* (1979). The pattern was calculated from the structure analysis for CuK$_\alpha$ radiation.

and 1.78, 1.78, and 1.79A in armangite (Moore and Araki, 1979b). The O–As–O′ average angles are 98.0° and 98.3° in paulmooreite, compared with 98.3° in magnussonite and 95.8°, 99.4°, and 96.3° in armangite.

Since $[As^{3+}O_3]^{3-}$ can be considered a mesodesmic anionic group, it is expected to form polymeric clusters as in the silicates and borates. In Figure 1 the dimeric $[As_2^{3+}O_5]^{4-}$ group is seen sharing the common O(3) corner. The cluster is not a flat dimer, but the triangular bases are oriented nearly normal to each other. The $[As_4^{3+}O_8]^{4-}$ tetrameric tetragonal ring arrangement occurs in stenhuggarite (Coda *et al.*, 1977). In claudetite, $[As_2^{3+}O_3]$, chains parallel to [001] further corner-link to form ${}^{2}_{\infty}[As_2^{3+}O_3]$ sheets parallel to {010}, explaining the perfect {010} cleavage in that mineral (Frueh, 1951).

Explanation of the cleavage in paulmooreite presented a problem initially, since Dunn *et al.* (1979) reported one perfect {100} cleavage (our orientation) yet, as seen in Figure 1, a continuous network of bonds extends along the [100] direction. The least number of broken bonds appeared to be along the [001] direction where the only strong bonds broken are –O(2)–Pb(1)–O(2)′–Pb(2) bonds, only four such bonds penetrating the {001} plane within the c-axial repeat, that is, an average of one bond per $c/4$ = 2.14A displacement. We were informed by Mr. Dunn that, due to an oversight in reorientation of their crystal cell, the plane of perfect cleavage is {001} in

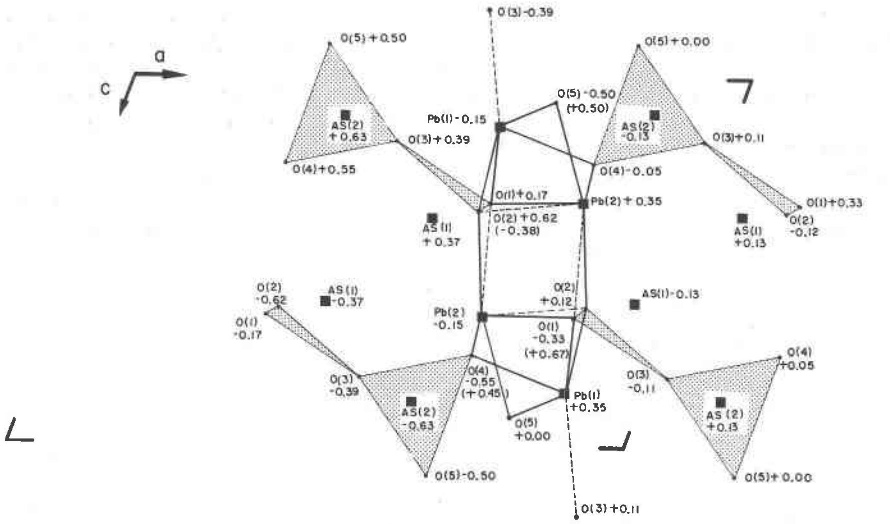

Fig. 1. Projection of the paulmooreite structure down [010]. The $[As_2O_5]^{4-}$ dimers are stippled. Pb–O bonds are drawn as spokes, the 4-coordinate Pb–O bonds drawn as solid lines. Longer Pb–O bonds (<3.8A) are drawn as dashed lines, for $^{[5]}$Pb(1) and $^{[6]}$Pb(2). Heights are given as fractional coordinates in *y*.

our orientation, and we appreciate his bringing this to our attention.

Bond strength–bond length relationships in Table 5 follow the procedure of Baur (1970). Two sets of results are presented, the first assuming $^{[4]}$Pb(1) and $^{[4]}$Pb(2), and the second with $^{[5]}$Pb(1) and $^{[6]}$Pb(2). Since Pb^{2+} does not occur in easily-defined coordination with respect to oxygen, ambiguity arises in the choice of coordination number. The first set (where all oxygens are electrostatically balanced) suggests that O(3), which links to As(1) and As(2), probably receives an extra bond from Pb(1). Although the second set offers better agreement between bond length–bond strength deviations, the results are not as convincing, as found in structures with regular coordination and a smaller range in individual bond distances. This certainly reflects the occurrence of lone-pair electrons for all the cations in paulmooreite's structure.

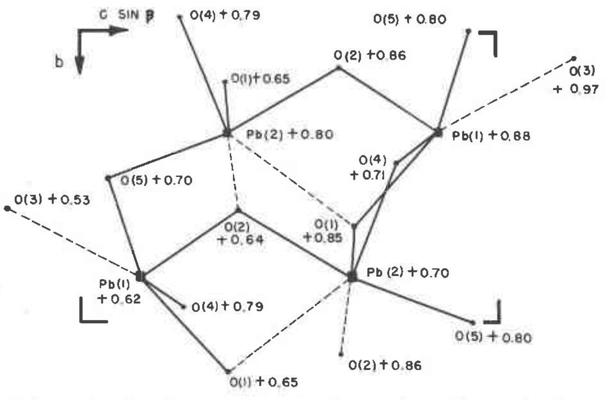

Fig. 2. Spoke diagram of Pb–O linkages in paulmooreite down [100] between $0.5 < x < 1.0$ See Fig. 1 caption for further information.

Finally, a calculated powder pattern based on the structure analysis is presented in Table 7. The agreement with the study of Dunn *et al.* (1979) is excellent, but more confidence can be placed in the choice of Miller indices. For complex patterns, a decided advantage exists in calculating the powder pattern directly from the structure results.

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