

The crystal structure of paulmooreite, $\text{Pb}_2[\text{As}_2\text{O}_5]$: dimeric arsenite groups

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Abstract

Paulmooreite, $\text{Pb}_2[\text{As}_2\text{O}_5]$, was studied in detail by three-dimensional X-ray diffractometry on a Picker four-circle goniostat using $\text{MoK}\alpha$ radiation. The new mineral is monoclinic, space group $P2_1$ or $P2_1/m$ including exceedingly weak reflections but refined in $P2_1/a$, $Z = 4$, $a = 13.584(4)$, $b = 5.650(2)$, $c = 8.551(3)\text{A}$, $\beta = 108.78(2)^\circ$. $R = 0.064$ ($R_w = 0.057$) for 2709 independent reflections. The structure was solved by Patterson, Fourier and least-squares refinement techniques.

The structure is based on $[\text{As}_2\text{O}_5]^{4-}$ corner-linked dimers which link to distorted Pb-O polyhedra, leading to the weakest links across $\{001\}$, the plane of perfect cleavage. For $^{[4]}\text{Pb}^{[3]}\text{As}_2\text{O}_5$, 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 $[\text{AsO}_3]^{3-}$ 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, $\text{Pb}_2\text{As}_2\text{O}_5$, 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 $0.059 \times 0.13 \times 0.10$ mm along its principal axes. Least-squares refinement employing 20 high-angle $\text{MoK}\alpha_1$ 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 $c = 8.551(3)\text{A}$, $\beta = 108.78(2)^\circ$.

Three-dimensional data were collected with unfiltered $\text{MoK}\alpha$ radiation, $\text{MoK}\beta$ 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 $2\theta = (3.3 \times 114.6 \Delta\lambda/\lambda)^\circ$. 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 $\mu_a = 755 \text{ cm}^{-1}$ assuming an arsenate-carbonate composition. The correct $\mu_a = 643 \text{ cm}^{-1}$ for $\text{Pb}_2[\text{As}_2\text{O}_5]$ 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 $(\sim 0, \sim 0, \sim \frac{1}{2})$, 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

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 ($\times 10^5$)†

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

and 5O in the asymmetric unit. Bond distance calculations led to the unambiguous assignment of atomic species and scattering curves.

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 $R_w = 0.057$ 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

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	\bar{z}	$\mu_{\bar{z}}$	$\theta_{\bar{z}a}$	$\theta_{\bar{z}b}$	$\theta_{\bar{z}c}$	Bequiv. $\bar{\lambda}^2$
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)	

† \bar{z} = i th principal axis; $\mu_{\bar{z}}$ = rms amplitude, $\theta_{\bar{z}a}$, $\theta_{\bar{z}b}$, $\theta_{\bar{z}c}$ = angles (deg.) between the i th 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 $[\text{As}_2^{3+}\text{O}_5]^{4-}$ 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 3.06 Å for values accepted within 3.8 Å. We have chosen 4-coordination by oxygen for Pb(1) and Pb(2), with distances between 2.26 and 2.55 Å, defining distorted tetragonal pyramids. The distances Pb(1)-O(3) 2.94, and Pb(2)-O(2) 2.80 and Pb(2)-O(1) 3.06 Å are also included in Table 4, and appear as dashed bonds in Figures 1 and 2. Accepting 4-coordination, the averages are $^{141}\text{Pb}(1)$ -O 2.38 and $^{141}\text{Pb}(2)$ -O 2.44 Å respectively, to be compared with $^{141}\text{Pb}(2)$ -O 2.36 and $^{141}\text{Pb}(3)$ -O 2.42 Å in alamosite, $\text{Pb}^{2+}\text{SiO}_3$ (Boucher and Peacor,

1968). In larsenite, $\text{Pb}^{2+}[\text{ZnSiO}_4]$, the $^{141}\text{Pb}(2)$ -O 2.47 Å 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 $^{141}\text{Pb}(1)$ -O distances range from 2.26 to 2.43 Å but three additional distances occur between 2.88 and 3.18 Å, and two additional Pb(2)-O 2.85 and 3.15 Å distances also occur.

The $^{141}\text{As}^{3+}$ -O 1.77 and 1.78 Å averages are close to 1.76 Å in magnussonite (Moore and Araki, 1979a), 1.78 and 1.79 Å in stenhuggerite (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	2.380	-O(1) ⁽¹⁾	3.055(9)
(inner 4)		average	2.436
grand average	2.492	(inner 4)	
		grand average	2.600

† Estimated standard errors refer to the last digit. Bond distances listed are those below 3.80 Å. The equivalent positions (referred to Table 1) in superscripts are (1) = $-x, -y, -z$; (2) = $\frac{1}{2}+x, \frac{1}{2}-y, z$; (5) = $\frac{1}{2}-x, \frac{1}{2}+y, -z$.

*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*

Anions	Coordinating Cations				Δp_o	Bond Length Deviations			
	Pb(1)	Pb(2)	As(1)	As(2)		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			Observed			Calculated		
I/Io	d(obs)	hkl	I/Io	d(calc)	hkl	I/Io	d(obs)	hkl	I/Io	d(calc)	hkl
30	6.45		21	6.430	200				8	1.716	413
30	6.12		16	6.078	201	15	1.691		6	1.691	324
50	4.26		27	4.244	210				2	1.689	124
40	4.06		17	4.066	202				4	1.684	801
			6	4.048	002	20	1.666		3	1.666	332
40	3.50		19	3.483	311				12	1.663	132
			8	3.468	211				5	1.631	803
50	3.42		25	3.409	112	10	1.612		4	1.614	811
100	3.30		100	3.291	012				5	1.610	415
20	3.22		14	3.215	400	5	1.596		6	1.594	721
			12	3.059	402	5	1.579		11	1.581	124
70	3.02		14	3.020	312				4	1.567	813
			31	3.005	112				4	1.557	513
80	2.905		50	2.904	411	10	1.553		2	1.555	605
			10	2.794	410				6	1.548	531
80	2.761		48	2.759	120	5	1.526		5	1.527	723
20	2.708		25	2.704	401	2	1.502		1	1.502	224
15	2.676		13	2.676	412	2	1.488		1	1.488	801
			8	2.661	212	2	1.439		4	1.439	811
1	2.565		2	2.562	221				2	1.418	613
			2	2.558	121				1	1.416	215
			1	2.534	213	5	1.415		1	1.415	206
15	2.506		15	2.501	403				4	1.413	040
20	2.453		14	2.448	511	2	1.405		2	1.405	334
15	2.360		4	2.359	320	5	1.380		2	1.382	316
			6	2.357	122	5	1.347		4	1.346	815
5	2.258		7	2.260	601	5	1.310		3	1.312	016
15	2.218		14	2.216	322				2	1.307	733
15	2.167		12	2.164	321	1	1.290		1	1.289	405
1	2.128		1	2.122	420	2	1.267		2	1.266	116
			3	2.047	412				1	1.257	415
			6	2.033	404	5	1.255		2	1.253	731
60	2.024		17	2.024	004				2	1.252	441
2	1.998		7	1.999	214	5	1.229		2	1.230	443
			3	1.978	314				4	1.228	533
10	1.954		9	1.956	323	1	1.207		1	1.207	921
			5	1.907	613				1	1.205	723
			5	1.897	322	1	1.198		1	1.196	541
2	1.867		1	1.863	130	5	1.160		2	1.160	735
			1	1.827	711	2	1.139		2	1.136	336
5b	1.818		2	1.822	611	2	1.130		1	1.130	12, 02
70	1.766		7	1.765	523				1	1.129	605
			15	1.761	521				2	1.109	525
			5	1.733	331	2	1.090		1	1.089	931
60b	1.725		3	1.728	713				2	1.074	727
			6	1.724	330	5	1.072		2	1.072	451
			7	1.724	132				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 armanigite (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 armanigite.

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 $\infty[As_2^{3+}O_3]$ 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

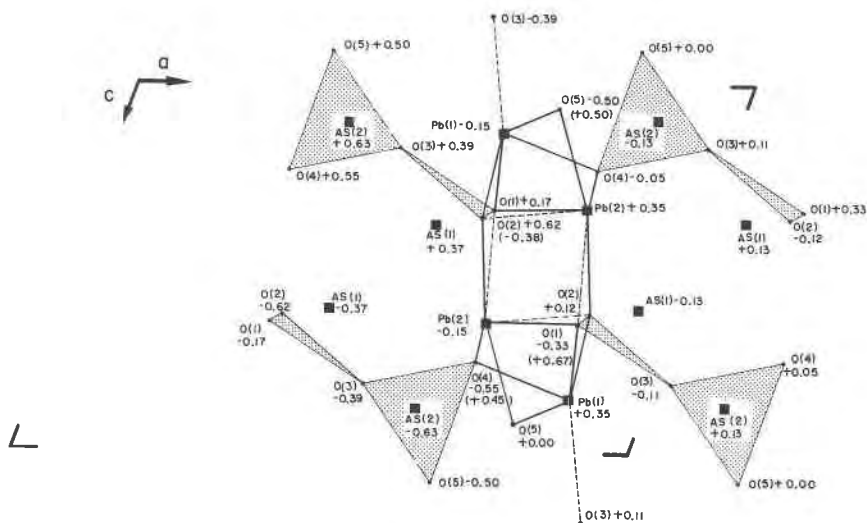


Fig. 1. Projection of the paulmooreite structure down [010]. The $[As_2O_5]^{4-}$ dimers are stippled. Pb-O bonds are drawn as spokes, the 4-coordinate Pb-O bonds drawn as solid lines. Longer Pb-O bonds ($<3.8\text{\AA}$) are drawn as dashed lines, for $^{15}Pb(1)$ and $^{16}Pb(2)$. Heights are given 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 $^{14}Pb(1)$ and $^{14}Pb(2)$, and the second with $^{15}Pb(1)$ and $^{16}Pb(2)$. 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 con-

vincing, 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.

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.

Acknowledgments

We appreciate a critical reading of the manuscript by Professor Donald R. Peacor. Portions of this study were supported by NSF grant EAR-19483 (Geochemistry).

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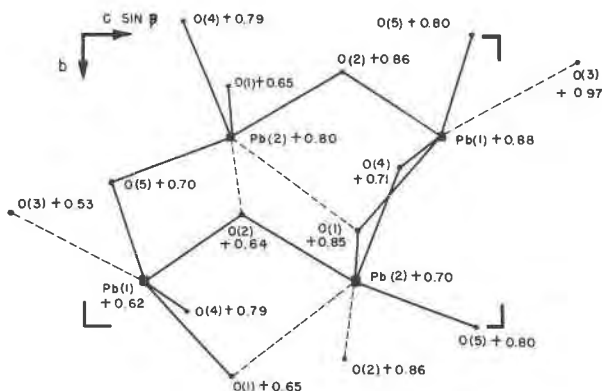


Fig. 2. Spoke diagram of Pb-O linkages in paulmooreite down [100] between $0.5 < x < 1.0$. See Fig. 1 caption for further information.

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Manuscript received, July 30, 1979;
accepted for publication, October 19, 1979.