

The Crystal Structure of Jagowerite: $\text{BaAl}_2\text{P}_2\text{O}_8(\text{OH})_2$ ¹

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Abstract

Jagowerite, $\text{BaAl}_2\text{P}_2\text{O}_8(\text{OH})_2$, is triclinic, $a = 6.049(2)$, $b = 6.964(3)$, $c = 4.971(2)$ Å, $\alpha = 116.51(4)$, $\beta = 86.06(4)$, $\gamma = 112.59(3)^\circ$, $Z = 1$. The structure was solved by Patterson and Fourier syntheses, and refinement in space group $P\bar{1}$ resulted in a final R -factor of 0.026. Space group symmetry $P1$ is a possibility, however, since the position of the hydrogen within the hydroxyl group was not determined.

The structure consists of a network of PO_4 tetrahedra sharing corners with $\text{Al}(\text{O},\text{OH})$ octahedra which in turn share edges in pairs. The barium is twelve-coordinated in a cavity formed by four pairs of edge-shared octahedra. The mean cation-oxygen distances are: P-O 1.535 Å, Al-(O,OH) 1.901 Å, Ba-(O,OH) 2.965 Å.

Introduction

Jagowerite is a new mineral, discovered in a quartz vein in the western central part of the Yukon Territory in 1968 and recently described by Meagher, Coates, and Aho (1973). These authors found the mineral to be triclinic with the following cell parameters: $a = 6.049(2)$ ³ Å, $b = 6.964(3)$ Å, $c = 4.971(2)$ Å, $\alpha = 116.51(4)^\circ$, $\beta = 86.06(4)^\circ$, $\gamma = 112.59(3)^\circ$. The reported specific gravity is 4.01 gm/cc, and the optical properties are: $\alpha = 1.672(3)$, $\beta = 1.693(3)$, and $\gamma = 1.710(3)$. The determined chemical formula for jagowerite based on ten oxygens is reported as $\text{Ba}_{1.07}\text{Al}_{2.15}\text{Fe}_{0.01}\text{P}_{1.89}\text{S}_{0.02}\text{O}_8(\text{OH})_2$ with $Z = 1$.

Experimental

A single crystal approximately cubic in shape and 0.07 mm on a side was aligned by standard precession photographic techniques. The cell parameters were refined by a least-squares procedure applied to the $\sin 2\theta$ values of 30 reflections measured on a

Datex-automated General Electric XRD 6 diffractometer using $\text{CuK}\alpha$ radiation and were found to be statistically identical to the values listed above.

The intensities of all reflections with $\sin \theta \leq 0.5$ were recorded on a Datex-automated scintillation-counter diffractometer using Zr-filtered Mo-radiation and a pulse height discriminator. For each reflection, a θ - 2θ scan was used with a scan speed of $1^\circ 2\theta$ per minute. Background counts of 40 seconds were recorded at the beginning and end of each scan. The data were monitored by recording a reference peak every two hours, and intensities were scaled as required. Of the 967 reflections scanned, the intensities of 910 were greater than $3\sigma(I)$ above background with $\sigma^2(I) = S + B + (0.05S)^2$, where S is the scan count and B is the background count. The remaining 57 reflections were classified as unobserved. The data were corrected for Lorentz and polarization effects, but no absorption corrections were applied.

Structure Determination

Because there is one formula unit of $\text{BaAl}_2\text{P}_2\text{O}_8(\text{OH})_2$ per unit cell, the barium ion must lie on a center of symmetry in space group $P\bar{1}$ or it can be arbitrarily placed at the origin for space group $P1$. A three-dimensional Patterson map clearly showed the Ba-

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³ Numbers in parentheses refer to one estimated standard deviation in terms of last significant digit.

TABLE 1. Calculated and Observed Structure Factors for Jagowite

H K L				F _o				F _c				H K L				F _o				F _c						
H	K	L	PO	F _o	F _c	RE	FL	F _o	F _c	RE	FL	H	K	L	PO	F _o	F _c	RE	FL	F _o	F _c	RE	FL			
0	0	0	1	14.20	13.84	2	1	499.93	499.59	0	-1	0	-1	15.69	15.22	1	0	2	17.89	18.87	1	3	23.30	25.07		
0	0	0	2	35.14	35	2	2	121.54	117.77	0	-2	0	-2	27.54	26.46	1	-2	2	21.16	20.40	0	1	33.67	33.04		
0	0	0	3	44.27	43.62	2	-1	5	19.57	19.70	0	-1	0	-1	26.59	25.84	1	-8	2	36.69	36.11	0	1	6.16	6.16	
0	0	0	4	42.80	43.87	2	2	0.00	0.00	0	0	0	0	0.00	0.00	1	-8	3	25.86	25.86	1	3	8.23	8.23		
0	0	0	5	15.61	15.14	2	-1	29.69	29.28	0	-1	0	-1	16.55	16.00	1	-8	4	17.13	17.47	1	1	11.97	13.30		
0	0	0	6	2.81*	3.88	3	-1	1.62	28.73	0	-1	0	-1	20.01	20.63	2	-8	0	34.26	34.72	1	1	66.24	65.78		
0	0	0	7	37.63	37.01	3	2	29.26	21.63	2	-8	0	0	0	0	0	0	0	0	34.26	34.72	1	1	61.17	61.28	
0	0	0	8	79.29	77.77	3	-1	3.73	-1.77	2	-8	0	0	0	0	0	0	0	0	34.26	34.72	1	1	11.97	12.86	
0	0	0	9	26.58	27.74	3	1	45.91	46.82	2	-8	0	0	0	0	0	0	0	0	34.26	34.72	1	1	20.66	21.83	
0	0	0	10	11.09	10.79	3	1	9.79	9.75	1	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	38.92	35.22	
0	0	0	11	35.15	35.50	4	-1	0	12.21	12.28	2	-8	0	0	0	0	0	0	0	34.26	34.72	1	1	32.00	31.57	
0	0	0	12	21.31	21.08	4	0	0	0	0	2	-8	0	0	0	0	0	0	0	34.26	34.72	1	1	43.59	45.20	
0	0	0	13	10.33	10.19	4	1	21.94	20.83	2	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	31.87	32.88	
0	0	0	14	19.43	19.85	4	1	3	20.11	19.43	2	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	16.24*	16.61
0	0	0	15	51.82	49.94	4	1	22.55	21.75	2	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	33.60	33.81	
0	0	0	16	31.40	31.15	4	-1	5	30.43	30.18	2	-7	0	0	0	0	0	0	0	34.26	34.72	1	2	10.31	10.17	
0	0	0	17	14.95	14.20	4	1	1	28.72	28.50	2	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	35.76	36.56	
0	0	0	18	62.88	62.81	5	-1	52.18	50.90	2	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	12.32	12.10	
0	0	0	19	39.66	38.38	5	1	11.83	11.88	2	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	26.08	23.85	
0	0	0	20	2.78*	0.88	5	-1	8	10.03	10.19	3	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	24.79	25.07	
0	0	0	21	86.07	85.48	5	1	17.32	17.81	3	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	2.61*	3.50	
0	0	0	22	18.29	18.55	5	1	16.24	15.58	3	-7	0	0	0	0	0	0	0	0	34.26	34.72	2	1	10.53	10.73	
0	0	0	23	13.22	13.44	6	-1	2	20.95	20.50	3	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	34.15	33.69	
0	0	0	24	43.63	43.45	6	1	18.03	18.87	3	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	15.88	15.88	
0	0	0	25	22.04	22.21	6	-1	2	20.95	20.50	3	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	16.63	16.58	
0	0	0	26	26.52	26.13	6	1	11.87	11.47	3	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	1	9.90	9.68	
0	0	0	27	15.00	14.62	6	-1	2	20.95	20.50	3	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	28.81	28.47	
0	0	0	28	22.44	22.21	6	1	8	19.08	18.55	3	-7	0	0	0	0	0	0	0	34.26	34.72	2	1	21.10	24.47	
0	0	0	29	43.63	42.44	7	-1	1	17.61	17.26	3	-7	0	0	0	0	0	0	0	34.26	34.72	2	1	2.48*	3.48	
0	0	0	30	25.00	24.62	7	1	3	32.53	33.63	3	-7	0	0	0	0	0	0	0	34.26	34.72	2	1	20.63	21.05	
0	0	0	31	8.95	8.95	7	-1	2	18.03	18.55	3	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	20.33	20.42	
0	0	0	32	23.07	22.97	7	1	1	30.89	31.37	3	-7	0	0	0	0	0	0	0	34.26	34.72	1	1	24.81	25.62	
0	0	0	33	19.79	19.19	7	0	11.88	13.11	4	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	5	28.09	28.59	
0	0	0	34	26.93	26.93	7	-1	3	38.78	38.86	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	6.66	6.66	
0	0	0	35	19.79	19.19	7	0	3	38.78	38.86	4	-7	0	0	0	0	0	0	0	0	34.26	34.72	1	5	33.11	33.98
0	0	0	36	26.93	26.93	7	-1	4	44.18	43.00	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	30.06	30.52	
0	0	0	37	19.70	19.57	7	0	5	21.51	21.48	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	29.71	24.85	
0	0	0	38	22.06	22.00	7	-2	6	39.07	32.81	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	21.76	23.77	
0	0	0	39	5.73*	4.57	7	-2	6	62.86	60.12	5	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	29.72	31.32	
0	0	0	40	10.69	10.69	7	1	1	18.59	18.59	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	22.73	23.82	
0	0	0	41	17.65	18.17	7	-1	2	16.05	15.75	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	12.96	13.07	
0	0	0	42	18.71	17.07	7	-1	2	15.21	15.99	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	37.26	38.35	
0	0	0	43	43.63	43.45	7	1	3	36.88	35.96	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	19.77	20.85	
0	0	0	44	22.44	22.21	7	1	4	45.91	46.82	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	9.07	9.68	
0	0	0	45	18.71	17.35	7	0	3	46.17	45.76	4	-7	0	0	0	0	0	0	0	34.26	34.72	2	3	16.26	16.59	
0	0	0	46	73.44	73.07	7	-2	6	20.15	19.99	4	-7	0	0	0	0	0	0	0	34.26	34.72	2	3	11.99	13.96	
0	0	0	47	8.19	8.19	7	1	3	46.88	45.96	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	30.99	30.99	
0	0	0	48	38.33	36.37	7	-2	2	24.88	23.86	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	10.00	10.79	
0	0	0	49	24.93	24.11	7	2	2	58.21	56.90	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	12.56	11.62	
0	0	0	50	38.29	38.29	7	-1	2	28.60	20.54	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	33.52	33.52	
0	0	0	51	30.91	30.19	7	2	3	11.14	11.24	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	12.42	11.78	
0	0	0	52	10.13	9.36	7	2	4	15.14	14.24	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	39.84	38.49	
0	0	0	53	10.63	9.36	7	-2	3	20.03	20.23	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	14.78	14.73	
0	0	0	54	10.63	9.36	7	-2	3	20.03	20.23	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	22.09	21.53	
0	0	0	55	26.88	25.04	7	-2	4	3.20	28.46	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	10.78	10.78	
0	0	0	56	26.88	25.04	7	-2	4	3.20	28.46	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	22.80	22.81	
0	0	0	57	26.88	25.04	7	-2	4	3.20	28.46	4	-7	0	0	0	0	0	0	0	34.26	34.72	1	5	11.99	10.78	
0	0	0	58	26.88	25.04	7	-2	4</																		

TABLE 2. Atomic Coordinates and Isotropic Temperature Factors for Jagowerite

Atom	x	y	z	B(\AA^2)*
Ba	0	0	0	0.76(1)
Al	0.3670(2)**	0.7484(2)	0.4257(2)	0.29(3)
P	0.8033(1)	0.5917(1)	0.2715(2)	0.23(2)
O(1)	0.7450(4)	0.5331(5)	-0.0573(6)	0.54(7)
O(2)	0.7665(4)	0.3707(4)	0.2985(6)	0.52(6)
O(3)	0.0666(4)	0.7729(4)	0.3842(6)	0.51(6)
O(4)	0.6514(4)	0.7156(4)	0.4795(6)	0.51(6)
OH	0.5280(4)	0.9419(4)	0.2389(5)	0.49(6)

*Isotropic equivalents of anisotropic temperature factors (Hamilton, 1959).

**Number in parentheses refers to one estimated standard deviation.

metal and Ba-oxygen vectors. A structure factor calculation for space group $P1$ based on the Patterson peak coordinates and using temperature factors derived from a Wilson plot, yielded a residual (R) factor of 0.23. A Fourier map based on $|F_{obs}|$ using the phases derived from the above structure factor calculation showed all peaks to be centrosymmetrically related, and the refinement was continued on the basis of $P\bar{1}$ symmetry.

The full-matrix least-squares refinement was carried out on an IBM 360/67 computer using the program BUCILS, a modified version of ORFLS (Busing, Martin, and Levy, 1962). The scattering curves for neutral atoms were taken from the *International Tables for X-ray Crystallography* (1962) and were corrected for the real part of the anomalous dispersion. Two cycles of refinement on the scale factor, atomic coordinates, and isotropic temperature factors with unit weights yielded an R -factor of 0.045. Two further cycles of refinement with anisotropic thermal parameters and weights derived from the counting statistics gave a final R -factor of 0.026. Observed and calculated structure factors are listed in Table 1. A difference Fourier map revealed no significant anomalies and no information regarding the position of the hydrogen atoms.

An attempt was made at this point to refine the structure in space group symmetry $P1$. In the initial model all atoms, with the exception of barium, were arbitrarily moved from their refined centric positions. The isotropic refinement was encumbered by high correlation between the positional parameters of those atoms which would be related by symmetry in space group $P\bar{1}$; however, the parameters did refine to values not significantly different from those determined in the centric refinement. The final atomic coordinates

TABLE 3. Anisotropic Temperature Factor Tensor Values for Jagowerite*

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ba	65(1)	57(1)	60(2)	14.4(7)	10.2(8)	15.9(9)
Al	18(3)	26(3)	38(4)	14(2)	4(5)	11(3)
P	16(2)	22(2)	26(4)	12(2)	5(2)	6(2)
O(1)	57(7)	49(7)	39(10)	25(6)	4(6)	18(7)
O(2)	45(7)	41(6)	66(11)	20(6)	7(7)	26(7)
O(3)	24(6)	39(6)	86(11)	15(5)	5(6)	20(7)
O(4)	35(6)	39(6)	66(11)	24(5)	3(6)	10(7)
OH	50(6)	35(6)	41(10)	15(5)	4(6)	10(6)

* Values are reported $\times 10^4$. The coefficients are of the form $(B_{11}h^2 + \dots + 2B_{12}hk + \dots)$.

and anisotropic thermal ellipsoid data for the $P1$ refinement are listed in Tables 2–4. Nevertheless, because the position of the hydrogen in the OH-group has not been determined, space group symmetry $P1$ for jagowerite remains a possibility.

Discussion of the Structure

A perspective drawing of the structure of jagowerite is shown in Figure 1. The phosphorus is tetrahedrally coordinated by the four non-equivalent oxygens, while the Al is octahedrally coordinated by four oxygens and two hydroxyls. The tetrahedra share each corner with an Al(O,OH) octahedron which in turn shares an OH-OH edge with an adjacent octahedron. This linkage results in an alternating network of PO_4 tetrahedra and of pairs of edge-

TABLE 4. Magnitudes and Orientation of Principal Axes of Thermal Ellipsoids in Jagowerite

Atom	Axis	rms displacement	Angle, in degrees, with respect to		
		$R(\sigma)$	$+a(\sigma)$	$+b(\sigma)$	$+c(\sigma)$
Ba	1	0.076(1)	96(1)	83(1)	34(1)
	2	0.095(1)	131(1)	117(1)	73(2)
	3	0.119(1)	139(1)	28(1)	118(1)
Al	1	0.045(5)	11(10)	120(6)	89(9)
	2	0.061(4)	99(11)	97(12)	141(13)
	3	0.073(3)	84(6)	31(6)	129(13)
P	1	0.038(5)	30(12)	120(6)	106(10)
	2	0.053(4)	119(12)	85(11)	139(11)
	3	0.066(3)	84(7)	30(6)	127(10)
O(1)	1	0.061(8)	85(11)	100(11)	19(10)
	2	0.087(6)	37(26)	148(25)	80(14)
	3	0.097(6)	53(26)	60(26)	105(9)
O(2)	1	0.075(7)	132(29)	22(28)	122(39)
	2	0.082(6)	72(64)	95(48)	148(39)
	3	0.086(6)	48(43)	68(28)	91(72)
O(3)	1	0.058(8)	4(11)	109(13)	89(8)
	2	0.080(7)	88(16)	140(15)	99(15)
	3	0.098(6)	67(7)	124(14)	9(15)
O(4)	1	0.058(9)	27(17)	131(9)	93(11)
	2	0.077(7)	116(18)	103(15)	124(12)
	3	0.100(5)	82(8)	43(8)	146(12)
OH	1	0.062(8)	93(11)	76(16)	42(16)
	2	0.082(7)	88(40)	155(33)	49(17)
	3	0.089(6)	4(25)	110(39)	85(27)

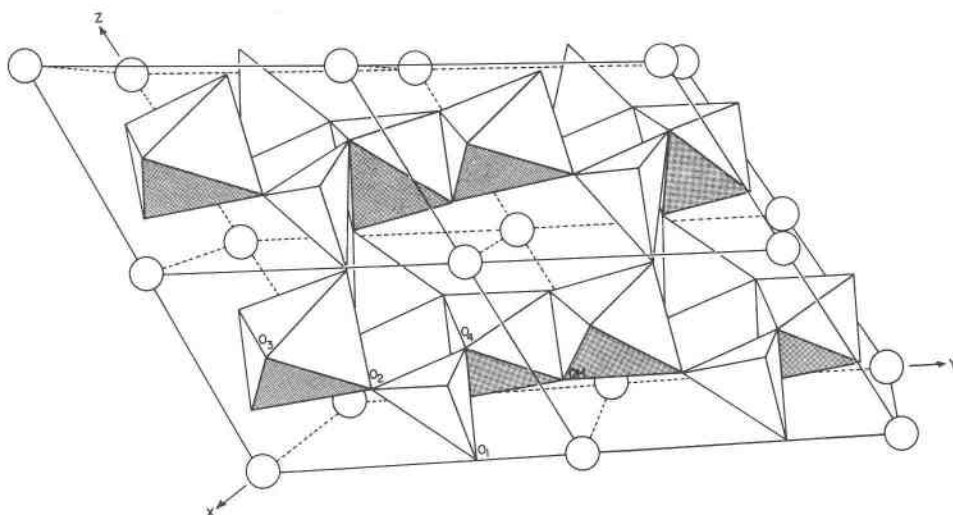


FIG. 1. A perspective drawing of the structure of jagowerite. Four unit cells are shown with the barium located at the origin. Each two Al(O,OH) octahedra share an OH-OH edge.

sharing Al(O,OH) octahedra. The barium ion occupies the void in the network between four pairs of edge-shared octahedra.

The PO_4 tetrahedron is slightly distorted with two of its edges, O(1)-O(3) and O(3)-O(4), being shared with the barium polyhedron. As predicted from electrostatic bonding principles, these edges are shorter and account for the smaller O-P-O tetrahedral angles (Table 6). The P-O distances range from 1.529 to 1.546 Å with a mean interatomic distance of 1.535 Å.

The mean Al-(O,OH) octahedral bond length is 1.901 Å with the mean Al-OH distance (1.914 Å) being significantly longer than the mean Al-O distance (1.895 Å), as would be expected. The octahedron is distorted as a result of the shortened, shared OH-OH edge which has a length of 2.392 Å.

TABLE 5. Interatomic Distances in Jagowerite

About P		About Ba*	
P-0(1) 1.529(3) Å	0(1)-0(2) 2.521(4) Å	Ba-0(1) 2.900(3) Å	
P-0(2) 1.534(3)	0(1)-0(3) 2.491(4)	Ba-0(2) 3.155(3)	
P-0(3) 1.546(3)	0(1)-0(4) 2.525(4)	Ba-0(3,1) 2.834(3)	
P-0(4) 1.531(3)	0(2)-0(3) 2.541(4)	Ba-0(3,2) 3.099(3)	
	0(2)-0(4) 2.516(4)	Ba-0(4) 2.833(2)	
	0(3)-0(4) 2.434(4)	Ba-(OH) 2.967(2)	
mean 1.535 Å		mean 2.965 Å	
About Al		About Ba*	
Al-0(1) 1.896(3) Å	0(1)-0(2) 2.894(4) Å	0(2)-(OH,2) 2.654(4) Å	
Al-0(2) 1.889(3)	0(1)-0(3) 2.645(4)	0(3)-(OH,1) 2.757(3)	
Al-0(3) 1.922(3)	0(1)-0(4) 2.722(4)	0(3)-(OH,2) 2.653(4)	
Al-0(4) 1.872(3)	0(1)-(OH,1) 2.798(4)	0(4)-(OH,1) 2.680(4)	
Al-(OH,1) 1.970(3)	0(2)-0(3) 2.629(4)	0(4)-(OH,2) 2.761(4)	
Al-(OH,2) 1.927(3)	0(2)-0(4) 2.648(4)	(OH,1)-(OH,2) 2.392(4)	
mean 1.901 Å			

*All have multiplicity of two.

The barium can be considered twelve-coordinated with a range of Ba-(O,OH) interatomic distances between 2.833 and 3.155 Å and a mean distance of 2.965 Å. The interatomic distances and angles are listed in Tables 5 and 6, respectively.

The O(1), O(2), O(4), and OH ions are three-coordinated while O(3) is four-coordinated by neighboring cations. The longest P-O distance in the tetrahedron (1.546 Å) and the longest Al-O distance in the octahedron (1.922 Å) are to the four-coordinated oxygen, O(3). The thermal vibrations of oxygens O(1), O(3), and O(4) are slightly anisotropic as indicated in Table 4 with the principal axis of the thermal ellipsoid being perpendicular to the Al-O-P bonds.

With the exception of the divalent cation, jagowerite is chemically similar to the lazulite group of minerals $(Mg,Fe)Al_2P_2O_8(OH)_2$ and to the mineral palermoite $SrAl_2P_2O_8(OH)_2$. They differ in the link-

TABLE 6. Interatomic Angles in Jagowerite

About P		About Al	
0(1)-P-0(2)	110.80(14)°	0(2)-Al-(OH,2)	88.13(11)°
0(1)-P-0(3)	108.27(14)	0(3)-Al-(OH,1)	92.76(11)
0(1)-P-0(4)	111.33(14)	0(3)-Al-(OH,2)	87.06(11)
		0(4)-Al-(OH,1)	90.52(11)
		0(4)-Al-(OH,2)	93.22(11)
		(OH,1)-Al-(OH,2)	77.30(12)
About P		About Al	
0(1)-Al-0(2)	99.65(11)°	0(2)-Al-(OH,2)	88.13(11)°
0(1)-Al-0(3)	87.68(11)	0(3)-Al-(OH,1)	92.76(11)
0(1)-Al-0(4)	92.49(11)	0(3)-Al-(OH,2)	87.06(11)
0(1)-Al-(OH,1)	94.92(11)	0(4)-Al-(OH,1)	90.52(11)
0(2)-Al-0(3)	87.21(11)	0(4)-Al-(OH,2)	93.22(11)
0(2)-Al-0(4)	89.50(11)	(OH,1)-Al-(OH,2)	77.30(12)

age of the Al(O,OH) octahedra and PO₄ tetrahedra, in apparent response to the variation of the size and coordination of the divalent cation. The coordination of Mg,Fe in lazulite is six (Lindberg and Christ, 1959), that of Sr in palermoite is eight (Strunz, 1960), while that of Ba in jagowerite is twelve.

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