

The crystal structure of tarbuttite, $\text{Zn}_2(\text{OH})\text{PO}_4$

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(Received October 15, 1965)

Auszug

Tarbuttite hat die Gitterkonstanten $a = 5,499 \text{ \AA}$, $b = 5,654 \text{ \AA}$, $c = 6,465 \text{ \AA}$, $\alpha = 102^\circ 51'$, $\beta = 102^\circ 46'$, $\gamma = 86^\circ 50'$. Die Elementarzelle enthält zwei Formeleinheiten $\text{Zn}_2(\text{OH})\text{PO}_4$. Raumgruppe ist $P\bar{1}$. Die Struktur wurde aus Patterson-Projektionen und mittels statistischer Methoden bestimmt. Dreibimensionale Verfeinerung führt zu $R = 0,12$.

Die Sauerstoff-Umgebung der Zn-Ionen ist eine nahezu regelmäßige trigonale Bipyramide mit dem durchschnittlichen Abstand von $2,04 \text{ \AA}$ zwischen Zn und O. Die PO_4 -Gruppe ist tetraedrisch, mit $1,54 \text{ \AA}$ als mittlerem Abstand P–O. Das Gerüst besteht aus zickzackförmigen Ketten von Zn_1 -Koordinationspolyedern längs der b -Achse; diese Ketten werden von einzelnen PO_4 -Tetraedern und von Paaren von Zn_2 -Polyedern zusammengehalten.

Abstract

Tarbuttite is triclinic, space group $P\bar{1}$. The cell parameters are: $a = 5.499 \text{ \AA}$, $b = 5.654 \text{ \AA}$, $c = 6.465 \text{ \AA}$, $\alpha = 102^\circ 51'$, $\beta = 102^\circ 46'$, $\gamma = 86^\circ 50'$. There are two formula units of $\text{Zn}_2(\text{OH})\text{PO}_4$ per unit cell.

The crystal structure has been solved from Patterson projections and statistical methods. Three-dimensional isotropic least-squares refinement yielded a final discrepancy index $R = 0.12$. The arrangement of oxygens about the Zn ions is a nearly regular trigonal bipyramid with average Zn–O distances of 2.04 \AA . The PO_4 configuration is a regular tetrahedron with a mean P–O bond length of 1.54 \AA . The framework consists of zig-zag chains of Zn_1 coordination polyhedra along b -axis direction, connected together by discrete PO_4 tetrahedra and pairs of Zn_2 coordination polyhedra.

Introduction and crystal data

Tarbuttite was originally investigated by SPENCER (1908) who assigned the mineral to the triclinic system from morphological studies. Later RICHMOND (1938) gave lattice constants based on x-ray investigation. Recently, as a preliminary to a structure analysis, FANFANI and ZANAZZI (1965) reported diffractometer data and

redetermined the lattice parameters with a new orientation of the elementary cell.

The unit-cell constants determined from rotation, Weissenberg and precession photographs, and refined by application of the least-squares method to diffractometer data, are:

$$\begin{array}{ll} a = 5.499 \text{ \AA} & \alpha = 102^\circ 51' \\ b = 5.654 & \beta = 102^\circ 46' \\ c = 6.465 & \gamma = 86^\circ 50'. \end{array}$$

The calculated density for two units of $\text{Zn}_2(\text{OH})\text{PO}_4$ per cell is $4.21 \text{ g} \cdot \text{cm}^{-3}$, in good agreement with the density $4.19 \text{ g} \cdot \text{cm}^{-3}$ given in A.S.T.M. card n° 12-200.

Tarbuttite is assigned to the centrosymmetrical space group $P\bar{1}$. This assumption was confirmed by the application of a statistical test (HOWELLS *et al.*, 1950), by absence of piezoelectric effects, and finally by the results of the structure analysis.

Experimental

The crystal used for the structure determination was a colourless and transparent tabular fragment from Broken Hill, Rhodesia. Equi-inclination multiple-film Weissenberg photographs were taken with Ni-filtered $\text{CuK}\alpha$ radiation. The crystal was rotated about the c axis for recording intensity data of $hk0$, $hk1$ and $hk2$ layers. The Buerger precession camera with Zr-filtered $\text{MoK}\alpha$ radiation was used to obtain $h0l$ and $0kl$ intensity data. The total number of independent reflections collected was 496. Of these, 106 were too weak to be observed.

Integrated intensities were measured by a Nonius microdensitometer. An empirical correction was applied for α_1, α_2 -doublet resolution. The F_{hkl}^2 were obtained by applying the Lorentz-polarization corrections using two programs written for IBM 1620 computer (ALBANO *et al.*, 1963; CATANI and ZANAZZI, 1965).

Structure determination

Patterson functions $P(xz)$ and $P(yz)$ were computed from $h0l$ and $0kl$ data. While the interpretation of Patterson maps was being made, a statistical method for the determination of the structure-factor signs according to the procedure described by DE VRIES (1965), was carried out for the 23 strongest $h0l$ reflections. Both methods enabled us to

locate the Zn and the P ions approximately. The phases from a set of structure factors obtained by locating the two Zn ions and the P ion in the asymmetric part of the unit cell were then used in computing the Fourier syntheses for the $\rho(xz)$, $\rho(yz)$ and $\rho(xy)$ projections. The oxygen sites, hardly detectable from the Patterson maps, were thus recognized.

At this stage the discrepancy index $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, was 0.21. For the structure-factor calculations the scattering-factor curves given by CROMER and WABER (1965) were used for Zn^{+2} and P. The scattering-factor values for O^{-1} are those reported in International Tables for X-ray Crystallography. The general isotropic temperature factor B was assumed to be 1.0 \AA^2 .

Refinement

The refinement was carried out by the least-squares method using all 390 observed reflections; this presented some difficulties because no absorption correction had been applied to the experimental data. The calculations were performed by an IBM 1620 computer program (ALBANO, BELLON, POMPA and SCATTURIN, 1963), using the following scheme for weighing the observed structure factors:

$$w(hkl) = 1/(a + F_o + cF_o^2)$$

where a is twice the minimum observed F_o and c is twice the reciprocal of the maximum observed F_o (CRUICKSHANK *et al.*, 1961).

After some refinement cycles, when the atomic positions remained virtually unchanged, the correction for secondary extinction errors was introduced, according to the semiempirical formula (HALL and MASLEN, 1965)

$$F_{o, \text{corr}}^2 = F_{o, \text{not corr}}^2 \exp(\varepsilon I_c).$$

The correction factor ε was estimated by least-squares calculation including the strongest reflections which showed extinction. After further refinement cycles the R index reached a final value of 0.12 for all the observed reflections.

Table 1 lists the observed and calculated structure factors. The final coordinates and the isotropic thermal parameters of non-equivalent atoms are shown in Table 2 together with their standard deviations.

Table 1. Observed and calculated structure factors

h	k	l	$10 \cdot F_o $	$10 \cdot F_c$	h	k	l	$10 \cdot F_o $	$10 \cdot F_c$	h	k	l	$10 \cdot F_o $	$10 \cdot F_c$	h	k	l	$10 \cdot F_o $	$10 \cdot F_c$	
0	1	0		2	1	-3	1	775	854	5	-1	1		-78	-2	6	2	190	-174	
0	2	0	1195	-1168	1	4	1	375	422	5	2	1	531	552	-2	-6	2		80	
0	3	0	213	226	1	4	1	529	294	5	-2	1	529	554		3	0	2	-12	
0	4	0	812	830	1	5	1	543	540	5	3	1		-88	3	1	2	464	-350	
0	5	0		-12	1	-5	1	301	-296	5	-3	1		78	3	-1	2	310	328	
0	6	0	492	-674	1	6	1	362	-328	5	4	1	290	-352	3	2	2	201	-146	
0	7	0	125	120	1	-6	1	228	-202	5	-4	1	471	-506	3	-2	2		-84	
1	0	0	285	354	1	-7	1	213	266	-5	0	1		-20	3	3	2		74	
1	1	0		-20	-1	0	1	386	384	-5	1	1		52	3	-3	2	242	-302	
1	2	0	311	-374	-1	1	1	67	-64	-5	-1	1		-98	3	4	2		62	
1	3	0	299	330	-1	-1	1		-6	-5	2	1		-62	3	-4	2		28	
1	4	0	268	274	-1	2	1	405	-492	-5	-2	1	240	-182	3	5	2		98	
1	5	0	167	-182	-1	-2	1	232	-284	-5	3	1		-70		3	-5	2	229	-270
1	6	0	239	-168	-1	3	1	84	-80	-5	-3	1	170	170	3	-6	2		-54	
1	7	0		90	-1	-3	1		-38	-5	4	1	242	188	-3	0	2	302	280	
-1	1	0	199	-198	-1	4	1	258	260	-5	-4	1	170	124	-3	1	2	908	832	
-1	2	0	269	-238	-1	-4	1		48	-5	-5	1	195	-208	-3	-1	2	749	-776	
-1	3	0		-24	-1	5	1	155	-90	-6	0	1	84	-122	-3	2	2		337	-286
-1	4	0	338	244	-1	-5	1	152	-112	6	1	1	261	334	-3	-2	2	185	-146	
-1	5	0		8	-1	6	1	313	-296	6	-1	1	399	-406	-3	3	2	526	-546	
-1	6	0	155	-102	-1	-6	1	152	-156	6	2	1		52	-3	-3	2	746	722	
-1	7	0	205	172	2	0	1	120	126	6	-2	1	195	194	-3	4	2	432	380	
2	0	0	555	940	2	2	1	150	182	-6	0	1	312	320		3	2		373	322
2	1	0	430	460	2	-1	1		-86	-6	1	1	339	-292	-3	5	2	582	528	
2	2	0	711	-648	2	2	1	170	-156	-6	-1	1	361	302	-3	-5	2	434	-398	
2	3	0	539	-664	2	-2	1		14	-6	2	1	410	-414	-3	-6	2		-52	
2	4	0	193	248	2	3	1	139	-114	-6	-2	1	384	-372	4	0	2	405	-386	
2	5	0		414	2	4	1		-18	0	1	1	344	-322	4	1	2		78	
2	6	0	306	-282	2	4	1		100	-6	-3	1	459	-390	4	-1	2	175	-186	
-2	1	0	731	-922	2	-4	1	110	-116	7	0	1		-104	4	2	2	405	468	
-2	2	0	651	-484	2	5	1		-26	-7	0	1	130	176	4	-2	2	333	396	
-2	3	0	774	776	2	-5	1		-74	0	0	2	166	-166	4	3	2	172	-168	
-2	4	0	287	254	2	6	1	254	-218	0	1	2	323	382	4	-3	2		248	
-2	5	0	705	-616	2	-6	1		46	0	-1	2	438	-458	4	4	2	402	-470	
-2	6	0	339	-286	-2	0	1	200	-180	0	2	2	129	-150	4	-4	2	421	-536	
3	0	0	547	604	-2	1	1	470	504	0	-2	2		-4	4	-5	2		-42	
3	1	0	96	-82	-2	-1	1	879	-996	0	3	2	396	-466	-4	0	2	309	-290	
3	2	0	580	-590	-2	2	1		22	0	-3	2	383	344	-4	1	2	248	204	
3	3	0	313	302	-2	-2	1	142	-138	0	4	2	120	140	-4	-1	2		-30	
3	4	0	216	298	-2	3	1	799	-788	0	-4	2		6	-4	2	2	374	306	
3	5	0	243	-244	-2	-3	1	961	972	0	5	2	377	356	-4	-2	2	241	234	
3	6	0	270	-276	-2	4	1		24	0	-5	2	213	-212	-4	3	2		-111	
-3	1	0		24	-3	1	1	209	-116	0	6	2		-36	-4	4	2		70	
-3	2	0	327	-344	-2	5	1	632	532	0	-6	2		48	-4	4	2		-74	
-3	3	0	284	-224	-2	-5	1	776	-650	0	7	2	228	-244	-4	-4	2	332	-316	
-3	4	0	164	192	-2	6	1	126	-112	0	-7	2		52	-4	-5	2	130	-138	
-3	5	0		58	-2	-6	1	198	116	1	0	2	568	-544	-4	-6	2	331	338	
-3	6	0	278	-260	3	0	1	362	-342	1	1	2	236	-188	-5	5	2		248	
4	0	0	145	-180	3	1	1	675	724	1	-1	2	446	564	5	1	2	268	244	
4	1	0	185	232	3	-1	1	608	-1140	1	2	2	898	880	5	-1	2	260	-246	
4	2	0	126	108	3	2	1	269	248	1	-2	2	573	718	5	2	2		14	
4	3	0		8	3	-2	1	181	214	1	3	2		38	5	-2	2		62	
4	4	0		58	3	3	1	647	-740	1	-3	2		-80	5	3	2	127	-128	
4	5	0		54	3	-3	1	631	794	1	4	2	452	-462	5	-3	2	120	110	
-4	1	0	186	-184	3	4	1	196	-210	1	-4	2	684	-704	-5	0	2	134	148	
-4	2	0	256	184	3	-4	1	382	-398	1	5	2		-10	-5	1	2	223	170	
-4	3	0	220	218	3	5	1	557	640	1	-5	2	218	182	-5	-1	2	139	-145	
-4	4	0		30	-3	-5	1	528	-556	1	6	2	275	282	-5	2	2	491	-422	
-4	5	0	143	-156	3	-6	1	227	248	1	-6	2	561	588	-5	-2	2	139	-144	
5	0	0	628	640	-3	0	1		8	1	-7	2	202	-226	-5	3	2	195	-178	
5	1	0	173	210	-3	1	1	196	154	-1	0	2	653	-702	-5	-3	2		32	
5	2	0	512	-534	-3	-1	1	93	94	-1	1	2	550	748	-5	4	2	237	264	
5	3	0		-114	-3	2	1	362	38	-1	-1	2	1325	-1060	-5	-4	2	151	158	
5	4	0	356	444	-3	-2	1	123	-112	-1	2	2	482	646	-5	-5	2	152	-166	
-5	1	0	161	-182	-3	3	1		2	-1	-2	2	314	326	6	0	2	299	-322	
-5	2	0	425	-386	-3	-3	1		60	-1	3	2	738	-794	6	1	2	192	-248	
-5	3	0	270	236	-3	4	1	267	206	-1	-3	2	787	704	6	-1	2	251	338	
-5	4	0	434	350	-3	-4	1	528	-556	-1	4	2	440	-428	6	-2	2	302	420	
6	0	0	121	88	-3	5	1	110	-106	-1	-4	2	806	-708	-6	0	2	198	-212	
6	1	0		14	-3	-5	1	209	-138	-1	5	2	574	524	-6	1	2	441	466	
6	2	0	237	-232	-3	6	1	183	-144	-1	-5	2	693	-566	-6	-1	2	645	-620	
6	3	0	85	90	-3	-6	1	160	138	-1	6	2	120	126	-6	2	2	139	108	
-6	1	0		20	4	0	1	110	124	-1	-6	2	530	492	-6	-2	2	207	180	
-6	2	0	155	-128	4	1	1	389	406	-1	-7	2	298	312	-6	3	2	380	-404	
-6	3	0	206	-144	4	-1	1	409	-424	2	0	2	142	-142	-6	-3	2	479	482	
7	0	0		12	4	2	1	212	-242	2	1	2	468	400	-6	-4	2	188	-206	
0	0	1	405	-472	4	-2	1	152	118	2	-1	2	387	-506	-7	0	2		36	
0	1	1	164	168	4	3	1	298	-314	2	2	2	353	326	0	0	3	938	-874	
0	-1	1	167	-132	4	-3	1	319	286	2	-2	2	187	256	0	1	3	179	-150	
0	2	1	629	722	4	4	1		94	2	3	2	202	-264	0	-1	3	149	160	
0	-2	1	275	290	4	-4	1		-30	2	-3	2	254	350	0	2	3	488	710	
0	3	1	95	-112	4	5	1	309	318	2	4	2	172	-182	0	-2	3	703	732	
0	-3	1	365	348	-4	-5	1	171	-190	2	-4	2	241	-234	0	3	3		-118	
0	4	1	104	-122	-4	0	1	881	876	2	5	2	335	368	0	-3	3	177	-164	
0	-4	1	456	-438	-4	1	1	433	342	2	-5	2		-38	0	4	3	422	-674	
0	5	1	111	142	-4	-1	1	241	-228	2	-6	2	203	220	0	-4	3	688	-734	
0	-5	1	177	-158	-4	2	1	762	-704	-2	0	2		22	0	5	3		4	
0	6	1		54	-4	-2	1	625	-610	-2	1	2	275	224	0	-5	3			

Table 1. (Continued)

h	k	l	10 ³ · F _o	10 ³ ·F _c	h	k	l	10 ³ · F _o	10 ³ ·F _c	h	k	l	10 ³ · F _o	10 ³ ·F _c	h	k	l	10 ³ · F _o	10 ³ ·F _c
1	0	3		102	4	0	4	203	-194	5	0	5	195	-160	0	-1	7	178	-140
4	0	3	340	-386	-4	0	4	408	-466	-5	0	5		-96	0	2	7	307	294
5	0	3	109	-140	5	0	4	332	366	-6	0	5	148	216	0	-2	7	384	340
-1	0	3	581	-644	-5	0	4	143	156	-7	0	5	72	-74	0	3	7	191	-146
1	0	3	169	148	-6	0	4	102	-142	0	0	6	599	538	0	-3	7	225	172
-4	0	3		-80	-7	0	4	115	-154	0	1	6	482	404	0	-4	7	399	-344
-7	0	3		-4	0	0	5	316	-280	0	-1	6	574	-442	0	-5	7	139	-112
1	0	4	497	472	0	1	5	328	-268	0	2	6	496	-442	0	-6	7	404	344
1	1	4	348	-340	0	-1	5	288	232	0	-2	6	321	-272	1	0	7		-38
0	-1	4	486	446	0	2	5		54	0	3	6	339	-268	-1	0	7	292	256
0	2	4	412	-446	0	-2	5	266	224	0	-3	6	618	508	2	0	7	338	-296
1	-2	4	757	-856	0	3	5	378	358	0	4	6	350	306	-2	0	7	213	-172
0	3	4	201	226	0	-3	5	289	-292	0	-4	6	336	326	3	0	7	641	-454
-1	-3	4	473	-484	0	4	5		-84	0	-5	6	356	-374	-3	0	7	161	-142
1	4	4	301	356	0	-4	5		4	0	-6	6	285	-280	-4	0	7	187	182
0	4	4	574	610	0	5	5	305	-314	1	0	6	137	-132	-5	0	7	138	-152
1	5	4	319	-322	0	-5	5	170	180	-1	0	6		24	0	0	8		48
1	-5	4	181	190	0	-6	5		78	2	0	6		-46	0	1	8		6
0	6	4	326	-290	0	-7	5		-14	-2	0	6	681	622	0	-1	8		-8
0	-6	4	396	-444	1	0	5	472	432	3	0	6	380	332	0	-2	8		-38
0	7	4	177	-206	-1	0	5	623	560	-3	0	6	455	474	0	-3	8	132	-82
1	0	4		-44	2	0	5	454	398	4	0	6	147	-108	0	-4	8		72
-1	0	4	346	-340	-2	0	5		16	-4	0	6		40	1	0	8	132	-114
2	0	4	178	184	3	0	5		56	-5	0	6	454	328	-1	0	8	533	-408
-2	0	4		-58	-3	0	5	153	139	-6	0	6		-32	-2	0	8	346	-248
3	0	4	300	354	4	0	5	408	466	0	0	7	211	-214	-3	0	8	204	-158
-3	0	4	159	-160	-4	0	5	467	366	0	1	7	286	246	-4	0	8	264	-232

Table 2. Fractional atomic coordinates, isotropic temperature factors and their standard deviations

Atom	<i>x</i>	10 ⁴ σ(<i>x</i>)	<i>y</i>	10 ⁴ σ(<i>y</i>)	<i>z</i>	10 ⁴ σ(<i>z</i>)	<i>B</i>	σ(<i>B</i>)
Zn ₁	.3866	6	.2481	5	.4923	6	.17	.05
Zn ₂	.0278	5	.7384	5	.1897	6	.05	.05
P	.8387	14	.2500	13	.2735	16	.20	.11
O ₁	.7724	36	.9917	36	.1482	42	.18	.33
O ₂	.9357	37	.3867	36	.1287	41	.22	.33
O ₃	.6034	36	.3817	35	.3338	41	.12	.33
O ₄	.9722	36	.7458	36	.5083	41	.25	.33
OH	.3661	37	.8850	36	.2990	40	.14	.34

Discussion of the structure

The lists of bond lengths and bond angles with their standard deviations are included in Tables 3 and 4. The standard deviations are estimated with Darlow formula (1961).

Table 3. Bond lengths and their standard deviations

P—O ₁	1.523 ± .018 Å	Zn ₂ —O ₁	1.971 ± .017 Å
—O ₂	1.530 .020	—O ₂	2.009 .016
—O ₃	1.539 .020	—O ₂ '	2.072 .021
—O ₄ '	1.553 .022	—O ₄	2.139 .021
		—OH	1.992 .019
Zn ₁ —O ₃	2.004 .019		
—O ₃ '	2.141 .017	OH—O ₁	2.769 .027
—O ₄ '	1.970 .019		
—OH	2.147 .017		
—OH'	1.941 .019		

Table 4. Bond angles and their standard deviations

O_1-P-O_2	$109.2^\circ \pm 1.2^\circ$		
O_1-O_3	$109.5^\circ \pm 1.1^\circ$		
O_1-O_4'	$111.7^\circ \pm 1.0^\circ$		
O_2-O_3	$108.2^\circ \pm 1.0^\circ$		
O_2-O_4'	$112.0^\circ \pm 1.1^\circ$		
O_3-O_4'	$106.0^\circ \pm 1.2^\circ$		
<hr/>			
$O_3-Zn_1-O_3'$	$81.5^\circ \pm 0.7^\circ$	$O_1-Zn_2-O_2$	$121.4^\circ \pm 0.8^\circ$
O_3-O_4'	$135.8^\circ \pm 0.8^\circ$	O_1-O_2'	$99.7^\circ \pm 0.8^\circ$
O_3-OH	$96.6^\circ \pm 0.7^\circ$	O_1-O_4	$91.7^\circ \pm 0.8^\circ$
O_3-OH'	$101.4^\circ \pm 0.8^\circ$	O_1-OH	$110.6^\circ \pm 0.7^\circ$
$O_3'-O_4'$	$87.0^\circ \pm 0.7^\circ$	O_2-O_2'	$77.1^\circ \pm 0.7^\circ$
$O_3'-OH$	$176.3^\circ \pm 0.7^\circ$	O_2-O_4	$84.5^\circ \pm 0.7^\circ$
$O_3'-OH'$	$98.7^\circ \pm 0.7^\circ$	O_2-OH	$128.0^\circ \pm 0.7^\circ$
$O_4'-OH$	$92.2^\circ \pm 0.7^\circ$	$O_2'-O_4$	$161.5^\circ \pm 0.6^\circ$
$O_4'-OH'$	$84.8^\circ \pm 0.7^\circ$	$O_2'-OH$	$95.9^\circ \pm 0.8^\circ$
$O_4'-OH'$	$122.5^\circ \pm 0.8^\circ$	O_4-OH	$93.6^\circ \pm 0.8^\circ$

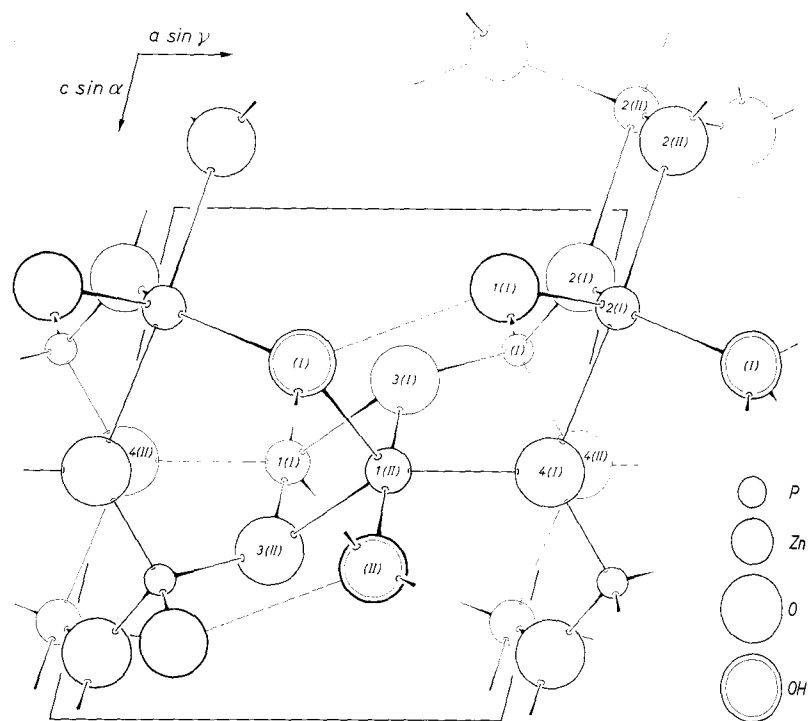
Fig. 1. Projection along the b axis of the structure

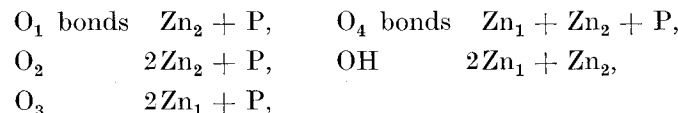
Figure 1 shows the arrangement of the two molecules in the unit cell, projected along b axis. In the structure there are independent regular tetrahedral $(PO_4)^{-3}$ complexes bound by the coordination polyhedra of the Zn^{+2} ions. The P—O bond lengths, whose average value is 1.54 Å, are in good agreement with those obtained in several determined structures containing discrete phosphate ions. The O—P—O angles, averaging 109.4°, do not differ significantly from the theoretical value.

The Zn ions are bonded to five oxygen atoms lying at the corners of a distorted trigonal bipyramid. A similar coordination has already been found in the mineral adamite (KOKKOROS, 1937). The average value for the Zn—O bond lengths is 2.04 Å.

Table 5. *Coordination-polyhedra edge lengths and their standard deviations*

PO ₄ -tetrahedron edge lengths			
O ₁ —O ₂	2.489 ± .022 Å	O ₂ —O ₃	2.487 ± .028 Å
O ₁ —O ₃	2.502 .025	O ₂ —O ₄ '	2.558 .028
O ₁ —O ₄ '	2.547 .028	O ₃ —O ₄ '	2.470 .026
Zn ₁ -coordination bipyramid-edge lengths		Zn ₂ -coordination bipyramid-edge lengths	
O ₃ —O ₃ '	2.708 ± .058 Å	O ₁ —O ₂	3.471 ± .022 Å
O ₃ —O ₁ '	3.683 .027	O ₁ —O ₂ '	3.090 .027
O ₃ —OH	3.101 .022	O ₁ —O ₄	2.951 .027
O ₃ —OH'	3.054 .026	O ₁ —OH	3.258 .027
O ₃ '—O ₄ '	2.832 .025	O ₂ —O ₂ '	2.544 .052
O ₃ '—OH'	3.100 .022	O ₂ —O ₄	2.791 .028
O ₄ '—OH	2.969 .026	O ₂ —OH	3.595 .024
O ₄ '—OH'	3.429 .027	O ₂ '—OH	3.019 .028
OH—OH'	2.761 .056	O ₄ —OH	3.014 .027

In Table 5 are listed the O—O distances in the coordination polyhedra. The oxygen atoms show the following coordination:



Considerations of electrostatic equilibrium and a study of the distances between OH and surrounding oxygens, led us to locate an hydrogen bond between OH and O₁.