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Crystal Structure of $\alpha Zn_2P_2O_7$

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$\alpha Zn_2P_2O_7$ is a hexpartite structure with a unit cell three times as long in the *a* direction and twice as long in the *c* direction as that of the parent $\beta Zn_2P_2O_7$. The crystal crystallizes with monoclinic symmetry with unit cell parameters of $a = 20.068(15)$ Å, $b = 8.259(6)$ Å, $c = 9.099(8)$ Å and $\beta = 106.35(5)°$, $Z = 12$ and the space group is I2/c. A total of 1841 reflections out of a total of 3740 considered had intensities strong enough to be measured. The structure was refined by full matrix least squares in both the possible space groups Ic and I2/c. The final reliability index is 0.080 for all the data. The coordination number of the cations to oxygen atoms are either 5 (for 2 Zn) or 6 (for 1 Zn) as compared to 6 for all cations in the β phase. All the anions shown nonlinear P—O—P bonds whereas in the β phase they appear linear because of disorder. The two independent anions have P—O—P angles of 139° and 148°. The average inner P—O bond length is 1.60 Å while the terminal bond average to 1.52 Å. The average error in the individual PO bond lengths is 0.008 Å. This structure can be characterized as composed of sequences of layers. A layer like that found in $\alpha Cu_2P_2O_7$ is followed by two layers like those found in $\alpha Mg_2P_2O_7$. The former layer has anions lying on two-fold axes and the cations are coordinated to five oxygen atoms while in the next two layers half of the cations are five coordinate while the anions in these layers show only approximate two-fold axes.

Introduction

Zinc pyrophosphate, $Zn_2P_2O_7$, is one of a family of divalent metal ion pyrophosphates which are isostructures in their high temperature (β) phase. The low temperature (α) phases fall into three groups each a multipartite, defined by Lefkowitz, Łukaszewicz, and Megaw (*1*), of its parent phase. These groups consist of $Cu_2P_2O_7$ which is bipartite along *c* (*2*), $Mg_2P_2O_7$ (*3*), $Ni_2P_2O_7$ (*4*), and $Co_2P_2O_7$, which are bipartite along both *c* and *a* and $Zn_2P_2O_7$ which is bipartite along *c* and tripartite along *a*. The structures of all the α phases except that of $Zn_2P_2O_7$ have been previously determined. The detail structure of the β phase of $Co_2P_2O_7$ has not been reported although magnetic measurements are consistent with its being isostructural to the other β phases in this series (*5*). In addition, the structure of $Mn_2P_2O_7$ (*6*) at room temperature has been refined by Calvo (*7*) and from NMR measurements on P^{31} it is known not to have a first order phase transformation between liquid He temperature and room temperature (*8*).

The transformation of $Zn_2P_2O_7$ doped with Mn^{2+} or Cu^{2+} has been monitored by electron spin resonance (*9*) and there appears to be a first order transition at 132°C and a gradual transformation of the second kind from this temperature to about 155°C. The detailed atomic changes occurring in this region are uncertain. The transformation of $Mg_2P_2O_7$ features a temperature range in which the high and low temperature phases coexist (*10*). The diffuse streaks found in the diffraction patterns of $Cu_2P_2O_7$ in the transition region suggests that its transformation may provide the most detailed information about the mechanism (*11*). In terms of the gross structure $\alpha Zn_2P_2O_7$ is the most complex of the series. An understanding of the phases and transformations of the entire series will be simplified by a study of each member of the series.

Experiments

A. Crystal Data

Crystals of $Zn_2P_2O_7$ were prepared from the melt obtained from the decomposition of precipitated $ZnNH_4PO_4$. The crystals were heated in a Vycor

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container to about 50°C above their melting temperature of 1020°C (*12*) and slowly cooled to about 900°C. They were then removed from the furnace and allowed to reach ambient temperature. Single crystals were selected for X-ray examination and were observed to show the general extinction conditions $h + k + l$ odd and l odd if k were zero. In addition, in an [100] zone photograph, only a very few l odd could be discerned and these were very weak.

Lattice parameters had been obtained by De Wolff (*13*) from powder data and reported based upon a *C* centered cell. We have chosen a body centered cell to preserve the same axial directions for the unit cell as in the β phase. Accurate parameters were obtained from a Debye–Sherrer pattern. Crystals were ground into a fine powder, mixed with a solution of acetone and fingernail polish and, when partially dried, drawn into thin fibers. One fiber was used to obtain a 4-day exposure. Sixteen lines were identified using De Wolff's lattice parameters as trial values and the new lattice parameters were obtained by a least squares fit. The lattice parameters are reported in Table I together with other crystal data.

TABLE I

CRYSTAL DATA

$a = 20.068(15)$ Å
$b = 8.259(6)$ Å
$c = 9.099(8)$ Å
$\beta = 106.35(5)° \; Z = 12$
$\rho_{exp} = 4.1$ gm/cm^3
$\rho_{calc} = 4.2$ gm/cm^3
μ (linear absorption coefficient) = 110 cm^{-1}

B. Intensity Data

A crystal of dimensions $0.13 \times 0.13 \times 0.35$ mm^3 was used to obtain data of the type hkn, $n = 0,1,2$, $0kl$ and hkk-$h/3$. MoKα radiation was employed together with an integrating precession camera, to record these data. The intensities of all reflections were measured with a Leeds and Northrup G1 microdensitometer and the intensities of symmetry equivalent reflections averaged.

A second crystal with dimensions $0.06 \times 0.06 \times 0.11$ mm^3 mounted parallel to the longest edge was used to record data of the type hnl, $n = 0,1,2,3,4,5$ with the Weissenberg camera. MoKα radiation was used to minimize the effects of absorption. Multiple exposures of each layer were taken and the intensities were estimated by visual comparison.

All the data were corrected for the Lorentz and polarization effects and absorption. The absorption corrections were approximate since the crystals were assumed to have idealized geometries. Since the linear absorption coefficient for MoKα radi-

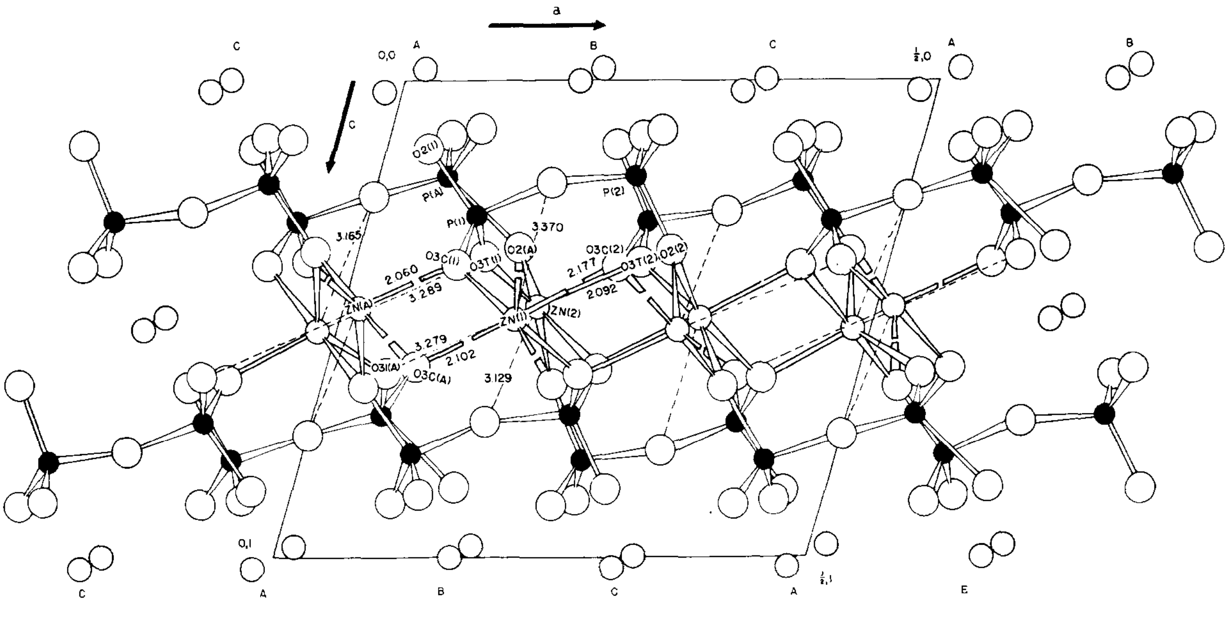

FIG. 1. The structure of $\alpha Zn_2P_2O_7$ in space group I2/c is shown projected onto the a–c plane. The layers are labeled A, B, and C. The oxygen atoms are represented by large open circles and the Zn atoms by small open circles. The filled circles represent phosphorus atom. The bond lengths are shown in Å units.

ation is 110 cm^{-1}, sizeable errors could be introduced for particular reflections for the former crystals, although the average error was estimated to be of the order to 5%. Standard errors for most of the reflections measured with the densitometer were initially assigned as a constant fraction of the intensity divided by the square root of the number of times it was observed. The standard error of the very weak reflections was increased by a factor accounting for their discrimination from background. The standard errors of the reflections measured visually were also assigned as a constant fraction of the intensity except that the errors for the very weak and the very strong reflections were increased by 50 or 100% depending upon the estimated accuracy with which the intensity could be observed.

The unit cell of $\alpha Zn_2P_2O_7$ contains 12 formula units and if the space group were Ic there would be three in the asymmetric unit. If the space group were I2/c, one of the anions would necessarily lie on a symmetry element, either a two-fold axis or a center of symmetry, and one pair of the cations would be related by a center of symmetry or would then lie on a two-fold axis, assuming the structural packing is similar to that in the β phase. The space group of lower symmetry was chosen for the initial trial in anticipation that if I2/c were the proper space group it would be recognized in the final atomic coordinates. This was considered to be the cautious approach despite the fact that statistical considerations using of the data of the [010] zone indicated that the structure was centrosymmetric. The

TABLE II

Atomic Parameters for $\alpha Zn_2P_2O_7$

(The estimated standard deviations are enclosed in parentheses.)

	x	y	z	$B(T)$
Zn(A)	0.01302(5)	0.31182(22)	−0.02382(11)	—
P(A)	0.06618(11)	0.02024(43)	0.20417(23)	—
01(A)	0	0.0886(17)	$\frac{1}{4}$	0.88(13)
02(A)	−0.12407(29)	0.0059(11)	0.1437(6)	0.47(7)
03C(A)	−0.08360(31)	0.1574(11)	0.3928(8)	0.54(8)
03T(A)	0.05120(37)	−0.1393(12)	0.1197(8)	0.95(10)
Zn(1)	0.16348(6)	0.18296(18)	0.00104(14)	—
Zn(2)	0.18239(5)	0.81089(19)	−0.02402(12)	—
P(1)	0.10189(11)	0.50679(45)	0.28423(22)	—
P(2)	0.23880(10)	0.51842(45)	0.20192(22)	—
01	0.16450(30)	0.5564(12)	0.2168(7)	0.60(8)
02(1)	0.04049(29)	0.4939(11)	0.1422(6)	0.31(6)
02(2)	0.28953(28)	0.5101(10)	0.3612(6)	0.51(7)
03C(1)	0.09400(33)	0.6513(11)	0.3829(8)	0.56(9)
03C(2)	0.25367(32)	0.6595(11)	0.1090(7)	0.64(8)
03T(1)	0.11792(39)	0.3550(12)	0.3758(9)	1.11(11)
03T(2)	0.23510(37)	0.3576(12)	0.1162(9)	0.89(10)

Anisotropic thermal parameters (Å)^2[a]

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn(A)	0.0072(4)	0.0052(9)	0.0056(4)	0.0004(5)	−0.0004(3)	0.0004(6)
P(A)	0.0047(7)	0.0049(18)	0.0025(6)	−0.0016(11)	0.0009(8)	0.0003(10)
Zn(1)	0.0056(3)	0.0063(8)	0.0056(3)	0.0009(6)	0.0003(2)	0.0003(6)
Zn(2)	0.0070(4)	0.0038(8)	0.0061(4)	0.0001(6)	−0.0011(3)	0.0001(8)
P(1)	0.0047(7)	0.0053(17)	0.0020(6)	−0.0003(9)	0.0003(5)	0.0010(10)
P(2)	0.0033(6)	0.0072(18)	0.0024(6)	0.0007(8)	0.0007(7)	0.0001(10)

[a] These values were obtained from $\beta_{ij} = 2\pi^2 b_i b_j U_{ij}$ where β_{ij}'s appear as a temperature effect through $\exp[-(\beta_{11}h^2 + 2\beta_{12}hk + \cdots)]$.

Table III Observed and Calculated Structure Factors for $\alpha Zn_2P_2O_7$

UNOBSERVEC REFLECTIONS ARE MARKED WITH AN ASTERISK (*), AND UNRELIAGLE REFLECTIONS WITH THE SYMBOL (0).

H	K	|FOBS|	FCALC
			L = 0
16	-10	23	-24
36	-6*	20	-4
34	-6	25	-23
32	-6*	19	-6
30	-6	31	-29
28	-6	81	-81
26	-6	17	14
24	-6	68	-73
22	-6	53	-53
20	-6	37	-37
18	-6	47	49
16	-6	16	-18
14	-6	41	-45
12	-6	69	-75
10	-6	21	-20
8	-6	82	-75
6	-6	78	84
4	-6	26	26
12	2	212	211
14	2	36	-38
16	2	15	17
18	2	32	33
20	2	37	-36
22	2	25	23
24	2	48	49
26	2	26	-24
28	2	22	-17
30	2	71	-68
32	2*	19	-4
34	2*	20	-20
36	2*	20	-2
38	2*	20	-12
40	2	30	-28
42	2*	19	-8
44	2*	17	15
46	2	27	-32
48	2*	14	-16
50	-4*	15	11
48	-4*	17	2
46	-4	33	-31
44	-4*	19	8
42	-4	18	18
40	-4	25	-24
38	-4*	20	2
36	-4*	20	-14
34	-4	77	-80
32	-4*	18	7
30	-4*	18	-6
4	-4	50	44
2	-4	61	-59
0	4	155	148
2	4	45	46
4	4	34	-35
6	4	293	338
8	4*	8	1
10	4	12	13
12	4	141	141
14	4*	10	-8
16	4	18	18
18	4	163	149
20	4	19	-18
22	4*	16	9
24	4	31	-33
26	4	20	-11
28	4*	19	-6
30	4	35	33
32	4*	20	-15
34	4*	20	-7
36	4*	20	-9
38	4	17	14
26	6	23	-22
28	6	23	24
30	6*	20	16
32	6*	20	-1
34	6*	20	-21
36	6	30	-29
38	6*	19	-13
40	6*	18	-2
42	6*	16	-6
50	-8*	15	1
48	-8	20	16
46	-8	30	-31
44	-8	20	12
42	-8	24	21
40	-8	22	-20
38	-8*	20	-3
36	-8*	20	3
34	-8	56	-47
32	-8	25	23
30	-8	29	-24
28	-8	65	-61
26	-8	25	-23
24	-8	34	31
22	-8	28	-28
20	-8	15	-8
18	-8	109	-99
16	-8	53	-60
14	-8	49	-56
12	-8	23	21
10	-8	27	32
8	-8	61	-66
6	-8	24	26
4	-8	11	13
2	-8	56	-59
0	8	122	123
2	8	41	41
6	8	179	159
8	8	43	39
10	8	15	-13
12	8	48	51
14	8*	16	-4
16	8*	17	-2
18	8	144	136
14	-10	40	-46
12	-10	17	-14
10	-10	55	-55
8	-10	20	-23
6	-10	16	-17
4	-10*	14	3
2	-10	100	-80
0	10	103	111
2	10	19	18
4	10	26	-28
6	10	19	-10
8	10*	16	-3
10	10	34	-34
12	10	167	167
14	10*	18	3
16	10*	18	2
18	10	72	67
20	10*	19	4
22	10*	20	4
24	10	34	39
26	10	22	-22
28	10*	20	5
30	10	37	38
32	10*	19	-4
34	10*	18	9
36	10*	16	0
38	10*	15	-7
40	10*	13	-8
50	-12*	13	4
48	-12	29	22
38	-16*	18	11
36	-16	23	24
34	-16	24	15
32	-16*	20	7
30	-16	26	26
28	-16	50	-55
26	-16*	20	14
24	-16*	20	0
22	-16*	20	-22
20	-16*	20	-1
18	-16*	20	0
16	-16	40	-37
14	-16*	20	8
12	-16	44	-43
10	-16	40	-41
8	-16*	20	-18
6	-16*	20	6
4	-16*	20	0
2	-16	24	-22
0	16*	20	-16
2	16*	20	-12
4	16*	20	-21
6	16*	20	-9
8	16*	20	10
10	16	33	-34
12	16	43	42
14	16*	20	14
16	16*	19	-8
18	16	29	29
20	16*	18	4
22	16*	17	-13
24	16	47	56
26	16*	13	7
28	16*	13	7
44	-18*	12	8
42	-18	20	23
40	-18*	15	12
38	-18*	16	0
36	-18	28	30
34	-18	28	-27
32	-18*	18	9
30	-18*	19	18
28	-18	23	-20
26	-18*	20	-5
24	-18	24	22
22	-18	26	-26
20	-18*	20	16
18	-18*	20	-12
16	-18	51	-50
14	-18*	20	-16
12	-18*	20	20
10	-18*	20	-12
8	-18*	20	-7
6	-18	37	-32
4	-18	42	-39
2	-18	22	-21
0	18	19	-14
2	18*	20	-1
4	18	32	-33
6	18*	19	5
8	18*	19	3
10	18*	19	-21
12	18*	18	12
14	18*	17	1
16	18	24	-29
18	18	37	39
20	18*	14	13
22	18*	13	-10
38	-20*	13	9
36	-20	16	17
34	-20*	15	-5
32	-20*	16	2
30	-20	20	20
4	1	27	-29
6	1	14	11
8	1	60	-59
10	1	68	-68
12	1	30	31
14	1	161	-169
16	1	63	-61
18	1	16	15
20	1	83	-86
22	1	21	-20
24	1	16	12
26	1	113	-103
28	1*	19	7
30	1*	20	3
32	1	58	-53
34	1*	21	7
36	1*	21	0
38	1	28	-31
40	1*	21	21
39	-2*	22	8
37	-2	34	36
35	-2*	21	-16
33	-2*	20	1
31	-2*	19	-3
-29	2*	22	17
-27	2	43	-38
25	-2	20	22
23	-2*	16	10
-21	2	66	67
-19	2	19	18
17	-2*	10	4
15	-2	82	-78
13	-2	41	-40
11	-2	55	57
-9	2	121	-135
7	-2*	6	-1
5	-2*	5	9
3	-2	70	-64
-1	2	19	-16
-1	-2	24	24
3	2	262	-263
5	2*	6	-2
7	2*	7	-2
9	2	45	41
11	2*	9	-1
13	2*	10	5
15	2	151	-155
17	2	24	25
19	2	14	-13
21	2*	16	2
23	2*	17	-12
25	2*	18	13
27	2*	19	6
29	2	23	16
31	2*	20	1
33	2*	21	-5
35	2*	21	-7
40	-3*	22	15
37	2*	22	23
38	-3*	21	-6
36	-3*	21	6
34	-3	38	37
32	-3	46	-45
30	-3*	19	2
28	-3*	18	16
26	-3	69	-67
24	-3*	16	6
22	-3*	15	13
20	-3	167	-162
18	-3	11	10
16	-3	17	-22
14	-3	136	-145
12	-3	15	16
2	-5	126	-97
0	-5*	8	4
2	5	44	47
4	5	24	24
6	5	11	11
8	5	11	-12
10	5	22	-20
12	5	11	14
14	5	15	-16
16	5	31	-35
18	5	20	21
20	5	99	-92
22	5	28	-30
24	5*	19	11
26	5	59	-52
28	5	22	-19
30	5*	21	9
32	5	67	-63
34	5*	22	3
36	5*	21	1
38	5	28	-35
40	5*	20	6
37	-6*	21	14
35	-6*	21	-5
33	-6	35	39
31	-6	46	42
29	-6*	19	-0
27	-6	26	-28
25	-6	23	-20
23	-6	19	15
21	-6	18	11
19	-6	35	40
17	-6*	11	13
15	-6*	11	-4
13	-6	14	-17
11	-6	43	42
9	-6	31	-29
7	-6	16	-15
5	-6	24	22
3	-6	11	-8
1	-6	20	-20
1	6	40	37
3	6	158	-164
5	6	31	-32
7	6	11	9
9	6	35	-35
11	6*	11	-4
13	6*	12	2
15	6	33	-33
17	6*	17	4
19	6*	17	-7
21	6	51	-53
23	6*	19	-7
25	6*	20	6
27	6*	21	12
29	6*	21	5
31	6*	21	-2
33	6	23	-27
35	6*	21	-2
37	6*	21	1
39	6	24	24
40	-7*	22	24
38	-7*	22	-3
36	-7*	21	9
34	-7*	21	21
32	-7*	20	-5
30	-7*	19	3
28	-7	52	48
26	-7	78	-66
24	-7*	16	2
22	-7	34	34
20	-7	67	-65
18	-7*	15	4
16	-7	21	22
8	-9	88	-90
6	-9*	11	8
4	-9	29	-28
-2	9	123	125
0	9*	9	-5
2	9	42	41
4	9	62	59
6	9*	16	0
8	9	32	32
10	9	25	26
12	9*	17	10
14	9*	18	-6
16	9*	19	-15
18	9*	19	13
20	9*	20	-10
22	9*	21	-20
24	9*	21	12
26	9	46	-42
28	9*	22	-14
30	9*	21	10
32	9	40	-40
34	9*	20	-13
36	9*	19	5
38	9	31	-39
18	0	70	69
20	0	18	-13
22	0	20	-18
24	0	14	-6
26	0	23	-27
28	0	20	-21
30	0*	18	7
32	0*	19	-1
34	0	33	-33
36	0	48	-47
38	0*	20	8
40	0	45	-47
42	0*	19	3
44	0*	18	-1
46	0	25	-25
48	0*	15	8
48	-2*	16	11
46	-2	44	-45
44	-2*	19	11
42	-2	33	-31
40	-2	32	-31
38	-2*	20	7
36	-2*	20	-1
34	-2	41	-40
32	-2*	19	-9
-30	2	50	-45
-28	2	51	-54
26	-2*	16	1
-24	2	22	-16
22	-2*	14	3
40	9*	15	-0
39	-10	26	-21
37	-10*	22	-6
35	-10*	21	4
33	-10*	21	-8
31	-10	33	30
29	-10*	20	-11
27	-10*	19	9
25	-10*	19	5
23	-10	23	73
21	-10*	18	0
19	-10	17	21
17	-10	19	-18
15	-10	50	55
13	-10	16	12
13	10*	19	1
11	-10	41	37
9	-10	88	-84
7	-10	27	-30
5	-10	17	16
15	12	69	-66
17	12*	21	-2
19	12*	21	-4
21	12*	22	11
23	12*	21	3
25	12*	21	5
29	12*	20	8
36	-13	23	18
34	-13*	22	21
32	-13*	21	6
30	-13*	21	11
28	-13*	21	21
26	-13*	21	3
24	-13*	20	9
22	-13	46	47
20	-13	25	-27
18	-13*	19	4
16	-13	38	38
14	-13	27	-37
12	-13*	18	6
10	-13	22	26
-8	13	85	82
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25	3•	16	15
27	3•	19	-12
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31	3•	21	-4
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37	3•	21	-0
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38	-4•	21	-11
36	-4•	21	7

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26	-4*	17	-13
24	-4	33	29
22	-4	12	10
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18	-4	28	-27
16	-4*	10	9
14	-4	19	16
12	-4	101	103
10	-4*	8	-3
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6	-4	226	-226
4	-4	46	-47
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0	4	114	-116
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4	4*	8	4
6	4	187	-140
8	4	17	17
10	4	21	-21
12	4	132	-125
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16	4	13	-15
18	4*	16	-9
20	4	30	27
22	4	17	-14
24	4	72	-70
26	4	19	17
28	4	20	-12
30	4	25	28
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34	4*	21	18
36	4	22	20
39	-5*	21	-7
37	-5*	21	-9
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27	-5*	18	-3
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9	-5	9	-8
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3	-5	10	-6
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1	5	111	-94
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13	5	24	25
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19	5	17	11
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25	5*	19	11
27	5*	20	-9
29	5	58	61
31	5*	21	-1
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21	-9*	17	-1
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16	-10	54	55
14	-10	13	13
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12	14	45	-43
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31	-15*	21	-20
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5	15*	21	-9
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26	-16*	21	3
24	-16*	21	-14

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-2	1	53	-53
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4	1*	9	6
6	1	13	-4
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10	1	26	23
12	1*	9	0
14	1	11	12
16	1*	11	-1
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22	1*	15	8
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26	1	29	31
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38	1*	22	17
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12	5	11	-8
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41	-6*	21	18
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9	-6	12	-5
7	-6	13	14
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11	6	13	-13
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15	6	123	119
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19	6*	18	10
21	6	38	40
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27	6	29	32
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14	-9	24	27
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10	-9*	12	2
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12	9*	18	-10
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25	-14	26	-29
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7	14	21	-21
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11	14*	21	0
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23	1	102	-90
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27	1	19	16
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29	1	82	-79
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33	1*	21	-1
35	1	39	-41
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39	1*	21	6
40	-2*	22	-8
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36	-2	22	21
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32	-2*	20	-3
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18	-2	11	-9
16	-2*	10	3
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8	-2	8	-10
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6	2	36	34
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10	2	9	10
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Table III (continued)

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24	-15*	22	-9
22	-15*	21	-9
20	-15*	21	-15
18	-15*	21	-8
-16	15	21	14
-14	15	28	-28
-12	15*	21	6
-10	15*	21	2
-8	15*	21	-18
-6	15*	21	3
-4	15*	21	20
-2	15*	21	-18
0	15*	21	6
2	15*	21	-7
4	15	36	-34
6	15*	21	-1
21	-16*	22	18
-19	16	60	52
-17	16*	21	-6
-15	16*	21	10
-13	16*	21	14
-11	16*	21	13
-9	16*	21	8
-7	16	26	24
-5	16*	21	6
-3	16	21	23
-1	16*	21	9
1	16	31	33
3	16*	22	-12
H	K		L = 6
0	0	242	305
2	0	15	-14
4	0*	7	0
6	0	24	22
8	0*	7	-5
10	0	10	9
12	0	83	81
14	0	54	-55
16	0	14	12
18	0	29	26
20	0	9	-5
22	0	14	-15
-25	1*	13	-4
-23	1	27	-27
-21	1*	15	6
-19	1*	15	-7
-17	1	107	-121
-15	1	16	16
-13	1	55	-57
-11	1	70	-74
-9	1	19	21
-7	1	22	-24
-5	1	15	-12
-3	1	10	15
-1	1	53	-53
1	1	36	-34
3	1*	13	9
5	1*	13	3
7	1	57	54
9	1	13	-6
11	1	91	90
13	1	23	19
15	1*	14	-0
17	1	34	32
19	1	27	28
21	1*	14	-11
23	1	73	81
-24	2*	22	6
-22	2*	22	-6
-20	2	40	-40
-18	2*	22	13
-16	2*	21	1
[illegible]	2	[illegible]	[illegible]
-9	2	24	18
-7	2	23	23
-5	2	28	-32
-3	2	103	109
-1	2	22	24
1	2*	19	4
3	2*	19	7
5	2*	19	0
7	2*	19	8
9	2	119	137
11	2*	20	-12
13	2*	20	15
15	2	26	-26
17	2*	22	4
19	2*	22	11
21	2*	22	23
23	2*	22	-22
0	3*	9	-12
12	3*	16	9
0	5*	9	5
3	6*	16	5
0	7*	16	-7
3	-8	60	-55
0	9*	7	-2
6	-9*	14	-3
9	4*	16	1
6	5*	16	10
H			K = 8
2	0	15	14
4	0	20	-18
6	0	177	-193
8	0	39	39
10	0	22	-19
12	0	95	-98
14	0	16	15
16	0	17	-11
18	0	18	-18
-19	1	21	22
-11	1	31	-30
-9	1	17	9
-7	1	36	33
-5	1	22	22
-1	1	12	-2
1	1	46	-45
5	1	34	32
7	1	27	25
11	1	19	19
13	1	40	-36
15	1	12	8
17	1	24	-20
23	1	24	35
-14	2	45	48
-12	2	91	-89
-10	2	25	-27
-8	2	33	32
-6	2	32	-27
0	2	181	-192
6	2	134	-149
10	2	30	-29
12	2	70	-73
14	2	40	35
16	2	25	-19
18	2	52	-51
0	4	138	-141
0	6	86	-83
0	8	61	-59
12	4	99	-110
6	6	101	-108
3	7	14	-7
15	3*	12	-14
-23	1*	11	7
-21	1*	13	3
-17	1*	14	1
-15	1*	15	4
-13	1*	15	-3
-3	1*	14	2
3	1*	14	7
9	1*	14	1
[illegible]	[illegible]	[illegible]	[illegible]
-11	1	54	56
-9	1	14	-10
-7	1	36	36
-5	1	54	52
-1	1	19	-15
11	1	34	-30
13	1	30	-40
17	1	78	-80
-8	2	32	-32
-6	2	90	98
0	2	44	47
6	2	89	90
12	2	55	50
0	4	98	92
0	6	63	64
2	0*	7	7
-13	1*	14	-1
-3	1*	15	-3
1	1*	15	-2
3	1*	15	4
5	1*	15	-5
7	1*	14	11
9	1*	14	6
15	1*	13	11
-16	2*	22	14
-14	2*	22	-15
-12	2*	22	20
-10	2*	22	13
-4	2*	22	20
-2	2*	22	-20
2	2*	22	5
4	2*	22	10
8	2*	22	-17
10	2*	22	-0
H			K = 11
3	0	105	-109
5	0	22	23
-10	1	29	30
-8	1	56	51
-6	1	15	-11
-4	1	36	38
-2	1	29	-30
8	1	16	13
10	1	17	-4
-15	2	24	-26
-11	2	25	26
-9	2	58	-55
-7	2	36	-25
-3	2	102	-106
3	2	88	-87
1	0*	6	-6
7	0*	5	-2
-12	1*	13	-0
0	1*	7	0
2	1*	14	-3
4	1*	14	-12
6	1*	14	-5
-13	2*	21	-10
-5	2*	22	3
-1	2*	22	-2
1	2*	22	11
5	2*	22	-6
0	3*	6	-4
H			K = 12
-10	2	24	-25
-6	2	25	30
-12	2*	19	3
-8	2*	21	-4
-4	2*	21	-3
-2	2*	21	-13
0	2*	21	-11

pseudo-symmetry apparent in the diffraction pattern suggested that this test may not be taken as reliable.

Since the reflections which distinguish the $\alpha Zn_2P_2O_7$ cell from that of the β phase were weak, small atomic displacements from the β structure should characterize the α phase. It was noted that the anisotropic thermal parameters of the atoms in $\beta Zn_2P_2O_7$ were similar to those in $\beta Cu_2P_2O_7$ (*14*) and therefore, $\alpha Zn_2P_2O_7$ was regarded tentatively as composed of three layers similar to those in $\alpha Cu_2P_2O_7$. These layers, $1/2\,a$ (of the β cell) thick and infinite in b and c, will be designated as layers A, B, and C. The broadening of the peaks in Patterson projections indicated that the major distortion was along the $[10\bar{3}]$ direction. The cation positions were determined by assuming that in layer A they were displaced from the β phase positions as in $\alpha Cu_2P_2O_7$. The remaining cations were split and one half displaced in the positive and the other in the negative $[10\bar{3}]$ direction. The multiplicity of each half cation was varied for one cycle of least squares where the value of

$$R_2\left(=\frac{\sum\omega(|Fo|-|Fc|)^2}{\sum\omega|Fo|^2}\right)^{1/2}$$

was minimized using a program written for the IBM 7040 by J. S. Stephens. The cation positions whose multiplicity had increased were then assigned to Zn^{2+} ions. The cations in layer C were located in this manner and those in layer B were found by the use of electron density projections. The cation positions were found to be curiously related to those of the β phase. In layer A they had moved by nearly equal and opposite amounts while one cation in each of the remaining layers had essentially remained in its β phase position. The other cations in these layers had moved toward each other with the major displacement being 0.3 Å in the $(10\bar{3})$ direction.

The anions were located by correlating the cationic displacements and that of the central oxygen atom of the anion in the same layers. As has been indicated (*2*), such a correlation exists because the oxygen atoms shared between the anion and the cation transfer the central oxygen atom displacements into a unique direction of rotation of the cations bonded to this anion. The axis of rotation essentially lies in the plane separating the cations and passes through the phosphorus atom on the near side of the anion. Electron density maps were used to refine these P and oxygen atoms positions. Scattering curves were obtained from the International Tables for X-ray Diffraction (*15*) and corrected for dispersion using tabulated values (*16*). No effort was made to distinguish the intensity of the pair of reflections *hkl* and *hkl*. Each layer was scaled independently and common reflections were averaged and assigned to the derived groups at random. After all the atoms had been located and satisfied reasonable chemical constraints as to bond lengths and angles, the zinc ions and the phosphorus atoms were assigned anisotropic thermal factor but those of the oxygen atoms remained isotropic. This latter restriction was necessary because of computer size and speed limitations. One least square cycle involving a maximum of 190 variables from a total of 218 parameters and 3470 reflections required 90 min. The weights now were chosen so that $|Fo - Fc|^2$ would be independent of the magnitude of Fo. Fractional values of the calculated parameter changes were applied. This was necessary since some of the atoms were highly correlated. Unobserved reflections whose calculated structure factor was less than the minimum observable value were left out of the refinement.

In the refined structure for this space group 8 of the 39 independent atoms had non-positive definite thermal parameters although in all but two cases the offending value was within one or two standard deviations of yielding positive definite tensors. The final R_2 value of 0.098 was obtained using all the data.

The structure obtained at this point appeared to be composed of an $\alpha Cu_2P_2O_7$-like layer followed by two $\alpha Mg_2P_2O_7$-like layers with the remaining structure generated by the I centering operation as shown in Fig. 1. The two cations in the A layer of $\alpha Zn_2P_2O_7$ were coordinated to five oxygen atoms with the sixth oxygen atom displaced along the axial direction of the supposed octahedron to a distance of 3.2 and 3.4 Å from its assigned cation. In $\alpha Cu_2P_2O_7$ the sixth oxygen atoms lie at 2.9 Å from its cation with the second cation related to the first by a center of symmetry. The other axial cation oxygen bond is 2.36 Å long in the latter compound compared to 2.0 and 2.1 Å found here for the unique axial cation oxygen atom bond to the two cations in layer A. The anion in the $\alpha Cu_2P_2O_7$ structure has a two-fold axis. In $\alpha Zn_2P_2O_7$, the anion's geometry in the A layer was highly irregular. The two central P—O bonds were 1.65 and 1.54 Å long. The P—O 3C bonds on the two halves of the anion had lengths of 1.59 and 1.49 Å with the longest bond on the same side as the longer P—O(—P) bond. The shorter P—O 3*T* bond, 1.46 Å, lay on this half of the anion however as compared to a value of 1.58 Å for this bond on the other half of the anion. Although the estimated standard deviations (e.s.d.'s) at 0.04 Å on

TABLE IV

Bond Distances and Angles in $\alpha Zn_2P_2O_7$

(Estimated standard deviations in parentheses.)

$P_2O_7^{4-}$ group

(a) Distances (Å)

"α-$Cu_2P_2O_7$-like" layer					
P(1)–01	1.603(6)	01(A)–02(A)	2.499(7)	02(A)–03C(A)	2.515(10)
–02(A)	1.541(6)	–03C(A)	2.460(8)	–03T(A)	2.537(9)
–03C(A)	1.535(9)	–03T(A)	2.586(13)	03C(A)–03T(A)	2.546(13)
–03T(A)	1.512(9)	P(A)–P′(A) =	3.000(3)		
"α-$Mg_2P_2O_7$-like" layers					
P(1)–01	1.599(8)	01–02(1)	2.443(8)	02(1)–03C(1)	2.513(10)
–02(1)	1.518(5)	–03C(1)	2.471(11)	–03T(1)	2.528(10)
–03C(1)	1.528(9)	–03T(1)	2.548(13)	03C(2)–03T(1)	2.498(14)
–03T(1)	1.489(10)				
P(2)–01	1.566(7)	01–02(2)	2.512(8)	02(2)–03C(2)	2.525(9)
–02(2)	1.520(5)	–03C(2)	2.424(11)	–03T(2)	2.525(10)
–03C(2)	1.518(9)	–03T(2)	2.504(13)	03C(2)–03T(2)	2.524(14)
–O3T(2)	1.531(10)	P(1)–P(2) = 3.046(3)			

(b) Angles (°)

"α-$Cu_2P_2O_7$-like layer"		
01–P–02		105.3(3)
–03C		103.2(5)
–03T		112.2(5)
02 –03C		109.7(4)
–03T		112.4(5)
03C–03T		113.3(5)
	P—O—P	138.7(7)°
"α-$Mg_2P_2O_7$-like layers"		
	Side 1	Side 2
01–P–02	103.2(4)	109.0(4)
–03C	104.4(5)	103.6(4)
–03T	111.1(5)	107.9(5)
02 –03C	111.2(4)	112.5(4)
–03T	114.4(5)	111.7(4)
03C –03T	*111.8(5)*	*111.8(5)*
	P—O—P 148.4(5)°	

Cation Environment

Zn(A)–02(I)	2.089(8)	Zn(1)–02(2)[d]	2.083(7)	Zn(2)–02(2)[d]	2.056(7)
–02(I)[a]	2.060(8)	–02(A)[a]	2.051(8)	–02(A)[a]	2.032(8)
–03CA[c]	2.024(7)	–03C(A)[c]	2.102(7)	–03C(2)	2.025(7)
–03TA[a]	1.956(8)	–03C(1)[b]	2.032(8)	–03T(2)	2.092(9)
–03C(I)[b]	2.060(8)	–03C(2)[e]	2.177(7)	–03T(1)[b]	1.929(9)
–03T(1)[b]	3.289(9)	–03T(2)	2.097(8)	–03C(A)	3.279(9)

[a] Generated by $\bar{x}\bar{y}\bar{z}$.

[b] Generated by $x\bar{y}1/2 + z$.

[c] Generated by $\bar{x}y1/2 - z$.

[d] Generated by $1/2 - x1/2 - y1/2 - z$.

[e] Generated by $1/2 - x1/2 + y - z$.

these bond lengths are high, the anion does appear to deviate significantly from a two-fold axis. These large e.s.d.'s reflect large correlation coefficients which in some cases were as great as 0.9.

The two adjacent $\alpha Mg_2P_2O_7$-like layers have cations occurring in pairs sharing two oxygen atoms. One of these cations is coordinated to six oxygen atoms while the second shows five-fold coordination. This dimer group is bonded to a similar group in the same layer through a pair of shared oxygen atoms. In $\alpha Mg_2P_2O_7$, these two dimers are related by a 2_1 axis lying in the sheet of the cations. In $\alpha Zn_2P_2O_7$, the B and C layers do not materially deviate from that found in $\alpha Mg_2P_2O_7$. Thus, if $\alpha Zn_2P_2O_7$ were to have symmetry I2/c then the cations in layer "A" should be related by a center of symmetry with the anion in the layer lying on the two-fold axis.

The refinement was completed in the higher symmetry space group with the two-fold axis through the anion in the A layer. The final value of R_2 obtained with weights chosen as $W = (43 - 1.4\ \mathrm{Fo} + 0.015\ Fo^2)^{-1}$ was 0.089 and all thermal ellipsoids were positive definite. The value of $R (= 0.080)$ was found to be a significant improvement over that obtained in space group IC. The bond geometries around the anion had improved in the sense that chemically equivalent bonds were more nearly equal.

A few additional cycles of refinement were carried out varying the anisotropic thermal parameters on the oxygen atoms. However ultimately the thermal ellipsoid became non-positive for 02(2) and 03A and thus this model was rejected.

The final atomic parameters are displayed in Table II while the observed and calculated structure factors for all the data are found in Table III.

Description of Structure

The gross features of the structures are as discussed for the refinement in the space group of lower symmetry. The bond distances and angles, collected in Table IV, have in fact shifted in a direction such as to yield chemically more reasonable anion geometries. The anion in layer A has a P—O—P bond angle of 139° with a bridging P—O bond of 1.603(6) Å and terminal P—O bonds averaging 1.53 Å. The bridging P—O bonds in the second anion are 1.599(8) and 1.566(7) Å with average terminal P—O bonds having values of 1.51 and 1.52 Å on side 1 and 2, respectively. Here the P—O—P bond angle is 148°. As has been found in $\alpha Mg_2P_2O_7$ the oxygen atom strongly bonded to only one cation, 03T, show the shortest terminal P—O bond length at 1.49(1) Å. Again as in $\alpha Mg_2P_2O_7$ the longest bridging P—O bond lies on the same side of the anion as the shortest-terminal P—O bond.

The cations showing six-fold coordination have remained in essentially the same place relative to the symmetry elements, as in the β phase. The remaining cations have been displaced largely along the direction of the axial bond and as a result, the bond to the oxygen atom in the direction opposite to this displacement is broken. This feature is also found in $\alpha Mg_2P_2O_7$ and $\alpha Cu_2P_2O_7$. The cationic displacements in the *a–c* plane from the analogous β phase positions are 0.27 Å in the $\alpha Cu_2P_2O_7$-like layer and 0.30 Å in the $\alpha Mg_2P_2O_7$-like layer.

Discussion

It is now apparent that the ordered structures in this series of compounds are intimately related. $\alpha Cu_2P_2O_7$ has a structure where the anion direction is the same for every anion in a sheet. A sheet is the region between planes separated by 1/2 *c* (of the α phase) and centered by the cations. In $\alpha Mg_2P_2O_7$ there is an anti-phase boundary after every two layers while in $\alpha Zn_2P_2O_7$ they occur after every third layer. In each case, a unit cell is defined after two such anti-phase boundaries. The transformation of $Cu_2P_2O_7$ indicates (*11*) that phase boundaries occur on the average after eight layers.

The cations in $\alpha Cu_2P_2O_7$ show five-fold coordination with the sixth oxygen atom displaced axially to a distance of 2.9 Å. In $\alpha Mg_2P_2O_7$ the symmetry is further reduced with the formation of a sixth additional bond to half the cations. The axial oxygen atom to the remaining cation lies displaced by over 3.3 Å. As has been indicated, the $\alpha Zn_2P_2O_7$ shows a mixture of the two structures with sequences defined by $\alpha Cu_2P_2O_7$-like layers separating a pair of $\alpha Mg_2P_2O_7$-like layers. This latter pair are symmetry-related as in $\alpha Mg_2P_2O_7$ whereas the $\alpha Cu_2P_2O_7$-like layer has the elements of symmetry of the layer in $\alpha Cu_2P_2O_7$. The $\alpha Zn_2P_2O_7$ structure suggests that the "up" "down" sequence of $\alpha Mg_2P_2O_7$-like layers should be regarded as the stabilized arrangement.

A detailed comparison of the anions, shown in Fig. 2, with those in the parent structures indicates a great deal of similarity. The bridging P—O bond length has increased from 1.576(7) Å in $\alpha Cu_2P_2O_7$ to 1.603(6) Å in $\alpha Zn_2P_2O_7$. This effect follows from decreased πp–πd bonding predicted by Cruickshank (*17*) as a result of the P—O—P angle decreasing from 157°, as found in $\alpha Cu_2P_2O_7$, to 139° as found in $\alpha Zn_2P_2O_7$. The O—P—O bond angles involving the terminal oxygen atoms are all larger than the

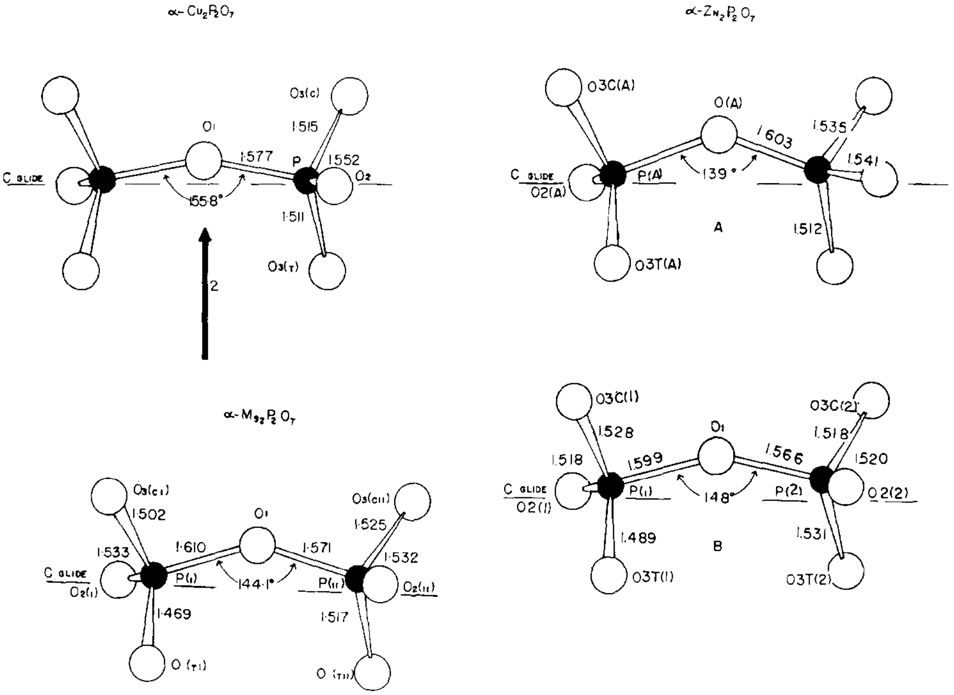

FIG. 2. The anions found in $\alpha Cu_2P_2O_7$ and $\alpha Mg_2P_2O_7$ are compared with those found in $\alpha Zn_2P_2O_7$. The open circles are oxygen atoms and the filled circles are phosphorus atom. The bond lengths are shown in Å units.

ideal tetrahedral angle as if the phosphorus atom has been displaced from the center of the tetrahedra to the face formed by the terminal oxygen atoms. In both compounds only the 01-P-03T exceeds the ideal tetrahedral value while the remaining bond angles involving 01 are substantially smaller than 109.5°.

The anion in the $\alpha Mg_2P_2O_7$-like layer shows a P—O—P angle of 148° as compared to 144° in $\alpha Mg_2P_2O_7$. Here the bridging P—O bond is 1.599(8) Å on the side showing the shortest P—O bond (1.489(10) Å). In $\alpha Mg_2P_2O_7$ these lengths are are 1.612(10) and 1.472(10) Å. The bridging P—O bond on the remaining side is 1.566(7) compared to 1.569(10) Å in $\alpha Mg_2P_2O_7$. Both tetrahedra show O—P—O bond angles involving terminal oxygen atom substantially larger than 109.5°. The bond angles involving 01 are quite different on the two sides, with a greater regularity, for those involved with the shorter bridging P—O bond.

The phase transformation at 132°C generates a $\beta Zn_2P_2O_7$ size cell but with two independent cation sites for the Mn^{2+} ion. Since the size of the resonance from the two sites seems to have equal amplitudes and the difference in the zero field splitting parameter changes relative to the β phase are comparable to those found in $\alpha Mg_2P_2O_7$, it appears that the structure transforms to one where half of the cations have five-fold coordination and the remainder have six-fold coordination. Since the line widths are very broad in the transformation region there appears to be a variation in the detailed topology about each of these cation sites.

Unfortunately there does not appear to be a structural reason for a change to equal numbers of five- and six-fold coordinated cations. Further the displacement from the high temperature resonance, where all cation sites are six-fold, is equal and opposite for the two sites. The zero field splitting parameters is primarily sensitive to fields produced by the near neighbor environment and thus the five coordinate site is expected to differ much more from the β phase than the six coordinate site. Of course we may in fact be seeing directly the effects of the distortions arising from the Mn^{2+} on the local environment in $\alpha Zn_2P_2O_7$. At any rate the molecular basis of the intermediate phase in $Zn_2P_2O_7$ is not understood.

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