Table 3. Cr–Al *distances and inter-bond angles in* $Cr_4Si_4Al_{13}$, $Mg_3Cr_2Al_{18}$ *and* θ(Cr–Al)

Phase	Al atom	Neighbours	Distances (Å)	Angle (°)
$Cr_4Si_4Al_{13}$	Al_1	2 Cr	2·46 (2)	166·2
	Al_2	2 Cr	2·77 (2)	60·5
$Mg_3Cr_2Al_{18}$	Al_f	2 Cr	2·58 (2)	173·2
	Al_g	1 Cr	2·81	—
θ(Cr–Al)	Al_0	4 Cr	2·58 (4)	180 (2)
	Al_7	2 Cr	2·47 (2)	167·9
	Al_8	2 Cr	2·48, 2·57	175·0
	Al_{11}	2 Cr	2·53, 2·59	162·7
	Al_{13}	2 Cr	2·48, 2·57	169·4
	Al_3	2 Cr	2·68 (2)	59·6
	Al_6	2 Cr	2·78 (2)	57·2
	Al_{14}	2 Cr	2·80, 2·91	102·4
	Al_{15}	2 Cr	2·77, 2·79	104·9
	Al_5	3 Cr	2·62 (2), 2·53	$\leqslant 180$
	Al_4	3 Cr	2·74 (2), 2·86	$\leqslant 180$
	others	1 Cr	> 2·59	—

Cr–Al distances in the three phases fall into two groups, one of which is significantly shorter than the sum of the twelve-co-ordinated radii of the atoms. These short distances indicate a stronger Cr–Al interaction which is associated with the sharing of corners between the icosahedra when the Cr–Al–Cr bond angle is near 180°. This suggests a directional character not usually associated with a purely metallic bond.

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The Crystal Structure of Sodium Triphosphate, Na5P3O10, Phase I

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The crystal structure of the high-temperature form of sodium triphosphate, $Na_5P_3O_{10}$, Phase I, has been determined by Fourier methods. The unit cell is monoclinic with

$$a = 9\cdot61, \quad b = 5\cdot34, \quad c = 19\cdot73 \text{ Å}; \quad \beta = 112°.$$

The space group is $C2/c$ and the unit cell contains 4 units of $Na_5P_3O_{10}$. The triphosphate ions have twofold axial symmetry with the central phosphorus atoms lying on twofold axes of the unit cell. Bond lengths are P–O (chain) $= 1\cdot62 \pm 0\cdot03$ (inner), $1\cdot66 \pm 0\cdot03$ (outer), P–O (mean, terminal) $1\cdot48 \pm 0\cdot03$ Å. The structure is generally more distorted than that found previously for the low-temperature form, Phase II. Some of the sodium ions are co-ordinated in distorted octahedral arrangements, while the remainder are involved in 4-fold co-ordination of an unusual type. A comparison of the structures of Phase I and Phase II suggests an explanation of some of their differences in properties.

Introduction

The crystalline forms of sodium triphosphate $Na_5P_3O_{10}$ and its hexahydrate are of theoretical interest and of importance in the production of modern detergent powders. A knowledge of the crystal structures of these salts is relevant to the explanation of many of the phenomena connected with their preparation, interconversion and hydration, which are at present only partially understood (Raistrick, 1948,; Van Wazer, 1958). In the present paper the structure of the high temperature anhydrous form, Phase I, is worked out and compared with that of the low temperature form, Phase II, which has been given previously (Davies & Corbridge, 1958).

Small crystals were obtained from a melt of composition 45% sodium pyrophosphate ($Na_4P_2O_7$) and

55% sodium trimetaphosphate ($Na_3P_3O_9$). About 30 g. of the mixture were melted, and cooled from 620 °C. to 580 °C. over a period of 8 hr. The contents were then quenched in liquid oxygen and the resulting mass yielded (from several preparations), some small ragged needles which were used for the investigation.

Unit cell and space group

Rotation and Weissenberg photographs showed the crystals to be monoclinic with

$$a = 9 \cdot 61 \pm 0 \cdot 03, \ b = 5 \cdot 34 \pm 0 \cdot 02, \ c = 19 \cdot 73 \pm 0 \cdot 05 \text{ Å};$$
$$\beta = 112 \pm 0 \cdot 5°.$$

Systematically absent reflections were hkl for $h+k$ odd and $h0l$ for l (and h) odd, which indicated the space group as $C2/c$ or C/c in accord with the data of Dymon & King (1951). The crystals were found to be non-pyroelectric and space group $C2/c$ was adopted. The density determined by flotation was 2·62 g.cm.$^{-3}$, and that calculated assuming 4 units of $Na_5P_3O_{10}$ per cell was 2·60 g.cm.$^{-3}$.

Intensity data

Intensity data were obtained by visual estimation of a and b axis Weissenberg photographs taken with Cu $K\alpha$ radiation. A multiple-film technique was used and the various photographs were related and corrected for geometrical and polarization factors by the usual methods. Absorption errors were minimized by choosing the smallest and best-formed crystals available. Because the crystals were poorly formed and usually twinned, many had to be selected before photographs satisfactory for intensity measurement could be obtained.

Structure determination

Sodium triphosphate Phase I has the same space group ($C2/c$) as Phase II (Davies & Corbridge, 1958); moreover the unit cells in each structure contain 4 molecules and have symmetry axes of nearly the same length. In both structures the $P_3O_{10}^{5-}$ ion lies on a twofold symmetry axis since it cannot lie on a centre of symmetry because of the tetrahedral disposition of oxygen round the central phosphorus atom. The central phosphorus atom, P_1, therefore lies on a twofold axis with the remaining atoms occupying sets of eightfold general positions. Similarly, one set of sodium ions (Na_1) lies on centres of symmetry as in the Phase II structure, or on twofold symmetry axes, and the remaining sodium ions Na_2 and Na_3 occupy two sets of general positions.

A Patterson synthesis was computed for the b axis projection in order to find the (x, z) co-ordinates of the phosphorus atom P_2. These co-ordinates were found only after some difficulty, since the P–P vectors did not give rise to outstandingly strong peaks. A

preliminary Fourier synthesis was calculated using signs determined by the phosphorus atoms P_1 and P_2 and oxygen atoms O_1 and O_2 placed in projected tetrahedral disposition round P_1. The results of this synthesis together with further trial and error work led to the assignment of approximate (x, z) co-ordinates to the remaining atoms in the structure. The structure was then refined by successive electron density and difference syntheses until no further reduction in the agreement factor R_{h0l} could be obtained.

The y co-ordinates

Bond lengths equivalent to those found in Phase II were assumed, and using these in conjunction with the (x, z) co-ordinates, an approximate set of y co-ordinates relative to the central phosphorus atom P_1 was derived. The unique sodium atom Na_1 was placed at $y = 0$ and a set of absolute y co-ordinates for the triphosphate ion could be obtained by moving the ion along the twofold axis to give a sixfold configuration of oxygen atoms round the sodium ion. Approximate y co-ordinates for the remaining sodium ions were deduced from packing considerations and the tentative structure was consistent with the results of a Patterson synthesis for the a projection. Refinement was then carried out by electron-density and difference syntheses until a minimum value of R_{0kl} was reached. The final electron-density difference maps for the two projections are shown in Fig. 1. After the minimum values of R_{h0l} and R_{0kl} had been obtained from the difference syntheses, further adjustment of the parameters of O_4, O_5 and Na_3 was carried out, but this only led to a deterioration in the structure-factor agreement. The final values of the agreement factors were $R_{h0l} = 14 \cdot 0\%$; and $R_{0kl} = 12 \cdot 3\%$; the final atomic co-ordinates are listed in Table 1.

Table 1. *Final atomic co-ordinates*

	x	y	z
P_1	0·000	0·655	0·250
P_2	0·070	0·523	0·400
O_1	0·143	0·806	0·267
O_2	0·013	0·448	0·312
O_3	0·980	0·329	0·420
O_4	0·035	0·790	0·405
O_5	0·232	0·533	0·438
Na_1	0	0	0
Na_2	0·357	0·552	0·326
Na_3	0·258	0·965	0·429

An initial temperature factor of $B = 3 \cdot 0$ Å^2 was used (as in Phase II), but subsequent comparison of observed and calculated structure factors indicated values of $B = 1 \cdot 5$ Å^2 for phosphorus, and $B = 2 \cdot 0$ Å^2 for sodium and oxygen, as being more satisfactory values.

Discussion of the structure

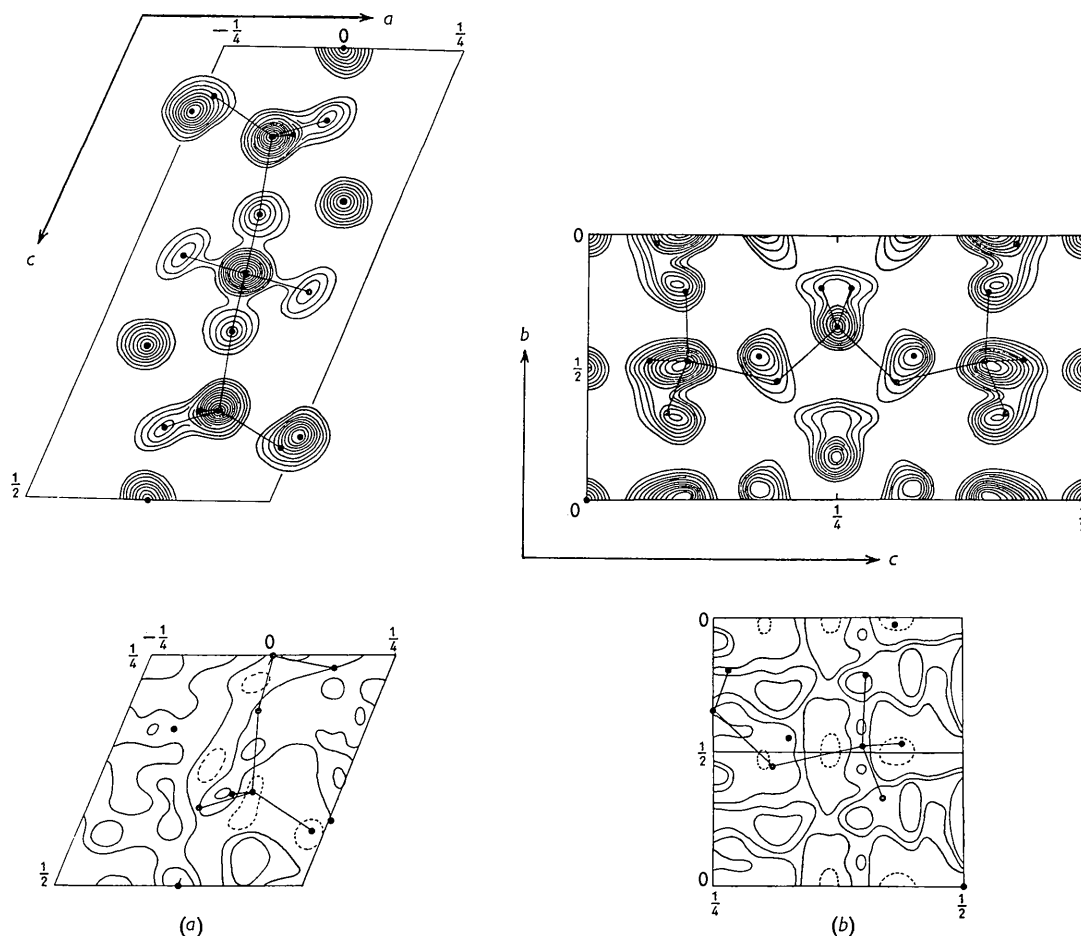A diagram of the structure in b projection is shown

Fig. 1. Projections (a) on (010), (b) on (100). Electron-density and difference syntheses, with contours drawn at arbitrary intervals. Contours on difference maps (lower figures) drawn at half the intervals as the corresponding electron-density maps (upper figures). Negative contours drawn in broken lines.
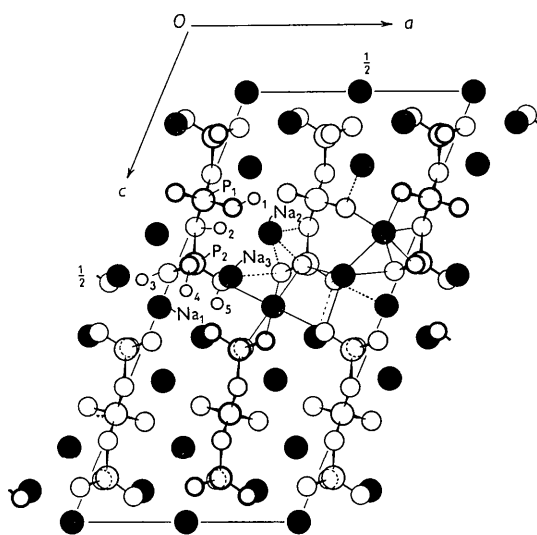

Fig. 2. Sodium triphosphate Phase I structure in b projection. Co-ordination of sodium ions shown in full lines and co-ordination of oxygen atoms completed by broken lines.

in Fig. 2. The triphosphate ion has a diad axis and the central phosphorus atom lies on a twofold axis of the unit cell, with the chain axis lying almost parallel to ($\bar{2}01$). Table 2 lists the interatomic distances and angles calculated from the data in Table 1.

Table 2. *Interatomic distances and angles in sodium triphosphate Phase I*

$P_1-O_1 = 1.519$ Å	$O_1-O_1' = 2.57$ Å	$P_1-O_2-P_2 = 121.8°$
$P_1-O_2 = 1.618$	$O_2-O_2' = 2.36$	$O_1-P_1-O_1' = 115.8$
$P_2-O_2 = 1.662$	$O_1'-O_2 = 2.61$	$O_1-P_1-O_2 = 112.8$
$P_2-O_3 = 1.494$	$O_2-O_1 = 2.56$	$O_1'-P_1-O_2 = 109.7$
$P_2-O_4 = 1.476$	$O_2-O_3 = 2.36$	$O_2'-P_1-O_2 = 93.8$
$P_2-O_5 = 1.454$	$O_2-O_4 = 2.54$	$O_2-P_2-O_3 = 96.4$
$P_1-P_2 = 2.87$	$O_2-O_5 = 2.63$	$O_2-P_2-O_5 = 114.7$
	$O_3-O_4 = 2.56$	$O_2-P_2-O_4 = 118.0$
	$O_3-O_5 = 2.56$	$O_3-P_2-O_4 = 118.9$
	$O_4-O_5 = 2.23$	$O_3-P_2-O_5 = 120.2$
		$O_4-P_2-O_5 = 99.0$

The accuracy of the structure was limited by the quality of the crystals which could be obtained, and the overlapping occurring in each projection. A cal-
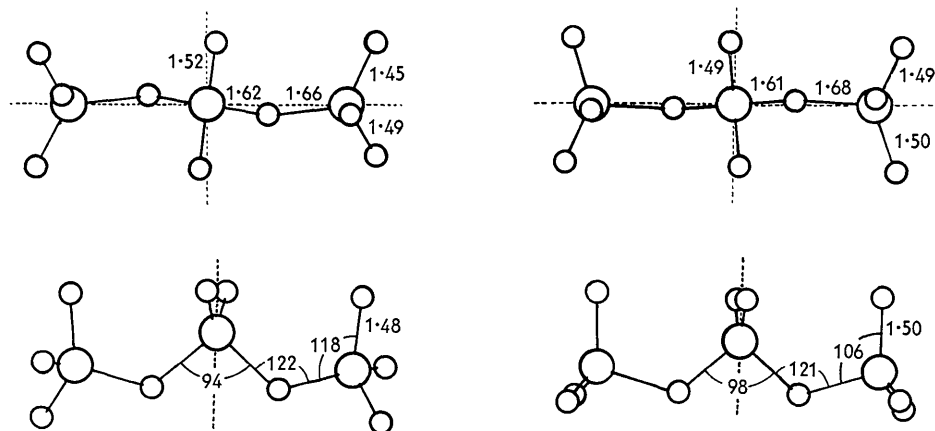
Fig. 3. Diagram of triphosphate ion in Phase I (left) and Phase II (right). Upper figures show ion viewed in b projection and lower figures, perpendicular to the $(\bar{2}01)$ and $(\bar{1}01)$ planes respectively. Mirror planes of a *trans* symmetrical configuration are shown in broken lines. Distances in Ångström units and angles in degrees. Glide plane related ions constitute enantiomorphic pairs in both Phase I and Phase II structures.

culation of the standard deviation of atomic co-ordinates by Cruickshank's method, for the (010) projection, gives $\sigma_x = \sigma_z \sim 0.03$ Å for the resolved oxygen atoms and $\sigma_x = \sigma_z \sim 0.01$ Å for the phosphorus atom. These figures suggest a standard deviation of about ± 0.03 Å in the P–O bond lengths, although the errors in the distances involving O_4 and O_5 could be somewhat greater. The differences between the inner and outer P–O chain distances are similar to those found in Phase II, but in the present structure these differences are probably within the limits of experimental error. In Fig. 3 the dimensions of the triphosphate ion in the two anhydrous forms of sodium triphosphate are compared. The distortion from a truly trans symmetrical configuration is greater in the present structure and considerable distortion of the terminal phosphate groups occurs.

Ionic co-ordination scheme

The ionic co-ordination scheme (Fig. 5) is generally less symmetrical than in Phase II. The sodium ions Na_1^+ and Na_2^+ are surrounded by oxygen in distorted octahedral arrangements, while the co-ordination of Na_3^+ is only fourfold. With the exception of two rather long contacts to Na_2, and excluding contacts greater than 3 Å, the Na–O distances are generally shorter than those found in Phase II, sodium pyrophosphate decahydrate (MacArthur & Beevers, 1957), and in other sixfold co-ordinated structures. The values in Table 3 may be

compared with the sum of the Pauling ionic radii (2·35 Å) and the octahedral values listed in Table 4.

Each Na_1^+ ion is linked to six different triphosphate anions and the octahedra form channels parallel to the b axis (Fig. 4). Pairs of triphosphate anions are linked 'end on', but unlike the corresponding arrangement in Phase II, the co-ordination octahedra do not share an edge in common with PO_4 tetrahedra. Three different anions are linked together by the Na_2^+ ions in a very unsymmetrical arrangement which involves the sharing of an octahedron edge with two oxygens (O_2 and O_3) of the same PO_4 group. Two of the anions are in successive unit cells along b and are linked together in a manner similar to a pair in the Phase II structure.

Table 3. *Sodium–oxygen distances in Phase I*

Na_1–O_3 = 2·32 Å	Na_2–O_1'''' = 2·26 Å	Na_3–O_4 = 2·22 Å
Na_1–O_4 = 2·31	Na_2–O_2' = 2·67	Na_3–O_5 = 2·33
Na_1–O_5' = 2·41	Na_2–O_4' = 2·31	Na_3–O_3' = 2·32
Na_1–O_5'' = 2·32	Na_2–O_3 = 2·32	Na_3–O_5''' = 2·59
Na_1–O_4'' = 2·31	Na_2–O_5 = 2·88	
Na_1–O_5''' = 2·41	Na_2–O_1 = 2·37	

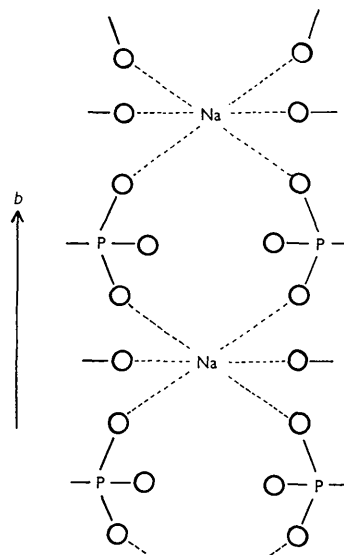Na_1–O(mean) = 2·35, Na_2–O(mean) = 2·47, Na_3–O(mean) = 2·37

Fig. 4. Co-ordination scheme for Na_1^+ forming continuous network parallel to b.

The sodium ions Na_3^+ form four short contacts in a rather 'one sided' arrangement involving three different anions. The remaining contacts, the shortest of which is 3·05 Å to O_5 in the cell above, presumably represent relatively weak attractions. One edge of the co-ordination polyhedron is shared with two oxygen atoms (O_4 and O_5) attached to the same PO_4 group which contributes to a very distorted arrangement.

The unsymmetrical co-ordination of Na_3^+ may be compared with the tetrahedral arrangement involving short contacts (2·30–2·41 Å) in sodium hydroxide monohydrate (Wunderlich, 1957), and the system found in sodium dithionite (Dunitz, 1956). In this latter structure the sodium ions make 4 short contacts (2·33–2·38 Å) in a one sided arrangement to a distorted square configuration of oxygen atoms, and this is balanced on the opposite side by two longer Na–O contacts (2·46 and 2·92 Å).
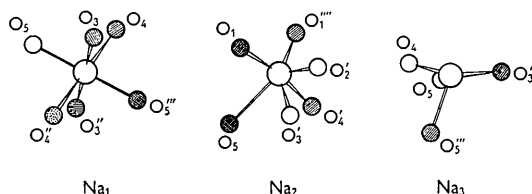

Fig. 5. Co-ordination of sodium ions viewed as in Fig. 2. Similar shading is used to denote oxygen atoms belonging to the same triphosphate ion in each co-ordination system.

Table 4. *Sodium–oxygen distances in ionic structures*

Salt	Range (Å)	Mean (Å)
6-fold co-ordination		
Sodium phosphoramidate	2·39–2·43	2·41
Sodium nitrite	2·46–2·54	2·50
Sodium chlorate	—	2·48
Sodium sulphate V	2·32–2·48	2·41
Sodium sulphate III (Na_1)	2·29–2·82	2·54
Sodium formate	2·35–2·50	2·44
Sodium oxalate	2·29–2·64	2·47
Sodium tropolonate	2·38–2·60	2·48
Sodium carbonate monohydrate	2·32–2·58	2·46
Sodium bicarbonate	2·35–2·57	2·47
Sodium sesquicarbonate	2·41–2·57	2·46, 2·44
Sodium zinc sulphato tetrahydrate	2·32–2·75	2·43
Sodium dithionate dihydrate	2·28–2·64	2·43
Sodium dithionite	2·32–2·92	2·46
Sodium pyrophosphate decahydrate	2·36–2·78	2·46, 2·55
Sodium triphosphate II	2·25–2·76	2·50, 2·47, 2·47
Sodium triphosphate I (Na_2)	2·26–2·88	2·47
5-fold co-ordination		
Sodium metasilicate	2·27–2·39	2·36
Sodium hydroxide tetrahydrate	2·35–2·38	2·36
4-fold co-ordination		
Sodium hydroxide monohydrate	2·30–2·41	2·36
Sodium triphosphate I (Na_3)	2·22–2·59	2·37
Close 6-fold co-ordination		
Sodium bromate	—	2·38
Sodium sulphate III (Na_2)	2·29–2·40	2·36
Sodium triphosphate I (Na_1)	2·31–2·41	2·35

Terminal atoms O_3 and O_4 are each co-ordinated to three sodium ions, and O_5 to four sodium ions. A continuous spiral parallel to b is formed by atoms of the O_1 type, each of which is linked to two sodium ions. Oxygen O_2 is linked on one side only to Na_2, the remaining contacts being greater than 3·3 Å. In Phase II the triphosphate ions are linked by O–Na–O contacts into sheets in the chain plane parallel to ($\bar{1}01$). In Phase I the corresponding sheet structure parallel to (100) is less well defined since relatively more ionic contacts are involved in inter-sheet linkages.

The expected decrease of co-ordination distance associated with a reduction of co-ordination number is illustrated for the case of sodium and oxygen in Table 4, which lists the more reliable data which are available. In octahedral configurations the mean Na–O distance usually lies in the range 2·40–2·50 Å, irrespective of the degree of distortion imposed by the rest of the structure which may result in some very short individual contacts. The mean (and individual) Na–O distances are near 2·36 Å in arrangements of lower co-ordination number. In the present structure the mean co-ordination distances involving Na_2^+ and Na_3^+ lie close to octahedral and lower co-ordination values respectively. The remaining sodium Na_1^+ is sixfold co-ordinated entirely by short contacts, like one of the sodium ions in the metastable form of sodium sulphate, Na_2SO_4 III (Frevel, 1940).

Relationship of structure and properties

The transition from Phase II to Phase I at about 415 °C. generally takes place more readily than the reverse process and there is evidence that the latter proceeds only through the amorphous phase (Topley, 1949; Van Wazer, 1958). Any transition between the two forms must involve considerable structural rearrangement, but the transition II → I might involve only a partial break up and re-orientation of the sheet-
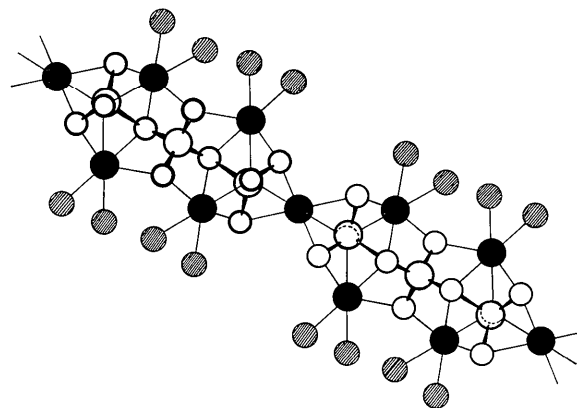

Fig. 6. Suggested hydrated sheet structure which may be present in concentrated solutions of Phase II. Viewed in (*b*) projection and formed by ($\bar{2}02$) cleavage of Phase II structure (ref. in text). Water molecules shown as shaded circles.

Table 5. Observed and calculated structure amplitudes

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
2 0 0	152	+144	4 0 16	22	+22	$\bar{4}$ 0 14	46	+33	0 2 7	<7	−6
4	134	+146	18	67	−53	16	151	+114	8	75	−87
6	14	+28				18	<20	+2	9	38	−50
8	62	+68	6 0 2	24	−27	20	26	+28	10	59	+56
10	18	−19	4	62	+62	22	61	−58	11	9	+10
			6	45	+46				12	41	+37
0 0 2	~20	+23	8	19	+26	$\bar{6}$ 0 2	168	−161	13	44	−37
4	39	−43	10	59	−42	4	158	+110	14	<10	−6
6	193	−195	12	60	+60	6	136	+105	15	40	+43
8	83	−80	14	16	−10	8	41	+42	16	16	+22
10	75	+68	8 0 2	37	−40	10	<13	+23	17	<12	+11
12	175	+166	4	45	+50	12	40	−27	18	38	+36
14	52	−42	6	21	+11	14	15	−35			
16	32	+32	8	<16	−24	16	103	+102	0 4 1	41	−40
18	19	+6	10	16	−22	18	<15	+3	2	47	+58
20	32	+20	12	16	+18				3	48	−44
			10 0 2	35	−39	$\bar{8}$ 0 2	<13	−1	4	53	−42
0 2 0	151	+177	4	<16	+10	4	76	+71	5	<13	+13
4	98	+94	6	24	+24	6	<13	+2	6	19	−19
6	42	+50				8	<13	−16	7	17	+14
			$\bar{2}$ 0 2	100	−93	10	76	−86	8	<13	−19
2 0 2	<9	−5	4	86	−100	12	77	+67	9	25	+28
4	77	+70	6	24	+13	14	41	+35	10	60	−56
6	33	−41	8	253	+247	16	77	+74	11	<13	−10
8	9	−2	10	30	+56	18	21	−19	12	20	+18
10	182	+160	12	35	+56				13	27	−34
12	75	+62	14	122	−112	$\bar{1}0$ 0 2	20	+20	14	<12	+9
14	35	−43	16	15	−8	4	77	+60	15	16	−12
16	16	−28	18	16	+18	6	<15	−7	16	16	−12
18	70	−56	20	106	+83				17	47	+43
20	53	+45	22	22	−20	$\bar{1}2$ 0 2	—	—	18	28	+27
22	50	+56				4	29	+35			
			$\bar{4}$ 0 2	<10	+6	6	34	−33	0 6 1	<12	+3
4 0 2	182	+193	4	<10	+7				2	<12	+10
4	35	+34	6	47	−65	0 2 1	<7	−1	3	<12	−19
6	112	−126	8	<12	+6	2	71	+82	4	<12	+7
8	51	−66	10	35	+40	3	57	+49	5	20	+25
10	24	−20	12	39	−42	4	60	−57	6	37	−42
12	112	+102				5	37	+30	7	12	−6
14	59	+62				6	38	+44	8	16	−23

like units already present in the structure. On the other hand, in the Phase I structure the relatively greater number of intersheet ionic attractions and the unsymmetrical co-ordination of Na$_3^+$ may favour a lattice break-up in all directions to form a completely amorphous phase prior to growth of a Phase II lattice.

Phase I is the more rapidly hydrating form of sodium triphosphate although both anhydrous forms are metastable and cannot be recrystallized from water. Phase I has a higher potential solubility than the low-temperature form, but solution is accompanied by the rapid formation of crystalline hexahydrate. Phase II on the other hand can be dissolved in water to form a two-fold supersaturated solution from which the hexa-hydrate crystallizes comparatively slowly (Van Wazer, 1958).

The greater ease of hydration of Phase I is presumably connected with the presence of 4 co-ordinated sodium ions (Na$_3^+$), which represent a relatively unstable arrangement. Structures with 4 or 5 co-ordinated sodium ions (Table 4) all have a strong affinity for water. The co-ordination instability of Na$_3^+$ and the less well defined sheet structure, probably favour a complete and ready break up of the lattice to give a high solubility, which may be great enough to initiate the growth of hexahydrate crystals. The rapid formation of crystalline hexahydrate from Phase I may also be facilitated by similarities in structure between the two salts and only when the structure of the hexahydrate is known will these phenomena be completely understood. The comparative reluctance of supersaturated solutions of Phase II to deposit hexahydrate crystals may be due to the presence of associated units whose structure is unfavourable for growth of the latter. An arrangement such as that shown in Fig. 6 might e.g. be formed by ionic cleavage to give hydrated 'polymeric' sheets.

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Short Communications

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Structure of morellin. By B. DAYAL and S. C. MATHUR, *Department of Physics, Banaras Hindu University, India*

Morellin is an antibiotic, extracted from the seeds of an Indian tropical evergreen Carcinia Morella (Mysore Gamboge tree); the yellow tetragonal crystals show positive birefringence, with marked elongation along [001] and a tendency to cleave very easily parallel to (110). The unit-cell dimensions, $a = 15.7$, $c = 11.7$ Å, are in good agreement with those given by Kartha (1954a). The empirical formula $C_{33}H_{38}O_7$ gives four molecules in the unit cell and the space group is $P4_1$ (Kartha, 1954b).

The provisional chemical formula suggested by Venkataraman in a private communication includes a chromene nucleus and an attached side-chain. The very marked yellow colour of the crystals suggests the presence of a chromophore such as a highly conjugated polycyclic system; the X-ray investigation briefly referred to in this communication confirms this view.

So far only Weissenberg photographs have been taken for $hk0$ and $0kl$ reflections and the intensities have been visually estimated. A very strong 430 reflection, together with the observed cleavage along (110) indicates that the flat ring system is lying nearly parallel to this plane with the longer axis of the molecule lying approximately parallel to the tetrad axis of the crystal. From packing considerations it was possible to give a sign to the 430 reflection and to a few others. An electron-density map calculated on this projection (Fig. 2) is consistent with the presence of a ring-system seen end-on and an additional group attached to the molecule.

A Patterson projection on (010) showed a strong maximum on the c axis at about 4 Å from the origin. This and other vector features were again consistent with a polycyclic ring system in spite of the overlapping molecules seen on this projected view of the crystal.

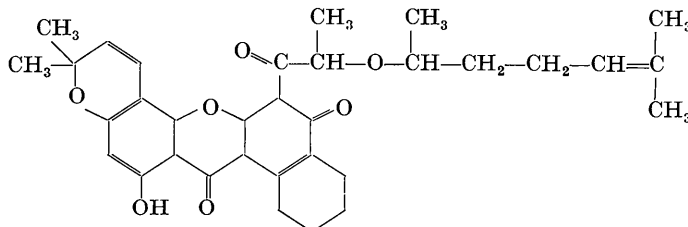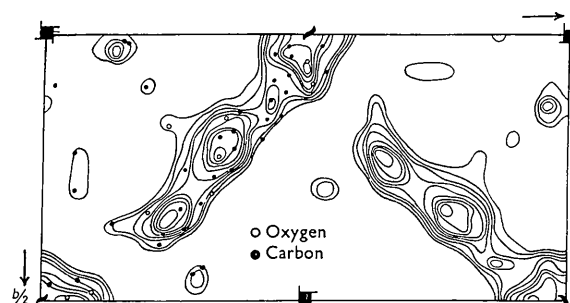Trials of atomic positions based on the formula of

Fig. 2. Fourier projection of morellin on the (001) plane along with the atoms of the quarter unit cell projected on the same plane, only half of the unit cell has been drawn.

Fig. 1 have shown reasonable agreement between calculated and observed structure factors but, owing to the complexity of the molecule and its awkward projections on (001) and (010), are not sensitive to further refinement. It is clear that the analysis needs to be carried out in three dimensions and this is now being done.

References

KARTHA, G. (1954a). *Current Sci.* **23**, 8.
KARTHA, G. (1954b). *Current Sci.* **23**, 216.

Fig. 1. Provisional chemical formula of morellin.

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