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The crystal structures of barium inosine-5′-phosphate and disodium inosine-5′-phosphate.

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The crystal structures of barium inosine-5′-phosphate ($C_{10}H_{11}O_8N_4P.Ba.6H_2O$) and disodium inosine-5′-phosphate ($C_{10}H_{11}O_8N_4P.Na_2.7{\cdot}5H_2O$) have been determined. The barium salt contains two crystallographically independent molecules in the structure of the space group $P2_12_12_1$. The structure of the sodium salt (space group, $C222_1$) has been deduced from that of the barium salt. The structural parameters defining the conformations of the molecules of the nucleotides are given as a preliminary report.

The crystal structures of barium inosine-5′-phosphate (Ba–IMP) and disodium inosine-5′-phosphate (Na–IMP) have been determined. The two structures are not isomorphous but they are homologous. Therefore, the result of the structure determination of Ba–IMP makes it possible to elucidate the structure of a Na–IMP.

Table 1. *Crystal data*

	Ba–IMP ($C_{10}H_{11}O_8N_4P.Ba.6H_2O$)	Na–IMP ($C_{10}H_{11}O_8N_4P.Na_2.7{\cdot}5H_2O$)
System	Orthorhombic	Orthorhombic
a	21·45 Å	23·06 Å
b	8·85	8·64
c	21·75	21·92
U	4128·9 Å^3	4367·4 Å^3
Z	8	8
Space group	$P2_12_12_1$	$C222_1$
D_m	1·935 g.cm^{-3}	1·62 g.cm^{-3}
D_x	1·928	1·616
Number of independent observed reflexions used for the structure determination.	2819	2165

Table 2. *Summary of the structural parameters for nucleotides*

	Nucleotide	φ_{OO}[a]	φ_{OC}[a]	Conformation about the C(4′)–C(5′) bond	φ_{CN}[c]	Displaced sugar atom[f]	φ_{OP}[e]
1	5′–TMP(Ca)	63°	57°	*gg*[b]	−48°	C(3′) endo (deoxyribose)	156°
2	5′–AMP	78	40	*gg*	−18	C(3′) endo	177
3	5′–UMP(Ba)	54	70	*gg*	−43	C(2′) endo	176
4	3′–CMP, orthorhombic form	74·7	43·8	*gg*	−42·1[d]	C(2′) endo	
5	3′–CMP, monoclinic form	73·7	45·5	*gg*	−39·3[d]	C(2′) endo	
6	3′–AMP	56·7	171·7	*gt*	− 3·9[d]	C(3′) endo	
7	AUP						
	adenosine residue	73	45	*gg*	−55	C(2′) endo	
	uridine residue	62	57	*gg*	−5	C(3′) endo	
8	5′–IMP(Ba)						
	molecule I	58	49	*gg*	−46[d]	C(2′) endo	170
	molecule II	57	51	*gg*	−34[d]	C(2′) endo	160
9	5′–IMP(2Na)	61	56	*gg*	−43[d]	C(2′) endo	172

[a] φ_{OO}: torsion angle O(1′)–C(4)–C(5′)–O(5′) and φ_{OC}: torsion angle C(3′)–C(4′)–C(5′)–O(5′), defined by Shefter & Trueblood (1965).

[b] Abbreviation of the torsion angles φ_{OO} and φ_{OC}, indicating the relative positions of the sugar and O(5′) atom. *g* and *t* denote the *gauche* and *trans* conformations, respectively.

[c] φ_{CN}: torsion angle about the glycosidic bond defined by Donohue & Trueblood (1960) and

[d] by Sundaralingam & Jensen (1965).

[e] φ_{OP}: torsion angle C(4′)–C(5′)–O(5′)–P.

[f] Sugars are ribofranose except 5′–TMP(Ca).

1. Calcium thymidylate (Trueblood, Horn & Luzzati, 1961).
2. Adenosine–5′-phosphate (Kraut & Jensen, 1963).
3. Barium uridine-5′-phosphate (Shefter & Trueblood, 1965).
4. Orthorhombic form of cytidine-3′-phosphate (Sundaralingam & Jensen, 1965).
5. Monoclinic form of cytidine-3′-phosphate (Bugg & Marsh, 1967).
6. Adenosine-3′-phosphate (Sundaralingam, 1966).
7. β-Adenosine-2′-β-uridine-5′-phosphoric acid (Shefter, Barlow, Sparks & Trueblood, 1964).
8. Barium inosine-5′-phosphate (present work).
9. Disodium inosine-5′-phosphate (present work).

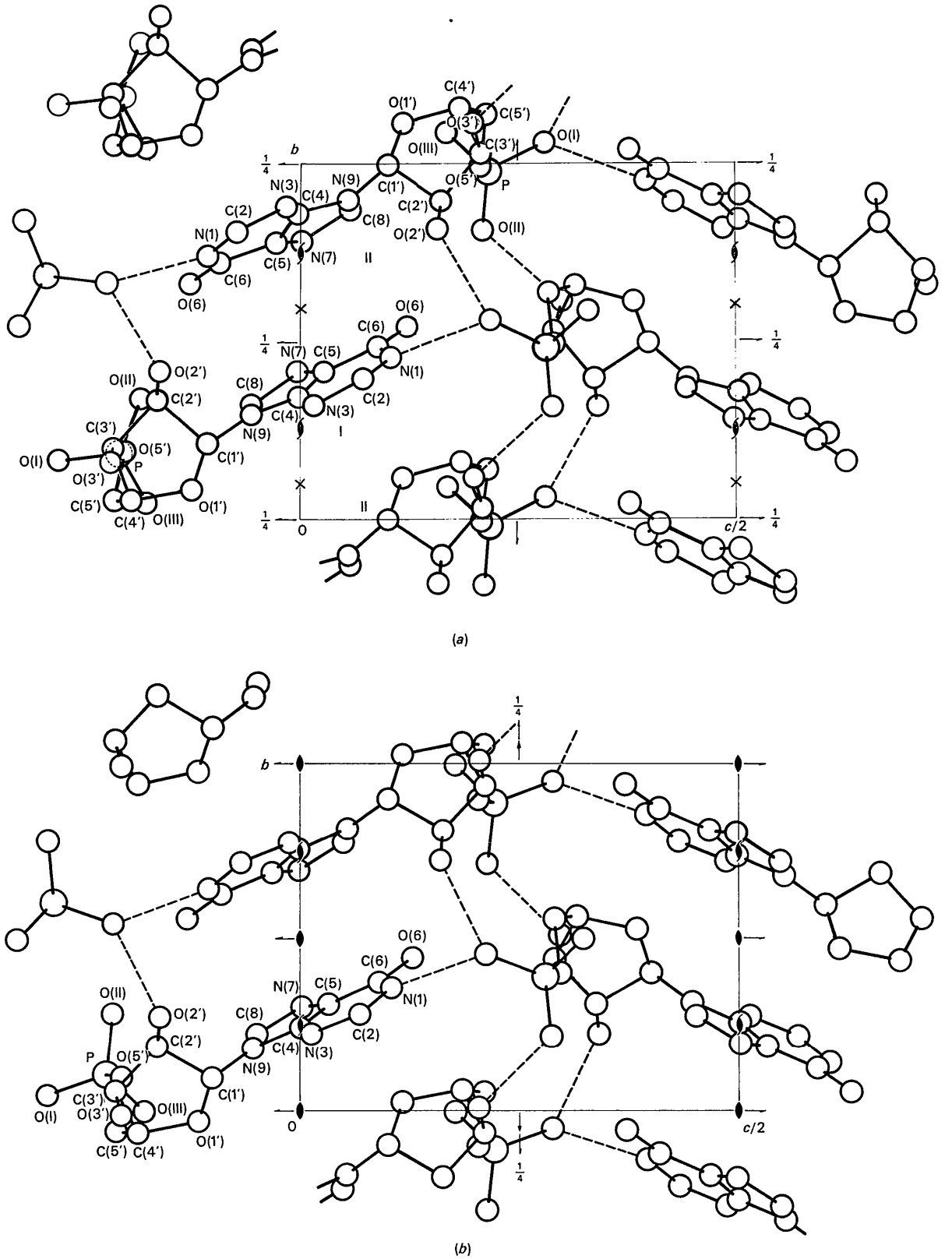

Fig. 1. Molecular packing viewed along the *a* axis. Metal ions and water molecules are omitted. Broken lines indicate intermolecular hydrogen bonds. (*a*) Ba–IMP (space group $P2_12_12_1$). Crosses (×) represent pseudo twofold rotation axes between molecules I and II. (*b*) Na–IMP (space group $C222_1$).

The unit-cell dimensions determined from precession photographs are shown in Table 1 together with other crystal data. Intensities were measured by visual estimation of the equiinclination Weissenberg photographs taken with Cu $K\alpha$ radiation. The structure of Ba–IMP determined by the heavy atom method was refined by block-matrix least-squares calculations, with anisotropic temperature factors, to an R value of 0·12. The a-axis projection of the structure is shown in Fig. 1(*a*). It is seen that the two crystallographically independent molecules (I and II) in the asymmetric unit take very similar conformations. However, they differ somewhat in the internal rotation angles such as those around the glycosidic bond (φ_{CN}) and the C(5′)–O(5′) bond (φ_{OP}). By inspection of Fig. 1 and disregarding the metal ions and water molecules, it is expected that a slight displacement of molecule I relative to molecule II would produce a twofold rotation axis (parallel to **a**) between them. If the molecules I and II moved so that the rotation axis passing through the point (0,0,0) was generated, then the space group of the structure would become $C222_1$. A gross feature of the structure of Na–IMP found in this way has been refined by difference Fourier syntheses followed by several cycles of block-matrix least-squares calculations. The R value at the present stage is 0·12. In Fig. 1(*b*) is shown the a-axis projection of the structure of Na–IMP.

Some of the well known structural parameters obtained for nucleotides are summarized in Table 2. A full account of the present work will be published elsewhere.

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