Crystal and Molecular Structure of Sodium Inosine 5′-Monophosphate, an Anticodon Nucleotide of Transfer Ribonucleic Acid

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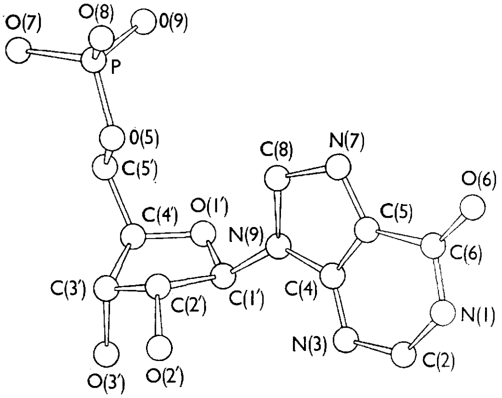
As part of our studies on the detailed molecular structures of the unusual components occurring in the anticodon loops of t-RNA, we have determined the crystal structure of the hydrated sodium salt of inosine 5′-monophosphate. The study also gave some indication of the mode of interaction and the stabilizing role of water molecules and alkali metal ions on the nucleic acids.

Crystals of the hydrated sodium salt of inosine 5′-monophosphate (5′-IMP) are orthorhombic, space group $C222_1$; $a = 8{\cdot}682 \pm 0{\cdot}003$, $b = 23{\cdot}216 \pm 0{\cdot}009$, and $c = 21{\cdot}917 \pm 0{\cdot}007$ Å, $D_m = 1{\cdot}576$ g.cm.$^{-3}$ (by flotation in $CHCl_3$–$CHBr_3$), $D_c = 1{\cdot}580$, $Z = 8$.

The intensities were measured on a Picker automatic diffractometer using nickel-filtered Cu-radiation ($\lambda = 1{\cdot}5418$) and the θ–2θ scan mode out to a 2θ value of 134°. The structure was obtained by the Patterson–Fourier technique using 1400 observed reflections. The refinement of the structure was carried through by the method of least-squares with isotropic and then anisotropic thermal parameters. The present discrepancy $R = 0{\cdot}10$.

A perspective drawing of the conformation of the nucleotide is shown in the Figure. The relative orientation of the base and the sugar defined by the torsion angle ϕ_{CN} around the glycosyl bond is $-44°$.[1] Thus the nucleotide displays the preferred *anti*-conformation.[2] The



FIGURE

D-ribose ring shows the C(2′)-*endo*-pucker,[3] with C(2′) displaced by 0·56 Å from the least-squares plane through the other ring atoms. The sugar-phosphate assumes the extended conformation.

The sodium ion has six near neighbours; four of them are water molecules and the remaining two are the ribose hydroxy-groups. The phosphate oxygens are thus not directly bound to the sodium ions, but bridged by the water molecules. There are nine independent sites for the water molecules per nucleotide. Five of these sites are fully occupied, of which two lie on the twofold axes. The remaining four sites are partially occupied, indicating disorder of these water molecules. The water content in the crystal turns out to be approximately six molecules by weight per nucleotide. However, the density of the crystal indicates the presence of eight molecules. It would thus appear that about two water molecules must have escaped during the process of data collection, as found in some other similar hydrated structures.[4] The structure is stabilized by an intricate scheme of hydrogen bonds with alternating layers of nucleotides and water channels in which the sodium ions are impregnated.

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[1] M. Sundaralingam and L. H. Jensen, *J. Mol. Biol.*, 1965, **13**, 914.
[2] J. Donohue and K. N. Trueblood, *J. Mol. Biol.*, 1960, **2**, 363.
[3] M. Sundaralingam, *J. Amer. Chem. Soc.*, 1965, **87**, 599.
[4] E. Shefter and K. N. Trueblood, *Acta Cryst.*, 1965, **18**, 1067.