X-RAY ANALYSIS OF MONOSODIUM CYTIDINE-5′-DIPHOSPHOETHANOLAMINE: $C_{11}H_{19}N_4O_{11}P_2Na.7H_2O$

We report here the molecular structure of monosodium salt of cytidine-5′-diphosphoethanolamine (CDP-ethanolamine) (Fig. 1) as determined from a three-dimensional single crystal X-ray analysis. CDP-derivatives play an important role in phospholipid metabolism. CDP ethanolamine, in particular, takes part in the biosynthesis of cephalin. The present study is in continuation of our X-ray analysis of nucleotide coenzymes (Viswamitra *et al.*[1]; Viswamitra *et al.*[2]).

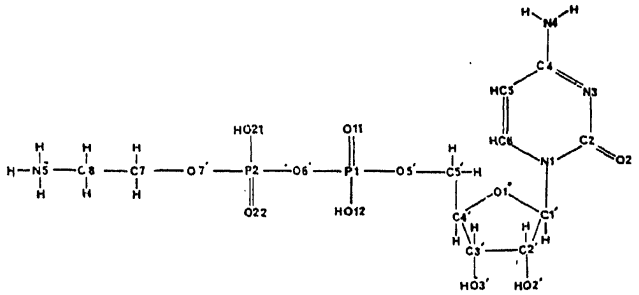

FIG. 1. Atom numbering scheme for CDP-ethanolamine molecule.

The monosodium salt of CDP ethanolamine (obtained from Boehringer Mannheim) is readily soluble in water giving neutral solution. Needle-shaped crystals of the compound were obtained from water-acetone solutions as in the case of nucleotide coenzymes[1, 2]. The crystal data were initially obtained from X-ray photographs and later refined on a Kappa-axis CAD-4 diffractometer.

$a = 6{\cdot}946$ Å, $b = 12{\cdot}503$ Å, $c = 28{\cdot}264$ Å,
$Z = 4$, $D_m = 1{\cdot}61$ gcm^{-3}, $D_{cal} = 1{\cdot}61$ gcm^{-3},
Space group: $P2_12_12_1$, $\lambda = 1{\cdot}5418$ Å.

The crystal (size $1{\cdot}95 \times 0{\cdot}15 \times 0{\cdot}025$ mm^3) mounted inside a Lindemann glass capillary along with a trace of mother-liquor was used for intensity data collection on the diffractometer. The reflections, 1454 in number, were retained as the observed ones out of a total of 2070 on the criterion that $I > 1{\cdot}5\sigma(I)$.

Structure Solution and Refinement

The structure was solved by direct methods using MULTAN (Main *et al.*[3]) followed by difference Fourier syntheses. Positional and the anisotropic thermal parameters were refined using structure factors least square techniques. The final R-factor for 1454 reflections was 10·4%.

Comments

The orientation of the base about the glycosidic N1–C1′ linkage is *anti* (C6–N1–C1′–O1′ = 62·8°). The ribose exhibits the uncommon C1′ *exo*–C2′ *endo* conformation. About the exocyclic C4′–C5′ and C5′–O5′ bonds the molecule has the usual *gauche*–*gauche* and *trans* conformations respectively (O1′–C4′–C5′–O5′ = − 66·3°, C3′–C4′–C5′–O5′ = 55·6°, C4′–C5′–O5′–P1 = 175·7°). The pyrophosphate has the characteristic staggered conformation (Fig. 2).

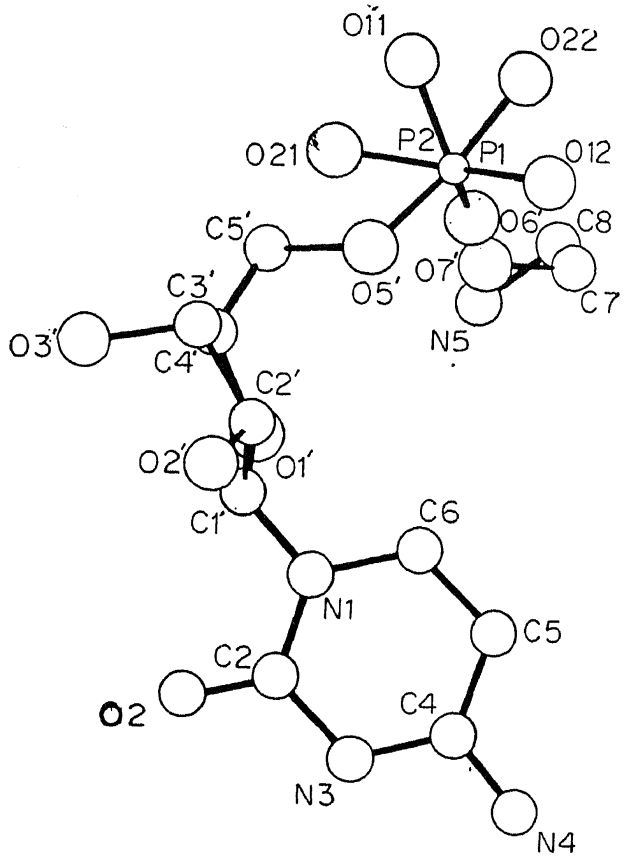

FIG. 2. View of the molecule down P1–P2 vector.

The bond lengths of the bridging oxygen O6′ to the two phosphorus atoms are different: P1–O6′ = 1·59 Å (0·01), P2–O6′ = 1·62 Å (0·01). Most of the torsion angles are similar to those of CDP–choline[1]. However, the torsion angle about P2–O7′ bond (− 102·7°) is significantly different from the corresponding angle in CDP–choline (71·3°) and this brings about a slightly extended structure for the former as compared to the highly folded one in the latter (Fig. 3). The intramolecular non-bonded N5···O7′ distance is 2·74 Å as a result of the *gauche* conformation about the C7–C8 bond (O7′–C7–C8–N5 = − 54·3°). The Na^+ ion is coordinated by five ligands from three indepedent CDP-ethanolamine molecules and does not link the base and the phosphate chain of the same molecule (Fig. 4). The distances of these ligands from Na^+ range from 2·20 Å to 2·45 Å. In the extended crystal structure the bases are not stacked. Three water molecules per nucleotide coenzyme have been presently identified. In the extended crystal structure the water molecules link up the phosphate and ethanolamine of the neighbouring molecules related by a 2_1-screw axis through hydrogen bonds. Details of the study will be published elsewhere.

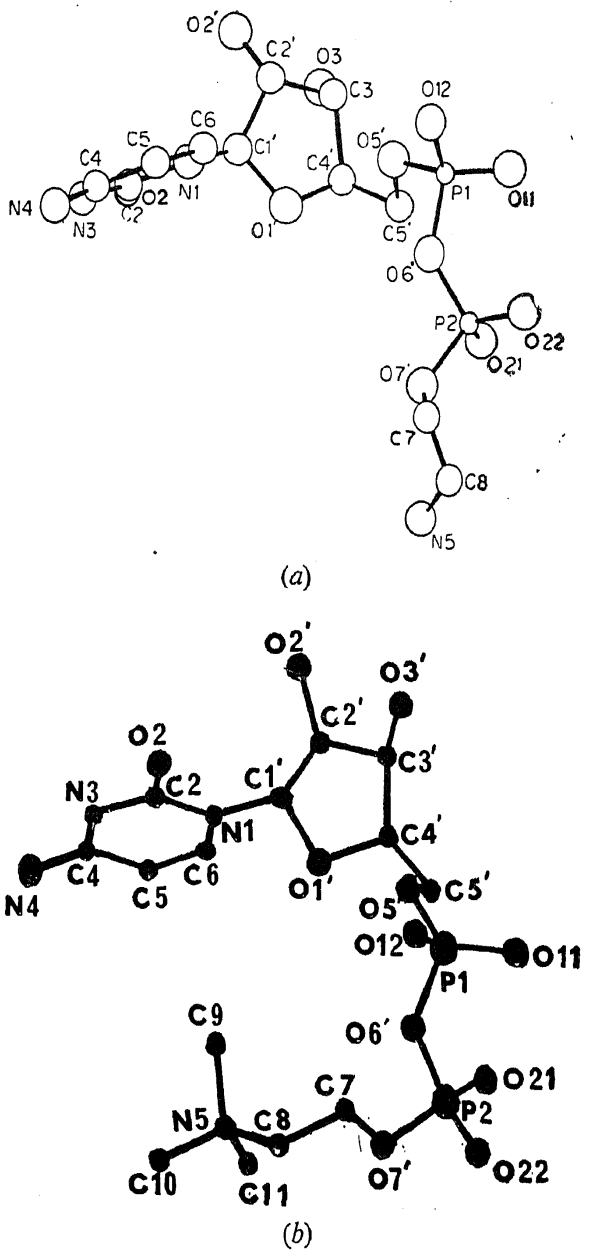

FIG. 3. Views of (*a*) CDP-ethanolamine and (*b*) CDP-choline almost perpendicular to the sugar.

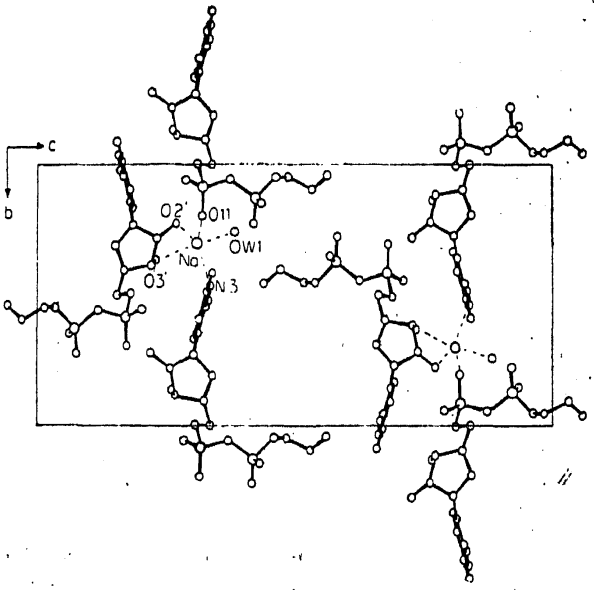

FIG. 4. Sodium ion binding to CDP-ethanolamine molecules as seen down *a*-axis.

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EFFECT OF SECTOR BOUNDARY PASSAGE ON THE DAILY VARIATION OF EQUATORIAL GEOMAGNETIC FIELD

SUBSTANTIAL evidence showing interesting relationships between terrestrial geomagnetic activity and the interplanetary magnetic field (IMF) direction in the ecliptic plane has been reported in literature in the wake of the discovery of the sector structure of IMF. Several articles reviewing the status of the knowledge on the topic have been written in recent times[1–4]. Rangarajan[5] recently examined the variation of the daily range of H-field at three stations in the Indian zone, spanning latitudes from the dip equator to near the Sq focus, in relation to sector boundary crossings using the sector boundary dates given by Svalgaard[6,7]. He noticed the mean daily range to show a conspicious increase on the day of the boundary crossing (irrespective of the type of boundary) at all the three stations, which feature was inferred by him to be essentially of non-ionospheric origin as the magnitude of the response at the three stations was found to be almost the same. This response of the daily range of H-field at equatorial latitudes to sector boundary passage was interpreted by him as due to a component of disturbance associated with sector boundary crossing. However, from a study of the behaviour of equatorial Dst in the vicinity of well defined sector boundaries, Kane[8] reported earlier that there is no definite and unambiguous relationships of equatorial Dst to solar magnetic sector structure. It is therefore felt worthwhile to re-examine the effect of sector boundary passage on the characteristics of the daily variation of H-field at equatorial latitudes using H-field data corrected for disturbance effects, to gain some insight into the origin of the effect of sector boundary passage noticed by Rangarajan[5]. In this brief communication, we present the results of such an analysis of H-field data at two stations in the Indian equatorial region.