fact that a_M is replaced by a in equation (1) and this approximation results in an error of 2 to 3%. Lack of accuracy in visual measurements of δ in those days (prior to 1952) may also contribute to this variation. Thus, within this limitation, the experimental and literature curves are agreeing very well. This, in turn, suggests general applicability of the method with reasonable accuracy. The chief advantage of this method is that MORD curves can be drawn theoretically for any system available in solid or liquid or liquid crystalline form without recourse to instrumentation of MORD. This involves less expensive equipment compared Magneto optic spectropolarimeter. The MORD is seen to have common origin of ORD by Dawber[5], and this suggests the utility of MORD for conformations (like ORD). Attempts to utilise MORD for conformations is in progress.

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X-RAY ANALYSIS OF THE MONOPOTASSIUM SALT OF ADENOSINE-5'-DIPHOSPHATE-DIHYDRATE $C_{10}H_{14}N_5O_{10}P_2K.2H_2O$

The ADP–ATP system plays a vital role in the energy transfer processes of a cell. Enzymatic reactions involving this system require the presence of various metal ions as cofactors. For example, the phosphorylation of ADP to ATP by the enzyme pyruvate kinase specifically demands the presence of monovalent K^+ ions along with Mg^{2+}. Detailed geometry of these coenzymes, when they are bound to K^+ and Mg^{2+} ions will therefore be of interest. We report here the molecular structure of the monopotassium salt of adenosine-5'-diphosphate (ADP-K) (Fig. 1) as obtained from the single crystal X-ray analysis.
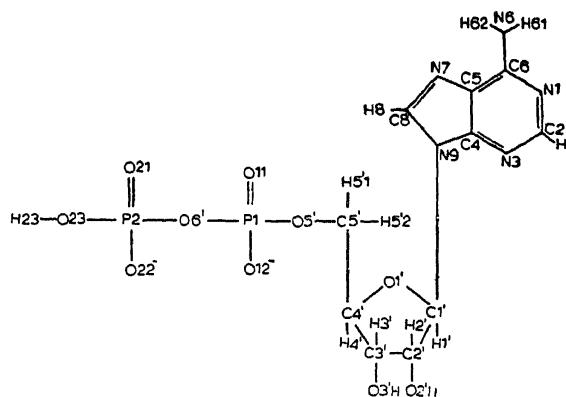

Fig. 1. Atom numbering scheme for ADP–molecule.

Crystal Data

Needle shaped crystals of ADP-K (obtained from Boehringer Mannheim) were grown by diffusion of isopropyl alcohol into its water solutions. The space group is $P2_12_12$ with $a = 28\cdot470$ Å, $b = 11\cdot449$ Å, $c = 6\cdot325$ Å, $Z = 4$, $D_m = 1\cdot81$ gcm^{-3}, $D_{cal} = 1\cdot82$ gcm^{-3}. A crystal (dimensions $0\cdot02 \times 0\cdot04 \times 0\cdot08$ mm^3) sealed inside a Lindemann glass capillary along with a drop of mother liquor was mounted on a CAD-4 automatic diffractometer. Three-dimensional intensity data, to a theta limit of 50° were collected using crystal monochromated copper $K\alpha$ radiation. Out of the 1190 reflections totally collected, those with $F > 2\sigma$ (F) were treated as observed reflections.

Structure Solution and Refinement

The cell dimensions of ADP-K are found to be very close to those of ADP-Rb in the same space group[1]. Hence the structure was solved using the coordinates of the ADP-Rb crystal structure, as the starting point with K^+ replacing Rb^+ ion. Block diagonal least squares refinement with individual isotropic temperature factors brought the R factor to $26\cdot3$%. A difference Fourier map at this stage revealed one water molecule, which again coincided with the one seen in ADP-Rb structure. Refinement including this water molecule and a subsequent difference Fourier showed up two peaks at special positions. These two were treated as water molecules with half the occupancy. During the final cycles of refinement K, P1 and P2 were given anisotropic temperature factors. The present R-factor is $16\cdot6$% for the observed reflections. Further refinement is in progress. The positional parameters for nonhydrogen atoms can be obtained from the authors.

Comments

The orientation of the base about the glycosidic C1'–N9 linkage is *anti* (C8–N9–C1'–O1' $= 42\cdot4°$). The ribose ring shows C2'-*endo* puckering. The conformation about C4'–C5' bond is *gauche-gauche* (C3'–C4'–C5'–O5'$=66\cdot5°$, O1'–C4'–C5'–O5' $=-67\cdot4°$)
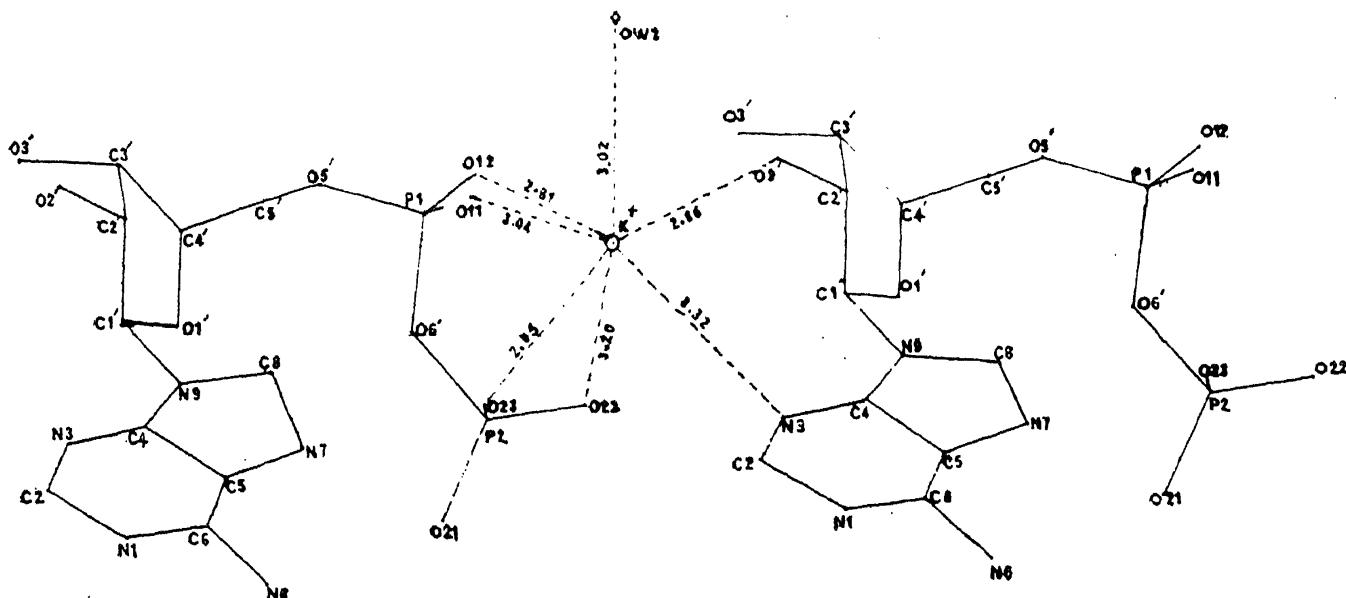
FIG. 2. View of the coordination sphere of potassium ion down c-axis (O11 bound to potassium belongs to the c-cell translated ADP molecule).

and that about C5′-O5′ bond is trans(C4′-C5′-O5′-P1 = 144·6°). The pyrophosphate moiety has a staggered geometry. K+ ion is in contact with three independent ADP molecules. Its coordination sphere consists of seven nearest neighbours with distances ranging from 2·8 Å to 3·3 Å as shown in the diagram (Fig. 2). In the extended crystal structure there is no self-association of bases either by base pairing or by base stacking. The main interactions between different molecules are pairs of hydrogen bonds between the adenine base and the pyrophosphate groups (Fig. 3). Similar interactions have been observed in ADP-free acid[2] and ADP-Rb structures also. The water molecules stabilise the structure by forming hydrogen bonds between two neighbouring molecules of ADP-K related by a two-fold axis.

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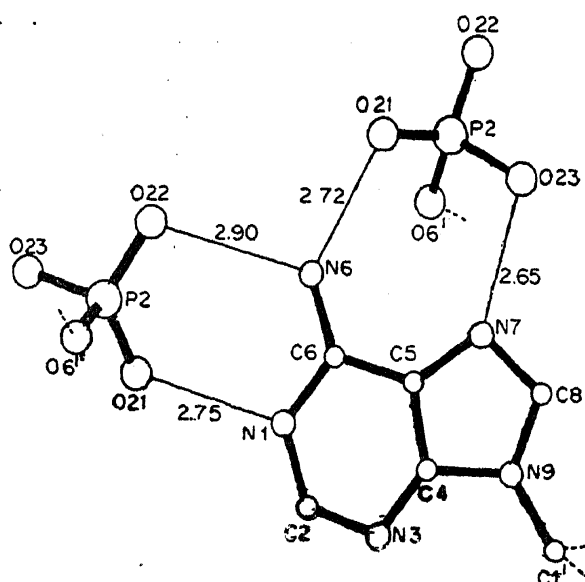2. Hosur, M. V. and Viswamitra, M. A., *Curr. Sci.*, 1979 (communicated).

FIG. 3. Hydrogen bonds between base and pyrophosphates.

KINETICS AND MECHANISM OF Ru(III) CATALYSED OXIDATION OF ALCOHOLS BY PERIODATE

TRANSITION metal complexes are known to act as good hydride ion abstracting agents both in acidic[1] as well as in basic[2] media. Under normal conditions monohydric alcohols do not undergo oxidation by periodate. It was therefore thought worthwhile to find out whether Ru(III) salts can act as catalysts in the oxidation of simple monohydric alcohols by periodate in basic medium.

All the chemicals used were of (BDH) AR grade or extra pure quality and purified by standard methods wherever necessary. A known volume of alcohol was added to the flask containing the required quantities of NaOH, RuCl₃ and NaIO₄ solutions after thermostating them for 30 min. Unreacted periodate at