Syntex $P2_1$ diffractometer of which 1,200 were significant on the basis of $F > 3\sigma(F)$. The data were of moderate accuracy due to the poor quality of the crystal specimen.

The structure was solved by the application of MULTAN[8] and a difference Fourier synthesis and refined anisotropically in a full-matrix least squares program to $R = 11.9\%$.

A view of the molecule, perpendicular to the base, is shown in Fig. 1. The orientation of the base about the glycosidic C1′–N9 linkage is *anti*, the only conformation so far observed in the crystal structures of nucleotides. The dihedral angles O1′–C1′–N9–C8 and C2′–C1′–N9–C8 are 40.3° and −75.8°.

In the ribose ring, C2′ is displaced by 0.54 Å from the mean plane through C3′, C4′, O1′, C1′ corresponding to a typical C2′-*endo* puckering. The conformation about the C4′–C5′ bond is *gauche gauche* with torsion angles O5′–C5′–C4′–C3′ = 57.0° and O5′–C5′–C4′–O1′ = −63.3°. The conformation about C5′–O5′ is *trans* (P1–O5′–C5′–C4′ = 147.1°). A similar conformation has also been proposed as the predominant structure of ADP in solution, from a Fourier transform nuclear magnetic resonance (NMR) study[9]. The pyrophosphate moiety has a staggered conformation. A striking feature of the structure is the observed difference of 0.10 Å between the lengths of the two bridging bonds in the high energy linkage, which seems to be significant at the level of accuracy attained in the present analysis. The values for P1–O6′ and P2–O6′ are 1.54 and 1.64 Å respectively with an estimated s.d. of 0.02 Å. The angle P1–O6′–P2 is 135° (e.s.d. 1°). Corresponding values in other nucleoside diphosphates recently determined by us are 1.60 and 1.64 Å and 133° in cytidine diphosphocholine and 1.58 and 1.62 Å and 128° in cytidine diphosphoric acid[10].

In the crystal structure, the ADP molecule is folded but there is no Rb^+ bridge between the phosphate and adenine groups of the same molecule. Nor is there any evidence of other types of intramolecular interactions such as hydrogen bonding or metal binding between the pyrophosphate chain and the base or sugar moiety. In this respect, the ADP structure resembles the conformations found in the crystal structures of the dipotassium salt of uridine-5′-diphosphate (M.A.V., M. L. Post and O.K., unpublished) and the monosodium salt of cytidine diphosphocholine[10]. These coenzyme molecules, which are in very different crystalline environments, are also folded without any intramolecular metal ligation. They seem to take up the folded conformation preferentially and it is likely that any binding involving metal ions merely helps to stabilise the folded structure. A recent NMR study of ATP bound to lanthanide cations in aqueous solution[11] has been interpreted in terms of a folded conformation, with the lanthanide ion bound only to the β and γ phosphates but with no direct interaction with the purine ring.

It is interesting to note that in contrast to the folded conformation reported here, difference electron density maps suggest that ADP is in the extended form when bound to either lactate dehydrogenase[1] or phosphoglycerate kinase (refs 2, 3 and H. C. Watson, personal communication).

The extended crystal structure shows no self association between the bases through either hydrogen bonding, or base stacking. Instead there are two pairs of hydrogen bonds linking the adenine base to phosphate group of two neighbouring molecules (Fig. 2). One of these pairs has the Watson–Crick geometry, while the other involves the amino group and the imidazole nitrogen N7. These interactions and the binding of Rb^+ to N3 may be relevant to the recognition of the base by polar side groups of amino acids and metal ions in biological systems (to be published). The role of similar interaction in the sequence specific recognition of nucleic acids by proteins has recently been discussed by Seeman *et al.*[12].

Figure 3 shows the role of the Rb^+ ions and the water molecules. Each Rb^+ ion is bound to two ADP molecules through the negatively charged α and β phosphate oxygen atoms. The four Rb · · · O distances range from 2.85 to 3.33 Å. The sixfold coordination around Rb^+ is completed by N3 of the adenyl base of a third molecule at 3.19 Å and the ribose hydroxyl atom of the same molecule at 2.91 Å.

The water molecules lie in sheets perpendicular to the *a* axis interlinking layers of Rb–nucleotide complexes through hydrogen bonding.

The investigation was supported by the Indian Council for Medical Research, the MRC and the SRC (visiting fellowship to M.A.V. and provision of the diffractometer).

M. A. Viswamitra
M. V. Hosur

ICMR Unit on Genetics and Cell Biology and Department of Physics, Indian Institute of Science, Bangalore-560012, India

Zippora Shakked
Olga Kennard*

University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, UK

Received January 30; accepted May 25, 1976

* External staff, Medical Research Council.

1 Chandrasekhar, K., Mcpherson, A., Jr, Adams, M. J., and Rossman, M. G., *J. molec. Biol.*, **76**, 503–517 (1973).
2 Bryant, T. N., Watson, H. C., Wendell, P. L., *Nature*, **247**, 14–17 (1974).
3 Blake, C. C. F., Evans, P. R., *J. molec. Biol.*, **84**, 585–601 (1974).
4 Kennard, O., *et al.*, *Proc. R. Soc.*, A325, 401–436 (1971).
5 Muller, F. A., Deluke, A. B., *Am. cryst. Ass., Abstr. Papers* (Winter Meeting), 26 (1971).
6 Sundaralingam, M., in *5th Jerusalem Symposium in Quantum Chemistry and Biochemistry* (edit. by Bergmann, E. D., and Pullman, B.), 417 (1973).
7 Happold, F. C., and Beechey, R. B., in *15th Biochemical Society Symposium* (edit. by Crook, G. M.) (Cambridge University Press, London, 1958).
8 Main, P., Woolfson, M. M., Lessinger, L., Germain, G., and Declerq, J. P., *MULTAN, A System of Computer Programmes for the Automatic Solution of Crystal Structures from X-ray Diffraction Data* (1974).
9 Sarma, R. H., Mynott, R. J., Hruska, F. E., and Wood, D. J., *Can. J. Chem.*, **51**, 1843–1851 (1973).
10 Viswamitra, M. A., Seshadri, T. P., Post, M. L., and Kennard, O., *Nature*, **258**, 497–501 (1975).
11 Tanswell, P., Thornton, J. M., Korda, A. V., and Williams, R. J. P., *Eur. J. Biochem.*, **57**, 135–145 (1975).
12 Seeman, N. C., Rosenberg, J. M., and Rich, A., *Proc. natn. Acad. Sci. U.S.A.*, **73**, 804–808 (1976).

Corrigendum

In the article "Two short lived X-ray transients at high galactic latitude" by B. A. Cooke (*Nature*, **261**, 564; 1976) the scale and legend to Fig. 2*a* are in error. The scale should read 13 h not 3 h and the source designation in the legend should be A1353−40 not A0353−40.

Errata

In the article "Extinction-free measurements in crystallography" by A. McL. Mathieson (*Nature*, **261**, 306; 1976), a sentence was omitted in the editing process. On line 12 of paragraph 1 mention of refs 5–7 should be deleted, and line 13 *et seq.* should read:
'. . . is applicable. The possibility exists of extrapolating to this condition, as a practical procedure, in relation to asymmetric reflection[5–7]. Starting with . . .'
In paragraph 4 line 7 of the right-hand column of page 307 'ref. 8' should be 'ref. 9', and in the caption to Fig. 2 the reference on the first line should be '5'.

In the article "Phosphorylation of yeast RNA polymerases" by G. Bell, P. Valenzuela and W. J. Rutter (*Nature*, **261**, 429; 1976) symbols were omitted from Fig. 1*a* which make it difficult to understand. The correct symbols are as follows. ^{32}P c.p.m. (○); RNA polymerase activity (●); Protein concentration (——).

In the article "Simple mathematical models with very complicated dynamics" by Robert May (*Nature*, **261**, 459–467; 1976) Figs 2 and 3 were transposed. The captions were in the correct position.