Watson model[4], this conformation is *gauche–trans* (GT). Crystal structures of 5′-nucleotides, dinucleosides and dinucleotides so far studied, however, have shown only the *gauche–gauche* (GG) conformation about this bond. The GG conformer is also the only one found in the refined models of the proposed structure of the double helical nucleic acids and polynucleotides[5-7]. The only nucleotide with a GT conformation is 6-azauridine-5′-phosphate[8] which is not a normal monomer unit of nucleic acids. It is also reported that 5′-dGMP assumes preferentially GT conformation in solution[9].

We wish to report here the molecular structure of the DNA monomer unit, deoxyguanydilic acid (dGMP-5′) as determined by a complete three-dimensional X-ray structure analysis. The nucleotide shows the GT conformation about the C-5′-C-4′ bond similar to that occurring in the Crick and Watson model.

Crystals of the disodium salt of deoxyguanosine 5′-phosphate were grown by slow diffusion of alcohol into aqueous solutions of the compound[10]. Thin platty crystals about 2 mm long were obtained in about 3 week. The crystal belongs to monoclinic system with space group $P2_1$. The unit cell dimensions are $a = 16.00$ Å; $b = 10.73$ Å; $c = 5.575$ Å; $\beta = 101.9°$; $d_{obs} = 1.64$ g cm^{-2}; $d_{cal} = 1.64$ g cm^{-2}; $Z = 2$. Density measurements carried out using carbon tertachloride-bromoform mixtures indicated the presence of four water molecules in the asymmetric unit. Intensity data were collected by multiple film, equiinclination, Weissenberg technique for hO1-h91 and hkO layers using CuK_α radiation. The data were measured visually by comparison with precalibrated graded intensity scale. A three-dimensional Patterson function was computed and the phosphorous atom was located from the Harker section. The structure was solved by symbolic addition

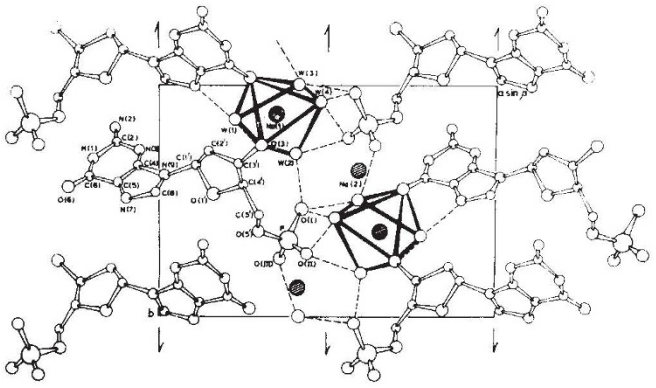

Fig. 1 Structure of dGMP-5′ Na_2 $4H_2O$ viewed down *c* axis. One of the sodium atoms (Na(1)) has an octahedral coordination shown by thick lines. Hydrogen bonds are indicated by broken lines. The stacking pattern of the bases belonging to molecules related by a 'c' cell translation is not shown for the sake of clarity.

method. Phases for 290 reflections were obtained using the program 'Multan'[11]. An E map was computed for the best set which gave a Karle *R* factor for 28.59%. The entire molecule with two sodium ions and one water oxygen atom were identified from the *E* map from a knowledge of the position of phosphorous atom and by model building approach. The current structure has an *R* factor of 9.0%. The view of the structure down *c* axis is given in Fig. 1.

The glycosidic torsional angle χ_{CN} is 52.6°. The relative orientation of the base with respect to the sugar is therefore, *anti*. The χ_{CN} value is within the range expected of β-purine nucleotides. The best four atom plane for the deoxyribose moiety passes through C1′-C2′-C3′-C4′. The O1′ atom shows an *endo* puckering, being displaced by 0.6 Å from this plane in striking contrast with the other three DNA monomers where the furanose ring is puckered either with C2′ or C3′ (refs 12–14).

The conformation about the C5′-C4′ bond is GT with $\phi_{O5'-O1'} = 62.5°$ and $\phi_{O5'-C3'} = 174.8°$. As mentioned earlier this is the first structure to show this conformation which is close to that found in Watson–Crick DNA model ($\phi_{oo} = 38°$, $\phi_{oc} = 155°$).

In model building studies and refinement on nucleic acid structures one tends to use the structural parameters and torsional angles within the constraints prescribed by the results of single crystal X-ray studies on nucleic acid constituents. It seems to us that the conformational features observed in dGMP-5′ have also to be considered in possible polynucleotide conformations and foldings particularly of the DNA. The GT conformer and the O1′ *endo* puckering of sugar ring are also of direct relevance to the concept of rigid nucleotide unit[15].

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Note added in proof:- An accurate independent X-ray analysis of this nucleotide has now been reported by Young, Tollin and Wilson[16,17]. Our findings are in close agreement with the conformational features reported by them.

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Errata

In the article "Volatilisation of mercury and organomercurials determined by inducible R-factor systems in enteric bacteria" by J. Schottel *et al.* (*Nature*, **251**, 335; 1974), in the last two lines of the legend to Fig. 1 and also in the penultimate line of para. 3, J53(471a) should read J53(R471a) on each occasion.

In the article "Subunit structure of chromatin" by M. Noll (*Nature*, **251**, 249; 1974) line 7 of the legend to Fig. 4 should read '. . . and $\underline{V}_m$=9.2 ml in 0.2 mM . . .' and not as originally printed.