On the Propeller Structure of Isolated Watson-Crick Base Pairs

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We consider the strongly nonplanar hydrogen bonding of nitrous bases in single Watson-Crick pairs to be due to pyramidal structure of their NH_2-groups.

The nucleotide sequence dependence of the DNA and RNA secondary structure is a problem of current interest in molecular biophysics. The key role of stacking interactions in determining this dependence is widely accepted [1, 2]. It is believed that the propeller twisting of base pairs, observed in the structure of both nucleic acids and crystals of nucleosides and nucleotides is a direct manifestation of these interactions.

Earlier we have revealed a nonplanar structure (with respect to the amino group) of adenine, guanine and cytosine molecules [3] using the quantum-chemical PCILO method. In these compounds the stable sp^3-hybridized character of the N atom valence bonds of the NH_2-group is responsible for the slope of the HNH plane of $\simeq 40^\circ$ to the molecule plane. The aim of this note is to demonstrate in terms of usual H-bonding how the propeller structure of the complementary base pairs can be realized without any stacking, only due to this feature of nitrous base geometry.

The conformation study of single Watson-Crick adenine-thymine (A−T) and guanine-cytosine (G−C) pairs has been carried out by the PCILO method. The variations of (i) the inter-base distances along the central hydrogen bond N−H···N and (ii) angle θ of the rotation of purine and pyrimidine base planes around this bond were considered. The main result is plotted in Fig. 1.

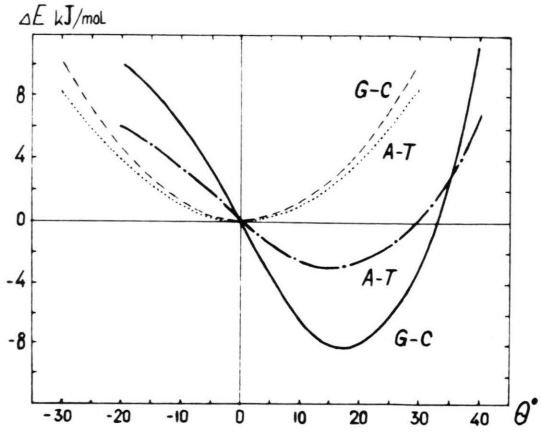

Fig. 1. Profiles of the potential energy surfaces of A−T and G−C pairs as a function of the angle θ of base plane rotation. (···), (− − −) = planar variant of the base structure, (−·−), (——) = nonplanar variant.

As seen from the curves, the base-pair propeller twist under such circumstances is not small and is $\theta \simeq 15^\circ$. It is in a good correlation with the estimated mean value of such a twisting in single nucleosides crystals [4]. The planar structure of nitrous bases causes only the coplanar type of pairing. The length of the central H-bond corresponding to the most stable conformation of these pairs is $R_{N-H\cdots N} \simeq 2.8$ Å and does not contradict the observed data [1]. The energy of hydrogen bonding for the two variations considered is 42 kJ/mol for the A−T pair and 63 kJ/mol for the G−C pair and comparable with the experimental values (54 kJ/mol and 88 kJ/mol respectively) [5].

Thus, the base-pair propeller twisting in the nucleic acid structure is an intrinsic property of the base pairs and is due to the primordially pyramidal structure of the amino groups participating in H-bonding. Along with stacking, it should crucially determine the base packing in DNA and RNA molecules.

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