

## **Susceptibility and conformation of nucleic acid bases**

V R Murthy, T V S Arun Murthy, D V Subbaiah and R N V Ranga Reddy

Molecular Biophysical Laboratories, Department of Physics,  
Sree Krishnadevaraya University, Anantapur-515 003, India

**Abstract:** The new method of determination of diamagnetic susceptibility from molecular vibration studies is extended to the study of susceptibilities of biopolymers in general and of the nucleic acid bases in particular. The bond diamagnetic susceptibilities are discussed in terms of the conformational aspects and the feasibility of using susceptibility as a dynamical variable in the study of conformation of biopolymers is explored. The present study lends satisfactory support to the suggestions of using susceptibility in conformational studies.

**Keywords:** Diamagnetic susceptibilities, nucleic acid bases.

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### **I. Introduction**

Nucleic acids are among several constituents of all the living cells. Uracil, cytosine, Thymine possess a common pyrimidine nucleus which plays a vital role in many biological processes. The reviews of Cheng (1969), Montgomery (1970), Suhadolnic (1970), Hitching and Elion (1965) give complete knowledge and application of nucleic acids in medicine and in other allied fields.

Diamagnetic susceptibilities have importance in stereo chemistry and electronic interactions.

There are various experimental and theoretical methods for determination of diamagnetic susceptibilities (Guy and Tilleu 1954, Baudet 1961, Haberditzal 1966, Gupta and Kumar 1983). But most of the available theoretical methods are either empirical or limited in their approach.

Any phenomenon be it, electrical, magnetic or electromagnetic is usually explained as due to the interaction of respective agency with outer valence electrons. Just as the force constant or mean amplitude of vibration is related to the relative orientation of the atoms results in bond susceptibility coefficients and hence a relation between bond susceptibility coefficients and molecular vibration parameters could be expected. The authors have developed two algebraic expressions between bond susceptibility coefficients and molecular vibration parameters.

## 2. Method

Two algebraic expressions have been developed between bond susceptibility coefficients and molecular vibration parameters based on the approaches of Rao and Murthy (1979), the details of which are as follows. The bond polarizability coefficients have been related to molecular vibration parameters by a method suggested by Rao and Murthy (1979). But the bond polarizabilities themselves are connected to bond susceptibility coefficients by another relation of Murthy and Naidu (1979) and Murthy and Ranga Reddy (1981). When these two approaches were compounded and analysed based on experimental data on molecular vibration parameters and susceptibilities, the following relation could be expected.

$$(\chi_L - \chi_T) = \eta \left[ (x_B x_O)^{1/2} \left( \frac{dN}{k-b} \right)^{2/3} \right]^3 \quad (1)$$

$$(\chi_L + 2\chi_T) = \eta/A.CP^j(j)^{\eta\sigma}\sigma_0^{1/2} \quad (2)$$

where  $\eta = Arm \sigma'$ ,  $\chi_L$  and  $\chi_T$  refer to longitudinal and transverse bond susceptibility coefficients. The necessary details are as in reference Murthy et al (1990a, 1990b).

The expressions (1) and (2) provide an opportunity to calculate anisotropic susceptibilities  $\chi_1$ ,  $\chi_2$ ,  $\chi_3$  and mean diamagnetic susceptibility following usual concept of additivity.

The above said method is successfully applied to biopolymers and a few liquid crystals (Murthy et al 1990a, 1990b).

The same method is used to measure the bond and mean molecular diamagnetic susceptibilities of nucleic acid bases.

The determination of principal and mean diamagnetic susceptibilities, however, need some correction. This is because of the fact that the outer valence electrons attached to an atom does not completely see (or feel the impact of) the impressed external magnetic field but will be screened to some extent due to neighbouring electrons in the atom. The screening is similar to the one experienced by a proton in NMR. The screening is estimated to a first order approximation by a parameter ' $\lambda$ ' called screening parameter, which when multiplied by  $\chi_x$  or  $\chi_x$  gives the true values of  $\chi_x$  where  $K = 1, 2, 3$ .

$$\lambda = [\sigma^1 c^{-\gamma/2}]^{1/2}$$

where  $\sigma^1 = [\sigma_1^1 \sigma_2^1 \dots \sigma_j^1]^{1/2}$ .  $\gamma$  is the saturation factor defined as in reference of Rao and Murthy (1979),  $\sigma_1^1, \sigma_2^1, \sigma_3^1, \dots, \sigma_j^1$  refer to the covalency factor of characteristic group in the system.

## 3. Results and discussion

The necessary data on force constants of the bonds present in nucleic acid bases (viz) Pyrimidine, Uracil, Cytosine, Thymine have been taken from the works of Sharma (1974), Susi and Ard (1971, 1973, 1974), Aruna (1983).

Table I. Molecular parameters.

Bond	Uracil		Cytocine		Thymine		Percentage of covalency $\sigma^1$
	K Dynes- $\text{cm} \times 10^5$	Mean ampli- tude of vibration $\text{\AA}$	K Dynes- $\text{cm} \times 10^5$	Mean ampli- tude of vibration $\text{\AA}$	K Dynes- $\text{cm} \times 10^5$	Mean ampli- tude of vibration $\text{\AA}$	
C-C	6.202	0.0438	6.202	0.0456	6.202	0.0449	1.0000
C=C	8.702	0.0421	8.702	0.0423	8.702	0.0423	1.0000
C-N	6.380	0.0459	6.380	0.0422	6.380	0.0459	0.9602
C-H	5.204	0.0764	5.289	0.0762	5.160	0.0768	0.9848
N-H	5.397	0.0756	5.604	0.0750	5.382	0.756	0.9637
2C=O	11.000	0.0386			11.000	0.0386	0.8824
4C=O	10.500	0.0381			10.500	0.0390	0.8824
C-NH <sub>2</sub>			7.570	0.0430			0.9692
N=C			10.550	0.0395			0.9692
C-CH <sub>3</sub>					4.889	0.0488	1.0000
C=O			7.340	0.0427			0.8824

The Table 1 presents the molecular vibration parameters of the nucleic acid bases. The Table 2 gives the diamagnetic susceptibilities of nucleic acid bases along with experimental values (Sastry 1985). The screening parameter in each system is given in the Table 2. The bonds' susceptibilities of  $C_s - C_s$  are also given Table 2.

**Table 2.** Diamagnetic susceptibilities of nucleic acid bases ( $\times 10$  CGS units).

	$\lambda$ Screening parameter	$\chi$ Present method	$\chi$ Expt. value
Pyrimidine	0.807	42.12	43.10
Uracil	0.773	45.89	44.23
Cytosine	0.842	50.87	55.69
Thymine	0.822	55.02	57.64
<u>Bond susceptibility of <math>C_s - C_s</math></u>			
Pyrimidine	5.688		
Uracil	5.472		
Cytosine	5.688		
Thymine	5.616		
Alkane	2.900		
Aromatics	6.520		

( $\pi$ -electron contribution in resonance structure also included).

The bond susceptibilities of C-C bond in alkanes is 2.93 where as in aromatics it is 6.52 (Gupta 1983).

The observation of the above results along with the bond susceptibilities in alkanes and aromatics one can infer the following.

The present value of bond susceptibilities in Pyrimidine, Uracil, Cytosine, Thymine varies as 5.68, 5.47, 5.68, 5.61. As it can be seen the values are in between the bond susceptibility values of alkanes and aromatics with a tendency towards the aromatic behaviour.

Thus this observation suggests that the bond susceptibility can be used for understanding the behaviour of carbon atom with respect to their reactivity.

This observation is in conformity with the observation of Subbiah et al on reactivity (Ramamurthy et al (1982), Subbaiah et al (1981, 1983)).

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