Indian J. Phys. **65B** (6), 535-539 (1991)

Molecular polarizabilities and diamagnetic susceptibilities of L-alanyl-L-alanine

R N V Ranga Reddy, D V Subbaiah, V R Murthy and
T V S Aruna Murthy
Department of Physics, Sri Krishnadevaraya University,
Anantapur-515 003, India

Abstract: The mean polarizability (α_M) of L-alanyl-L-alanine (L-A-L-A) is evaluated by Molecular vibration method of Rao and Murthy (1979) and Lippincott-δ-function potential model (Rao and Murthy 1972 *Curr. Sci.* **41** 16). From the estimated polarizability the diamagnetic susceptibility of L-alanyl-L-alanine (L-A-L-A) is calculated by using Rao and Murthy's method. The diamagnetic susceptibility of the oligomer is evaluated by Pascal's method also. The additivity of polarizability and susceptibility in oligomers is established.

Keywords: Molecular polarizability, diamagnetic susceptibility, L-alanyl-L-alanine, bio-polymers.

PACS No: 87.15.Mi

1. Introduction

Bio-polymers play a vital role in understanding the basic principles of cell structure, metabolism and other physiological phenomena. A study of their properties is very useful in understanding the molecular configurations and the nature of hydrogen bondings in the molecule. The conformation of such bio-polymers is usually studied by physical techniques like X-ray diffraction, NMR, ORD, CD, IR and Resonance Raman spectroscopy. Recently attempts are made by Rao and Murthy to utilise the molecular polarizability in conformation of bio-polymers, though its application to simple molecules has been done extensively by LeFevre School. In this direction (Rao *et al* 1977) and Murthy *et al* (1977, 1979, 1980) have studied the molecular polarizabilities of a few bio-polymers and liquid crystals and applied successfully molecular polarizability in the conformational analysis of bio-polymers (Murthy 1979). The molecular polarizability is found to be useful in evaluating London dispersion forces also.

In the present investigation the mean polarizability of L-alanyl-L-alanine is reported by using (i) Molecular vibration method and (ii) Lippincott-δ-function method. The diamagnetic susceptibility of L-A-L-A is also estimated from the knowledge of polarizability data and compared with the one obtained from Pascal's method (Pascal 1910, Pacault 1948).

3. Results and discussion

The values of $(b_L - b_T)$, $(b_L + 2b_T)$ (as calculated from eqs. 1 and 2) b_L and b_T are presented in Table 1. The values of $\Sigma\alpha_{l\parallel}$, $\Sigma\alpha_{l\perp}$, $\Sigma 2\alpha_{\perp}$ and α_M obtained from

Table 1. Bond polarizabilities of L-A-L-A ($\times 10^{23}$ cm^3).

Bond	$(b_L - b_T)$	$(b_L + 2b_T)$	b_L	b_T
$N^+ - H$	0.089	0.192	0.123	0.034
$N^+ - C_\alpha$	0.008	0.487	0.168	0.160
$C_\alpha - H$	0.070	0.199	0.113	0.043
$C_\alpha - C$	0.017	0.614	0.216	0.199
C – O	0.013	0.260	0.095	0.082
$CH_3 - C_\alpha$	0.006	0.622	0.211	0.205
C – H	0.071	0.198	0.113	0.042
C – N	0.010	0.449	0.156	0.146
N – H	0.076	0.192	0.114	0.038
$N - C_\alpha$	0.009	0.520	0.180	0.170
C – O	0.014	0.242	0.090	0.076

Lippincott method are presented in Table 2. The mean polarizability of L-A-L-A obtained from the two methods are presented in Table 3. The values of

Table 2. Molecular polarizability ($\times 10^{23}$ cm^3) of L-A-L-A from Lippincott method.

$\Sigma\alpha_l$	$\Sigma\alpha_{l\parallel}$	$\Sigma 2\alpha$	α_M
2.464	0.168	1.606	1.413

diamagnetic susceptibility of L-A-L-A obtained from Rao and Murthy's method and Pascal's method is presented in Table 4.

Table 3. Comparison of the mean molecular polarizability ($\times 10^{23}$cm^3) of L-A-L-A.

Molecular vibration method	Lippincott method
1.398	1.413

From Table 3, it is found that there is a very good agreement between the values of α_M obtained from molecular vibration method and Lippincott method.

From Table 4, it is found that the diamagnetic susceptibility of L-A-L-A obtained from Rao and Murthy's method and Pascal's method are agreeing very well.

Table 4. Diamagnetic susceptibility ($\times 10^6$ CGS emu/mol) of L-A-L-A.

$-\chi_M{}^a$	$-\chi_M{}^b$	$-\chi_M{}^c$
75.48	76.208	79.116

[a]Estimated from Rao and Murthy's method by using α_M of molecular vibration method.

[b]Estimated from Rao and Murthy's method by using α_M of Lippincott method.

[c]Estimated from Pascal's method.

References

Gupta M K and Gupta V D 1978 *Indian J. Biochem. Biophys.* **15** 413

Murthy V R 1970 *Ph.D. Thesis* (S V University, Tirupati, India)

——1979 *Indian J. Biochem. Biophys.* **16** 32

Murthy V R, Subbaiah D V and Naidu S V 1977 *Ind. J. Chem.* **1**

——1979 *Indian J. Biochem. Biophys.* **16** 43

Murthy V R, Naidu S V and Ranga Reddy R N V 1980 *Mol. Cryst. Liq. Cryst.* **59** 27

Pacault A 1948 *Rev. Sci.* **86** 38

Pascal P 1910 *Ann. Chem. Phys.* **19** 5

Rao B P and Murthy V R 1972 *Curr. Sci.* **41** 15

Rao B P, Murthy V R and Subbaiah D V 1976 *Indian J. Pure and Appl. Phys.* **14** 276

——1977 *Indian J. Biochem. Biophys.* **14** 181

Rao B P and Murthy V R 1979 *Indian J. Chem.* **13** 17

Selwood P W 1960 *Techniques of Organic Chemistry* (New York: Wiley-Interscience) Vol I, Part IV p 28