

## LETTERS TO THE EDITOR

MAGNETO OPTIC ROTATION FROM  
REFRACTIVITY STUDIES

The conformations of polymers and biopolymers are studied by physical techniques such as X-ray diffraction, NMR, ORD, CD, etc. Recently Rao and others<sup>1-4</sup> have attempted to see if molecular polarizability ( $a_M$ ) and magneto optic rotatory dispersion (MORD) could be used as tools in conformation of these macromolecules. In an attempt to test the feasibility of using MORD in conjunction with ORD in conformational analysis, the authors have developed an expression for magneto optic rotation (Verdet constant) in terms of refractive index ( $n$ ). The details of the derivation are given below.

Rao and Murthy<sup>5</sup> developed a method of evaluating mean molecular polarizability ( $a_M$ ) from Verdet constant starting from Malleman's principle and the expression for  $a_M$  reads as

$$a_M = \left[ \frac{9e\lambda^2}{8\pi^3N} \frac{nMp\delta}{\rho(n^2+2)^2 \left(1 - \frac{\Delta^*}{2}\right)} \right]^{1/2} \quad (1)$$

The significance of Various terms in equation (1) is given in Ref. (5).  $\Delta^*$ , the optical anisotropy in most molecules is less than 0.04 and hence can be neglected. On rearranging the terms, and simplifying, equation (1) can be rewritten as

$$\delta = \left[ K \frac{M}{\rho} \frac{(n^2-1)^2}{n\lambda^2} \right] \quad (2)$$

Where  $a_M$  is replaced by  $a$  and Lorentz-Lorenz expression is used for  $a$ . The error in this approximation will be less than 0.5% in most cases.  $K$  is a constant equal to

$$\frac{\pi}{2eN} = 1.8674 \times 10^{-11}.$$

$\delta$  is given in minutes/gauss/cm.

Using this equation, the Verdet constants of alkyl halides, substituted benzenes, naphthalenes and phenols were calculated taking data on  $M$ ,  $\rho$  and  $n$  from 55th edition of *Hand Book of Chemistry and Physics*, Chemical Rubber Company, Ohio, U.S.A. and are given in Table I. The values of  $p$ , the effective number of electrons are calculated by the method outlined in reference (5). The calculated Verdet constants are

compared with the values reported in literature. From Table I, it can be seen that there is very good agreement between values of  $\delta$ . This, in turn, suggests general applicability of the method with reasonable accuracy. The chief advantage of this method is that the MORD curves can be drawn theoretically for any molecular systems, without recourse to experiment. It has been found by authors that MORD simulates ORD curves in visible region for ketones and this leads to systematic study of MORD. Theoretical expressions for MORD analogous to two term Drude's expression has been derived by the authors. Efforts to apply MORD in conjunction with ORD for conformational analysis are under progress.

TABLE I  
Verdet constants ( $\delta \times 10^5$  mts/meter/gauss)

| Molecule                     | $p$ | Verdet constant ( $\delta$ ) Calculated | ( $\delta$ ) at 5893° A Reported |
|------------------------------|-----|---|----------------------------------|
| Dibromomethane               | 16  | 2.89                                    | 2.74                             |
| Bromoform                    | 22  | 3.22                                    | 3.13                             |
| ethyl bromide                | 16  | 1.86                                    | 1.82                             |
| ethyl Iodide                 | 16  | 2.98                                    | 2.95                             |
| chloro benzene               | 22  | 2.86                                    | 2.92                             |
| Bromo benzene                | 22  | 3.38                                    | 3.26                             |
| Iodo benzene                 | 22  | 4.43                                    | 4.06                             |
| P-Xylene                     | 28  | 2.42                                    | 2.46                             |
| P-chloro Toluene             | 28  | 2.51                                    | 2.65                             |
| P-Bromo Toluene              | 28  | 2.94                                    | 2.88                             |
| Trimethyl benzene            | 35  | 2.22                                    | 2.28                             |
| Naphthalene                  | 24  | 4.26                                    | 4.47                             |
| $\alpha$ -chloro naphthalene | 27  | 4.61                                    | 4.91                             |
| $\alpha$ -Bromo naphthalene  | 27  | 5.13                                    | 5.19                             |
| $m$ -Cresol                  | 28  | 2.43                                    | 2.89                             |
| Phenol                       | 22  | 2.73                                    | 3.21                             |
| P-Cresol                     | 28  | 2.41                                    | 2.91                             |

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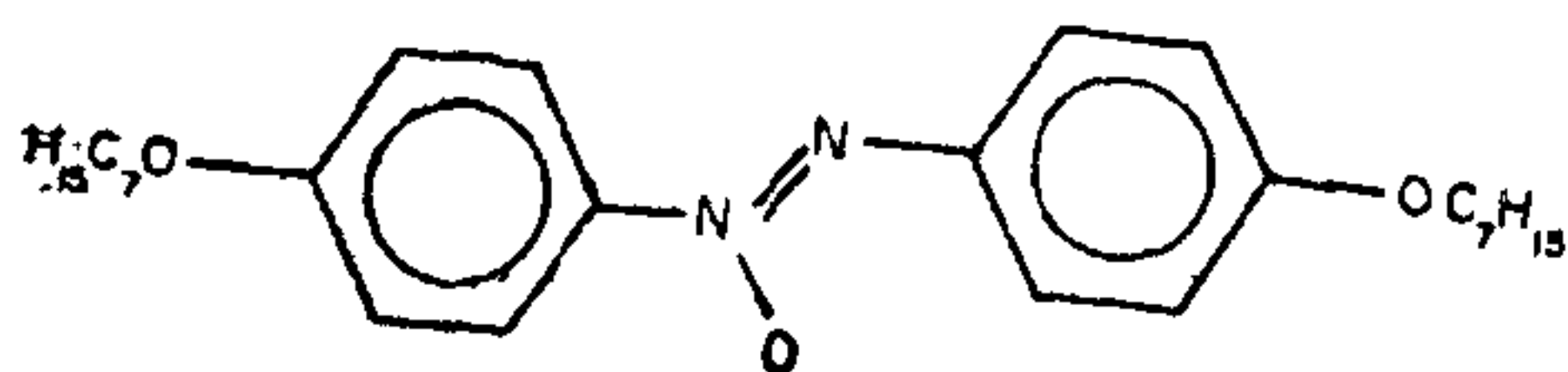
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#### CRYSTALLOGRAPHIC DATA OF MESOGENIC 4, 4'-BIS (HEPTYLOXY) AZOXYBENZENE

THE mesogenic compound 4, 4'-bis (heptyloxy) azoxybenzene with the structural formula



4-4'-bis (heptyloxy) azoxybenzene

exhibits, on heating, the following liquid crystalline phases :

Solid 73°C smectic (C) 95°C nematic 123°C isotropic.

This has been confirmed from our observation on the phase transition of this substance using a hot stage in conjunction with a polarizing microscope as well as from X-ray Laue Photograph studies. The refractive indices and densities at different temperatures have been determined and already reported<sup>1</sup>. Presently we have carried out preliminary X-ray investigations on these crystals.

Large rectangular plaque type yellow crystals were grown from benzene solution. Rotation and Weissenberg photographs along different axes were recorded using optically homogeneous crystals (as verified by observing the crystals under a polarising microscope). From these photographs the unit cell dimensions and space group were determined using the standard

techniques<sup>2</sup>. The relevant crystal data thus obtained are :

Molecular formula:  $C_{26}H_{38}N_2O_3$ , Molecular weight: 426.6, Space group: P1 or  $P\bar{1}$ ,  $a = 8.61 \pm 0.04 \text{ \AA}$ ,  $b = 10.82 \pm 0.04 \text{ \AA}$ ,  $c = 14.70 \pm 0.04 \text{ \AA}$ ,  $\alpha = 98^\circ 48'$ ,  $\beta = 102^\circ 18'$ ,  $\gamma = 95^\circ 31'$ ,  $z = 2$ ,  $\rho_{\text{exp.}} = 1.13 \text{ g/cc}$ ,  $\rho_{\text{cal.}} = 1.08 \text{ g/cc}$ .

The crystal belongs to space group P1 or  $P\bar{1}$ , which is explainable<sup>3</sup> on the basis of imbricated packing as there are two molecules per unit cell.

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#### ESTIMATION OF URANIUM IN PLANT AND WATER SAMPLES

ESTIMATION of traces of uranium in plant and water samples is carried out by using fission track technique. The uranium content in plants varies from 0.26 ppm to 15 ppm with its maximum concentration in hydrophytes. Water samples show a variation in uranium content from 1 ppb to 19 ppb.

##### Introduction

It is well known that trace quantities of uranium are present in almost all substances. Fission track technique provides an ingenious method for trace estimation of uranium in plant and water samples. The technique first developed by Price and Walker<sup>1-2</sup> was applied with success by Fleischer and Lovett<sup>3</sup> for uranium estimation in water and by Nagpal *et al.*<sup>4</sup> for uranium estimation in plants.

Our present investigations are based on the study of eight plant samples collected from the different ecological habitats in the Punjabi University campus and three water samples collected from the Manikaran and Deng hot water springs and from the University water supply.