

## NOTE

## Polarizabilities, Susceptibilities and Electron Ionization Cross-sections of Some Organic Monoazides

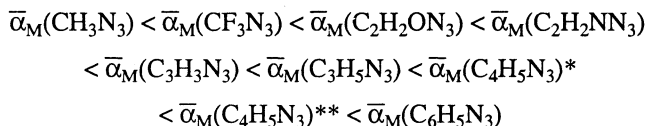
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A semi-empirical delta-function potential model of chemical binding has been employed to compute mean molecular polarizabilities, diamagnetic susceptibilities and electron ionization cross-sections of some organic monoazides. The results are briefly discussed.

Recently Klæboe *et al.*<sup>1</sup> have shown that —NNN, azide group in organic azides R—NNN (R = CH<sub>3</sub>, CF<sub>3</sub>, C<sub>2</sub>H<sub>2</sub>N, C<sub>2</sub>H<sub>3</sub>, C<sub>3</sub>H<sub>5</sub>, C<sub>6</sub>H<sub>5</sub>) has many interesting bond and molecular properties. Therefore in the present communication, it is aimed to study the molecular parameters such as mean molecular polarizability, diamagnetic susceptibility and electron ionization cross-section of some organic monoazides whose structural data have currently been reported in literature.<sup>1</sup> The mean molecular polarizability ( $\bar{\alpha}_M$ ) has been calculated using the relation of Lippincott and Stutman.<sup>2</sup> In the computation of  $\bar{\alpha}_M$ , the values of  $\delta$ -function strengths of the atoms, reported by Verma and Pandey,<sup>3</sup> have been used. The results thus obtained have been further utilised to evaluate diamagnetic susceptibility ( $\psi_M$ ) and electron ionization cross-section ( $Q_i$ ) using the relation given by Rao and Murthy<sup>4</sup> and Beran and Kevan<sup>5</sup> respectively. The results of the present communication are summarized in Table-1, according to their residual atomic polarizability,  $nd_f$ . It is apparent from Table-1 that  $\alpha_M$  increases in the order:



*i.e.*  $\bar{\alpha}_M$  increases as the lighter atom is replaced by heavier atom as expected.<sup>6</sup> A comparison of calculated and available experimental values shows that the two values are in excellent agreement. This indicates the accuracy of the present computation. A similar trend is further observed for  $\psi_M$  and  $Q_i$  as expected.<sup>4,5</sup> The polarizability data will be useful for the interpretation of Raman intensities and allied experimental data, and data on  $\psi_M$  and  $Q_i$  will be of great help in stereochemical analysis and positive ion chemistry data whenever available for these compounds.

TABLE-1  
 MEAN MOLECULAR POLARIZABILITY  $\bar{\alpha}_M$  ( $10^{-25} \text{ cm}^3$ ) DIAMAGNETIC  
 SUSCEPTIBILITY  $\psi_M$  (in  $10^{-6} \text{ cgs emu mole}^{-1}$ ) AND ELECTRON IONIZATION  
 CROSS-SECTION  $Q_i$  (in  $10^{16} \text{ cm}^2$ ) OF SOME ORGANIC MONOAZIDES

Molecule	nd <sub>f</sub>	$\bar{\alpha}_M$	$-\psi_M$	$Q_i$
CH <sub>3</sub> N <sub>3</sub>	9	52.70	29.20	9.41
CF <sub>3</sub> N <sub>3</sub>	9	54.96	23.45	9.81
C <sub>2</sub> H <sub>2</sub> NN <sub>3</sub>	10	75.16	37.13	13.43
C <sub>2</sub> H <sub>3</sub> ON <sub>3</sub>	11	74.41	34.86	13.28
C <sub>3</sub> H <sub>3</sub> N <sub>3</sub>	13	75.88 (78.44) <sup>a</sup>	37.83	13.55
C <sub>3</sub> H <sub>5</sub> N <sub>3</sub>	13	80.57	40.18	14.39
*C <sub>4</sub> H <sub>5</sub> N <sub>3</sub>	14	85.25	38.26	15.21
†C <sub>4</sub> H <sub>5</sub> N <sub>3</sub>	14	85.38	42.57	15.24
C <sub>6</sub> H <sub>5</sub> N <sub>3</sub>	18	103.51	41.80	18.48 (19 in C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> ) <sup>b</sup>

Values in parentheses are observed values.

\*2-azido-1,3 butadiene, †1-azido-2-butyne <sup>a</sup>ref. 7 <sup>b</sup>ref. 8

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