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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 Klaeboe *et al.*[1] have shown that —NNN, azide group in organic azides R—NNN (R = CH_3, CF_3, C_2H_2N, C_2H_3, C_3H_5, C_6H_5) 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.[1] The mean molecular polarisability ($\bar{\alpha}_M$) has been calculated using the relation of Lippincott and Stutman.[2] In the computation of $\bar{\alpha}_M$, the values of δ-funcftion strengths of the atoms, reported by Verma and Pandey,[3] have been used. The results thus obtained have been further utilised to evaluate diamagnetic susceptibility(ψ_M) and electron ionization cross-secdtion (Q_i) using the relation given by Rao and Murthy[4] and Beran and Kevan[5] 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 α_M increases in the order:

$$\bar{\alpha}_M(CH_3N_3) < \bar{\alpha}_M(CF_3N_3) < \bar{\alpha}_M(C_2H_2ON_3) < \bar{\alpha}_M(C_2H_2NN_3)$$
$$< \bar{\alpha}_M(C_3H_3N_3) < \bar{\alpha}_M(C_3H_5N_3) < \bar{\alpha}_M(C_4H_5N_3)^*$$
$$< \bar{\alpha}_M(C_4H_5N_3)^{**} < \bar{\alpha}_M(C_6H_5N_3)$$

i.e. $\bar{\alpha}_M$ increases as the lighter atom is replaced by heavier atom as expected.[6] 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 ψ_M and Q_i as expected.[4, 5] The polarizability data will be useful for the interpretation of Raman intensities and allied experimental data, and data on ψ_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 MOLECUALR POLARIZABILITY $\bar{\alpha}_M$ ($10^{-25}cm^3$) DIAMAGNETIC SUSCEPTIBILITY ψ_M (in 10^{-6} cgs emu $mole^{-1}$) AND ELECTRON IONIZATION CROSS-SECTION Q_i (in 10^{16} cm^2) OF SOME ORGANIC MONOAZIDES

Molecule	nd_f	$\bar{\alpha}_M$	$-\psi_M$	Q_i
CH_3N_3	9	52.70	29.20	9.41
CF_3N_3	9	54.96	23.45	9.81
$C_2H_2NN_3$	10	75.16	37.13	13.43
$C_2H_3ON_3$	11	74.41	34.86	13.28
$C_3H_3N_3$	13	75.88 (78.44)[a]	37.83	13.55
$C_3H_5N_3$	13	80.57	40.18	14.39
*$C_4H_5N_3$	14	85.25	38.26	15.21
†$C_4H_5N_3$	14	85.38	42.57	15.24
$C_6H_5N_3$	18	103.51	41.80	18.48 (19 in $C_6H_5N_3$)[b]

Values in parentheses are observed values.

*2-azido-1,3 butadiene, †1-azido-2-butyne [a]ref. 7 [b]ref. 8

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