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Soviet-era science, translated into English

# LETTER TO THE EDITOR

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## Abstract

## Full Text

# LETTER TO THE EDITOR

In my article (R. M. Aminova, “On the molecular-orbital theory of the diamagnetism of cyclic molecules. Calculation of the magnetic anisotropy of cyclopropane” ), published in DAN, vol. 157, no. 6, 1964, the following corrections must be made.

In formulas (14), (16), and (19) one should read  $(\chi_p)_{\alpha\beta} = 0$ ; in formula (21) one should read  $\Delta\chi_p^{\text{C}_3\text{H}_6} = 0$ , in connection with which the arguments concerning the paramagnetism of interatomic contributions should be regarded as invalid. Formula (12) should read:

$$L_{\mu\nu}^2 = (e^2/4\hbar^2c^2) H_\alpha H_\beta (\mathbf{R}_\mu \times \mathbf{R}_\nu)_\alpha (\mathbf{R}_\mu \times \mathbf{R}_\nu)_\beta. \quad (12)$$

Then formulas (15), (18), (20) should read:

$$(\chi_d)_{\alpha\beta} = (Ne^2/2\hbar^2c^2) \sum_{\mu<\nu} P_{\mu\nu} (\mathbf{R}_\mu \times \mathbf{R}_\nu)_\alpha (\mathbf{R}_\mu \times \mathbf{R}_\nu)_\beta \mathcal{H}_{\mu\nu}^{(0)}; \quad (15)$$

$$(\chi_d^{A-B})_{\alpha\beta} = (Ne^2/2\hbar^2c^2) \sum_{\mu<\nu}^{A-B} P_{\mu A\nu B} (\mathbf{R}_A \times \mathbf{R}_B)_\alpha (\mathbf{R}_A \times \mathbf{R}_B)_\beta \mathcal{H}_{\mu A\nu B}^{(0)}; \quad (18)$$

$$\Delta\chi_d^{\text{C}_3\text{H}_6} = \chi_{\parallel} - \chi_{\perp} = \chi_{zz} = \frac{2Ne^2}{\hbar^2c^2} \sum_{\text{bonds}} \sum_{\mu<\nu}^{A-B} S_{AB}^2 P_{\mu A\nu B} \mathcal{H}_{\mu A\nu B}^{(0)}. \quad (20)$$

If  $\mathcal{H}_{\mu A\nu B}^{(0)}$  is found semiempirically, taking  $\mathcal{H}_{ij} = 0.5K(\mathcal{H}_{ii} + \mathcal{H}_{jj})S'_{ij}{}^{(1)}$  ( $S'_{ij}$  is the overlap integral), and adopting  $\mathcal{H}_{ii}(C \cdot 2p\sigma) = -11.17$  eV,  $\mathcal{H}_{ii}(C \cdot 2p\pi) = -9.44$  eV,  $\mathcal{H}_{ii}(C \cdot 2s) = -21.4$  eV<sup>(2)</sup>, then the interatomic contribution to the anisotropy of the cyclopropane ring will be equal to

$$\Delta\chi_d^{\text{C}_3\text{H}_6} = -23.5 \cdot 10^{-6} \text{ cm}^3/\text{mol}.$$

R. M. Aminova

## CITED LITERATURE

<sup>1</sup> R. Hoffmann, J. Chem. Phys., **39**, no. 6, 1397 (1963). <sup>2</sup> R. Mulliken, J. Chem. Phys., **2**, no. 11, 782 (1934).

*Note: Figure translations are in progress. See original paper for figures.*

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