Theoret. chim. Acta (Berl.) 1, 468 (1963)

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# Erratum

## Studies of Delocalized Electron Bonding

Theoret. chim. Acta (Berl.) **1**, 133, 222 (1963)

By

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An error has been noted in the solution of the secular equations affecting the calculations of paper I [Theoret. chim. Acta (Berl.) **1**, 133 (1963)] and paper II [Theoret. chim. Acta (Berl.) **1**, 222 (1963)]. Tab. 2 of paper I should read:

| $\varphi$ | $E$(*Kcal/mole*) | $c_1$ | $c_2$ | $c_3$ | $c_4$, $c_5$ | $J_{HH'}$ (c.p.s.) |
|---|---|---|---|---|---|---|
| 0° | —278.6857 | 0.99059 | 0.05748 | —0.00310 | —0.02008 | 26.84 |
| 15° | —278.8212 | 0.99113 | 0.05650 | —0.00300 | —0.02012 | 26.38 |
| 30° | —279.1855 | 0.99260 | 0.05382 | —0.00272 | —0.02021 | 25.13 |
| 45° | —279.6730 | 0.99471 | 0.04996 | —0.00233 | —0.02034 | 23.35 |
| 60° | —280.1202 | 0.99721 | 0.04535 | —0.00187 | —0.02050 | 21.21 |
| 75° | —280.4003 | 0.99989 | 0.04037 | —0.00138 | —0.02066 | 18.92 |
| 90° | —280.4166 | 1.00255 | 0.03541 | —0.00089 | —0.02083 | 16.64 |
| 105° | —280.1771 | 1.00524 | 0.03035 | —0.00039 | —0.02100 | 14.33 |
| 120° | —279.7019 | 1.00774 | 0.02562 | 0.00009 | —0.02116 | 12.18 |
| 135° | —279.1349 | 1.01003 | 0.02127 | 0.00053 | —0.02131 | 10.22 |
| 150° | —278.5886 | 1.01185 | 0.01781 | 0.00089 | —0.02143 | 8.66 |
| 165° | —278.1997 | 1.01305 | 0.01551 | 0.00113 | —0.02152 | 7.62 |
| 180° | —278.0577 | 1.01346 | 0.01474 | 0.00121 | —0.02154 | 7.28 |

These corrected solutions lead to a calculated rotation barrier of 0.63 Kcal/mole favoring the staggered configuration. The $\delta$ integral for 105° listed in Tab. 1 of Paper I was erroneously listed as +4.78 rather than +3.78.

Equations (1), III, paper II, are,

III: $W = -16.6843$ e.v.;

$$\Psi = 1.0818\,\psi_{ab,\,cd,\,ef,\,gh} - 0.0278\,(\psi_{ab,\,ch,\,dg,\,ef} + \psi_{af,\,be,\,cd,\,gh})$$
$$- 0.0286\,(\psi_{ah,\,bg,\,cd,\,ef} + \psi_{ab,\,cd,\,eh,\,fg} + \psi_{ad,\,bc,\,ef,\,gh} + \psi_{ab,\,cf,\,de,\,gh})$$
$$+ 0.0008\,(\psi_{ah,\,bc,\,dg,\,ef} + \psi_{ab,\,ch,\,de,\,fg} + \psi_{af,\,bc,\,de,\,gh} + \psi_{ah,\,be,\,cd,\,fg})$$
$$- 0.0016\,\psi_{ah,\,bc,\,de,\,fg} + 0.0016\,(\psi_{ah,\,bg,\,cf,\,de} + \psi_{ad,\,bc,\,eh,\,fg}),$$

and the last row of the table in Paper II should read:

| Calculation | Number of Electrons | Number of v. b. Structures | $\Delta W_{res}$ (e. v.) | $J_{HH'}$ (c. p. s.) | $\eta_{HH'}$ (exchange order) | $P_{HH'}$ (bond order) |
|---|---|---|---|---|---|---|
| III | 8 | 14 | 0.0563 | 12.55 | —0.4595 | 0.0270 |

These corrections do not substantially alter the discussion and conclusions of either Paper I or II.

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