# Erratum: Stability Criterion for the Localization of an Excess Electron in a Nonpolar Fluid

B. E. Springett, Joshua Jortner and Morrel H. Cohen

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SCF wavefunction for this molecule and have examined the bonding scheme as described in the localized orbital picture. In Table I we have listed the localized orbitals for ketene. The formaldehyde localized orbitals are also listed for comparison. The coordinate system used in these calculations is the same as that of Ref. 1, with the exception that the direction of our $z$ axis is reversed. From Table I we note in particular, the similarities in the C–H bonds of both molecules and in the $sp$ hybrid orbitals containing the nonbonded electrons. In formaldehyde, there is a second pair of nonbonded electrons, which occupies the oxygen $p_y$ orbital. In contrast, in ketene, there is an additional "$\pi_y$"-type bond between carbon and oxygen in the molecular $yz$ plane. In this plane therefore, there are two localized C–O bonds, the $\sigma$ C–O, and the highly polarized "$\pi_y$".

The amount of triple bond character in the C–O bond can then be measured by the amount of participation of the two $p_x$ electrons of the oxygen atom in the molecular $\pi_x$ system. We see from Table I that orbitals (7) and (8) represent $\pi$ bonds, (7) primarily between $C_1$ and $C_2$, and (8) between $C_2$ and O. The total $\pi$ bond order between $C_2$ and O is 0.588, which represents a weakened $\pi$ bond when compared with the C–O $\pi$ bond order of formaldehyde, 0.968. However, this bond order is a direct measure of the triple-bond character of the classical C–O double bond in ketene and in this sense, is significant. Thus, the triple-bond character of the C–O bond suggested in Ref. 1 is described directly and quite explicitly in terms of localized CNDO orbitals, in spite of their approximate nature.

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[2] J. Del Bene and H. H. Jaffé, J. Chem. Phys. **50**, 1126 (1969).
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[4] C. Trindle and O. Sinanoğlu, J. Chem. Phys. **49**, 65 (1968).

# Errata

### Erratum: Stability Criterion for the Localization of an Excess Electron in a Nonpolar Fluid

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D. L. Dexter has brought some numerical errors to our attention. They are as follows. In Table I the entries under $U_p$ should read $-0.38$, $-1.47$, and $-3.00$ and under $V_0$ (theory) the entries should read $+1.26$, $+0.45$ and $-1.13$, both in descending order. The next to last sentence in the left-hand column, page 2725, should read "Now, from the experimental density data[37] at 19°K we get $r_s = 2.23$ Å and hence from Eqs. (25) and (27) we get $T = 3.57$ eV, $U_p = -1.41$ eV, and $V_0 = +2.16$ eV."

Table II should be revised as follows, reading from left to right: $H_2$, 19°K, 2.17, 2.15, 2.16, $0.138 \times 10^{-2}$, 0.029; $D_2$, 19°K, 2.59, 2.15, 3.00, $0.072 \times 10^{-2}$, 0.015; $^3$He, 3°K, 1.29, 0.02, 0.65, $0.023 \times 10^{-2}$, 0.005; $^3$He, 1°K, 0.40, 0.85, $0.124 \times 10^{-2}$, 0.026; $^4$He, 3°K, 2.13, 0.21, 1.24, $0.042 \times 10^{-2}$, 0.009; $^4$He, 1°K, 2.18, 0.35, 1.26, $0.065 \times 10^{-2}$, 0.014; Ne, 25°K, 3.72, 5.5, 0.45, $8.44 \times 10^{-2}$, 1.79. The heading to column 6 in Table II should read $4\pi\beta\gamma/V_0^2$. The second sentence in the last paragraph of the right-hand column on page 2729 should have 0.6 replaced by 1.8.

Our original conclusions remain unaltered.

### Erratum: Electron Correlation and the Nuclear Spin–Spin Coupling Constant. II. The Generalized Product Approximation with Intergroup Configuration Interaction

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Equation (2) should be written,

$$\rho_1(\lambda\mu \mid 1; 1') = P_1(\lambda\mu \mid \overset{\alpha}{1}; \overset{\alpha}{1'})\alpha(1)\alpha^*(1')$$
$$+ P_1(\lambda\mu \mid \overset{\alpha}{1}; \overset{\beta}{1'})\alpha(1)\beta^*(1') + \cdots. \quad (2)$$

The summation in Eq. (4) is over the triplet states, $\kappa$. Equation (12) is given by

$$Q_1(0\tau_0 \mid 1; 1')$$
$$= \sum_{t_0}[c_0 c_{t_0} - (1/\sqrt{3})\sum_{R \neq T} c_{rt}c_{\tau_0,r_0}]Q_1(0t_0 \mid 1; 1')$$
$$+ \sum_{R \neq T}[c_0 c_{\tau_0,r_0} - (1/\sqrt{3})\sum_{t_0}c_{t_0}c_{rt}]Q_1(0r_0 \mid 1; 1'). \quad (12)$$

Reference 15 should be deleted. Equation (23) is given by

$$H_{RS,RS} = \sum_T H^T(tt) + H_{\text{eff}}^R(r_{+1}r_{+1}) + H_{\text{eff}}^S(s_{+1}s_{+1})$$
$$+ J^{RS}(r_{+1}r_{+1}, s_{+1}s_{+1}) - K_0^{RS}(r_{+1}r_{+1}, s_{+1}s_{+1})$$
$$+ 2k^{RS}(r_{+1}r_{+1}, s_{+1}s_{+1}), \quad (23)$$

where, for example,

$$H_{eff}^{R}(r_{+1}r_{+1}) = H^{R}(r_{+1}r_{+1})$$
$$+ \sum_{T \neq R, S} [J^{RT}(r_{+1}r_{+1}, tt) - K^{RT}(r_{+1}r_{+1}, tt)].$$

The factors of $\frac{1}{2}$ should be deleted from Eqs. (24) and (29). Equation (52) is written,

$$k^{AB}(a_{+1}a_{+1}, b_{+1}b_{+1}) = \frac{1}{2} \sum_{jklm} c_{a_0 j} c_{a_0 k} c_{b_0 l} c_{b_0 m}$$
$$\times (\tfrac{1}{2})^{2n - i_{jk} - i_{lm}} \sum_{a,b} g_{jk}{}^{a} g_{lm}{}^{b} K(a, b). \quad (52)$$

These corrections do not affect the numerical results reported in Sec. V.

## Erratum: Dielectric Relaxation, Far-Infrared Absorption, and Intermolecular Forces in Nonpolar Liquids

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The second sentence in the last paragraph on page 2559 has become garbled during the printing or editing process, and is meaningless at present. It should read "The low-frequency side of the band was assumed to drop linearly from the absorption at 17 cm⁻¹ to zero absorption, which it reached at about 10 cm⁻¹."

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## Erratum: Physical Properties of Aromatic Hydrocarbons. IV. An Analysis of the Temperature Dependence of the Viscosity and the Compliance of 1,3,5-Tri-α-naphthylbenzene

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Equation (5), page 3680, should read

$$\ln \eta = (7.804 \times 10^{3}) - (5.764 \times 10^{5} T^{-1}) - 4.176T$$
$$+ 0.115 T^{2} - (1.740 \times 10^{-4} T^{3}) + (1.375 \times 10^{-7} T^{4})$$
$$- (4.453 \times 10^{-11} T^{5}) \cdots. \quad (5)$$