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Erratum

Extension of the MNDO formalism to *d* orbitals: Integral approximations and preliminary numerical results

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Table 2 of the title article [1] lists the absolute values of the coefficients $c_{lm}^{\mu\nu}$ and does not specify their sign. The following 12 coefficients with labels (μ, ν, l, m) are negative:

$$(p_\pi, p_\pi, 2, 0), (p_{\bar{\pi}}, p_{\bar{\pi}}, 2, 0), (p_{\bar{\pi}}, p_{\bar{\pi}}, 2, 2), (p_\pi, d_\sigma, 1, 1), (p_{\bar{\pi}}, d_\sigma, 1, -1),$$
$$(p_{\bar{\pi}}, d_\delta, 1, -1), (d_\sigma, d_\delta, 2, 2), (d_\sigma, d_{\bar{\delta}}, 2, -2), (d_{\bar{\pi}}, d_{\bar{\pi}}, 2, 2), (d_{\bar{\pi}}, d_\delta, 2, -1),$$
$$(d_\delta, d_\delta, 2, 0), (d_{\bar{\delta}}, d_{\bar{\delta}}, 2, 0).$$

Equations (22)–(26) in [1] contain typographical errors. They should read:

$$(\rho_1^{sp})^{-1} - [(\rho_1^{sp})^2 + (D_1^{sp})^2]^{-1/2} = 4G_{sp}^1/3 = 4h_{sp}, \quad (22)$$

$$(\rho_1^{pd})^{-1} - [(\rho_1^{pd})^2 + (D_1^{pd})^2]^{-1/2} = 16G_{pd}^1/15, \quad (23)$$

$$(\rho_2^{pp})^{-1} - 2[(\rho_2^{pp})^2 + (D_2^{pp})^2]^{-1/2} + [(\rho_2^{pp})^2 + 2(D_2^{pp})^2]^{-1/2} = 24\,F_{pp}^2/25 = 8h_{pp}, \quad (24)$$

$$(\rho_2^{sd})^{-1} - 2[(\rho_2^{sd})^2 + (D_2^{sd})^2]^{-1/2} + [(\rho_2^{sd})^2 + 2(D_2^{sd})^2]^{-1/2} = 8G_{sd}^2/5 = 8h_{sd}, \quad (25)$$

$$(\rho_2^{dd})^{-1} - 2[(\rho_2^{dd})^2 + (D_2^{dd})^2]^{-1/2} + [(\rho_2^{dd})^2 + 2(D_2^{dd})^2]^{-1/2} = 24F_{dd}^2/49. \quad (26)$$

The right-hand side of Eqs. (23) and (26) can be expressed as $4h_{p_\sigma d_\sigma}$ and $8h_{d_\pi d_\delta}$, respectively, if multipole interactions beyond the quadrupole are neglected (otherwise only by linear combinations of one-center exchange integrals). In the spirit of the original derivation, an alternative choice for the right-hand side of Eq. (23) would be $4\,G_{pd}^1/5$ which would lead to minor changes in the numerical results that can be absorbed by a very slight adjustment of the α parameter.

In summary, the MNDO/*d* integral formalism is defined by the original formulas [1] with the modifications listed above (concerning the signs of the coefficients $c_{lm}^{\mu\nu}$ and Eqs. (22)–(26)). Our computational implementation [2] of MNDO/*d* has always been based on this definition. Hence, the published numerical results [3–5] remain valid.

References

1. Thiel W, Voityuk AA (1992) Theor Chim Acta 81:391
2. Thiel W (1993) Program MNDO93 and later versions
3. Thiel W, Voityuk AA (1992) Int J Quantum Chem 44:807
4. Thiel W, Voityuk AA (1994) J Mol Struct 313:141
5. Thiel W, Voityuk AA (1996) J Phys Chem 100:616