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Erratum: “Polarized Molecular Orbital Chemistry. 2. The PMO Method”

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With this Erratum, we provide a clear definition of the core-core energy term between pairs of oxygen atoms that is used in the PMOv1 method presented in the original publication.¹

This clarification does not alter any of the results or conclusions shown in the paper.

The core-core energy term² between pairs of oxygen atoms, A and B, in PMO version 1 is:

$$E_{AB}^{\text{core}} = 36 \left(S^A S^A, S^B S^B \right) \left[1 + 2e^{-\hat{\alpha}^O R_{AB}} - 2e^{-\alpha^O R_{AB}} + 2R_{AB} e^{-\alpha^O R_{AB}} \right]$$

The values of α^O and $\hat{\alpha}^O$ are given in Tables 1 and 2, respectively.

References

- (1). Zhang P, Fiedler L, Leverentz HR, Truhlar DG, Gao J. *J. Chem. Theory Comput.* 2011; 7:857. [PubMed: 23378824]
- (2). Dewar MJS, Thiel W. *J. Am. Chem. Soc.* 1977; 99:4899.