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Erratum

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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 term[2] between pairs of oxygen atoms, A and B, in PMO version 1 is

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

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

REFERENCES

(1) Zhang, P.; Fiedler, L.; Leverentz, H. R.; Truhlar, D. G.; Gao, J. J. *Chem. Theory Comput.* **2011**, *7*, 857.

(2) Dewar, M. J. S.; Thiel, W. *J. Am. Chem. Soc.* **1977**, *99*, 4899.

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