Errata

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Erratum: Water molecule interactions

[J. Chem. Phys. 53, 4544 (1970)]

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In the calculation of the total energy of the water monmer, $E(1)$, we inadvertently included an additional D-type function on the oxygen atom [the $(x^2+y^2+z^2)$ combination which has S-type symmetry]. This function was not included in the oxygen atom basis sets for the dimer, $E(1,2)$, or trimer, $E(1,2,3)$, total energy calculations. The corrected monomer energy is -76.041361 a.u. or a change of 0.14023 kcal/mole. The dimer pair interaction energies $V^{(2)}$ should be corrected by -0.28046 kcal/mole while the three molecule nonadditivities $V^{(3)}$ should be corrected by $+0.42069$ kcal/mole.

All qualitative conclusions remain the same. The principal effect is to increase all nonadditivities by a constant amount. The distance variation of the trimer nonadditivities, Fig. 7, now extrapolates correctly to zero at infinite separation. In addition, the role of $V^{(3)}$ in the bonding energy of ice is now computed to be -1.708 kcal/mole.

We thank B. R. Lentz and H. A. Scheraga for bringing this error to our attention.

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Erratum: Mulliken type MO calculations with exact kinetic energy

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The following corrected values for the C–C and C–H bond populations, respectively, should be substituted in Table I. Values determined by the exact K. E. Mulliken method are for C_2H_2: 2.02174 and 0.66974; for C_2H_4: 1.42298 and 0.76974; for C_2H_6: 0.84720 and 0.77819. Values determined by the empirical K. E. Mulliken method are for C_2H_2: 1.62189 and 0.76164; for C_2H_4: 1.10761 and 0.78322; for C_2H_6: 0.69756 and 0.76226.

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Erratum: Dickinson energy of H_2^+

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Tables I and II inadvertently list values of $c'=cR/2$ in place of the parameter c of the text. Thanks are due Dr. M. P. Melrose and Mr. Wm. Mott of King's College, University of London, for pointing out this error.