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ERRATA

Erratum: "Comparative assessment of a new nonempirical density functional: Molecules and hydrogen-bonded complexes" [J. Chem. Phys. 119, 12129 (2003)]

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TPSSh vibrational frequencies were inadvertently computed using the TPSS functional at the TPSSh geometries. The mistake affects the last row in Table VIII and the TPSSh dissociation energies (D_0) of hydrogen-bonded complexes in Table IX.

The last row in Table VIII should be replaced by the following:

Method	ME	MAE	Max (+)	Max (−)
TPSSh	6.6	26.7	141.4 (F_2^+)	−78.0 (HF^+)

The TPSSh D_0 values in Table IX should be

	D_0 (kcal/mol)	
Method	ME	MAE
TPSSh	0.06	0.46

This makes TPSSh the second best functional for H-bond energetics. TPSSh remains the best functional for harmonic vibrational frequencies of molecules. TPSSh results for other properties are not affected.

Also, the LSDA energies of Cl, P^+, Ar^+, HCl^+, S^-, and O_2^- used in calculations of standard enthalpies of formation, ionization potentials, and electron affinities were not fully converged, because the default SCF algorithm fails to produce self-consistent LSDA solutions for these systems. The quadratically convergent SCF algorithm (the option SCF =QC) may be used as a remedy. The correction slightly affects the results reported in Tables I and II, where the ME and MAE for LSDA should be replaced with the following. Table I: ME=−83.27, MAE=83.27 (G2/97); ME =−196.57, MAE=196.57 (G3-3); ME=−121.38, MAE =121.38 (G3/99). Table II: ME=0.047, MAE=0.231. These changes are very small and in no way affect any of the conclusions.

TPSSh ω_e and D_0 values in Tables S6 and S7, and LSDA values for the affected atoms and molecules in Tables S1, S2, and S3 of EPAPS Document No. E-JCPSA6-119-302348 (Ref. 51) have been corrected. The old EPAPS files have been replaced with new ones.

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