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Department of Chemistry, University of Southern California, Los Angeles, California 90089-0482: Effect of a Heteroatom on Bonding Patterns and Triradical Stabilization Energies of 2,4,6-Tridehydropyridine versus 1,3,5-Tridehydrobenzene

Page 2591. An incorrect value for the doublet—quartet gap of the 1,3,5-tridehydrobenzene was reported because of a mistake in the calculations. The values in Table 2 and the respective discussion should be corrected as follows:

- (1) In the abstract: The adiabatic doublet—quartet gap of 2,4,6-tridehydropyridine is smaller than that of 1,3,5-tridehydrobenzene by 0.08 eV; the respective values are 1.223 and 1.302 eV.
- (2) The last two columns (the ΔE^a_{13} and ΔE^a_{23} values) in Table 2 are corrected in Table 1.

TABLE 1: 1,3,5-Tridehydrobenzene: Total Energy (hartree) for the Ground $(^2A_1)$ State and Vertical and Adiabatic Excitation Energies (eV) of the 2B_2 and 4B_2 States Using the EOM-SF Methods and the cc-pVTZ Basis Set^a

method	ΔE_{13}^a	ΔE_{23}^a
CCSD	1.141	1.131
CCSD(fT)	1.277	1.259
CCSD(dT)	1.302	1.286

^a The superscripts 1, 2, and 3 correspond to the ${}^{2}A_{1}$, ${}^{2}B_{2}$, and ${}^{4}B_{2}$ states, respectively.

This error does not affect the rest of the properties presented in the article. The TSE values for 1,3,5-tridehydrobenzene discussed in the text are from the previous work and are based on the correct doublet—quartet gap. P.U.M. apologizes for the mistake and is grateful to Prof. Michael Winkler for pointing it out to us.

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