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Addition/Correction

Correction to "Heptazine, Cyclazine, and Related Compounds: Chemically-Accurate Estimates of the Inverted Singlet−Triplet Gap"

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An error was found in he CIS(D), ADC(2) and CC2 results for compound **10**. See the SI for details and corrected values. This error does not affect the reference values. However, as can be seen below in Table 1, that replaces the Table 4 of our original work,[1] this tunes the statistics for these three methods, with now very small standard deviation of the errors (SDEs) for both ADC(2) and CC2. The statistics for the singlet and triplet energies can be found in the present SI.

Table 1. MSE, MAE, and SDE (in eV) Determined for the STG, Considering the TBEs[a]

Method	MSE	MAE	SDE
CIS(D)	−0.241	0.241	0.073
ADC(2)	−0.021	0.021	0.011
SOS-ADC(2)	−0.193	0.193	0.089
SCS-ADC(2)	−0.115	0.115	0.019
CC2	−0.014	0.015	0.009
SOS-CC2	−0.165	0.165	0.031
SCS-CC2	−0.111	0.111	0.021
CCSD	+0.081	0.081	0.014
PBE0−2[b]	−0.066	0.114	0.235
SOS-PBE-QIDH	−0.073	0.075	0.084
SCS-PBE-QIDH	−0.033	0.055	0.085
SOS-RSX-QIDH	−0.084	0.105	0.121

[a]See ref 1 for details. [b]For PBE0−2, **6** is a clear outlier due to a strong orbital mixing in the triplet state (see the SI of the original work). Removing it yields MSE, MAE, and SDE of 0.006, 0.046, and 0.056 eV, respectively. Note, however, that removing this challenging compound would improve the statistics of all other double-hybrid functionals.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jpclett.5c00462.

Computational tests with several codes for **10**; corrected statistical values (PDF)

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■ REFERENCES

(1) Loos, P.-F.; Lipparini, F.; Jacquemin, D. Heptazine, Cyclazine, and Related Compounds: Chemically-Accurate Estimates of the Inverted Singlet−Triplet Gap. *J. Phys. Chem. Lett.* **2023**, *14*, 11069−11075.

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