THE JOURNAL OF PHYSICAL CHEMISTRY LETTERS
A JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

pubs.acs.org/JPCL

Addition/Correction

Correction to "Noncovalent Interactions from Models for the Møller–Plesset Adiabatic Connection"

Timothy J. Daas, Eduardo Fabiano, Fabio Della Sala, Paola Gori-Giorgi, and Stefan Vuckovic*

J. Phys. Chem. Lett. **2021**, *12* (20), 4867−4875. DOI: 10.1021/acs.jpclett.1c01157

Cite This: *J. Phys. Chem. Lett.* 2023, 14, 1478−1478

Read Online

ACCESS | Metrics & More | Article Recommendations

We correct an error in Table 1 of the Letter[1] regarding the reference data of B3LYP-D3 for S22 and S66. The mean absolute errors (MAEs) in the Letter are 0.15 and 0.18 for S22 and S66, respectively, which are actually the MAEs of B2PLYP-D3. The correct MAEs of B3LYP-D3 are 0.31 and 0.26 instead, which can be found in the Supporting Information of ref 2. For clarity, we include the updated table with the correct data (Table 1). This error does not change any of our calculations or the conclusions of the Letter.

Table 1. MAE in kcal/mol of Different Methods for the S22, CT7, DI6, S66, and L7 Datasets from the Existing Literature[a]

set	MP2	SPL	SPL2	MPACF-1	B3LYP-D3
NGD8	0.04	0.05	**0.03**	**0.03**	0.08
CT7	0.92	0.57	**0.45**	0.60	1.48
DI6	0.48	0.27	**0.18**	0.20	0.46
S22	0.88	0.38	**0.15**	0.19	0.31
S66	0.47	0.35	**0.21**	0.26	0.26
L7	8.74	3.83	**0.89**	2.32	1.78

[a]Best results are highlighted in bold. NGD8 is a set of eight noble gas dimers (Ar_2, He_2, Kr_2, Ne_2, ArKr, C_6H_6−Ne, CH_4Ne, and HeAr) that we construct here.

REFERENCES

(1) Daas, T. J.; Fabiano, E.; Della Sala, F.; Gori-Giorgi, P.; Vuckovic, S. Noncovalent Interactions from Models for the Møller-Plesset Adiabatic Connection. *J. Phys. Chem. Lett.* **2021**, *12*, 4867−4875. PMID: 34003655.

(2) Goerigk, L.; Hansen, A.; Bauer, C.; Ehrlich, S.; Najibi, A.; Grimme, S. A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. *Phys. Chem. Chem. Phys.* **2017**, *19*, 32184−32215.

Published: February 6, 2023