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Erratum

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Correction to Comprehensive Benchmark of Association (Free) Energies of Realistic Host–Guest Complexes

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On page 3797 of the original article, we wrote: "OM2-D3 also shows a large MAD of about 10 kcal mol^{-1}. This is due to the bad description of the anionic systems **29** and **30**. For these two complexes, ΔE is off by a factor of 2 (overbinding). If **29** and **30** are disregarded from the statistics, the MAD drops to a reasonable value of 5.3 kcal mol^{-1}."

The OM2-D3 association energies reported for anionic systems **29** and **30** are wrong due to incorrect charges. The correct values are −47.6 and −43.4 kcal mol^{-1}, respectively, which is in good agreement with the reference values of −53.5 and −49.3 kcal mol^{-1}. Thus, the OM2-D3 method has a correct overall MAD of 5.3 kcal mol^{-1} with respect to the reference values and performs even better than PM6-D3H2. Therefore, Figure 11 should be replaced with Figure 1 provided here.

■ ACKNOWLEDGMENTS

We thank Dr. Pavlo Dral for pointing out this error to us.

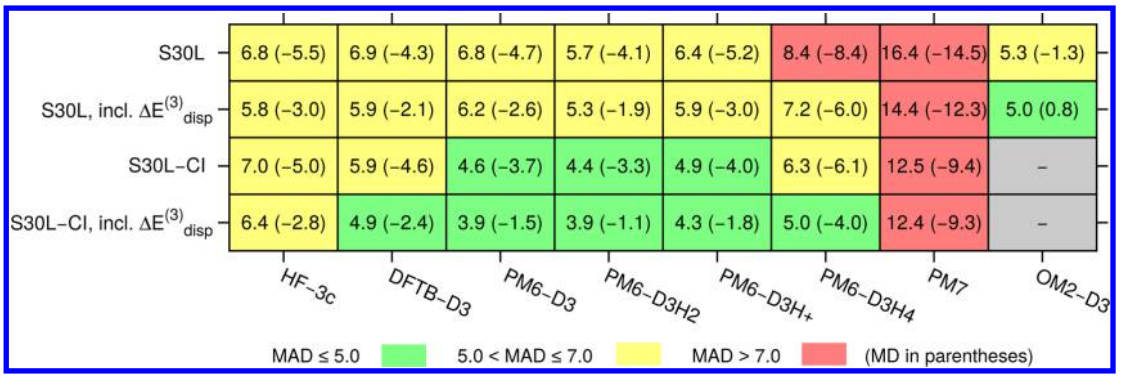

Figure 1. MADs (and MDs) for calculated ΔE of S30L and S30L-CI for several semiempirical methods w.r.t. ΔE^{emp} in kcal mol^{-1}. The values are given with and without inclusion of the three-body dispersion term $\Delta E^{(3)}_{disp}$. For OM2-D3 six complexes of the S30L had to be disregarded due to missing parameters.

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