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Erratum

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# Erratum: Accurate Prediction of Noncovalent Interaction Energies with the Effective Fragment Potential Method: Comparison of Energy Components to Symmetry-Adapted Perturbation Theory for the S22 Test Set

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Our previous paper[1] reports SAPT energies for the S22 data set presented in Figure 2 and Table S1 (in the Supporting Information). However, while the paper states that the SAPT results were obtained at the SAPT2+(3)/aug-cc-pVTZ level of theory, the presented data correspond to the SAPT2+/aug-cc-pVDZ level of theory. The correct SAPT2+(3)/aug-cc-pVTZ data, corresponding to Sherrill group best values, modern PSI4 SAPT code with exchange scaling[2] applied, are shown in Figure 1 and Table S1 in this Erratum.

Although nominally a better level of theory, SAPT2+(3)/aug-cc-pVTZ performs very similarly to SAPT2+/aug-cc-pVDZ in comparison to coupled-cluster benchmarks for interaction energy (both have a mean absolute error of 0.32 kcal/mol over the S22 data set), with the former excelling for dispersion-dominated systems and the latter for hydrogen-bonded and mixed-influence complexes.[2] The comparison of energy

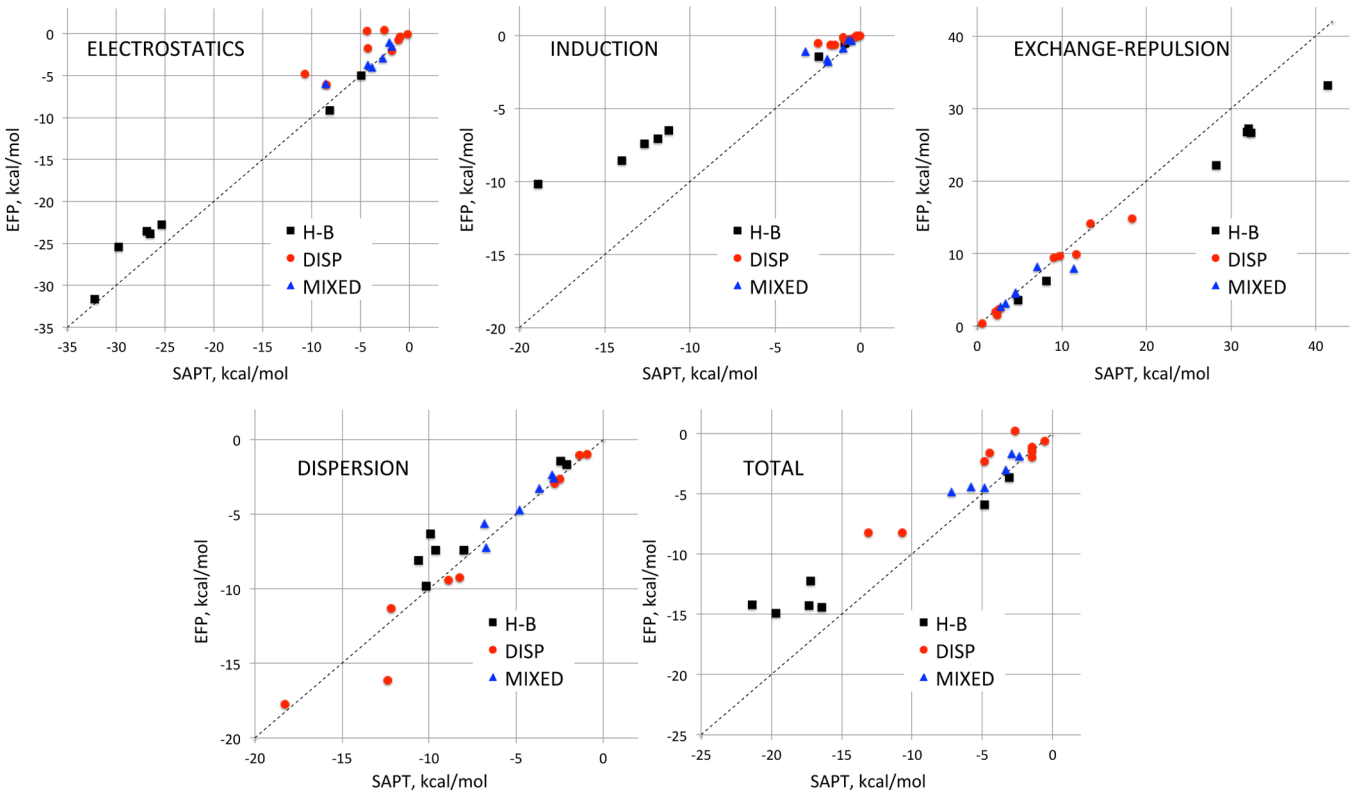


**Figure 1.** Comparison of EFP and SAPT energy components for the S22 data set dimers: hydrogen bonded (H−B), dispersion dominated (DISP), and mixed (MIXED) dimers.

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**Table S1. Comparison of SAPT and EFP Energy Components for S22 Data Set (kcal/mol)**

| | electrostatics | | exchange-repulsion | | induction (polarization) | | dispersion | | total | |
|---|---|---|---|---|---|---|---|---|---|---|
| | SAPT | EFP | SAPT | EFP | SAPT | EFP | SAPT | EFP | SAPT | EFP |
| hydrogen bonded complexes | | | | | | | | | | |
| ammonia dimer | −4.89 | −5.01 | 4.82 | 3.63 | −0.91 | −0.56 | −2.08 | −1.70 | −3.06 | −3.63 |
| water dimer | −8.10 | −9.17 | 8.15 | 6.19 | −2.45 | −1.44 | −2.42 | −1.46 | −4.81 | −5.88 |
| formic acid dimer | −32.22 | −31.66 | 41.38 | 33.19 | −18.94 | −10.14 | −9.89 | −6.33 | −19.67 | −14.94 |
| formamide dimer | −25.36 | −22.75 | 28.19 | 22.23 | −11.26 | −6.48 | −8.01 | −7.43 | −16.44 | −14.44 |
| uracil H-bonded dimer | −29.79 | −25.46 | 32.06 | 27.25 | −14.01 | −8.59 | −9.63 | −7.42 | −21.38 | −14.22 |
| 2-pyridone 2-aminopyridine dimer | −26.91 | −23.57 | 32.39 | 26.60 | −12.65 | −7.45 | −10.17 | −9.84 | −17.34 | −14.25 |
| adenine-thymine WC | −26.58 | −23.85 | 31.83 | 26.75 | −11.88 | −7.07 | −10.60 | −8.09 | −17.21 | −12.26 |
| dispersion dominated complexes | | | | | | | | | | |
| methane dimer | −0.15 | −0.04 | 0.59 | 0.41 | −0.03 | 0.00 | −0.94 | −0.99 | −0.53 | −0.62 |
| ethene dimer | −1.13 | −0.79 | 2.38 | 1.48 | −0.23 | −0.02 | −2.48 | −2.65 | −1.46 | −1.97 |
| benzene-methane | −0.96 | −0.39 | 2.61 | 2.37 | −0.31 | −0.13 | −2.79 | −2.93 | −1.46 | −1.08 |
| benzene stack dimer | −2.54 | 0.39 | 9.04 | 9.42 | −0.93 | −0.36 | −8.24 | −9.23 | −2.67 | 0.23 |
| pyrazine dimer | −4.27 | −1.73 | 9.71 | 9.68 | −1.02 | −0.12 | −8.90 | −9.44 | −4.47 | −1.60 |
| uracil stack | −8.52 | −6.12 | 11.72 | 9.87 | −1.75 | −0.65 | −12.17 | −11.30 | −10.72 | −8.20 |
| indole-benzene stack | −4.31 | 0.31 | 13.36 | 14.16 | −1.48 | −0.63 | −12.40 | −16.16 | −4.83 | −2.31 |
| adenine-thymine stack | −10.66 | −4.85 | 18.30 | 14.87 | −2.49 | −0.54 | −18.27 | −17.72 | −13.12 | −8.25 |
| mixed complexes | | | | | | | | | | |
| ethene-ethyne dimer | −1.77 | −2.08 | 2.21 | 1.95 | −0.57 | −0.26 | −1.36 | −1.07 | −1.48 | −1.46 |
| benzene-water | −2.71 | −2.95 | 3.32 | 3.12 | −1.00 | −0.86 | −2.91 | −2.35 | −3.30 | −3.04 |
| benzene-ammonia | −1.74 | −1.61 | 2.76 | 2.71 | −0.53 | −0.36 | −2.82 | −2.63 | −2.33 | −1.89 |
| benzene-HCN | −3.84 | −4.03 | 4.55 | 4.60 | −1.91 | −1.79 | −3.67 | −3.28 | −4.86 | −4.49 |
| benzene dimer T-shaped | −2.00 | −1.11 | 4.58 | 4.51 | −0.70 | −0.31 | −4.78 | −4.75 | −2.90 | −1.65 |
| indole-benzene T-shaped | −4.25 | −3.69 | 7.11 | 8.16 | −1.95 | −1.61 | −6.70 | −7.28 | −5.79 | −4.42 |
| phenol dimer | −8.57 | −6.02 | 11.38 | 7.94 | −3.22 | −1.10 | −6.79 | −5.64 | −7.20 | −4.82 |

components between EFP and these two levels of SAPT does not change qualitatively, and all main conclusions of the paper remain valid.

## AUTHOR INFORMATION


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## REFERENCES


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