Benchmark Interaction Energies for Biologically Relevant Noncovalent Complexes Containing Divalent Sulfur

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DOE/Office of Science/Biological & Environmental Research

Objective

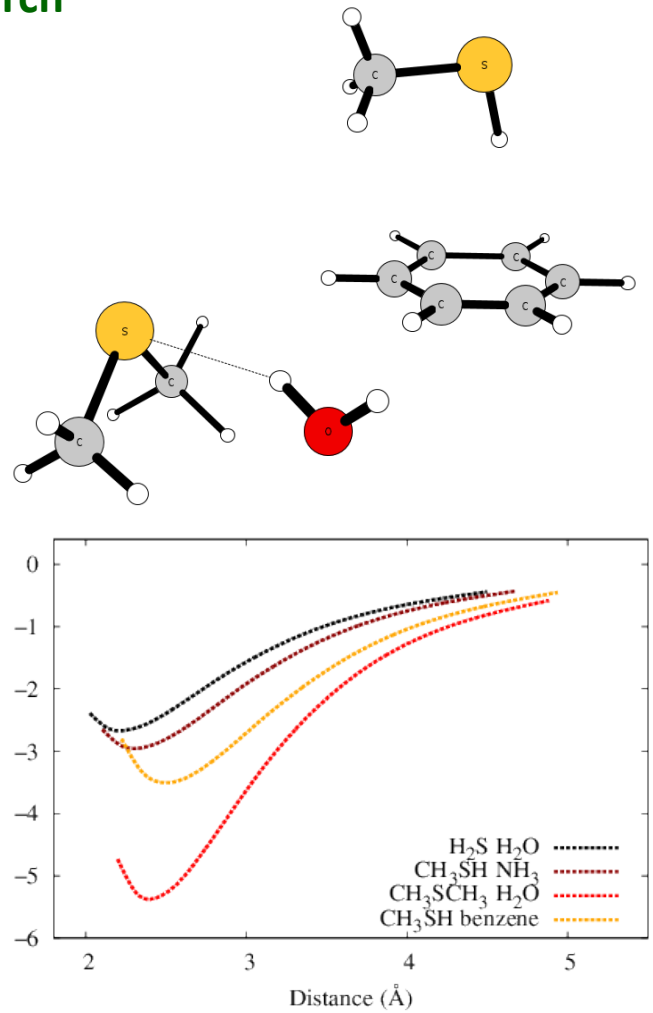
- Using *ab initio* quantum chemical calculations, compute highly accurate non-covalent interaction energies for biologically relevant model complexes that contain sulfur.

New Science

- Interaction energies are among the most accurate to date for sulfur-containing complexes bound by hydrogen bonding or dispersion. These effects play important roles in determining the structure and function of proteins and other biomolecules.

Significance

- Results will be useful for developing and assessing the accuracy of quantum chemical and classical methods that are more computationally efficient and therefore applicable to much larger molecular systems, including mercury sulfide chemistry.



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Molecules containing divalent sulfur can participate in significant noncovalent interactions. Computing accurate noncovalent interaction energies using ab initio quantum chemical methods requires a proper description of electron correlation effects. Coupled-cluster theory with single and double substitutions and perturbative triple substitutions, CCSD(T), using extrapolation to the complete basis set (CBS) limit has become the method of choice for computing accurate interaction energies of noncovalently bound complexes. Here, interaction energies are computed for several biologically relevant hydrogen-bonded and dispersion-bound complexes that contain divalent sulfur. Eight-point estimated CCSD(T)/CBS dissociation curves along the noncovalent interaction vector are computed for each complex. As a comparison of high-accuracy *ab initio* methods, interaction energies are also calculated for each complex using the correlation-consistent Composite Approach (ccCA). We find that, on average, the two methods yield energies within 0.1 kcal/mol of each other. The interaction energies provided here should be useful for developing and assessing the accuracy of more approximate *ab initio*, density functional theory, semi-empirical, and classical force field approaches.

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