Chelate Effect: Quantum Chemical Modelling of an Entropy Effect in Aqueous Solution

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As the name implies continuum solvation models (CSMs) were designed to predict the solvation energies, and related properties, of ions/molecules in solvent media. While the common CSMs, IEFPCM and SMD, are routinely used in the prediction of the solvation properties of small molecules, there are, however, some shortcomings in the prediction of solvation properties for ions in water. As part of a series of projects in the East group dedicated to fixing the challenges of popular CSMs in predicting reaction free energies in aqueous solutions, this work is focused on reproducing the experimental free energy of the chelate effect, an entropic effect, in water. Computations of the aqueous reaction free energy ($\Delta_{rxn}G$) for $Zn(NH_3)_4^{2+}$ + 2 en → $Zn(en)_2^{2+}$ + 4 NH_3 (en = 1,2-ethylenediamine) are performed, demonstrating that the two most common means of computing $\Delta_{rxn}G$ here are not accurate enough to properly reproduce the chelate effect. Until improved CSMs become available, an ad hoc fix is proposed.