Quantitative Solvation Energies from Gas-Phase Calculations: First Principles Charge Transfer and Perturbation Approaches

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These results were generated using the solvation_fit.py, solvation_cv.py, and solvation_cv_output.py modules.

- solvation_fit.py: provides the functionality to fit the experimental data using C-DFT methods.
- solvation_cv.py: allows to run the cross-validation tests.
- solvation_cv_output.py :generates the output files.

The structure of the output files is the following:

- The first 7 lines include the details of the systems considered.
- dXs indicates the solvation enthalpy (dHs) or Gibbs free energy (dGs).
- dX-+ indicates the anion/cation difference in enthalpy (dH-+) or Gibbs free energy (dG-+).
- Ref dXs, Ref dX-+: experimental values.
- The methods are as follows: “allparams” (γ, ξ, m, b), “gamma” (γ, m, b), “zeta” (ξ, m, b), “simple” (m, b).
- The statistical error measures are: MAE mean unsigned error, RMSD root mean square deviation, AIC Akaike information criterion, dAIC Akaike information criterion relative to the minimum, AICc Akaike information criterion for small datasets, dAICc Akaike information criterion for small datasets relative to the minimum.

The experimental data used to perform the fits is available upon request.