

Simple one- and two-parameter models for calculating atomic charges in molecules

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The concept of *atomic charges* in molecules is widely used by chemists to qualitatively describe molecular properties and reactivity. Nevertheless, there is no unique way to define a charge of an atom in a molecule. Hence, many alternative schemes exist that differ in the way how the molecular electron density is partitioned among the atoms.

We propose two new atomic-charge methods, the *Adjusted Charge Partitioning* (ACP) [1] and its iterative version, *Iterative ACP* [2]. To partition the valence electronic density into atomic components, Slater-type weighting factors $c_A r^{2n-2} e^{-\alpha_A r}$ are used. Within the *ACP method*, both c_A and α_A are fixed parameters reflecting atomic electronegativity and atomic size, respectively. The parameters are adjusted to reproduce molecular dipole moments in the best way. In the *Iterative ACP*, only α_A is fixed, while the coefficient c_A is determined iteratively in every calculation.

The advantage of the ACP method is that it is non-iterative, thus fast and reliable. The Iterative ACP is more accurate, flexible and easier to parameterize, but a little bit more computationally demanding.

Extensive numerical tests show that the resulting atomic charges accurately reproduce experimental dipole moments, are insensitive to basis sets used and chemically consistent.

Possible applications of the ACP and Iterative ACP schemes for calculating solvation energies of neutral molecules are shown.

References

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