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Atomic charges for reproducing the dependence of molecular dipole moment on conformation

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A modification of the principal component regression model is proposed for obtaining a fixed set of atomic charges (referred to as dipole-derived charges) optimized for reproducing the dipole moment of a conformationally rich
molecule, i.e., a molecule with multiple local minima on the potential energy surface. The method requires geometry of the conformers, their dipole moments and APT charges (which only depend on the derivatives of the dipole moments with respect to the atomic coordinates) in each of the conformers as input data, and produces a single set of fixed charges suitable for accurate representation of both the dipole moment vector of all conformers and its variations resulting from small changes in molecular geometry (e.g., caused by vibrations) [1]. The peculiar feature of the method is that it requires neither adjustable empirical parameters, nor averaging over conformers or any other post-processing of the obtained charges. The input data used in the proposed method are obtained from ab initio calculations which also do not require empirical parameters.
The proposed method has been applied to canonical 2'-deoxyribonucleotides, the model DNA monomers, and the dipole-derived charges have been shown to outperform both the averaged APT and RESP charges in reproducing the dipole moments of large sets of conformers, thus demonstrating a potential usefulness of the dipole-derived charges as a 'reference point' for modeling polarization effects in conformationally rich molecules, parameterizing non-polarizable force fields and for developing novel polarizable force fields for classical MD simulations.

[1] T.Yu.Nikolaienko and L.A.Bulavin, Phys. Chem. Chem. Phys, 20, 2890-2903 (2018).

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