# Atomic Charge Calculator II – a web service for calculating partial atomic charges

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Partial atomic charges are a theoretical concept simplifying the electron density in a molecule to a set of point charges. Charges were proven useful in many research areas, e.g., computational chemistry or structural bioinformatics. Since they are not physical observables, their values must be computed via a suitable method. Standard approaches employ quantum mechanics (QM) principles, but their high computational complexity limits their use to small systems. On the other hand, empirical methods can reproduce the results from the QM calculations with high accuracy within a fraction of the original time. Unfortunately, implementations of most empirical methods are not available to the users. Therefore, we developed a web service Atomic Charge Calculator II (ACC II) [1], to make the most important empirical methods accessible to the community. ACC II features 20 empirical methods with parameter sets gathered from the literature. It can be used interactively in a web browser providing charge visualizations, or automatically in user-defined workflows utilizing an API. ACC II is freely available at [https://acc2.ncbr.muni.cz](https://acc2.ncbr.muni.cz/).

[1] Raček, T., Schindler, O., Toušek, D., Horský, V., Berka, K., Koča, J., & Svobodová, R. (2020). Atomic Charge Calculator II: web-based tool for the calculation of partial atomic charges. Nucleic acids research, 48(W1), W591-W596.