

Poster Presentation

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Invariom point charges

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The invariom database [1] is known to provide aspherical scattering factors for atoms in different chemical environments. It contains more than 1450 geometry optimized model compounds. Underlying the database is a formalism of assigning the atoms according to their local bonding situation. An atom in such a specific intramolecular environment is called an invariom (invariant atom) because the properties related to it are invariant of the molecule. Besides aspherical scattering factors this formalism, combined with a model compound database, automatically provides point charges for atoms in common organic compounds as soon as 3D-coordinates are available. This could be especially useful for improving molecular mechanics simulations based on force fields like AMBER [2] in drug development, where point charges often have to be established manually. The invariom classification accounts for a more detailed description than a general atom force field, especially for hydrogen atoms. These are closest to the molecular surface and have a big impact on intermolecular interactions. Since the database already contains optimized structures of model compounds and their electron density, it only takes a restrained fit to the electrostatic potential (resp) [3] to obtain charges, which were designed to be transferable and are therefore ideally suited for application in force fields. Amber suggests the use of hf/6-31g* resp computations. The model compounds in the invariom database have been optimized using more extensive basis sets and DFT (M06/TZVP). A revision of the database that can in principle cover elements up to Krypton will be provided. Results from invariom point charges are compared with those from existing methods. Furthermore, some improvements to the invariom notation will be discussed.

[1] B. Dittrich, C. B. Hübschle, K. Pröpper, F. Dietrich, T. Stolper, J. J. Holstein, *Acta Cryst.* (2013), B69, 91-104., [2] W. D. Cornell, P. Cieplak, C. I. Bayly, I. R. Gould, K. M. Merz, D. M. Ferguson, D. C. Spellmeyer, T. Fox, J. W. Caldwell, P. A. Kollman, *J. Am. Chem. Soc.*, (1995), 117 (19), 5179–5197., [3] C. I. Bayly, P. Cieplak, W. D. Cornell, P. A. Kollman, *J. Phys. Chem.* (1993), 97, 10269-100280.

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