Advances in Charge Density and Electrostatic Interaction Analyses

Christian Jelsch, Angelique Lagoutte, Benoit Guillot, Virginie Pichon-Pesme, Claude Lecomte,*LCM3B CNRS UHP Faculte des Sciences. Vandoeuvre les Nancy*. E-mail: christian.jelsch@lcm3b.uhp-nancy.fr

The number of high resolution biological macromolecules X-ray structures increases regularly. Feasibility of multipolar refinement of protein structures has been proved [1, 2], assuming subatomic resolution and sufficiently low thermal motion. The high resolution crystallographic refinement program MoPro employs a multipolar representation of the electron density, the latest functionalities will be described [3,4].

Electrostatic properties are of major importance in numerous biological and molecular recognition. Three methods are employed in the VMoPro software to calculate the accurate electrostatic potential and the interaction energy:

* numerical grid integration
* Buckingham summation of charges & multipoles interaction
* coulombic energy using real and virtual spherical atoms.

The electron density parameters are obtained either from a crystallographic refinement or from a database transfer [5]. The applications go from small compounds crystals to protein–ligand complexes.

[1] Muzet N., Guillot B., Jelsch C., Howard E., Lecomte C., *PNAS*, 2003, **100**, 8742. [2] Jelsch C., Teeter M.M., Lamzin V., Pichon-Pesme V., Blessing R.H., Lecomte C., *PNAS*, 2000, **97**, 3171-3176. [3] Jelsch C., Guillot B., Lagoutte A., Lecomte C., *J. Appl. Cryst.* A, 2005, **38**, 38-54. [4] Guillot B., Viry L., Guillot R., Lecomte C., Jelsch C., *J. Appl. Cryst.*, 2001, **34,** 214. [5] Pichon-Pesme V., Jelsch C., Guillot B., Lecomte C., *Acta Cryst.*, 2004, **A60**, 204-208.

Keywords: charge density, protein, database