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Reactivity of Molecules through their Electrostatic Properties. Nour Eddine Ghermani[a], Nouzha Bouhmaida[b], Jean-Michel Gillet[c]. [a,c]*Laboratoire Physico-Chimie-Pharmacotechnie-Biopharmacie, UMR CNRS 8612, Université Paris-Sud 11, Faculté de Pharmacie, 5 rue Jean-Baptiste Clément, 92296. Châtenay-Malabry, France.* [b]*Laboratoire des Sciences des Matériaux, Université Cadi Ayyad, Faculté des Sciences Semlalia, boulevard Prince Moulay Abdallah, BP 2390, 40000 Marrakech, Morocco.* [c]*Laboratoire Structures et Propriétés des Matériaux Solides, UMR CNRS 8580, Ecole Centrale Paris, Grande Voie des Vignes, 92290 Châtenay-Malabry, France.*
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Once the electron density is determined experimentally or theoretically, it is possible to derive the electrostatic properties of isolated or crystal embedded molecules. The property of importance is the electrostatic potential emphasizing nucleophilic and electrophilic regions (possible chemical attacks) of the chemical system. Last researches were devoted to the topological features of the electrostatic potential of molecules in crystals in complementary to electron density topology. Features of the electric field (minus gradient of the electrostatic potential) were highlighted and the critical points of the electrostatic potential were carefully analyzed.[1] The electric field can be used, applying the Gauss's law, to evaluate the forces between atoms in the bonds.[2] All these properties including electrostatic potential at the nuclei, Feynman and Ehrenfest forces, Fukui functions are strictly related to the molecular reactivity. These can be used as predictable indices of the chemical reactions. This is what we will try to demonstrate.

[1] N. Bouhmaida, M. Dutheil, N. E. Ghermani and P. Becker, *J. Chem. Phys. B,* 2002, 116, 6196. [2] N. Bouhmaida and N.E. Ghermani, *Physical Chemistry Chemical Physics,* 2008, *10*, 3934.

Keywords: electron density, electrostatics, reactivity.

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Characterization of a Non-Nuclear Attractor in a dimeric Magnesium(I) compound. Jacob Overgaard[a], Cameron Jones[b], Jamie Platts[c]. [a]*Department of Chemistry, Aarhus University, Denmark* [b]*School of Chemistry, Monash University, Australia.* [c]*School of Chemistry, Cardiff University, Wales.*
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High-resolution X-ray diffraction data coupled with theoretical calculations are used to demonstrate the presence of a non-nuclear local maximum in the electron density of a dimeric Mg(I) molecule. Multipole refinement of high-resolution X-ray data, allied to density functional theoretical data, reveals the first unambiguous evidence of such a feature in a stable molecule. The properties of the Mg-Mg bond are therefore qualitatively different to "typical" metal-metal bonds, with each Mg(I) ion bound to a pseudoatom associated with the non-nuclear attractor. This pseudoatom encompasses almost an entire electron within its basin, and acts as the electronic glue binding the Mg ions. The electron density located within the pseudoatom is only weakly held and strongly delocalized over the remainder of the molecule, properties that have clear implications for the chemistry of this class of molecules.

Keywords: topological properties of charge distribution, electron density studies, chemical bonding

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Electron Densities of Macromolecules from Synchrotron Experiments and Databases. Peter Luger[a], Roman Kalinowski[a], Stefan Mebs[a], Anja Lüth[a], Armin Wagner[b], Alke Meents[c], Birger Dittrich[d]. [a]*Free University Berlin, Germany,* [b]*Diamond Light Source, Didcot, UK,* [c]*Hasylab, Hamburg, Germany, University Goettingen, Germany.*
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The understanding of mutual recognition of biological interacting systems on an atomic scale is of paramount importance in the Life Sciences. Electron density (ED) distributions that can be obtained from high-resolution X-ray diffraction experiments can provide – in addition to steric information – intra and intermolecular electronic properties of the species involved in these interactions. Macromolecules e.g. proteins/drug-receptor complexes are of great interest for ED studies but represent a major challenge with respect to various unfavorable properties which make an accurate high-resolution X-ray diffraction experiment almost impossible. Database applications can help to overcome the experimental shortcomings. One concept is given by the invariom [1] formalism, an aspherical scattering model which assigns fixed multipole populations from theoretical calculations to each atom of a structure. The corresponding database entries are then assigned to the building blocks of a given macromolecule to generate additively the ED of the entire molecule. The invariom formalism was applied to the aspherical modelling of three protein structures: (i) the 11.6 kDa dimer of rhombohedral insulin (0.90 Å data set from synchrotron beam line I03, Diamond Light Source); (ii) the 14.3 kDa structure of tetragonal lysozyme (0.80 Å data set from synchrotron beam line X10SA, Swiss Light Source); (iii) the triclinic form of lysozyme (0.65 Å data kindly provided by the group of Z. Dauter, Argonne, USA, PDB entry 2VB1 [2]). Functional relations between the aspherical model and the initial spherical parameters were examined, among them were the R-values before and after aspherical invariom refinement and the change of other properties, as residual densities, displacement parameters etc. The conclusion is at present that all considered properties indicated that only small improvements resulted from the aspherical ED models although high quality atomic resolution data from 3rd generation synchrotrons were used.
In an attempt to avoid the above mentioned limitations we examined drug-receptor complexes which were reduced to appropriate substructures around the active center. In an easy-to-use procedure the combination of experimental X-ray structure information and aspherical atomic ED data from the invariom library resulted in properties like the electrostatic potential and the Hirshfeld surface in the active site region which allowed a study of electronic complementarity and the identification of sites and strengths of drug receptor interactions. Applications were considered for three examples: The anilinoquinazoline Gefitinib (Iressa®) which belongs to a new class of anticancer drugs; the interaction of epoxid