Oral presentation

Atomic ionisation determined by dynamical kappa refinement against 3D electron diffraction data

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Advancements in accurate structure refinement from three-dimensional electron diffraction (3D ED) have increased the method's popularity, especially when dealing with very small crystals [1]. However, better approaches have to be developed to extract information on atomic interaction, and charge transfer to fully leverage the advantages of the 3D ED method in the field of material science for designing new functional materials with improved physical properties. The conventional refinement strategies used for 3D ED data assume a spherical atomic model called the *Independent atom model* (IAM) which disregards the bonding effects between the atoms in the molecule. This model is chemically rudimental and the refined structure parameters can be biased or inaccurate [2].

We performed *dynamical kappa refinement,* which takes into consideration the dynamical diffraction effects and assumes a simple spherical atom model for extracting the information on atomic bonding effects[3,4]. We performed multiple tests on different organic and inorganic structures varying in the type of chemical bonding, centrosymmetry, crystal morphology, and atomic number of the constituting atoms to test the general applicability of the method for extracting the charge density information. Despite not considering the aspherical part of the Hassens-Coppens multipolar model, results showed significant improvements in the structure parameters of the studied compounds (especially for compounds with light atoms) all the while extracting meaningful charge density information.

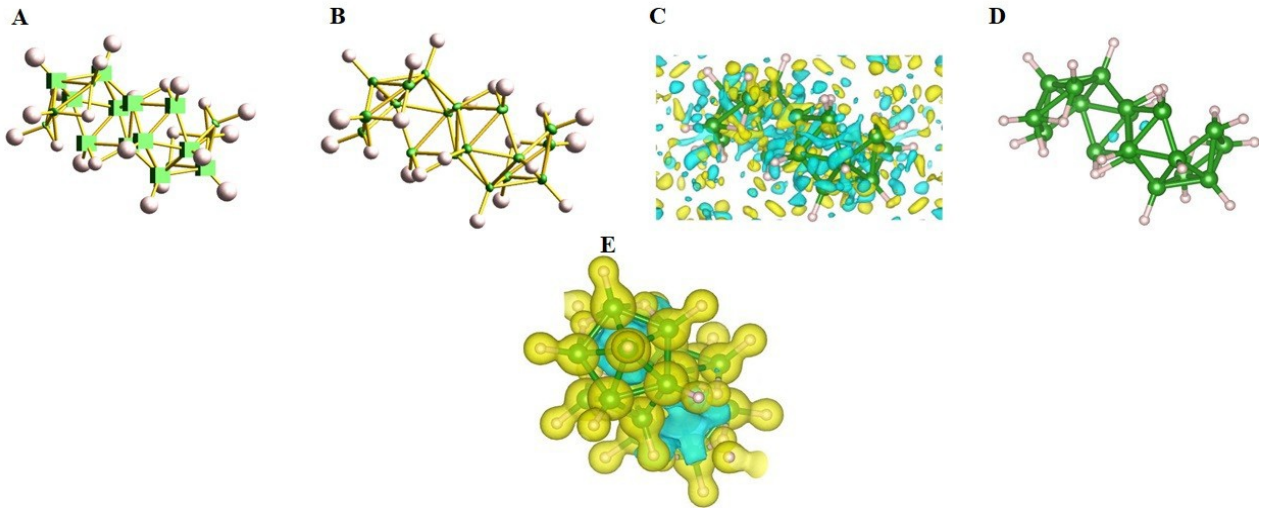

Figure 1. Evaluation of quality of refinements for borane ($B_{18}H_{22}$). Structure model of the molecule before (A) and after (B) charge density refinements. The 3D difference Fourier maps before (C) and after (D) charge density refinements plotted at the same isosurface value (0.12 e $Å^{-1}$). The static deformation map (E) of the molecule after the charge density refinement. Positive and negative isosurfaces are plotted in yellow and blue, respectively.

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