Model Wave Function for Glycyl-L-Alanine from Experimental Diffraction Data

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The XCW method is a relatively new technique for analysing X-ray diffraction experiments [1-5]. Rather than using the more common pseudo-atom expansion of the electron density [6], the X-ray diffraction data are introduced directly into the calculation of the quantum mechanical molecular wave function in such a way that the wave function is constrained to reproduce the X-ray data, at the expense of the smallest possible change in the quantum mechanical energy. The XCW method has been applied to a number of small-molecule organic crystals [2-4] showing, for example, that the constrained wave functions could model the effects of higher level calculations, simply by including experimental data or that the effects of the crystal lattice could be incorporated [2]and that a number of derived properties, such as electrostatic potentials and multipole moments could be obtained [3-4]. In order to address the limitations of the XCW method as compared to other forms of analysis of the electron distribution in crystals, like the pseudo-atom model, and to extend the application of the XCW method to more complex systems for which ab-initio calculations cannot be expect to give very accurate results (e.g. for proteins), synchrotron and neutron diffraction data have been measured on the model dipeptide Glycyl-L-Alanine at multiple-temperatures in the range 10 to 295K. The multi-temperature data were used in a molecular Einstein model [5] to get a more complete description of the thermal motion in the crystal and to recover information on the atomic correlation of motion. These latter were then included in the XCW fitting procedure to see their influence on the predicted structure factors and on the derived electronic properties. The neutron data where essential to evaluate the contribution of the motion of the hydrogen atoms to the final XCW-derived electron density.

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