Topological Properties from Conventional Fourier Maps

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The last step of a crystal structure determination that requires human intervention is the interpretation of Fourier maps, displayed as peaks in a favourable projection. Crystallographers usually infer bonding by empirically assigning bonds between peaks via geometrical criteria. The location all critical points were suggested as a new method [1], based on the topological properties of the charge density, to avoid human intervention on the Fourier maps interpretation. The molecular structure can be defined by means of the topology of the electron density which is reflected by means of its critical points. This algorithm for the full analysis of critical points and recognition of the molecular graph in Fourier maps has been developed and implemented into the package DIRDIF [2].

We have applied this procedure to a variety of crystal structures and, in the most cases, the complete structure is recovered and the connectivity matrix is constructed without any user intervention.

In this communication, we will show some recent results obtained by the application of our procedure to standard data sets of crystal structures of a wide family of oxines, with interesting H-bonding properties. Furthermore, we are currently exploring the effectiveness of the application of our procedure to medium size proteins. Preliminary results of the analysis of trypsin data will be presented.

[1] Menéndez-Velázquez A., García-Granda S., *J. Appl. Cryst*., 2003, **36**, 193-205. [2] Beurskens P. T., Beurskens G., De Gelder R., García-Granda S., Israel R., Gould R. O., Smits J. M. M., *The DIRDIF-99 program system*, Crystallography Laboratory, University of Nijmegen, The Netherlands, 1999.

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