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Bijvoet revisited. A Python class to check Friedel pairs

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Keywords: absolute configuration, graphical interface, Bijvoet, Friedel pairs

The determination of absolute configurations is a task of major importance on the characterization of optically active molecules. The use of X-ray to 'ab initio' assign absolute configurations was first explored by Bijvoet.Nowadays the Rogers's parameter [1] and mainly the Flack's parameter [2] are used to determine the right absolute configurations.
In spite of the Flack's parameter is strong and reliable, in some cases the comparison of a strong set of Friedel's pairs is in our experience very useful to solve the uncertainly resulted from the Flack ś parameter calculation. In order to check the Friedel pairs for a particular crystal the Dirdif package [3] uses the Bijvoet program[4] develop some time ago by professor Paul Beurskens.
A Python based graphical interface has been developed to use Bijvoet as an independent tool. This procedure will be presented along with a collection of test cases where the combination of Flack ś parameter weak indications are solved, based on the direct investigation of the Friedel pairs through the Bijvoet coeficient (B).

[1] Rogers, D., *Acta Cryst.*, 1981, A37, 734.
[2] Flack, H. D., *Acta Cryst.,* 1983, A39, 876.
[3] Beurskens, G; Noordik, J. H.; Beurskens, P. T., Cryst. Struct. Commun., 1980, 9, 23.
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The CRYSTALBUILDER project: an easy way for single crystal structure analysis

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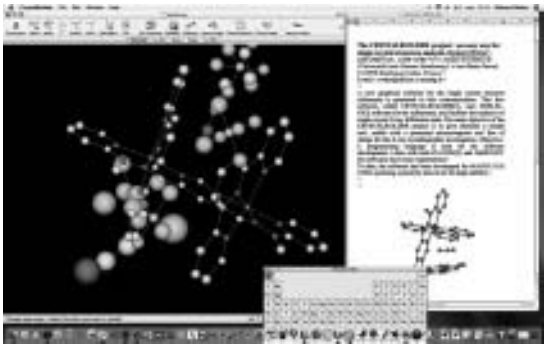
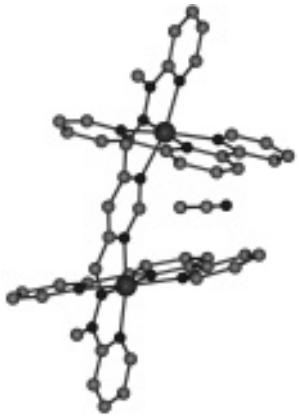
Keywords: single X-ray diffraction, molecular visualisation, free academic software

A new graphical software for the single crystal structure refinement is presented in this communication. This free software, called CRYSTALBUILDER[1], uses SHELXL-97[2] software for the refinement, and facilites the analysis of single crystal X-ray diffraction data. The main objective of the CRYSTALBUILDER project is to give chemists a simple tool, usable with a personnal microcomputer and free of charge for the X-ray crystallographic investigation. Objective-C programming language is used for the software development. Links with both PLATON[3] and MERCURY [4] softwares have been implemented.
To date, the software has been developped for MACOS 10.X UNIX operating system[5], known for his high stability.



Screen view of CRYSTALBUILDER during a refinement process



Pov-Ray image generated by CRYSTALBUILDER

[1] http://www-chimie.u strasbg.fr/~decomet.
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[4] Bruno I. J.;, Cole J. C.; Edgington P. R.; Kessler M. K.; Macrae C. F.; McCabe P.; Pearson J.; Taylor R. *Acta Crystallogr.*, 2002 389-397, B58.
[5] http://www.apple.com/macosx/