EdMol: A Graphical Molecular Editor

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EdMol is a graphical molecular editor tool for the input of molecular structures in 2D or 3D. The format of output coordinates (Z-Matrix, Spherical, Fractional or Cartesian are some of the options presently implemented) can be selected by the user as input for other programs, as FullProf [1], Expo2004 [2] or StructRes, in order to aid the structure solution, mainly from powder diffraction, using global optimisation as Simulated Annealing, Genetic algorithms or any other algorithm or method as Patterson or Direct Methods.

EdMol is written in Fortran95 using the CrysFML [3] (Crystallographic Fortran Module Library) and X/Winteracter [4] libraries for Linux (x86) and Windows 9X/NT/2K/XP versions. The use of EdMol is totally free for the scientific community and it is distributed within the FullProf Suite package or as a stand-alone program in the FullProf Suite Web site[5].

[1] Rodriguez-Carvajal J., *Physica B*, 1993, **192**, 55. [2] Altomare A., Caliandro R., Camalli M., Cuocci C., da Silva I., Giacovazzo C., Moliterni A. G. G., Rizzi R., *J. Appl. Cryst.*, *submitted*. [3] Rodriguez-Carvajal J., Gonzalez-Platas J., *Compcomm Newsletter*, 2003, **1**, 90. [4] *Winteracter. The Fortran 9X GUI Toolset* http://www.winteracter.com [5] *FullProf Suite Web* http://valmap.dfis.ull.es/fullprof

Keywords: computer applications, computer software, computer graphics molecular