s3.m1.p1 **MarchingCubeELD - electron density visualization program for small molecules and its application on cyclosporins structures investigation**. M. Hušák , J. Cejka, *Department of Solid State Chemistry, Institute of Chemical Technolgy, Technická 5, 166 28 Prague 6, Czech Republic*.
Keywords: computing, hot topics.

Several methods of modern computer graphic were used for developing a program for fast 3D electron densities visualization:

a) OpenGL graphic language[1] – a computer API originally designed by SGI company for communication between software and graphic hardware nowadays widely supported on PC platform.

b) Marching cube algorithm – a mathematical algorithm for voxelized data visualization like results of X-ray tomography in medicine. Application of this algorithm to ELD map leads to very fast construction of 3D objects which can represent those ELD map.

c) Stereoscopic visualization[2]. The program supports interlaced and HW page flipped stereoscopic output suitable for watching by the help of LCD glasses.

All described methods are combined in Marching Cube ELD program. The program is able to directly read output from CRYSTLALS[3] crystallographic package, moreover in cooperation with WinGX[4] interface it can process SHELX refinement output as well. The POVRAY raytracing file with the ELD map could be produced as one of the output graphic options.

The program is widely used for visual interpretation of solvated Cyclosporines[5] ELD maps in our laboratory. It was found a very powerful tool for correct disordered solvents characterization.

The software is available from the CCP14 mirror page: http://www.ccp14.ac.uk/tutorial/marchingcube/ index.htm.

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s3.m1.p2 **Comparing Polymorphs of Crystal Structures of Small Organic Molecules.** J.P.M. Lommerse. *Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, United Kingdom.*
Keywords: structure comparison, coordination sphere, clustering.

The comparison of two different crystal structures can be a tricky problem. Most methods are based on comparison of cell dimensions. A popular method is conversion into a reduced cell [1]. Other methods include conversion into standard settings which may be compared directly [2]. These are complicated methods and always an uncertainty about the final similarity between two crystal structures remains.

For molecules with Z'=1, the environment around each molecule in the crystal structure is identical. A new algorithm has been developed which does not compare the cell dimensions, but rather the coordination sphere of molecules around a central molecule in the crystal structure. The method is based on original ideas of Gavezzotti [3].

In general, a molecule in a crystal structure is fully enclosed by 14 surrounding molecules [4], which fully determines the unique structure in a particular crystal. Therefore, it is sufficient to superimpose the coordinates of a central molecule plus its 14 nearest neighbours of one crystal structure on top of the coordination sphere of a second crystal structure. In order to get the best RMSD for the superimposition, however, one has to try all possible permutations, which is 14!, more than 87 billion times. This would make the method extremely slow. The number of superimpositions has been reduced dramatically by using predefined distance and orientation criteria. This makes the algorithm fast and accurate results in terms of a optimum RMSD for the superimposition are obtained.

The main advantage of the new algorithm is that it does not depend on space group symmetry. Polymorphs in different space groups can be remarkably similar. The method can be used for clustering in crystal structure prediction calculations, and assessment of final results. Investigations are on their way to judge how (dis)similar environments are of the independent molecules in Z'=2 and higher.

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