s13.m36.o3 **Mogul: Rapid Retrieval of Molecular Geometry Information From a Crystallographic Database**. Susan Robertson, *Cambridge Crystallographic Data Centre (CCDC), 12 Union Rd, Cambridge, CB2 1EZ, UK. E-mail: robertson@ccdc.cam.ac.uk*

Keywords: Knowledge Bases; Crystallographic Databases; Molecular Geometry

The Cambridge Structural Database (CSD) currently contains over 310,000 structure determinations for small molecule organic and organometallic compounds, and thus is a good source of information on molecular geometries and conformational preferences. The program Mogul (Molecular Geometry Library) has been developed by the CCDC to provide rapid access to this information with full statistics.

To retrieve information on a bond length, valence angle or acyclic torsion, the user inputs a molecule of interest into Mogul and selects the geometric feature to be investigated. The molecular environment of the selected fragment is used to generate atom- and bond-based "keys", which are then used to retrieve all relevant CSD hits. The use of a search tree optimises search speeds without the need for graph-based atom-by-atom matching typically used by other retrieval programs such as ConQuest [1]. Key statistics and histograms are derived and displayed along with an indication of how well the geometry of the feature in the input molecule matches observed geometries in the CSD. Mogul searches can be run automatically via an instructions file with results written to an output file, allowing easy integration with other programs. Mogul has already been integrated with CRYSTALS [2] in this way to allow validation of molecular geometries of newly refined crystal structures; a similar use is envisaged with DASH [3], which aids the solving of structures from powder diffraction data. Other potential applications will be discussed.

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s13.m36.o4 **Comparing Structures with *Z*'=2 Using *CRYSTALS*.** A. Collins, R.I. Cooper, *Chemical Crystallography, Chemistry Research Laboratory, University of Oxford, Mansfield Rd, Oxford, OX1 3TA, UK. E-mail: anna.collins@chem.ox.ac.uk*

Keywords: *Z*-prime > 1; Pseudosymmetry; Software

Approximately 11% of organic structures in the CSD [1] have more than one molecule in the asymmetric unit ($Z'>1$), of which almost 90% have $Z'=2$. A sizeable proportion of these structures are thought to exhibit pseudosymmetry, but establishing the extent of the deviation from true symmetry is problematic. Two situations need to be distinguished: pseudosymmetry arising from small differences in conformation of molecules otherwise related by a true crystallographic operator (which would require a higher symmetry space group); and molecules with identical conformations that are related by an arbitrary operator which is incompatible with the space group symmetry.

Conformational similarity of crystallographically-independent molecules has been the subject of several studies, e.g. by Sona and Gautham [2,3] where the RMS deviation was used as a measure of similarity. Although this is a very useful comparison, it does not allow the relationship between molecules - and thus the extent of pseudosymmetry - to be established. *CRYSTALS* [4] has been used to evaluate 7064 recent $Z'=2$ structures in the CSD. The MATCH routine has been adapted to find a pseudo-operator that relates the independent molecules. This operator is tested to see if it forms a closed set with the space group operators and is compatible with the metric symmetry of the cell. Together these two factors provide a measure of compatibility. A high measure of compatibility is indicative of pseudosymmetry, and, in combination with the RMS deviation, allows the extent of pseudosymmetry to be assessed.

PLATON [5] has been used to verify the success of this method. Structures with small RMS deviation and high compatibility scores are frequently found to have missing additional symmetry by ADDSYM, which may indicate that the structure has been determined in the incorrect space group in some cases. Our measure allows evaluation of the degree of pseudosymmetry for a larger range of deviations from ideal higher symmetry, and hence provides an insight into the frequency of occurrence of pseudosymmetry in crystalline materials.

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