

## VALIDATING CRYSTAL STRUCTURES SOLVED FROM POWDER DIFFRACTION DATA USING THE dSNAP SOFTWARE

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The rapid increase in the number of organic and organometallic structures solved and refined using powder diffraction data has increased considerably over the past five years. New techniques of structure solution have also been able to solve structures with relatively low resolution data and a paucity of independent intensity measurements. With this success comes the potential problem of errors in the structure and the need for validation. We present here a method based on cluster analysis, multivariate statistics and the use of the Cambridge Structural Database [1] as implemented in the dSNAP computer program [2].

The Cambridge Structural Database (CSD) currently (2006) holds 366,866 crystal structures for organic and metal-organic compounds whose 3D structures have been determined using either X-ray or neutron diffraction. It is a superb repository of structural data, and is an obvious source of structures that can be used in a validation environment. The question is how best to utilise this information.

The computer program that does this is dSNAP [2]. This software has been used to classify structural fragments derived from the CSD in an easy way (see, for example, [2] ), but here we work as follows:

1. Define a key fragment or fragments for the structure to be validated *e.g.* functional groups.
2. Search the CSD; dSNAP can work with bonded and/or non-bonded geometries.
3. Export the solved crystal structures from powder data to CIF files.
4. The CIF and the CSD results are provided as combined input into dSNAP.
5. The output is examined for potential outlier behaviour, which may indicate errors in the determined structures.

In the last step (5) a correlation matrix is generated in which all the fragments are correlated with each other, and this is used to generate a dendrogram and a multidimensional metric scaling plot of the data where any outliers will be obvious. An example using sulphonamides will be presented.

The modified dSNAP software is available free of charge to all interested researchers from Bruker-AXS. Go to the web site <http://www.chem.gla.ac.uk/snap> and follow the instructions. A licence key is also required and this is obtained by emailing [snap@chem.gla.ac.uk](mailto:snap@chem.gla.ac.uk).

1. Allen, F.H., *Acta Crystallogr.* 2002, **B58**, 380-388.
2. G. Barr, W. Dong, C. J. Gilmore, A. Parkin and C. C. Wilson, *J. Appl. Cryst.*, 2005, **38**, 833-841.
3. Parkin A, Barr, G., Gilmore, C.J. & Wilson, C.C., 2006, *CrystEngComm*, **8**, 257-264.