ISOBASEmm: Isostructurality in the Protein Data Bank

Jan M.M. Smits, R. de Gelder, *Molecular Materials, Institute for Molecules and Materials, Radboud University Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands*. E-mail: R.deGelder@science.ru.nl.

The ISOQUEST program [1,2], a method for the comparison of crystal structures based on pattern matching techniques [3], has recently been applied to analyse the Cambridge Structural Database (CSD) [4]. A full analysis of all entries in the CSD led to ISOBASE, a database which contains all isostructurality relations in the CSD. Investigation of this ISOBASE shows that many classes of identical or closely related structures can be found, although the chemistry within those classes can vary considerably. This information can be used to extract crystal packing rules that otherwise can not be revealed.

To extend the range of applicability of the ISOQUEST method an analogous approach was chosen to analyse the collection of all macromolecular structures present in the Protein Data Bank (PDB) [5]. This poster presents the resulting macromolecular database ISOBASEmm and examples of structural relations in the PDB that can be extracted from this database.

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