

New Organic Subfiles in PDF-4/Organics 2010

A. Gindhart, S. Kabekkodu, V. Bosnic
International Centre for Diffraction Data
Newtown Square, PA 19073

One of the key features of the Powder Diffraction File's search/match option is the ability to search by common classes of materials. These subfiles are vital to the continued growth of the database. After adding the subfile classifications to our other products, we have now extended subfiles to the organics product as well. In the new release of PDF-4/Organics 2010 we have incorporated seven new subfiles to better distinguish the classes of compounds. We used the chemical classes first supplied by the Cambridge Structural Database (CSD) as a foundation and then inserted, where appropriate, our existing experimental set into those various classes. To identify the rest of the experimental database into each subfile we combined a semi-automated approach that included a review of the chemistry of similar materials by query-based assignment and a more manual approach that involved the effort of the ICDD's editorial team. This poster focuses on the new subfiles located in the PDF-4/Organics 2010.