News about the Inorganic Crystal Structure Database ICSD

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With the 2nd update 2004 82,876 entries are included in ICSD, including about 11,00 mineral structures. For about 22,000 structures a cross-reference to the Powder Diffraction File PDF is given. Inorganic structures don't contain C-H bonds together with C-C bonds in any residue. So some overlapping with organic structures is possible (e.g. with oxalate anions or tetramethylammonium cations). In addition organic residues are allowed in *zeolites and in* minerals.

For the introduction of **Structure types** the Pearson-symbols were unified as to get only one symbol per Bravais-type. The single-side centred cells were united under the letter "S". The remaining 14 symbols are: aP, mP, mS, oP, oS, oI, oF, tP, tI, hP, hR, cP, cI, cF. The number of atoms in the Pearson-symbol always refers to the standard setting, which for the rhombohedral structures is that of the rhombohedral primitive cell. The remarks of the prototype entries (one per structure type) will contain further information about the structure type in question, e.g. the "atomic environment types" of Daams & Villars [1]. The first about 100 structure types are ready to be incorporated into the first update of 2005.

Authors can easily help to complete the database ICSD! Just check your publication list against the entries in ICSD. Structures only published in a doctoral thesis or presented as a poster can be included into ICSD too.

[1] a) *J. Alloys Comp*., 1992-97, **182**, 1-33; b) *J. Alloys Comp*., 1992-97, **197**, 243-269; c) *J. Alloys Comp*., 1992-97, **215**, 1-34; d) *J. Alloys Comp*., 1992-97, **252**, 110-142

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