

How aggregate water molecules in organic crystal structures?

The importance of weak intermolecular interactions for aggregation and solvation of small molecules in solid state

One of central question of RESOLV is how influence water or solvents the aggregation of compounds and how aggregate water or a solvent with itself? A deeper insight of the aggregation can be an analysis of the situation of aggregated compounds with water/solvents in solid state. The fixed position of atoms in solid state allows a detailed investigation of geometrical and topological parameters of the "captured" aggregation form. This is exactly the approach how we will try to learn more about molecular aggregation depending of water and solvents. After a (short) theoretical introduction you will investigate the aggregation of compounds with and without solvens/water in solid state - "in silico" - by your own.

By using the Crystal Structure Database (CSD) with more than 500.000 (!) crystal structures of organic compounds and the visualization software Mercury you will pursue the question if general rules, or interesting exceptions, of aggregation of molecules in the presence of solvens/water.