

Symmetry and Asymmetry in the Associations of Molecular Crystals, Mátyás Czugler, *X-ray Diffraction Department, Chemistry Institute, Chemical Research Center, 1525 Budapest POB 17, Hungary*, E-mail: czugler@chemres.hu

Keywords: molecular symmetry, crystal structures, association properties

Recently some successful design strategies employ host molecules possessing special molecular symmetries, often coupled to the ideas of rigidity and to bulk. Crystal engineering also often touches upon the molecular symmetry theme[1] as mediated by prime intermolecular actions[2]. If one considers that symmetries must bring about operator- (and of course van der Waals radii) dependent forbidden volumes in crystals then incorporation of symmetries into molecules may lead to interesting consequences. Several crystal structures from our laboratory will be enumerated in which host molecules have two-, three-, four- and even six-fold molecular symmetry. These symmetries are employed more or less efficiently in building crystal structures of the associate molecular crystals in a range of space groups such as mainly from the trigonal, from tetragonal and from the hexagonal crystal systems. In going through these examples several interesting phenomena will be encountered such as Pasteur resolution, success and failure of chiral molecular recognition and like. We relate presence of the specific molecular symmetry to the macroscopic phenomenon in question. Discriminating effects as reflected by distances will be analyzed. Exploring into the CSD [3] V5.25 indicated over 38.000 crystal structures complying with the $Z' < 1$ AND $No. of entities > 1$ criteria thus indicating further research possibilities into the issues of molecular symmetry, space group symmetry and associate formation[4]. Financial support from OTKA-T042642 is acknowledged.

References

- [1] J.W. Steed, *Cryst.Eng.Comm.*, 2003, **5**, 169-179
- [2] R.F.M. Lange, F.H. Beijer, R.P. Sijbesma, R. W.W. Hooft, H. Kooijman, A.L. Spek, J. Kroon, E.W. Meijer, *Angew. Chem. Int. Ed. Eng.*, 1997, **36**, 969-971
- [3] F.H. Allen, *Acta Cryst.*, 2002, **B58**, 380-388.
- [4] E. Pidcock, W.D.S. Motherwell, J.J. Cole, *Acta Cryst.*, 2003, **B59**, 634-640