

Poster Presentations

[MS38-P07] Effect of size of organic molecules on aggregation into the crystalline state
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It is shown that organic and metal-organic molecules which have been retrieved from the Cambridge Crystal Structure Database [1] cease to arrange in a crystalline state for reduced unit-cell volumes with 8000-9000 Å³. This volume corresponds to about 500 non-hydrogen atoms -see [2] where 18 Å³ per non-hydrogen atom has been assessed for structures which are composed of molecules containing C, H, N, O at most. The structures with more constituting molecules (residues) as well as those composed of metal-organic molecules tend to crystallize in larger unit cells than homomolecular structures where the van der Waals forces are the main cohesion forces. It is also shown that proportion of the structures crystallizing in *Pbca* is considerably increasing towards large unit-cell volumes [3]. This means that relation between the symmetry of the molecules and the symmetry of the corresponding crystal is also dependent on the size of the molecules. *Tendency* for decreasing ability of large organic and metal-organic molecules to arrange in a crystalline state due to their size is manifested by increasing occurrence of a positional disorder in the structures of organic and metal-organic molecules in large unit cells. This means that large organic molecules tend to be less tightly packed in the crystal structures [4, cf. 5]. These empiric results provoke considerations about the origin of life since *e.g.* proteins are giant molecules which usually do not crystallize in organisms.

[1] Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.

[2] Kempster, C. J. E & Lipson, H. (1972). *Acta Cryst.* **B28**, 3674.

[3] Fábry, J. & Krupková, R. (2008). *Ferroelectrics* **375**, 59-73.

[4] Fábry, J., Kopeck••, M. & Krupková, R. (2012). *Helvetica Chimica Acta* **95**, 1202-1216.

[5] Kitajgorodskij, A. I. (1955). *Organicheskaja Kristalloghimija*, Moscow: Izdatel'stvo Akademii Nauk SSSR.

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