

Poster Presentations

[MS25-P10] C₆F₁₀ at 4.2K -Crystal Structure and Theoretical Analysis of Weak Interactions

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The crystal structure of 1,2,3,3,4,4,5,5,6,6-decafluorocyclohex-1-ene (decafluorocyclohex-1-ene, C₆F₁₀), is solved in direct space from neutron powder diffraction data previously collected at 4.2K [Pawley, G.S. *J. Appl. Crystallogr.* (1981). **14**, 357-361] and refined by energy minimization in the solid state. To optimize the positions of the 64 atoms in the monoclinic computational cell the PBESOL and hybrid PBE0 functionals were used. The crystal structure of the title compound, which is liquid at RT, is built of antiparallel pairs of molecules assembled into molecular columns stacked along the *a*-axis. Analysis of bonding conditions in the structure by theoretical molecular calculations showed that electrostatic interactions does not play any important role in stabilization of the crystal structure and the dominating the crystal-building forces are weak non-directional intermolecular dispersion interactions. Bonding conditions in the structure were analysed by theoretical molecular calculations of representative next-neighbour molecular dimers done using dispersion-corrected DFT functionals and the SCS-MP2 wave function method. The largest interaction energy is of the order of 4 kcal/mol, i.e. somewhere between the interaction energies of a benzene dimer (2.7 kcal/mol) and a water dimer (5.0 kcal/mol). The interaction energy for the second most stable dimer can be compared to either that of a benzene dimer or of

a C-H... p hydrogen bond. The remaining five weakly interacting dimers (~1-2 kcal/mol) can be characterized as stronger interactions than those of methane dimers (0.53 kcal/mol), but weaker than for instance that of benzene molecules pair or weak C-H...C interactions [1].

[1] L. Smrčok, P. Mach and A. Le Bail (2013). *Acta Cryst.* **B69**. In press..

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