Appendix F. Deposited as an electronic file only

Table 4. The main concepts introduced when preliminary considering crystal structures of organic compounds

Compounds	Examples of problems discussed	Concepts introduced	References (see Appendix C)
Different classes of organic compounds (relevant for the courses of organic chemistry and for the course of biochemistry)	Work interactively with the crystal structures of choice retrieved from the Cambridge structural database and get the values of bond lengths and angles in the common functional groups. Apply MOGUL to make statistics.	Molecular crystals (revisited and extended). Intra- and intermolecular interactions.	Robertson, 2004 Allen and Motherwell, 2002; Galek *et al*., 2009, 2010; Milner-White et al., 2004; Orpen, 2002; Pidcock and Motherwell, 2005; Weng *et al.*, 2008; Wood *et al*., 2008; Yao *et al*., 2002
	Compare the geometry of the same fragments and the same molecules in different crystalline environments (examples: biphenyl family in the gas phase, and in different crystal structures, conformational polymorphs of pharmaceuticals).	Effect of crystalline environment on the intramolecular geometry.	
	Compare the crystal structures of paraffines with the close-packed structures of balls. Which properties of a solid can depend on the packing efficiency?	Statistical analysis of the molecular conformations, intramolecular bond lengths and bond angles in different crystal structures, as a method of studying intermolecular non-covalent interactions.	
	Consider the reasons of the non-monotonic change in the melting temperatures in a series of the alkane hydrocarbons CH_3-$(CH_2)_n$-CH_3 vs. *n* in terms of the efficiency of the close packing, which can be achieved for the molecules with odd and with even number of the methylene groups in the chain.		Boese *et al*., 1999
	Which features of a structure may suggest that van der Waals interactions play a smaller relative role, than intermolecular hydrogen bonds? Does this really happen often? Why is the density of ice lower than that of liquid water?	Analysis of crystal structures as a method of revealing the nature of the intermolecular interactions at ambient and non-ambient conditions. Directional / non-directional, specific / non-specific interactions (revisited).	Görbitz, 2002,
	Which role do van der Waals interactions and hydrogen bonds play in gas hydrates? Compare the mechanism of crystallization of a gas hydrate with a template synthesis.	Open framework structures based on hydrogen bonds (ices, dipeptides, etc.).	
	Why does acetic acid form very stable dimers in the gas phase and in the liquid state, but infinite chains in the crystal structure?	Host-guest compounds.	
	Compare the H-bonding patterns in classes of compounds (alcohols, carbonic and dicarbonic acids, amino acids, etc.). Interpret the results.	"Structure-forming unit", "synthone", "H-bonded motif".	
	Consider the crystal structures of the aromatic and halogen-containing compounds.	CH-π , π -π , or Hal-Hal interactions	
	Compare the ambient-conditions structures with those at low / high temperature or high pressure. Compare the response to mechanical treatment. What can this information teach us about the intermolecular interactions and the factors determining the crystal structures? Try to predict the anisotropy of properties from crystal structure.		Boldyreva, 2008 Reddy *et al*., 2005, 2006, a,b 2003, 2007
	Analyze selected multi-component structures and suggest which interactions hold the species together.	Multicomponent crystals / co-crystals / solid solutions	