3.7.8. Crystallography Open Database (COD) (with Saulius Gražulis)

The Crystallography Open Database (COD) project (http://www.crystallography.net/cod/; Gražulis *et al.*, 2009, 2012) aims at collecting in a single open-access database all organic, inorganic and organometallic structures, except for the structures of biological macromolecules, which are available in the Protein Data Bank (Berman *et al.*, 2003, 2011). The database was founded by Armel Le Bail, Lachlan Cranswick, Michael Berndt, Luca Lutterotti and Robert M. Downs in February 2003 as a response to Michael Berndt's letter published on the Structure Determination by Powder Diffractometry (SDPD) mailing list (Berndt, 2003). Since December 2007, the main database server has been maintained and new software has been developed by Saulius Gražulis and Andrius Merkys at the Institute of Biotechnology of Vilnius University (VU). Currently, the database includes more than 376 000 entries describing structures of small molecules and small-to-medium-sized unit-cell materials as published in IUCr journals and other major crystallographic and peer-reviewed journals, as well as contributions by crystallographers from major laboratories. Most of the mineral data are obtained from the American Mineralogist Structure Database (Rajan *et al.*, 2006) and are donated by its maintainer and COD co-founder Robert M. Downs.

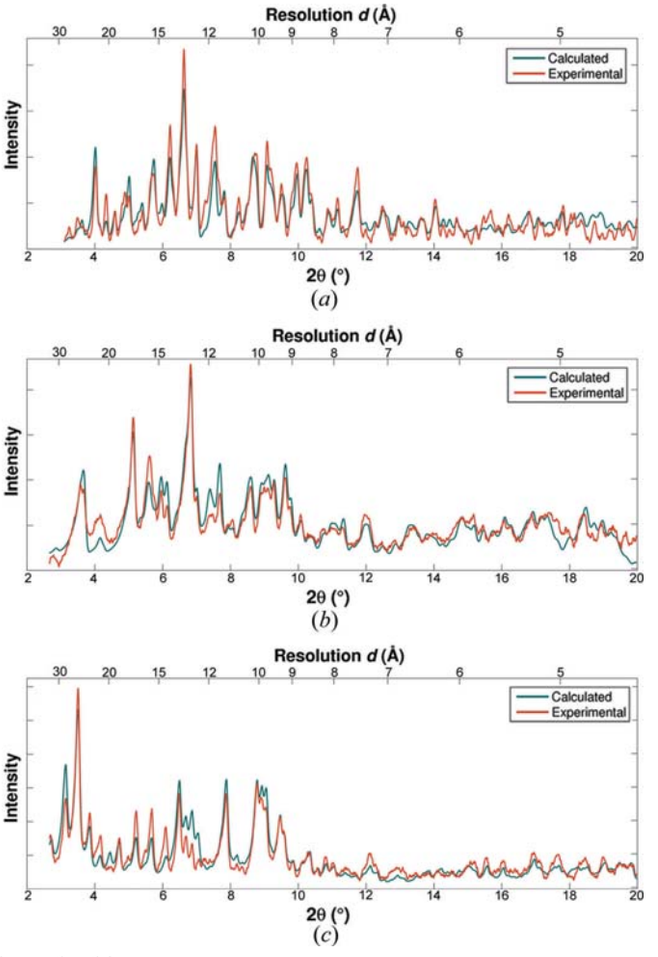
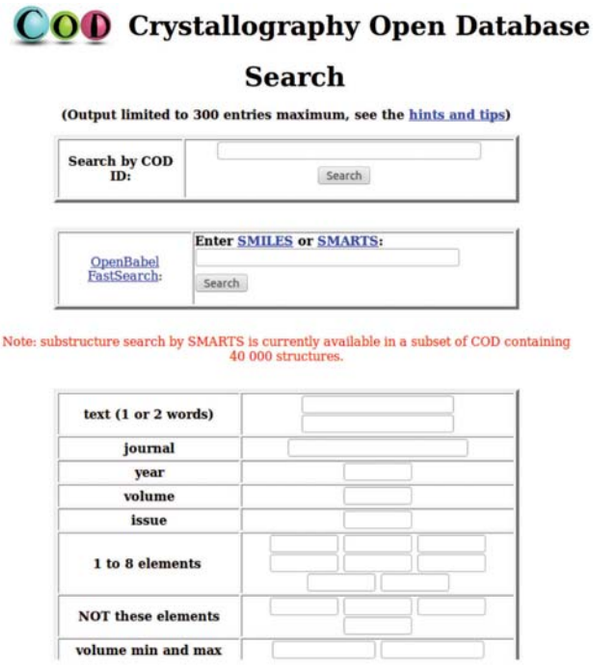
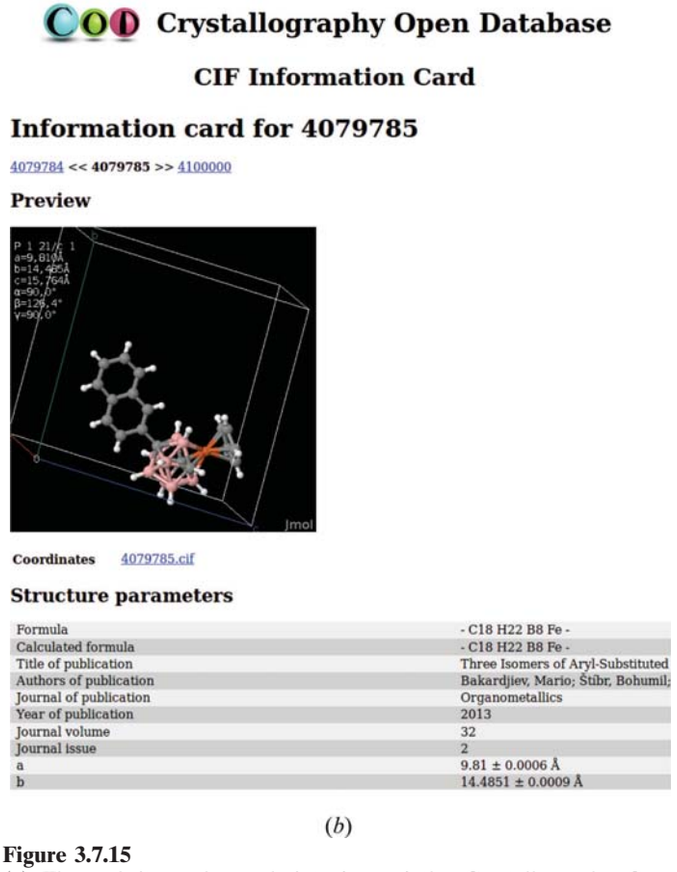


Figure 3.7.14
Calculated and experimental powder patterns for (*a*) lysozyme, (*b*) trigonal insulin and (*c*) cubic insulin. The calculated patterns (blue) are corrected for bulk-solvent and geometrical effects using the revised Lorentz factor. From Hartmann *et al.* (2010).

The database is an internet resource (Fig. 3.7.15) with data-search and download capabilities designed by Armel Le Bail and Michael Berndt. In addition, registered users may deposit new data, whether from previous publications or as personal communications, using the deposition web site designed at VU by



(*a*)



(*b*)

Figure 3.7.15
(*a*) The website and search interface of the Crystallography Open Database (COD) permits searches of crystallographic data by a range of parameters and unrestricted retrieval of the found data. (*b*) Data can be viewed online in the interactive *Jmol* applet (Hanson, 2010, 2013) or downloaded for further processing either one record at a time or in bulk.