Chapter 34

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34.1 Molecular Models

We wish to thank the Cambridge Crystallographic Data Centre (CCDC) and the Fachinformationszentrum Karlsruhe (FIZ Karlsruhe) for allowing Imagineering Media Services (IMS) to access their databases of atomic coordinates for experimentally determined three-dimensional structures. CCDC's **Cambridge Structural Database (CSD)** is the world repository of small molecule crystal structures (distributed as part of the CSD System), and in FIZ Karlsruhe's **Inorganic Crystal Structure Database (ICSD)** is the world's largest inorganic crystal structure database. The coordinates of organic and organometallic compounds in CSD and inorganic and intermetallic compounds in ICSD were invaluable in ensuring the accuracy of the molecular models produced by IMS for this textbook. The authors, the publisher, and IMS gratefully acknowledge the assistance of both organizations. Any errors in the molecular models in this text are entirely the responsibility of the authors, the publisher, and IMS.

The CSD System: The Cambridge Structural Database: a quarter of a million crystal structures and rising. Allen, F.H., *Acta Cryst*. (2002), **B58,** 380–388. *ConQuest:* New Software for searching the Cambridge Structural Database and visualizing crystal structures. Bruno, I.J., Cole, J.C., Edgington, P.R., Kessler, M., Macrae, C.F., McCabe, P., Pearson, J., Taylor, R., *Acta Cryst*. (2002), **B58,** 389–397. *IsoStar:* IsoStar: A Library of Information about Nonbonded Interactions. Bruno, I.J., Cole, J.C., Lommerse, J.P.M., Rowland, R.S., Taylor, R., Verdonk, M., *Journal of Computer-Aided Molecular Design* (1997), **11-6,** 525–537.

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