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High-Temperature and High-Pressure Crystal Chemistry

Robert M. Hazen and Robert T. Downs, Editors

Chapter 1. PRINCIPLES OF COMPARATIVE CRYSTAL CHEMISTRY

Robert M. Hazen, Robert T. Downs and Charles T. Prewitt

- **XtalDraw** is an interactive computer program that draws crystal and molecular structures as ball and stick, polyhedral, or as thermal ellipsoid representations. It comes with a large set of data files. The program runs in Win95/98/00/NT. Not only does it use the XtalDraw data files, but it can also use the *American Mineralogist* Crystal Structure Data Base files with the extension *.amc. Download the programs and datafiles . The software also reports tables of bond lengths, angles, polyhedral volumes, thermal parameters, distortion parameters, etc. that are computed with the METRIC software written by Boisen, Gibbs, Bartelmehs and Downs.
- The Collaborative Computational Project Number 14 (CCP14) has an extensive listing of crystallographic software free for public use.
- STRAIN by Ohashi, Y. (1982) A program to calculate the strain tensor from two sets of unit-cell parameters. In Hazen, R. M. and Finger, L. W., Comparative Crystal Chemistry. NY, Wiley, pp. 92-102.
- ANHARM: Software to deal with anharmonic treatments of thermal motion is available from Dr. Boysen.
- Prometheus: Refinement software that incorporates anharmonic treatments of thermal motion is available from Dr. Kuhs .

Chapter 2. EQUATIONS OF STATE

Ross J. Angel

- EosFit : to fit and manipulate Equations of state, and other software for collecting and processing high-pressure single-crystal diffraction data.
- STRAIN by Ohashi, Y. (1982) A program to calculate the strain tensor from two sets of unit-cell parameters. In Hazen, R. M. and Finger, L. W., *Comparative Crystal Chemistry*. NY, Wiley, pp. 92-102.

Chapter 3. ANALYSIS OF HARMONIC DISPLACEMENT FACTORS

Robert T. Downs

- The PEANUT software can be obtained from Jurg Hauser at Universitat Bern.
- The TLS program was used to compute the rigid body corrections for quartz. It can be obtained with the quartz sample datafile.

Chapter 4. ANIMATION OF CRYSTAL STRUCTURE VARIATIONS WITH PRESSURE, TEMPERATURE, AND COMPOSITION

Robert T. Downs and Paul J. Heese

- American Mineralogist Crystal Structure Database : This is a set of all the crystal structure data ever published in American Mineralogist, and is maintained by Bob Downs for the Mineralogical Society of America. It is a source of digital data files used to construct images and can be found at /xtal-cgi/test
- **XtalDraw**: This software, written by Bob Downs, Kurt Bartelmehs, and Kausik Sinnaswamy can be used to make images of crystal structures. It is available with a large set of data files at /xtal/personal.html. More details are provided in the links for Chapter 1.
- Movie Gear : Shareware to construct animated GIF89 files that display the mineral movies on both the PC and on the Internet. We do not control access to this software, but as of this publication date, it can be obtained from http://www.gamani.com
- Examples and detailed instructions to make crystal structure movies can be found at /xtal/movies/crystal_movies.html