*American Mineralogist, Volume 88, pages 247–250, 2003*

# The *American Mineralogist* crystal structure database

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## ABSTRACT

A database has been constructed that contains all the crystal structures previously published in the American Mineralogist. The database is called "The American Mineralogist Crystal Structure Database" and is freely accessible from the websites of the Mineralogical Society of America at http://www.minsocam.org/MSA/Crystal_Database.html and the University of Arizona. In addition to the database, a suite of interactive software is provided that can be used to view and manipulate the crystal structures and compute different properties of a crystal such as geometry, diffraction patterns, and procrystal electron densities. The database is set up so that the data can be easily incorporated into other software packages. Included at the website is an evolving set of guides to instruct the user and help with classroom education.

## INTRODUCTION

The structure of a crystal represents a minimum energy configuration adopted by a collection of atoms at a given temperature and pressure. In principle, all the physical and chemical properties of any crystalline substance can be computed from knowledge of its crystal structure. The determination of crystal structures and the deduction and understanding of these computational algorithms constitutes a major part of scientific research in physics, chemistry, biology, medicine, mineralogy, geology, and material sciences. As such, crystal structure data represent one of the most important resources for developing our scientific knowledge and thus should be archived in ways that make them easy to access and preserve. However, this data is often cumbersome to retrieve and verify from the literature and even more difficult to analyze for many scientists for whom crystallography is not their primary discipline. Thus, the Mineralogical Society of America and the University of Arizona have established a collection of mineralogically important crystallographic data sets that are freely accessible through the Internet. This database is an important resource to the Mineralogical Society of America and the Society is committed to maintain it as part of its outreach program (Alex Speer, the Executive Director of MSA, personal communication).

## THE DATABASE

The database contains every experimentally determined crystal structure reported in the American Mineralogist. Including the data published through the end of the 2001 calendar year, we have collected 2627 individual data sets representing 1007 unique mineral and chemical species. The data represent structures determined at ambient conditions as well as at temperature or pressure. Constructing the database is a multi-step process that includes: (1) examining each volume of the American Mineralogist to identify all papers that report crystal structures; (2) manually entering the reported data in the database; (3) verifying the consistency of the data with reported crystal chemical parameters; (4) contacting the authors about irresolvable inconsistencies between reported and computed parameters; (5) incorporating comments from either the original authors or ourselves when changes are made to the originally published data. Each record in the database consists of a bibliographic reference, cell parameters, symmetry, atomic positions, displacement parameters, and site occupancies. An example of a data set is provided in Figure 1.

The first part of each data set contains identifying information, bibliography and notes, while the second part contains the crystallographic parameters. The first line of a data file contains an identifier, such as the name of the mineral or formula of the chemical species. The next line(s) contain the names of the authors, each separated by a comma. This is followed by the journal reference, title of the paper, and additional notes. The crystallographic data begins with a listing of the cell parameters and space group. If the data is given with respect to a non-standard space group origin then an asterisk precedes the space group symbol and the next line contains the translation vector from the standard origin. The 1952 edition of the *International Tables for X-ray Crystallography* are used to define the standard origin. The rest of the data set is a fixed-formatted listing of the atoms, their positional and displacement parameters, and occupancies. A header is provided that defines right-justified columns. The name of each atom identifies the occupying elements, with additional identifiers added when appropriate. For instance, "Oco" identifies a particular oxygen atom in the albite structure. Some data sets report a crystallographic site occupied by molecular species rather than elemental, such as OH, water or methane. In most of these cases the atom name is denoted by molecular formula. For example, "CH4" denotes methane, and "Wat" denotes water. The displacement factors are tabulated in one of two formats, *U*'s or b's

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Spinel - (Mg,Fe)2Si04
Hazen R M, Downs R T, Finger L W
American Mineralogist 78 (1993) 1320-1323
Crystal chemistry of ferromagnesian silicate spinels: Evidence for
Mg-Si disorder.
Sample: SUNY 1102
8.2059 8.2059 8.2059 90 90 90 Fd3m
atom     x     y     z  occ B(1,1) B(2,2) B(3,3) B(1,2) B(1,3) B(2,3)
Si    .125  .125  .125      .00157 .00157 .00157      0      0      0
Mg      .5    .5    .5 .218 .00208 .00208 .00208 .00002 .00002 .00002
Fe      .5    .5    .5 .782 .00208 .00208 .00208 .00002 .00002 .00002
O    .2418 .2418 .2418      .00212 .00212 .00212 .00037 .00037 .00037
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**FIGURE 1.** An example of the crystallographic data included in the database.

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(see Downs 2000 for further details on displacement factors).

Quality control is an area of major concern and effort in construction of the database. Each data set must be verified for accuracy and omissions before being added to the database. We use METRIC, a software program developed by Bartelmehs, Gibbs, Boisen, and Downs (1993) at Virginia Tech. This program was written using the matrix methods and group theory outlined in Boisen and Gibbs (1990) to compute the crystal chemical parameters that are typically found in many crystal structure publications. The crystal chemical parameters include bond lengths, angles, polyhedral volumes, distortion indices, displacement parameter details, rigid-body motion parameters, and such, as recently reviewed in Hazen et al. (2000). The software has been widely used for crystal structure research and educational purposes (Bartelmehs et al. 1993). Comparing the crystal chemical parameters calculated by METRIC with those included in the original publication provides a check of the internal consistency of the data. If a discrepancy is found then we try to determine its source and correct it. Many errors are typographical, while others are more complex. The authors are contacted to correct an error when possible. The database contains only the corrected data set. The METRIC software that we use to check the data is freely available and is distributed on the website.

Our experience has shown that the number of publications with errors in their data is large. We estimate that at least 50% of the published data have errors of one sort or another that require deducing the problem and contacting the authors. To address this problem, the American Mineralogist has appointed a crystal structure technical editor (currently R.T. Downs). The editor checks the internal consistency of the data for each structure that is being reported in a submitted manuscript using the METRIC software. The results of the check are forwarded to both the primary editor and the authors so that the manuscript can be corrected before publication. We estimate that 75% of all submitted manuscripts have errors of one sort or another in their crystallographic tables. Anne Hofmeister, recent editor of American Mineralogist, and Robert Martin, editor of the Canadian Mineralogist, can corroborate this high percentage of errors (personal communications).

## THE ANCILLARY SOFTWARE

A suite of software visualization and analysis tools has been developed to make the database more useful as a scientific and educational tool. Two key applications are XtalDraw, an application that creates multiple representations of a crystal structure, and METRIC, described above.

The XtalDraw and METRIC modules, with their options and interface, are the result of many years of development. The software was written for DOS systems in 1986 at Virginia Tech (Bartelmehs et al. 1993) for two purposes: (1) to aid teaching in the Geosciences, Material Sciences, and Mathematics programs at the university, and (2) to facilitate research. These goals have been maintained over the years. Through interaction with undergraduates who use the software in class, the interface algorithms have been streamlined to be simpler and more intuitive, however, these refinements serve the professional scientist as well.

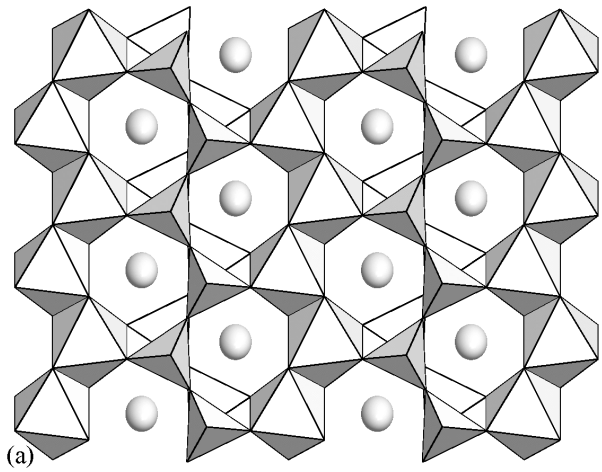
While powerful, they still are not completely user-friendly and may often require significant experience or oversight by an instructor to use them in a classroom setting. Furthermore, the applications are not fully compatible with the crystal structure database nor do they provide for seamless data analysis. With a grant from the National Science Foundation, we are working to transform these powerful applications into a more user-friendly visualization and analysis tool set, fully integrated with the crystal structure database. This will make the database more useful and accessible. Below we describe the existing software and provide insight into how it will evolve.

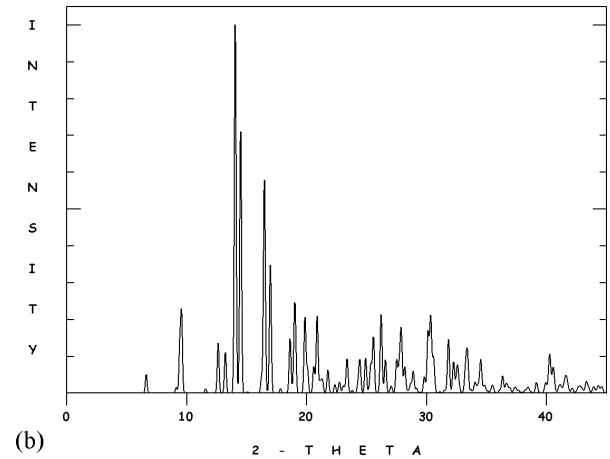
When completed, students and scientists of all disciplines will be able to explore and analyze crystal structure data with a state-of-the-art Windows-based software. The basic features of the software will include default settings that allow a range of users, from the high school student in chemistry to the professional mineralogist, to investigate fundamental properties of minerals including: (1) crystal chemical parameters such as bond lengths and angles, polyhedral volumes and distortions, thermal vibration amplitudes, and rigid body motion parameters; (2) fixed wavelength or energy dispersive X-ray and neutron powder diffraction patterns; and (3) electron densities and bonding analyses.

Crystallographic parameters are the foundation of research in material properties and being able to visualize and manipulate crystal structures is fundamental to understanding them. Thus, when a crystal structure in the database is accessed, it can automatically be displayed with the XtalDraw module (Bartelmehs et al. 1993; Downs and Bartelmehs 1996; Hazen and Downs 1996; Downs 1998; Hazen et al. 2000). Currently, this stand-alone software contains options to draw the crystal structure with ball and stick, polyhedral, and thermal ellipsoidal renderings (Fig. 2). The user can rotate the image with the arrow keys, or manually enter directions of view in direct or reciprocal space coordinates. They can expand or shrink the image, and add or delete atoms from the field of view. The number of displayed atoms will depend only upon available computer memory. Users can change the colors of atoms, their sizes, the bonds, and so forth. The software produces publication quality bitmaps of any desired size. Carefully selected default viewing parameters are one very powerful feature of XtalDraw that make it easy to use. For instance, after a data file is read, the structure is initially displayed with **c*** coming out of the screen, in a default orientation established by the International Tables for Crystallography. The atoms are drawn in a set of colors suggested by Lipson and Cochran (1957) to represent elemental species, and in sizes that scale to the Shannon and Prewitt (1969) radii. The user has the option to change these settings at any time and to establish their own default settings. The software can also be used to make animations of crystal structures that change with temperature, pressures, or composition (Downs and Heese 2000).

The database software module also integrates the ability to calculate many of the important crystal chemical parameters that are used by today's researchers, such as bond lengths and angles, polyhedral volumes and distortion parameters, vibrational amplitudes and orientations (Hazen et al. 2000) using the METRIC module.

Another important property of a crystal that can be computed from its structural data is its diffraction pattern. Neutron



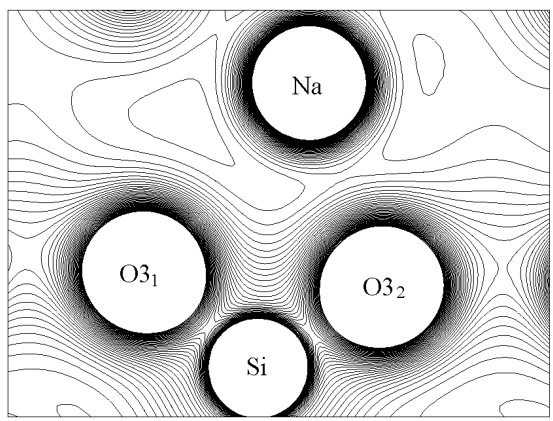




**FIGURE 2.** An example of interactive displays that can be created by the software associated with the American Mineralogist Crystal Structure Database. The example includes images of (**a**) the crystal structure of jadeite in a combined polyhedral and ellipsoidal rendering made with XtalDraw; (**b**) the powder diffraction pattern of jadeite using Mo$K\alpha$ radiation made with XPOW; and (**c**) an electron density map of the plane through Na and bridging O atoms in jadeite made with SPEEDEN.

and X-ray powder diffraction patterns, generated from a fixed source or from an energy dispersive source, such as at a synchrotron, can be computed with the software XPOW (Downs et al. 1993). Currently, XPOW calculates the diffraction pattern for any crystalline substance and provides an interactive display of the pattern, as it would be generated by a conventional powder diffractometer (Fig. 2). The user can alter the radiation source wavelength, the peak widths, limits and orientation of the display. It provides a way to learn about the relationship between a crystal structure and a diffraction pattern by allowing the user to adjust parameters and view the changes. It is also of great use in identifying unknown materials by providing a complete diffraction pattern, and not just the few *d*-spacings listed in a search-match table.

SPEEDEN, a program that can produce a standardized electron density distribution for a given crystal structure, will also be integrated in the software package. The electron density is generally very difficult and time-consuming to obtain from experiment, and expensive and time consuming to compute. However, the procrystal model (also known as the independent atom model, IAM) of the electron density is surprisingly simple to obtain (Gibbs et al. 1992). Functions for spherically averaged electron densities are placed at the observed positions of the atoms in a crystal and the electron density for the crystal is computed by the superposition principle. This model provides a quite accurate description of the true electron density, especially around the heavier atoms (Coppens 1997; Downs et al. 2002).

Recent work pioneered by Bader (1995) and co-workers provides algorithms for analysis of the topology of the electron density. In particular, a pair of atoms is bonded if and only if a ridge of electron density joins the pair and there is a saddle point at the minimum between the atoms. Thus, for the first time, we have an unambiguous way to determine if two atoms are bonded. Downs et al. (2002) shows that the procrystal model provides a determination of bonding that is consistent with that produced by full quantum calculations for a large number of inorganic structures. The analysis and use of electron density to determine bonding is still a new tool in the mineralogical community (Downs et al. 1996; Downs et al. 1999; Gibbs et al. 1992, 1998; Rakovan et al. 1999) and so this software will be of great use to researchers. The SPEEDEN (SPhErically averaged Electron DENsity program) module was originally coded by two high-school students, Andalman and Hudasko, who won the First Place Grand Award at the 1995 International Science and Engineering Fair with this project (Andalman et al. 1995; Downs et al. 1996). Figure 2 shows a contour map of the electron density in a part of the structure of jadeite. This image was generated by computing a grid of electron density data with SPEEDEN, and then importing the grid into commercial contouring software.

As this project progresses, additional software will be developed and made accessible from the database website. We invite other researchers to also contribute their software and forward suggestions for improving our existing software.

## ACCESSING THE DATABASE INFORMATION

A good database should be comprehensive, accurate, easily accessed, and easily analyzed. When completed, the Crystal

Structure database will meet all of these criteria. Currently, access is provided through a search procedure that consists of drop-down list boxes containing the names of the minerals or chemical species, the authors and titles of the relevant journal articles, as well as fields for chemistry, unit-cell dimensions, and space group symmetry. There is also a field to enter a general search for words or phrases. These fields can be combined with the logical conditions *or* and *and* in a search.

The search algorithm uses MYSQL with the following scheme. Each data set is stored as a separate file, identified by volume number and page number of the reference with the file extension *.amc. Associated with each filename are entries in the database that correspond to *mineral name*, *authors*, *title*, *chemical elements* present in the data set, *cell parameters*, and *space group*. The website interface is constructed dynamically using php programming.

After the search criteria are defined and the search is initialized, the php program collates the contents of the pertinent data files and displays them on a new screen. The user has several options. They can cut-and-paste the relevant text, or select an individual data set, or select the entire set of data. Since the data files are stored on an ftp server, the user can then download the selected files to their own computer through an ftp hyperlink. If the file extension of the data, *.amc, has been associated with an application on the user's local computer, then the application will be launched and should automatically open the file. For instance, XtalDraw can be launched in this manner, so that choosing a data set of the website opens up an interactive drawing of the crystal structure on a PC. This feature is modeled after the *.pdf interface with Adobe Acrobat Reader.

In addition to accessing data through the web-based interface described above, a search can be initialized from any web page by sending a php query to the website. A successful search would bring up the data without going through our search interface. This method for accessing the data is currently being used by databases such as http://www.webmineral.com and would be a good way to provide access to the data through education web pages. The details for constructing this type of search can be found at the website.

## THE EDUCATIONAL COMPONENT

Our current database provides fast and easy access to crystal structure data in a tabular format. In its current form, this data is most useful to the professional mineralogist who has a good understanding of crystallography or for those in an educational setting where some training may be provided. Implementing the software enhancements will greatly improve the ease of use and create a seamless interface between the data and each software module. This will open the door to a much wider audience of users. To complete the outreach goals of the database, a set of instructional modules or guides are being developed to provide tutorials that explain how to use the software, as well as an exploration of the data and fundamental properties of crystals. In particular, guides will be designed for: (1) analysis of the structural systematics of pyroxenes as a means to learn how to use the XtalDraw module; (2) analysis of the behavior of pyroxenes as a function of temperature as a means to learn how to make animations (Downs and Heese 2000); (3) investigation of the relationship between crystal structure and diffraction pattern as a way to learn how to use the XPOW diffraction module; (4) analysis of the bonding changes displayed by the pyroxene structure as it transforms from one symmetry to another, as a means to learn how to use the electron density module, SPEEDEN.

These guides will be also be turned into complete lesson plans so that high school teachers and university faculty can use them to introduce students to the software. The lesson plans will be tested in the classroom in the natural course of teaching mineralogy at the University of Arizona prior to publication.

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MANUSCRIPT RECEIVED MAY 8, 2002
MANUSCRIPT ACCEPTED JULY 26, 2002
MANUSCRIPT HANDLED BY LEE A. GROAT