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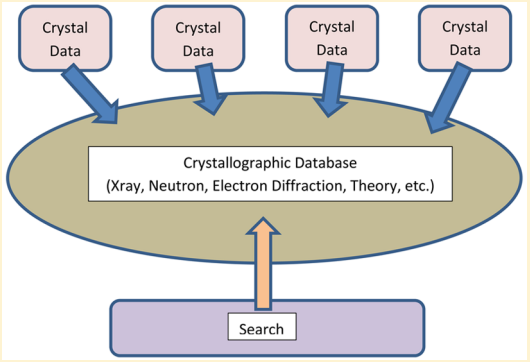
Crystallographic Information Resources

Leslie Glasser*

Nanochemistry Research Institute, Department of Chemistry, Curtin University, GPO Box U1987, Perth, Western Australia 6845, Australia

ABSTRACT: Crystallographic information provides the fundamental basis for understanding the properties and behavior of materials. This data, such as chemical composition, unit cell dimensions, space group, and atomic positions, derives from the primary literature—that is, from published experimental measurement or theoretical calculation. Although the major crystallographic journals provide their published data in the form of computer-readable *.cif text files, finding and accessing this material directly is often difficult and certainly time-consuming. On the other hand, we are fortunate to have ready access through the Internet to extensive crystallographic databases, both academic/commercial and free, where the former databases are critically compiled and of the highest quality. The available databases generally specialize, as for inorganic or organic materials, or minerals, etc. The current paper is directed at the occasional user of crystallographic information, and examines methods of searching for and obtaining crystallographic information (mainly inorganic and minerals, but also organic, biological and metallic) from some important free databases; namely: NIMS AtomWorks for inorganics; the Crystallography Open Database (COD) for both inorganics and organics; WWW-Mincryst for minerals; the Protein Databank (PDB) for proteins and nucleic acids; and the Database of Zeolite Structures. An example of a search repeatedly used here demonstrates the changes in information provided from the first X-ray structural determination (of halite by the father-and-son Braggs) to modern representations. The professional researcher is best served by the academic/commercial databases: Inorganic Crystal Structure Database (ICSD); Cambridge Structure Database (CSD) for organics; Pearson's Crystal Data (PCD) for inorganics; Crystmet for metallic systems, etc. However, free demonstration versions of these important databases provide user introductions and, indeed, usable data for a limited range of materials. A Table provides information and rapid access details for 11 of the major crystallographic databases. This text is directed toward the search for data, but some indication is given as to how the data collected may be used.



KEYWORDS: *Continuing Education, Graduate Education/Research, Internet/Web-Based Learning, Chemoinformatics, Crystals/Crystallography, Enrichment/Review Materials, X-ray Crystallography, Solids*

INTRODUCTION

Fundamental information regarding a solid material is its chemical structure, and this is enshrined in its crystallography: that is, its chemical formula, the spatial arrangement of its atoms or ions, and their repetitions in space (the unit cell axial lengths and angles, the number of chemical units involved, and the space group). These data tell us of the bonds that are formed, the groupings that form, the energetics and thus stability of the material, and the relationship of the material to others of like kind. With this information, we are in a position to consider the synthesis, reactions and decomposition of the material, its physical properties, its applications, and its possible dangers.

The study of crystalline materials has a long history, originating from the fascinating shapes which can be exhibited by individual crystals. Indeed, the origins of scientific crystallography can be traced back to René Just Haüy[1] (1743−1822), who became interested in explaining, on the basis of packing of simple rhombohedral units, the geometrically simple fragments remaining after he damaged a friend's calcite sample. Haüy's Law of Rational Indices derives from the fact that the densest layers are exposed on cleavage of crystals.

Until the development of X-ray and (later) electron and neutron diffraction methods, crystal geometry was characterized by the angles between displayed surfaces, using devices such as reflection goniometers. Modern crystallography provides information on the dimensions of the unit cell, the chemical contents of the unit cell, and the placement of those contents in space through the space group, which describes the symmetry of the contents in space,[2] assuming that the unit cell is strictly repeated (periodic) in space. There are 17 two-dimensional plane and 230 three-dimensional space groups, which can be extended to 1651 magnetic space groups—where magnetically active ions (such as iron) may display parallel and antiparallel orientations while otherwise identical. (These are also called black-and-white or color space groups.) In very recent times, it has been realized that some materials are quasicrystalline, which means that their structures, while ordered to fill space, are not strictly periodic through space.[3]

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Table 1. Principal Crystallographic Databases Considered

Subject Area	Database Title	No. of Records	Cost	Demo. Version	Producer	URL
inorganics	Inorganic Crystal Structure Database (ICSD Web)	>177 000	various	Free with Registration	FIZ Karlsruhe (Leibniz-Institut für Informations-infrastruktur)	http://www2.fiz-karlsruhe.de/icsd_web.html
inorganics	Pearson's Crystal Data (PCD)	>258 000	various	Available for down-loading	ASM International	http://www.crystalimpact.com/pcd/
inorganics, metals	Inorganic Material Database (AtomWork)	>82 000 crystal structures >55 000 material properties >15 000 phase diagrams	Free with Registration		National Institute for Materials Science (NIMS)	http://crystdb.nims.go.jp/index_en.html
minerals, inorganics	American Mineralogist Crystal Structure Database	>4000	Free		American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy, Physics and Chemistry of Minerals, as well as selected data sets from other journals	http://ammin.geoscienceworld.org/ http://rruff.geo.arizona.edu/AMS/amcsd.php
organics inorganics, metal−organics minerals	Crystallography Open Database (COD)	>330 000	Free		"All data on this site have been placed in the public domain by the contributors."	http://www.crystallography.net/
minerals	Mineralogy Database	>4500	Free		D. Barthelmy	http://webmineral.com
biological macromolecular structures	RCSB Protein Data Bank (includes Nucleic Acid Database)	>110 000	Free		Research Collaboratory for Structural Bioinformatics (Rutgers University, UC San Diego)	http://www.rcsb.org/pdb/home/home.do http://ndb-mirror-2.rutgers.edu/
small-molecule organics, metal−organics	Cambridge Structural Database (CSD)	>750 000	Institution based	Available	Cambridge Crystallographic Data Centre (CCDC)	http://www.ccdc.cam.ac.uk/products/csd/
organics	CSD Teaching Database	733	Free			http://webcsd.ccdc.cam.ac.uk/teaching_database_demo.php
metals, alloys, intermetallics minerals	CRYSTMET	>161 000	various	Available for down-loading	Toth Information Systems	http://www.tothcanada.com/databases.htm
zeolites	Database of Zeolite Structures	all approved Zeolite Framework Types	Free		Ch. Baerlocher L. B. McCusker	http://www.iza-structure.org/databases/

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Structural parameters of $InFeMO_4$, where M = Mg, Co and Ni, as obtained from Rietveld refinement and Mössbauer spectroscopy data

Structural parameters	M		
	Mg	Co	Ni
Space group	*Fd*-3*m*	*Fd*-3*m*	*Fd*-3*m*
a/b (Å)	8.63432(5)	8.63967(6)	8.60300(7)
V (Å^3)	643.70	644.89	636.72
A site composition (%) [In, Fe, M]	[66,34,0]	[54,36,10]	[58,35,7]
B site composition (%) [In, Fe, M]	[18,32,50]	[22,30,48]	[21,32,47]
Oxygen site x	0.26012	0.2625	0.2593
R_p (%)	9.57	7.47	10.4
R_{wp} (%)	11.7	9.54	12.1
χ^2	8.11	4.23	14.3

Atomic positions are 8*a* (1/8,1/8,1/8) for A site, 16*d* (1/2,1/2,1/2) for B site and 32*e* (x, x, x) for oxygen.

Figure 1. Summary crystallographic information on $InFeMO_4$[20] from the primary literature. Although the number, Z, of $InFeMO_4$ units in the unit cell is not stated explicitly, it may be inferred from the footnote stating that there are 32 oxygen atoms in the Wyckoff *e* symmetry position, implying that there are 32/4 = 8 of $InFeMO_4$ units in the unit cell. Reproduced with permission from ref 20. Copyright 2007 Elsevier.

CRYSTALLOGRAPHIC RESOURCES

Access to crystallographic information today is relatively simple and often free. It is the purpose of the present communication to introduce the occasional user to such facilities, providing some indication as to how to access and search for the desired information.[4] Searches may be initiated via free search sites such as Google, Google Scholar, Bing, etc., or commercial sites such as SciFinder, Web of Science, Scopus, ScienceDirect, etc., but a direct search through one of the sites listed in Table 1 is likely to be more efficient and productive.

The principal theoretical basis for crystallography is provided y the *International Tables for Crystallography*, currently available in eight printed volumes,[5] or in online open access[6] for the Space Group Tables, also printed as volume A.[7] The Bilbao Crystallographic Server[8] provides comprehensive links to basic symmetry information, from point groups to magnetic space groups. The textbook *Structure of Materials*,[9] has a Web site with rather comprehensive information; an online appendix (under the title "Additional Material")[10] provides excellent graphic representations of 106 prototype crystal structures as well as a link to graphics of the magnetic point groups.

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#------------------------------------------------------------------------------
#
# This file is available in the Crystallography Open Database (COD),
# http://www.crystallography.net/
#
# All data on this site have been placed in the public domain by the
# contributors.
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    C1 C4+ 2 a 0. 0. 0. 1. 0 d
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    O2- -2.000
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Figure 2. *cod/1010928* cif file for the calcite structure of $CaCO_3$ from the Crystallography Open Database (COD),[27] based upon an X-ray structural analysis of $CaCO_3$,[28] and here presented in two columns for space conservation. The file has also here been divided into sections for ease of reference: highlighted section 1 contains bibliographic information, section 2 describes the unit cell, while highlighted section 3 contains the symmetry information and fractional coordinate values to locate atom centers in the unit cell. Reproduced with the permission of the COD Advisory Board.

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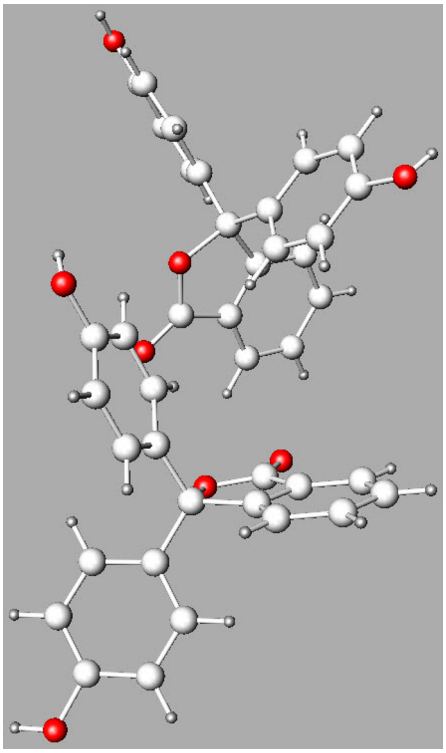

Figure 3. Snagit screen-shot[29] of the orthorhombic crystal structure of phenolphthalein, $C_{20}H_{14}O_4$.[30] The two symmetry-independent molecules within the set of eight in the unit cell ($Z = 8$) are depicted. Data is derived from COD[27] file *2007144.cif* and visualized using the interactive ATOMS 6.4 graphics program.[24a]

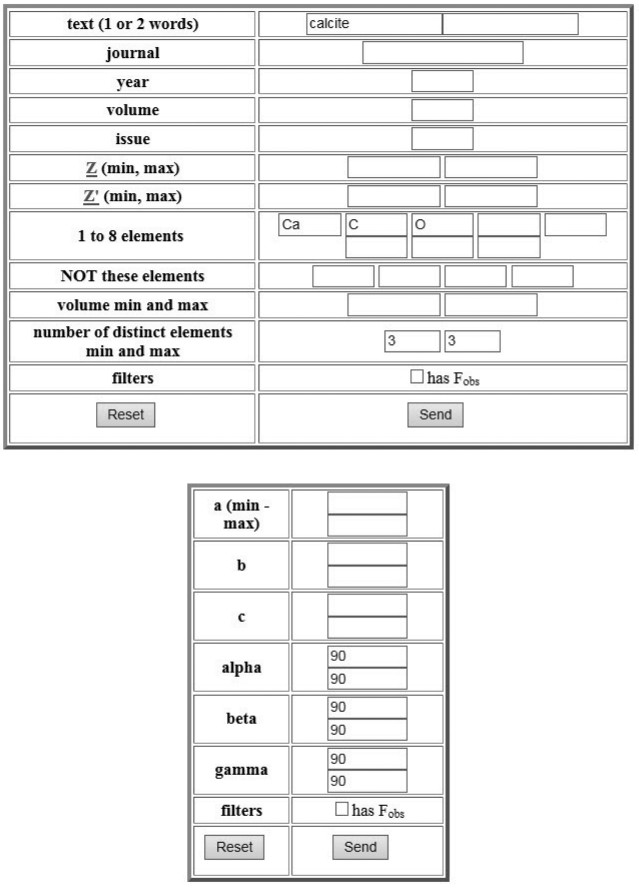

Figure 4. Search panel for calcite on the COD.[27] Reproduced with the permission of the COD Advisory Board.

The book "*Solid state chemistry and its applications (student edition)*" (2nd ed.) by A. R. West[11] has a Web site[12] containing a free, downloadable version of the *CrystalViewer* software with a set of more than one hundred displayable inorganic structures; this material is free for private study and teaching purposes. The "Open Acess Crystallography" site[13] has useful links to other interactive display sites.

Data for individual materials can be found in the primary literature. The professional literature (such as *Acta Crystallographica*,[14] *American Mineralogist*,[15] etc.) provides the data free and online in the form of *Crystallographic Information Files* (.cif—see below). However, this is by no means the favored direction for search, since many of the online databases also provide such .cif files together with additional information such as graphic displays, often rotatable with the user's mouse by means of online Java-based Jmol software.[16] In the following, we illustrate the information provided by various sources, from the primary literature to current database providers.

DATA FROM THE PRIMARY LITERATURE

Data from the older primary literature may sometimes be incomplete. As a unique example, consider this report (1913) of the very first crystal structure determination, by the Nobel-winning Bragg father-and-son team,[17] of the halite structure of sodium chloride (DOI 10.1098/rspa.1913.0040):

"... taking as a unit of the point system-

(1) The group 4NaCl, the smallest complete unit of the crystal pattern.

(2) The individual atom of either nature, associated with only one-eighth of the volume of the complete unit."

"...the point system which the diffracting centres form has as element of its pattern that suggested above, a cube with a point at each corner and one at the centre of each face. Of the three elementary cubic space lattices, this is the only one in which the distance between the (111) planes is greater than that between any other of the planes of the system." This rather wordy elaboration was supplemented in the following year by a more complete description, including a diagram of the structure (DOI 10.1098/rspa.1914.0015).[18] This research is discussed in a marvelous series of videos presented on the Royal Institution's *RI Channel*.[19a] This year (2015) is the centenary of the award of the Nobel prize to the Braggs.[19b]

Clearly, the modern literature has a more complete description than that above, although particular needs may require an abbreviated presentation[20] (for example, omitting an explicit value for Z, the number of asymmetric units contained in the unit cell,[21] as in Figure 1).

Current practice generally provides comprehensive information, as for example for the newly identified mineral, pauloabibite, in a recent issue of *American Mineralogist*.[22]

*.CIF FILES

The primary literature and many databases now provide their data most conveniently in .cif files,[23] which condense the information into a human- and computer-readable text format (see Figure 2). Many crystallographic programs can, in turn, directly read .cif files and extract the information which they require for their particular purposes—such as drawing a three-dimensional

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representation of the crystal structure (see Figure 3),[24] or even for 3D-printing of unit cells.[25] It is important, then, that the data within the .cif file is supplied in a standard format so that it is correctly interpreted on input to a computer program. As a consequence, programs are available which check the format of .cif files as well as the completeness and correctness of the information that they contain.[26]

DATABASES

We here show the varied methods by which some of the more significant free crystallographic databases[31] provide search capabilities by which their data may be located. Emphasis is placed on the free online databases accessible to the occasional user, but indications are provided as to the availability of free demonstration versions of the academic/commercial databases.

Crystallographic Open Database (COD)

COD is an open-access collection of crystal structures of organic, inorganic, metal−organic compounds, and minerals, excluding biopolymers. All data on the site have been placed in the public domain by the contributors.

Figure 4 below shows a simple COD search for the calcite structure of calcium carbonate, where the additional input of elemental information avoids the detection of other materials with the calcite structure, such as $NaNO_3$ or more complex materials.

NIMS AtomWorks

In Figure 5 below, from the Japanese-Swiss *National Institute for Materials Science* AtomWork Web site, we have deliberately selected the original definitive analysis of NaCl by the 22-year old son, W. L. Bragg. This database also contains 17 other more recent determinations of the NaCl halite structure (as well as two for the less-stable CsCl structure).

The Mineralogy Database and the WWW-Mincryst Database

A very extensive listing of basic mineralogical crystallographic information is available as the *Mineralogy Database*.[35]

The *Institute of Experimental Mineralogy* of the Russian Academy of Sciences provides the important mineralogical database, WWW-Mincryst. A simple search using the name "perovskite" for the material $CaTiO_3$ yields 80 structural determinations (plus another four for $BaTiO_3$) for various perovskite structures, as well as for perovskite itself under various conditions of temperature and pressure. Much more detailed information is also available from this site in an associated file ("Full Information Card"). In Figure 6, we display only the basic information, while the full file contains information on the data source, basic crystallographic data, an exhaustive set of atomic coordinates in the unit cell, interatomic distances, and X-ray diffraction pattern (derived in this case from data contained in the early collection by R. W. G. Wyckoff[36]). An estimated lattice energy, based upon the molar volume of the material,[37] is also available.

Database of Zeolite Structures

The free *Database of Zeolite Structures*[39] provides structural information on all of the Zeolite Framework Types that have been approved by the Structure Commission of the International Zeolite Association (IZA-SC).

PDB—Protein Data Bank and NDB—Nucleic Acid Database

The Protein Data Bank[40] is a free archive of information concerning the three-dimensional structures of proteins, nucleic acids, and complex assemblies. It is managed by the Worldwide PDB (wwPDB) organization. Figure 7 depicts insulin, in a cartoon format which clearly illustrates the secondary

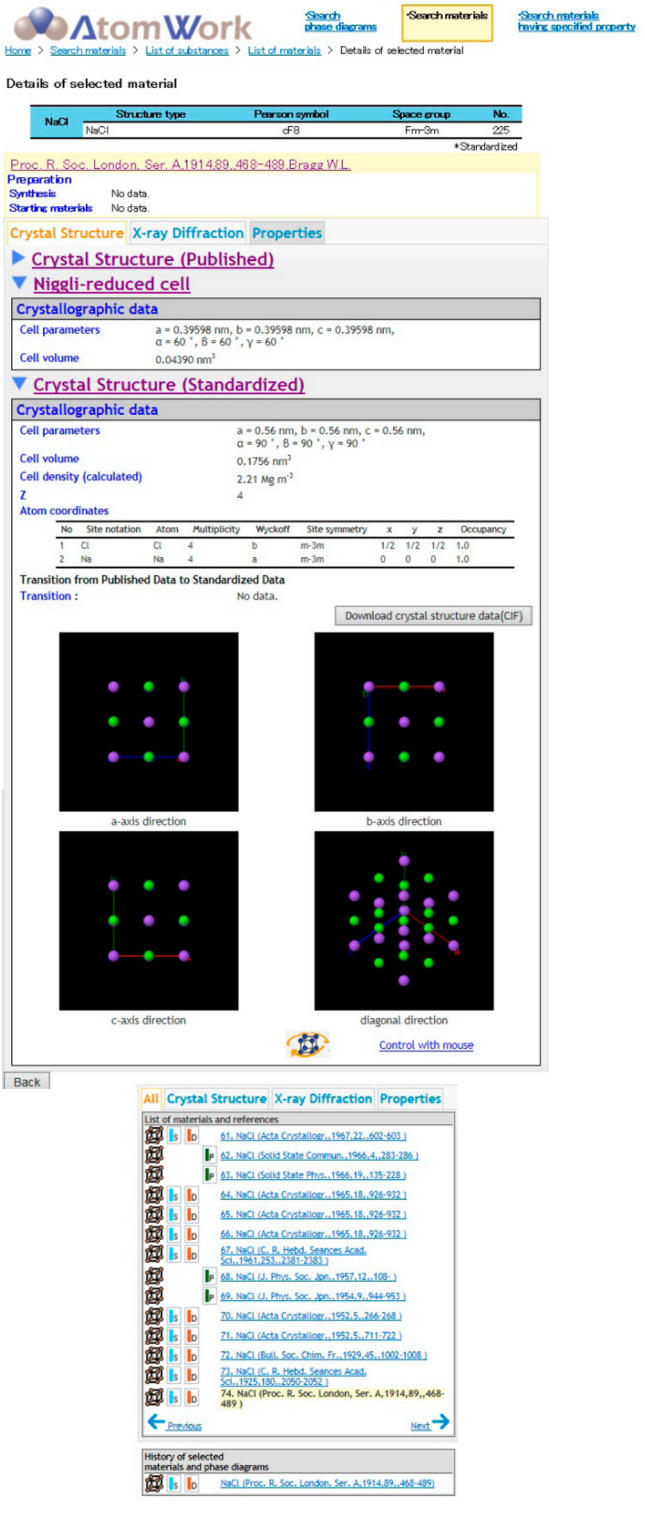

Figure 5. Output from the NIMS AtomWork database[32] for the original Bragg[18] determination of the halite (NaCl) structure, with the "Crystal Structure" option selected. The structure diagram is interactive (using Jmol[33]), and activated with the "Control with mouse" option at the bottom-right of the screen. The Java Runtime Environment[34] needs to be installed on the local computer for this purpose. Figure reproduced with permission from the Inorganic Material Database (AtomWork), http://crystdb.nims.go.jp/ [accessed 2015-03-16].

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Name:	**PEROVSKITE**		
Specification:	[2], structure type - perovskite		
Formula:	$CaTiO_3$		
Symmetry Class:	orthorhombic		
Space Group:	P bnm		
Unit Cell Parameters:	a = 5.3700 | b = 5.4400 | c = 7.6400		
Number of Formula Unit:	**Z** = 4	*Unit Cell Volume, Å³:*	$\mathbf{V_c}$ = 223.19
Number of Atomic Position per full Unit Cell:	**P/U** = 20	*Molar Volume, cm³/mol:*	$\mathbf{V_m}$ = 33.61
Number of Reflexes used in Structure Determination:	-	*X-ray density, g/cm³:*	**ρ** = 4.05
R-factor:	-	*MU, 1/cm:*	**μ** = 506.009
Wave Length for Calculated Powder Diffraction Patterns:	Cu=1.54056	*Mass attenuation coefficient, cm²/g:*	**μ/ρ** = 125.081
Theta-Interval for CPDP:	**T/I** = 1-45		

Figure 6. Output for $CaTiO_3$ (perovskite) from the WWW-Mincryst database.[38] Reproduced with permission.

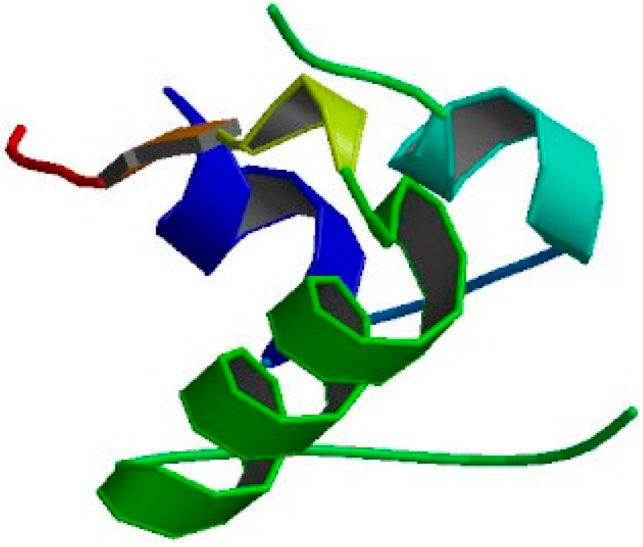

Figure 7. Example of a protein structural "cartoon"—insulin.[43] The structure depicted is that of PDB entry 1trz.[42] The α-helices are clearly represented. This structure is discussed in the RCSB "Molecule of the Month" newsletter—Insulin. Reproduced with permission from Research Collaboratory for Structural Bioinformatics (RCSB).

features of the protein—only α-helices in this case, but also β-sheets, etc.

The Nucleic Acid Database (NDB)[41] contains information about experimentally determined nucleic acids and complex assemblies, in the form of both DNA and RNA. It currently contains over 6600 structures. The current PDB links directly through to the NDB.

ICSD—Inorganic Crystal Structure Database and CSD—Cambridge Structural Database

The principal source of inorganic crystal data is ICSD,[44] containing more than 177 000 peer-reviewed data entries. It is an academic/commercial database maintained by FIZ Karlsruhe, Germany, and the National Institute of Standards & Technology (NIST), Gaithersburg, USA, but a free demonstration version is available. Similarly, CSD[45] is the academic/commercial repository for small-molecule organic and metal−organic crystal structures, with over half a million entries, and it also provides a free teaching-subset of 500 of its data for demonstration purposes as WebCSD.[46]

CRYSTMET

CRYSTMET[47] is an academic/commercial database of critically evaluated crystallographic data for metals, including alloys, intermetallics, and minerals. A free demonstration version is available.

PCD—Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds

Pearson's Crystal Data[48] is an academic/commercial collaboration between ASM International and Material Phases Data System, Vitznau, Switzerland (MPDS), aiming to create and maintain the world's largest critically evaluated "nonorganic database". It currently contains nearly 258 500 entries for about 150 000 different chemical formulas. A free demonstration version is available.

APPLICATIONS OF CRYSTALLOGRAPHIC DATA

Crystallographic data provide information on the composition of materials, their phases, three-dimensional structures, bond lengths, bond angles, atomic contacts, stereochemistry, and so forth. For example, the Braggs were able to reject the hypothesis of the existence of NaCl molecules in halite on the direct observational basis that the constituent atoms did not pair. The bond valence model[49] provides the basis for chemical understanding of the bonding within inorganic materials, and relies on structural information to draw its conclusions. Our current understanding of the structures of biological molecules depends critically on X-ray (and related) studies, as notably illustrated by the demonstration by Watson and Crick[50] of the double-helical (strictly, double-helicoidal) structure of DNA,[51] based upon the X-ray data of Rosalind Franklin.[52] A current *J. Chem. Educ.* paper[53] demonstrates the possibility of determining stereochemistry, which cannot be elucidated by IR and ^{1}H NMR spectroscopy, using X-ray structure analysis.

CONCLUSIONS

We have here provided links to many sources of crystallographic information and data, much of it readily accessible online and free, in both textual, graphical, and interactive forms. We have demonstrated some of the methods used to search for information on the great variety of materials which have been investigated, including inorganics, organics, metallics, zeolites, and biological materials.

These rich resources provide the basic information required for the investigation of the properties and behaviors of a huge range of materials.

AUTHOR INFORMATION

Corresponding Author

*E-mail: l.glasser@curtin.edu.au.

Notes

The author declares no competing financial interest.

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