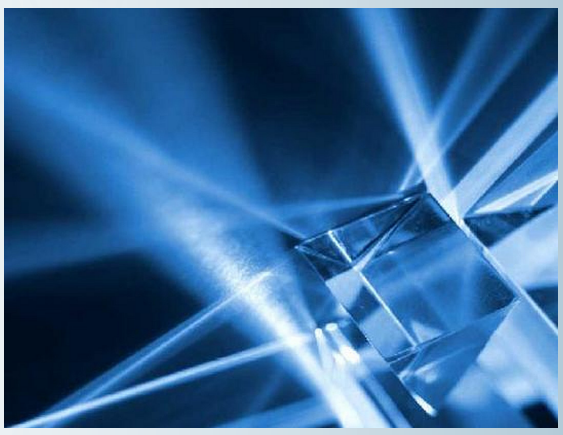
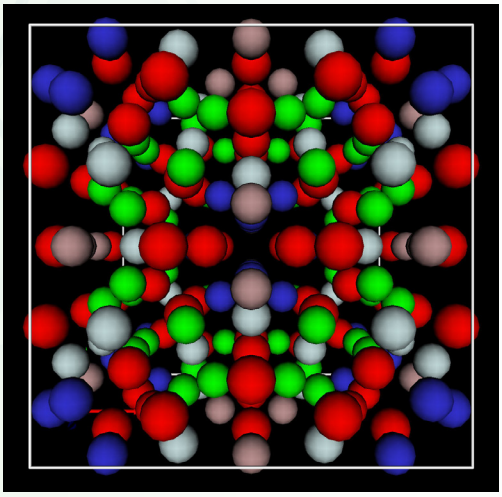
Crystallographic Databases

Objective

Components and devices used in a broad spectrum of technology sectors such as health care, communications, energy and electronics are manufactured from crystalline materials. The development of advanced crystalline materials requires accurate crystal-structure data. The objective of this project is to provide critically evaluated, comprehensive crystal-structure databases that enable phase identification required for the development of advanced inorganic materials and devices depending on them. NIST designs, populates, evaluates and disseminates NIST Standard Reference Databases SRD 3 (NIST Crystal Data), SRD 83 (NIST Metals Structural Database, NSD) and SRD 84 (FIZ/NIST Inorganic Crystal Structure Database, ICSD).



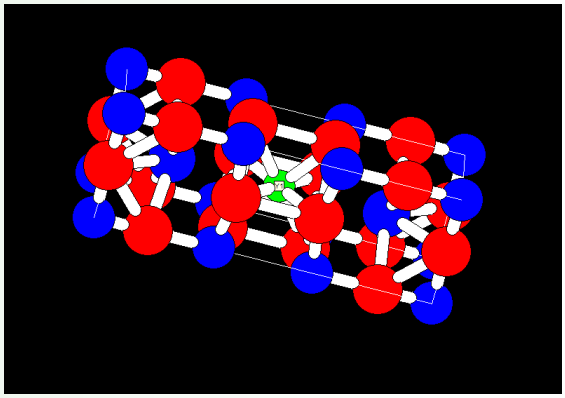


Impact and Customers

Materials with new or improved properties are continually being developed to meet demands for increased functionality of components and devices at decreased costs. Examples of multi-million dollar industries driven by materials advances are solid-state lighting (GaN-based devices), automotive (Pt-alloy catalytic converters) and prosthetic devices (ceramic dental crowns).

Crystalline compounds can be identified by their characteristic diffraction patterns using X-rays, neutrons and electrons. An estimated 20,000 X-ray diffractometers and a comparable number of electron microscopes are used daily in materials research and development laboratories for this purpose. The inclusion of the Material Measurement Laboratory's comprehensive crystal structure databases in diffraction instruments will greatly increase the number of materials that can be identified, improve the ability to discriminate between materials with similar structures, and is expected to result in increased instrument sales.

Customers and beneficiaries include diffraction instrument vendors (Oxford Instruments, PANalytical, Rigaku, EDAX) and materials developers and researchers in industry, academia and government.



ICSD #63,483: 3D Model Render

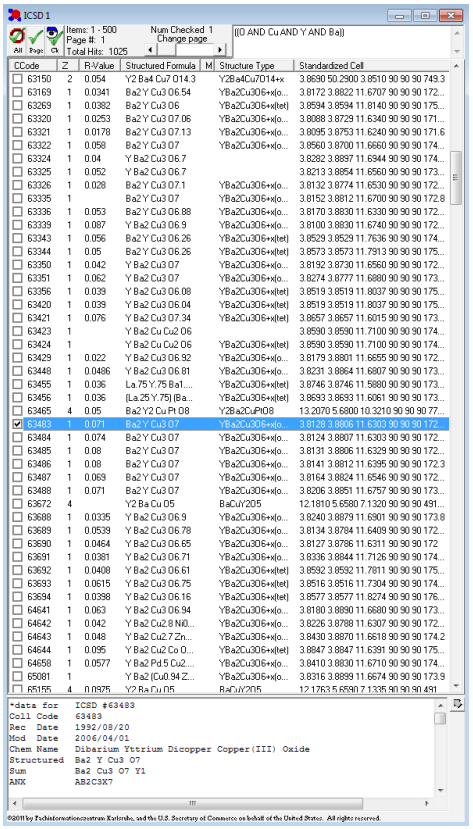
Approach

The FIZ/NIST Inorganic Crystal Structure Database is a collection of crystal structure entries for non-organic compounds including inorganics, ceramics, minerals, pure elements, metals and intermetallics. The database is produced cooperatively with FIZ-Karlsruhe, Germany, and includes information published since 1913. It is updated twice a year, with each update comprising about 2,000 to 10,000 new or re-evaluated entries. Each structure determination reported in the literature yields a separate entry in the database and all data are recorded by experts and checked several times (in an iterative manner). Apart from updating, data integrity and completeness are critical objectives. Incorporation of missing structures and evaluation and correction of data with the help of authors, users and experts are ongoing activities. NIST develops software tools for the calculation and standardization of derived data items and modules for the intelligent access of these data, and provides access through modern user interfaces and networking capabilities.

Accomplishments

The FIZ/NIST Inorganic Crystal Structure Database (SRD 84) has been expanded to cover all categories of non-organic materials including inorganics, metals, intermetallics and minerals as we work toward the formation of a single, comprehensive database for all non-organic materials. Twice a year, content updates to the Inorganic Crystal Structure Database are made and delivered to individuals, institutions, instrument companies and software vendors. The March 2012 Release of the FIZ/NIST Inorganic Crystal Structure Database contains more than 142,000 critically evaluated entries.

ISCD search for compounds containing Y, Cu, Ba, & O



By way of illustration, searching the ICSD database for yttrium-barium-copper-oxide, a common superconducting material, yields 1,025 crystal structures. ICSD # 63,483 provides the crystal structure, models, and simulated powder diffraction data for superconducting YCBO (see below).

A free demonstration CD is available upon request or can be downloaded from the website http://www.nist.gov/srd/.

ICSD #63,483: Example of search results

ICSD #63483

Coll Code: 63483
Rec Date: 1992/08/20
Mod Date: 2006/04/01
Chem Name: Dibarium Yttrium Dicopper Copper(III) Oxide
Structured: Ba_2 Y Cu_3 O_7
Sum: Ba_2 Cu_3 O_7 Y
ANX: AB2C3X7
D(calc): 6.43
Title: Structure of the 100 K superconductor Ba_2 Y Cu_3 O_7 between (5-300) K by neutron powder diffraction
Author(s): Capponi, J.J.; Chaillout, C.; Hewat, A.W.; Lejay, P.; Marezio, M.; Nguyen, N.; Raveau, B.; Soubeyroux, J.L.; Tholence, J.L.; Tournier, R.
Reference: Europhysics Letters (1987), 3, 1301-1307
Golden Book of Phase Transitions, Wroclaw (2002), 1, 1-123
Unit Cell: 3.8128(1) 3.8806(2) 11.6303(5) 90. 90. 90.
Vol: 172.08 Z: 1
Space Group: P m m m SG Number: 47
Cryst Sys: orthorhombic Pearson: oP13
Wyckoff: t s r q2 h e a R Value: 0.071
Red Cell: P 3.812 3.880 11.630 90 90 90 172.081
Trans Red: 1.000 0.000 0.000 / 0.000 1.000 0.000 / 0.000 0.000 1.000
Comments:
Stable up to 1640 K (2nd ref., Tomaszewski), above P21/c Neutron diffraction (powder)
The structure has been assigned a PDF number (calculated powder diffraction data): 01-078-2269
The structure has been assigned a PDF number (experimental powder diffraction data): 41-227
Rietveld profile refinement applied
Temperature in Kelvin: 5
Structure type : $YBa_2Cu_3O_6$+x(orh)
At least one temperature factor is implausible or meaningless but agrees with the value given in the paper.

ICSD #63,483: Atomic Position Information

Atom	#	OX	SITE	x	y	z	SOF	H	ITF(B)
Ba	1	+2	2t	0.5	0.5	0.1826(5)	1.	0	0.14(10)
Y	1	+3	1h	0.5	0.5	0.5	1.	0	0.61(11)
Cu	1	+2.333	1a	0	0	0	1.	0	0.01(11)
Cu	2	+2.333	2q	0	0	0.3542(3)	1.	0	0.37(3)
O	1	-2	2q	0	0	0.1595(4)	1.	0	0.37(14)
O	2	-2	2s	0.5	0	0.3773(4)	1.	0	0.0(1)
O	3	-2	2r	0	0.5	0.3769(5)	1.	0	0.43(11)
O	4	-2	1e	0	0.5	0	1.	0	0

Learn More

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http://www.nist.gov/srd/

Publications

'NIST Standard Reference Database 84' - FIZ/NIST Inorganic Crystal Structure Database; Release 2011/2 (March 2012; 142,179 entries); NIST contributors: VL Karen, and X Li

GR Desiraju, Chair, Committee for Crystallographic Databases, International Union of Crystallography (Members: F Allen, H Berman, B Duax, J Faber, VL Karen, G Kostorz, B McMahon, J Rodgers, P Villars), Report of the Executive Committee for 2006, Acta Cryst. **A63**, 484-508, (2007).

CJ Long, D Bunker, X Li, VL Karen, and I Takeuchi, Rapid Identification of Structural Phases in Combinatorial Thin-Film Libraries using X-Ray Diffraction and Non-Negative Matrix Factorization, Review of Scientific Instruments, **80**, 103902 (2009).

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