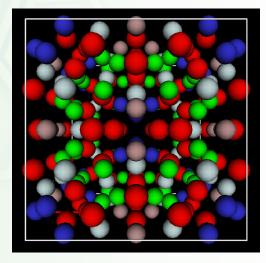
## **ADVANCED MATERIALS**

# **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).



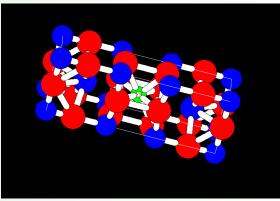


#### **Impact and Customers**

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

LCSD 1					2
	Items: 1 - 500 Page #: 1	Num Checked 1 Change page	((0 AND Cu AN	D Y AND Bajj	
	Total Hits: 102		•		
Code Z	R-Value	Structured Formula M	Structure Type	Standardized Cell	
63150	2 0.054	Y2 Ba4 Cu7 014.3	Y28a4Cu7014+x	3.8690 50.2900 3.8510 90 90 97	19.3
63169	1 0.0341	Ba2 Y Cu3 06.54	YBa2Cu306+x(o	3.8172 3.8822 11.6707 90 90 90 13	72
63269	1 0.0382	Ba2 Y Cu3 06	YBa2Cu306+x(tet)	3.8594 3.8594 11.8140 90 90 90 12	75
	1 0.0253	Ba2 Y Cu3 07.06	YBa2Cu3O6+x(o	3.8088 3.8729 11.6340 90 90 90 1	
	1 0.0178	Ba2 Y Cu3 07.13	YBa2Cu3O6+x(o	3.8095 3.8753 11.6240 90 90 90 1	
	1 0.058	Ba2 Y Cu3 07	YBa2Cu3O6+x(o	3.8560 3.8700 11.6660 90 90 90 1	
	1 0.04	Y Ba2 Cu3 06.7		3.8282 3.8897 11.6944 90 90 90 1	
	1 0.052	Y Ba2 Cu3 06.7		3.8213 3.8854 11.6560 90 90 90 1	
	1 0.028	Ba2 Y Cu3 07.1	YBa2Cu306+x(o	3.8132 3.8774 11.6530 90 90 90 1	
	1	Ba2 Y Cu3 07	YBa2Cu3O6+x(o	3.8152 3.8812 11.6700 90 90 90 1	
	1 0.053	Ba2 Y Cu3 06.88	YBa2Cu306+x(o	3.8170 3.8830 11.6330 90 90 90 17	
	1 0.087	Y Ba2 Cu3 06.9 Ba2 Y Cu3 06.26	YBa2Cu306+x(o YBa2Cu306+x(tet)	3.8100 3.8830 11.6740 90 90 90 17 3.8529 3.8529 11.7636 90 90 90 17	
	1 0.056	Ba2 Y Cu3 06.26 Ba2 Y Cu3 06.26		3.8573 3.8573 11.7913 90 90 90 1	
	1 0.05	Ba2 Y Cu3 06.26 Y Ba2 Cu3 07	YBa2Cu306+x(tet) YBa2Cu306+x(o	3.8573 3.8573 11.7513 50 50 50 11 3.8192 3.8730 11.6560 50 50 50 11	
	1 0.042	Y Ba2 Cu3 07 Y Ba2 Cu3 07	YBa2Cu306+x[o	3.8274 3.8777 11.6880 90 90 90 1	
	1 0.039	Y Ba2 Cu3 06.08	YBa2Cu306+x[tet]	3.8519 3.8519 11.8037 90 90 90 17	
	1 0.039	Y Ba2 Cu3 06.04	YBa2Cu306+x[tet]	3.8519 3.8519 11.8037 90 90 90 17	
	1 0.076	Y Ba2 Cu3 07.34	YBa2Cu3O6+x[tet]	3.8657 3.8657 11.6015 90 90 90 1	
	1	Y Ba2 Cu Cu2 06		3 8590 3 8590 11 7100 90 90 90 1	
63424	1	Y Ba2 Cu Cu2 06	YBa2Cu306+x[tet]	3,8590 3,8590 11,7100 90 90 90 1	74
63429	1 0.022	Y Ba2 Cu3 06.92	YBa2Cu306+x[o	3.8179 3.8801 11.6655 90 90 90 12	72
	1 0.0486	Y Ba2 Cu3 06.81	YBa2Cu306+x(o	3.8231 3.8864 11.6807 90 90 90 1	
63455	1 0.036	La.75 Y.75 Ba1	YBa2Cu306+x(tet)	3.8746 3.8746 11.5880 90 90 90 1	73
63456	1 0.036	(La.25 Y.75) (Ba	YBa2Cu306+x(tet)	3.8693 3.8693 11.6061 90 90 90 17	73
63465	4 0.05	Ba2 Y2 Cu Pt 08	Y28a2CuPt08	13.2070 5.6800 10.3210 90 90 90	77
63483	1 0.071	Ba2 Y Cu3 07	YBa2Cu306+x(o	3.8128 3.8806 11.6303 90 90 90 13	72
	1 0.074	Ba2 Y Cu3 07	YBa2Cu306+x(o	3.8124 3.8807 11.6303 90 90 90 1	
	1 0.08	Ba2 Y Cu3 07	YBa2Cu3O6+x(o	3.8131 3.8806 11.6329 90 90 90 1	
	1 0.08	Ba2 Y Cu3 07	YBa2Cu3O6+x(o	3.8141 3.8812 11.6395 90 90 90 1	
	1 0.069	Ba2 Y Cu3 07	YBa2Cu3O6+x(o	3.8164 3.8824 11.6546 90 90 90 1	
	1 0.071	Ba2 Y Cu3 07	YBa2Cu3O6+x(o	3.8206 3.8851 11.6757 90 90 90 1	
	4	Y2 Ba Cu 05	BaCuY205	12.1810 5.6580 7.1320 90 90 90 4	
	1 0.0335	Y Ba2 Cu3 06.9	YBa2Cu306+x(o	3.8240 3.8879 11.6901 90 90 90 1	
	1 0.0539 1 0.0464	Y Ba2 Cu3 06.78 Y Ba2 Cu3 06.65	YBa2Cu306+x(o YBa2Cu306+x(o	3.8134 3.8784 11.6409 90 90 90 1 3.8127 3.8786 11.6311 90 90 90 1	
	1 0.0464	Y Ba2 Cu3 06.65 Y Ba2 Cu3 06.71	YBa2Cu306+x[o	3.8336 3.8844 11.7126 90 90 90 1	
	1 0.0381	Y Ba2 Cu3 06.61 Y Ba2 Cu3 06.61	YBa2Cu306+x[o YBa2Cu306+x[tet]	3.8592 3.8592 11.7811 90 90 90 1	
	1 0.0408	Y Ba2 Cu3 06.61 Y Ba2 Cu3 06.75	YBa2Cu306+x(tet)	3.8516 3.8516 11.7304 90 90 90 1	
	1 0.0398	Y Ba2 Cu3 06.16	YBa2Cu306+x(tet)	3.8577 3.8577 11.8274 90 90 90 17	
	1 0.063	Y Ba2 Cu3 06.94	YBa2Cu306+x(cer)	3.8180 3.8890 11.6680 90 90 90 1	
	1 0.063	Y Ba2 Cu2 8 Ni0	YBa2Cu306+x[0	3.8226 3.8788 11.6307 90 90 90 17	
	1 0.042	Y Ba2 Cu2.7 Zn	YBa2Cu306+x[o	3.8430 3.8870 11.6618 90 90 90 17	
	1 0.095	Y Ba2 Cu2 Co 0	YBa2Cu306+x[tet]	3.8847 3.8847 11.6391 90 90 90 17	
	1 0.0577	Y Ba2 Pd 5 Cu2	YBa2Cu306+x[o	3.8410 3.8830 11.6710 90 90 90 1	
	1	Y Ba2 (Cu0.94 Z	YBa2Cu3O6+x[o	3.8316 3.8899 11.6674 90 90 90 1	
	4 0.0975	Y2 Ba Cu 05	BaCuY205	12 1763 5 6590 7 1335 90 90 90 4	
data for	ICSD #634				
oll Code	63483				in '
ec Date	1992/08/2				
od Date hem Name	2006/04/0 Dibarium	)1 Yttrium Dicopper	Copper(III) Or	ide	
tructured	Ba2 Y Cu:		oopper(iii) on	200	
	Ba2 Cu3 (	07 Y1			
	AB2C3X7				-
um NX	AB2C3X7			4	Ŧ

Learn More

Vicky Lynn Karen **Research Chemist** 301-975-6255 vicky.karen@nist.gov

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

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).

ICSD #63,483: Example of search results

Ва	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)
0	1	-2	2q	0	0	0.1595(4)	1.	0	0.37(14)
0	2	-2	2s	0.5	0	0.3773(4)	1.	0	0.0(1)
0	3	-2	2r	0	0.5	0.3769(5)	1.	0	0.43(11)
0	4	-2	1e	0	0.5	0	1.	0	0

### Publications

2f\_amat-11/12

'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).



## **ADVANCED MATERIALS**

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