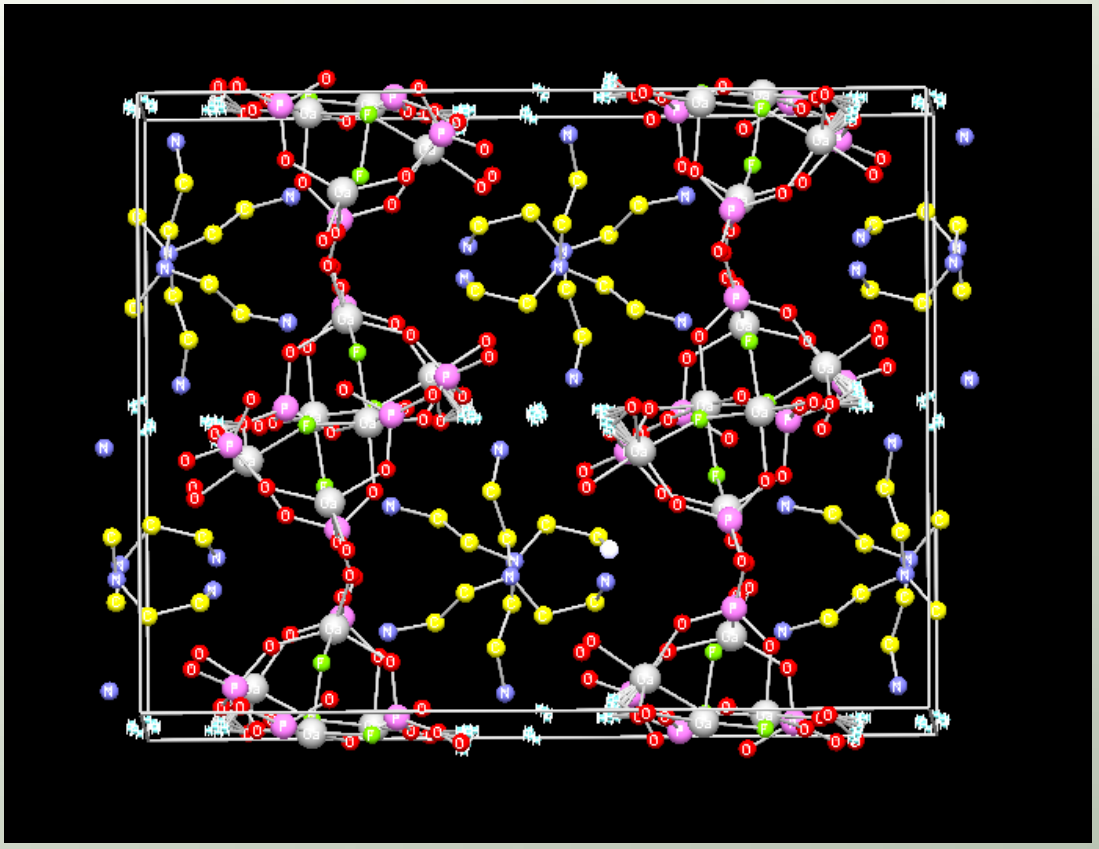
Molecular Graphics

Molecular Graphics

What?

PDF 00-057-0248

ULM-8
A microporous florinated gallium phosphate with $N_4C_6H_{19}$ in the pores



PDF-4 products contain data sets with atomic coordinates. Two molecular graphic packages embedded in the product allows molecules to be displayed (above). Data can also be exported for use in other graphics utility programs.

Molecular Graphics

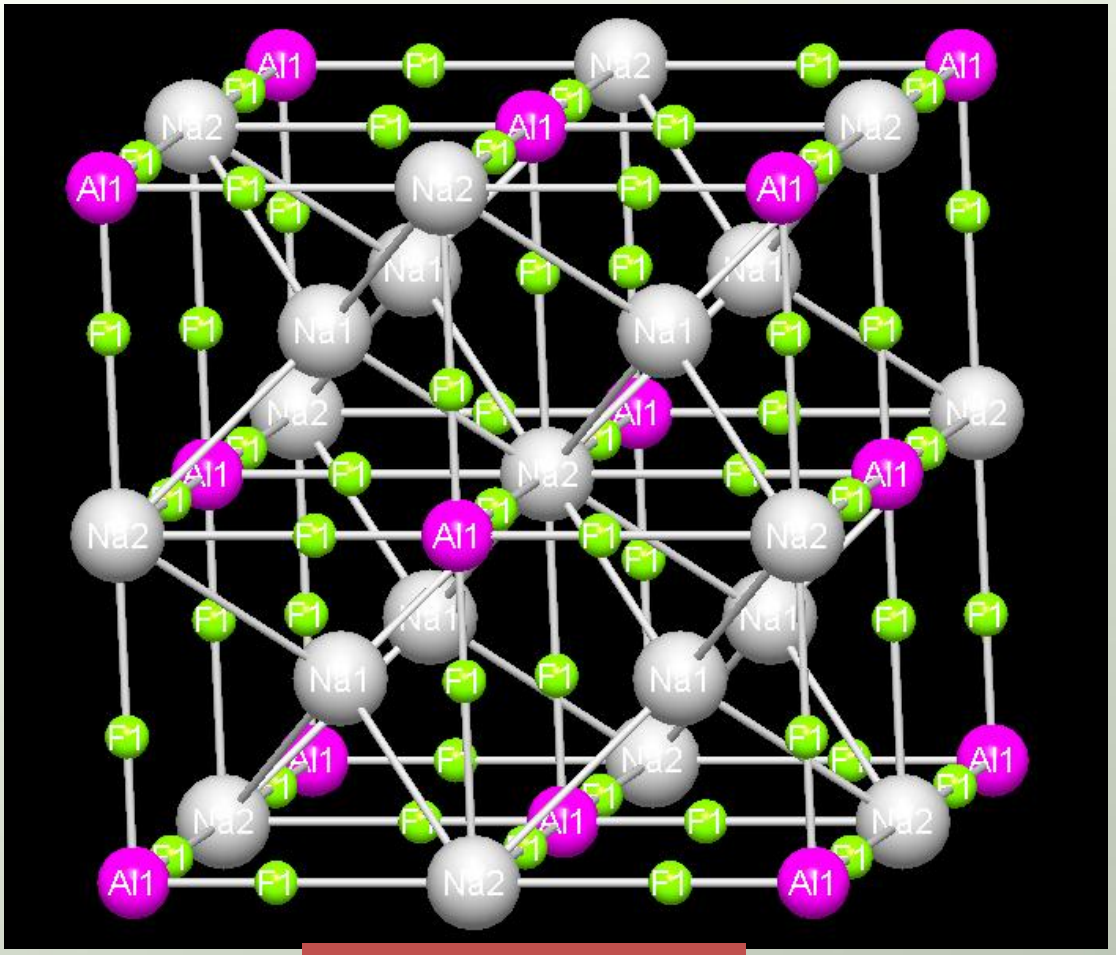
Why?

Through the use of molecular graphics, molecules can be visualized and examined for their conformation. This is important in understanding how materials react and interact.

The particular molecular graphics package employed in PDF-4 was originally developed by a team at Crystal Impact, as part of the Linus Pauling Project, headed by Dr. Pierre Villars, President of Material Phases Data System (MPDS). This package also examines the "atomic environment" around each atom as a means of studying molecular "building blocks" and determining structural prototypes. This graphic package is explained in this tutorial.

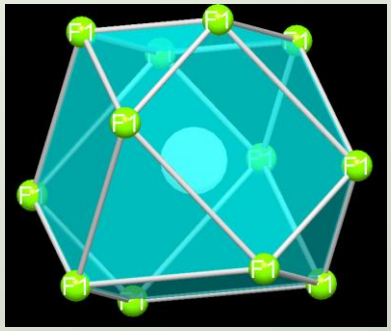
In PDF-4 Release 2011, a second graphics package was added called Jmol (www.jmol.org). This package can plot multiple unit cells, autorotate the molecules, and express the molecules as polyhedra. This graphics package is explained in the tutorial "Use 3D Structure Capabilities".

Unit Cell Cryolite
Na_3AlF_6

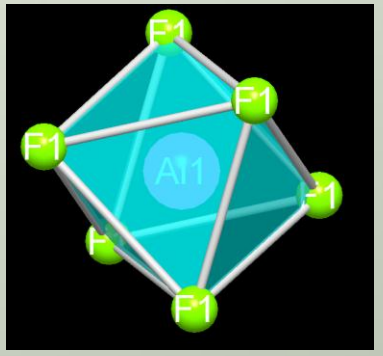


PDF 04-007-8587

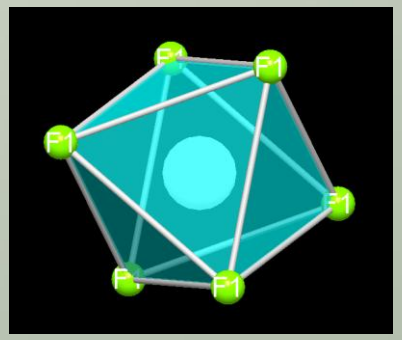
Atomic Environments (AE)



Na (1)



Al

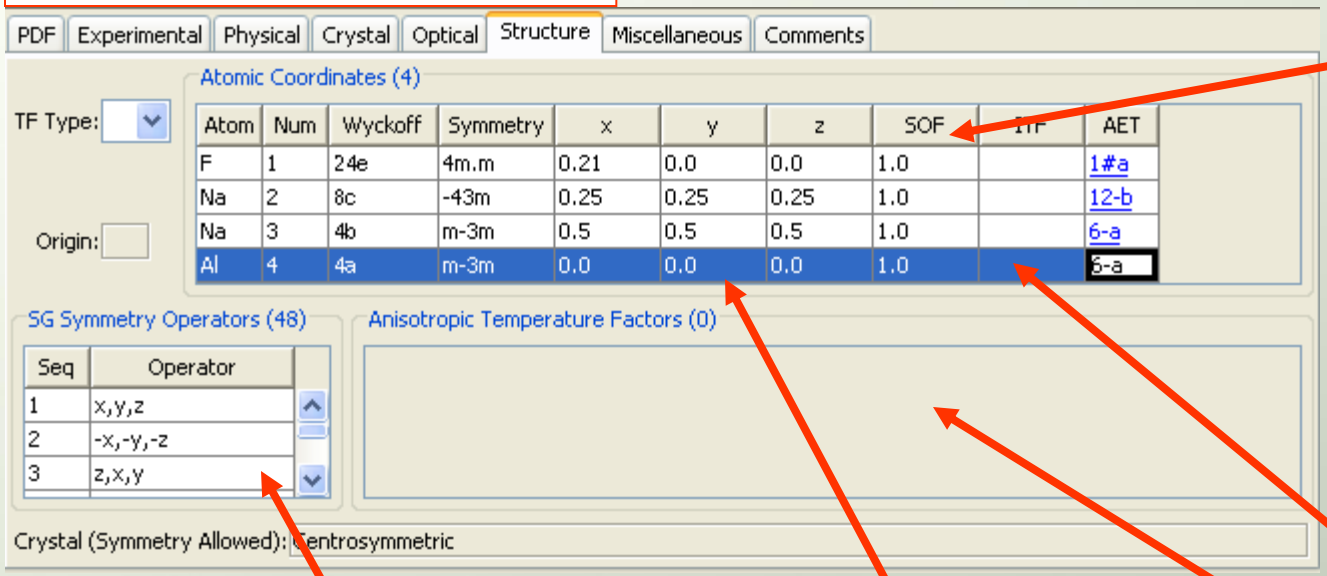


Na (2)

Molecular Graphics

How?

PDF 04-007-8587, Cryolite



Site Occupancy Factor (SOF)

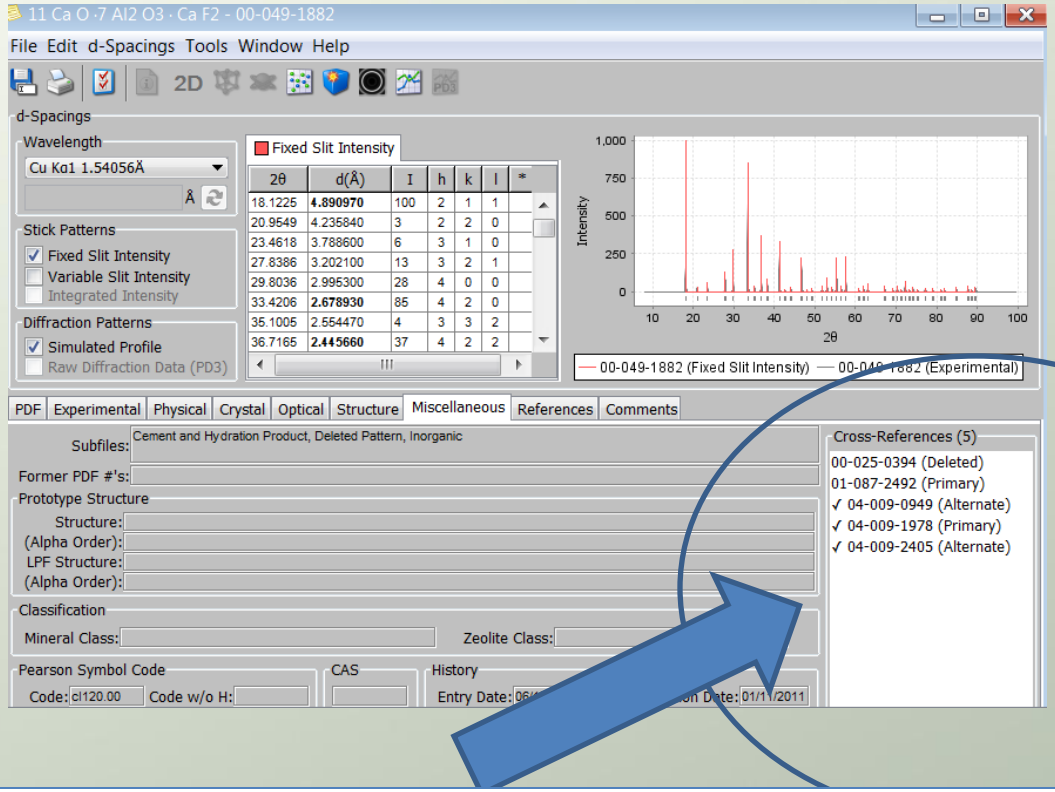
Temperature Factors
ITF = Isotropic (shown)
Table provided for anisotropic factors

Symmetry Operators

Atomic Coordinates
Symmetry
Wyckoff Notation
Atom Designations

Molecular graphics are calculated from the atomic parameters and symmetry operators shown in the Structure tab of a PDF Card. The unit cell parameters in the Crystal tab are also used.

Cross References



Some entries, especially those from powder data, may not have atomic coordinates under the Structure Tab. In the Miscellaneous Tab of every entry, cross references where the formula and unit cells match the entry, are listed. The entries with atomic coordinates are listed with a check mark. To find the appropriate set of atomic coordinates just double click on the entry number.

Getting Started

To display molecules and atomic environments, you need to have atomic parameters, space groups and a unit cell. Space groups and unit cells are published for most data in the PDF. In PDF-4+, Web PDF-4 and PDF-4/Minerals the majority of entries have atomic coordinates or cross referenced atomic coordinates. In PDF-4/Organics >30,000 entries have atomic coordinates.

Data Sources for the PDF

Source of Data	Coordinates in the PDF-4	Reference*
LPF	Yes, All Data	Yes
ICSD	Select data	Yes
CSD	Select data	Yes
ICDD	Select data	Yes
NIST	Majority	Yes

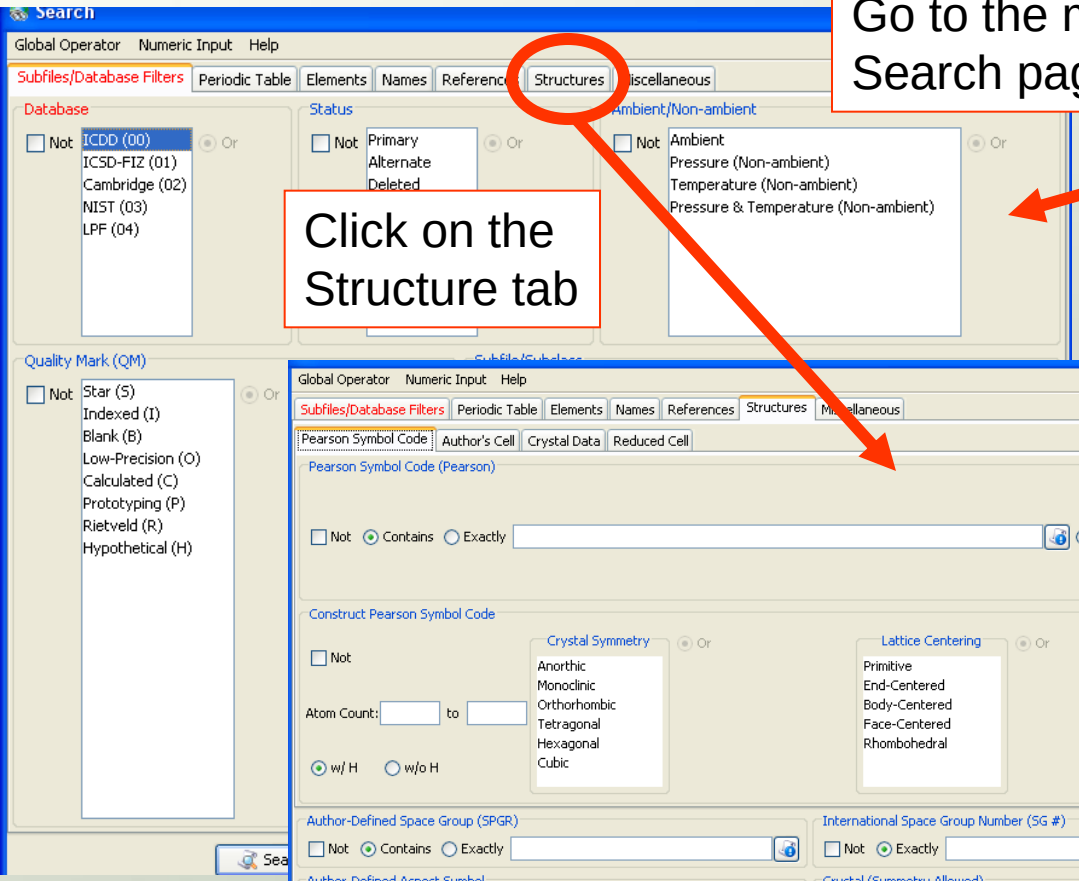
* All references contain both a reference to the single crystal source data (ICSD, NIST, CSD, LPF) and a primary literature reference.

PDF-4+ contains over 200,000 entries with atomic coordinate sets or direct cross references to atomic coordinate sets.

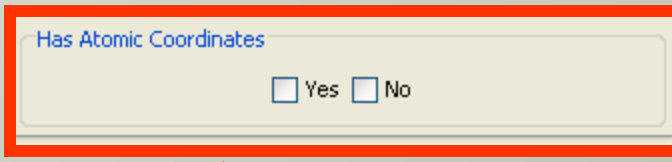
Finding Entries with Atomic Coordinates

Go to the main Search page

Click Search on the toolbar



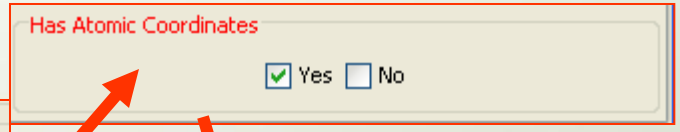
Click on the Structure tab

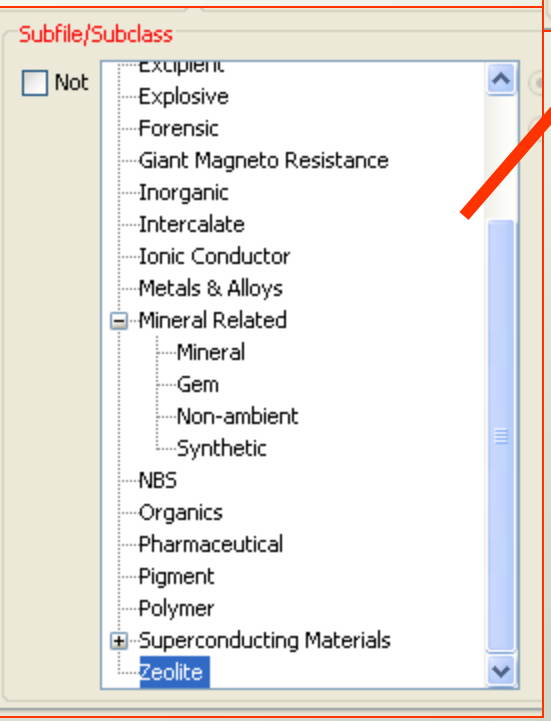


Use the "Has Atomic Coordinates" search

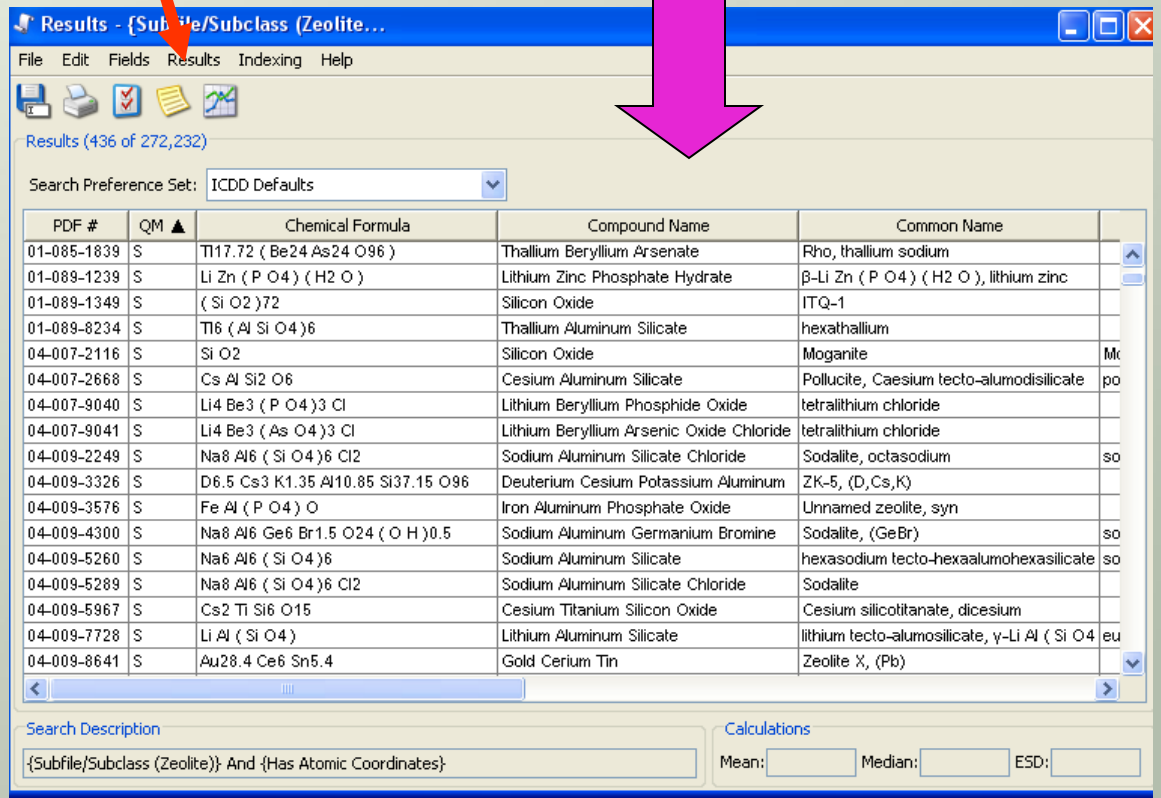
This search can be combined with any other search.

Finding Entries with Atomic Coordinates





A search of zeolites having atomic coordinates finds 436 entries.

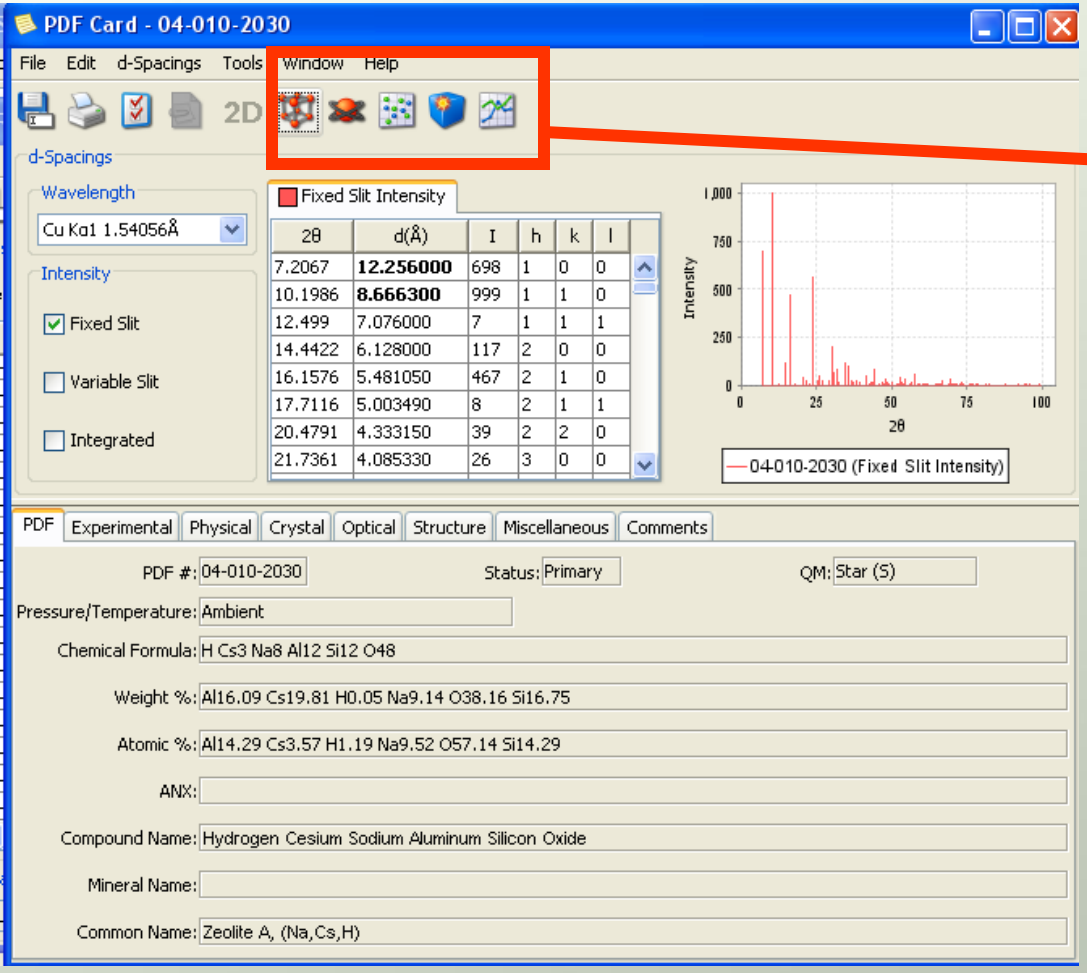


PDF #	QM ▲	Chemical Formula	Compound Name	Common Name	
01-085-1839	S	Tl17.72 (Be24 As24 O96)	Thallium Beryllium Arsenate	Rho, thallium sodium	
01-089-1239	S	Li Zn (P O4) (H2 O)	Lithium Zinc Phosphate Hydrate	β-Li Zn (P O4) (H2 O), lithium zinc	
01-089-1349	S	(Si O2)72	Silicon Oxide	ITQ-1	
01-089-8234	S	Tl6 (Al Si O4)6	Thallium Aluminum Silicate	hexathallium	
04-007-2116	S	Si O2	Silicon Oxide	Moganite	Mo
04-007-2668	S	Cs Al Si2 O6	Cesium Aluminum Silicate	Pollucite, Caesium tecto-alumodisilicate	po
04-007-9040	S	Li4 Be3 (P O4)3 Cl	Lithium Beryllium Phosphide Oxide	tetralithium chloride	
04-007-9041	S	Li4 Be3 (As O4)3 Cl	Lithium Beryllium Arsenic Oxide Chloride	tetralithium chloride	
04-009-2249	S	Na8 Al6 (Si O4)6 Cl2	Sodium Aluminum Silicate Chloride	Sodalite, octasodium	so
04-009-3326	S	D6.5 Cs3 K1.35 Al10.85 Si37.15 O96	Deuterium Cesium Potassium Aluminum	ZK-5, (D,Cs,K)	
04-009-3576	S	Fe Al (P O4) O	Iron Aluminum Phosphate Oxide	Unnamed zeolite, syn	
04-009-4300	S	Na8 Al6 Ge6 Br1.5 O24 (O H)0.5	Sodium Aluminum Germanium Bromine	Sodalite, (GeBr)	so
04-009-5260	S	Na6 Al6 (Si O4)6	Sodium Aluminum Silicate	hexasodium tecto-hexaalumohexasilicate	so
04-009-5289	S	Na8 Al6 (Si O4)6 Cl2	Sodium Aluminum Silicate Chloride	Sodalite	
04-009-5967	S	Cs2 Ti Si6 O15	Cesium Titanium Silicon Oxide	Cesium silicotitanate, dicesium	
04-009-7728	S	Li Al (Si O4)	Lithium Aluminum Silicate	lithium tecto-alumosilicate, γ-Li Al (Si O4	eu
04-009-8641	S	Au28.4 Ce6 Sn5.4	Gold Cerium Tin	Zeolite X, (Pb)	

Finding Entries with Atomic Coordinates

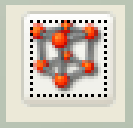
In recent years, the box on the left has been replaced with the box on the right. In PDF-4+, the >160,000 entries with atomic coordinates are supplemented by another >40,000 entries with cross references.

Molecular Graphics From an Entry

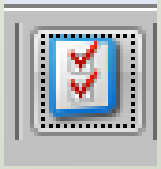


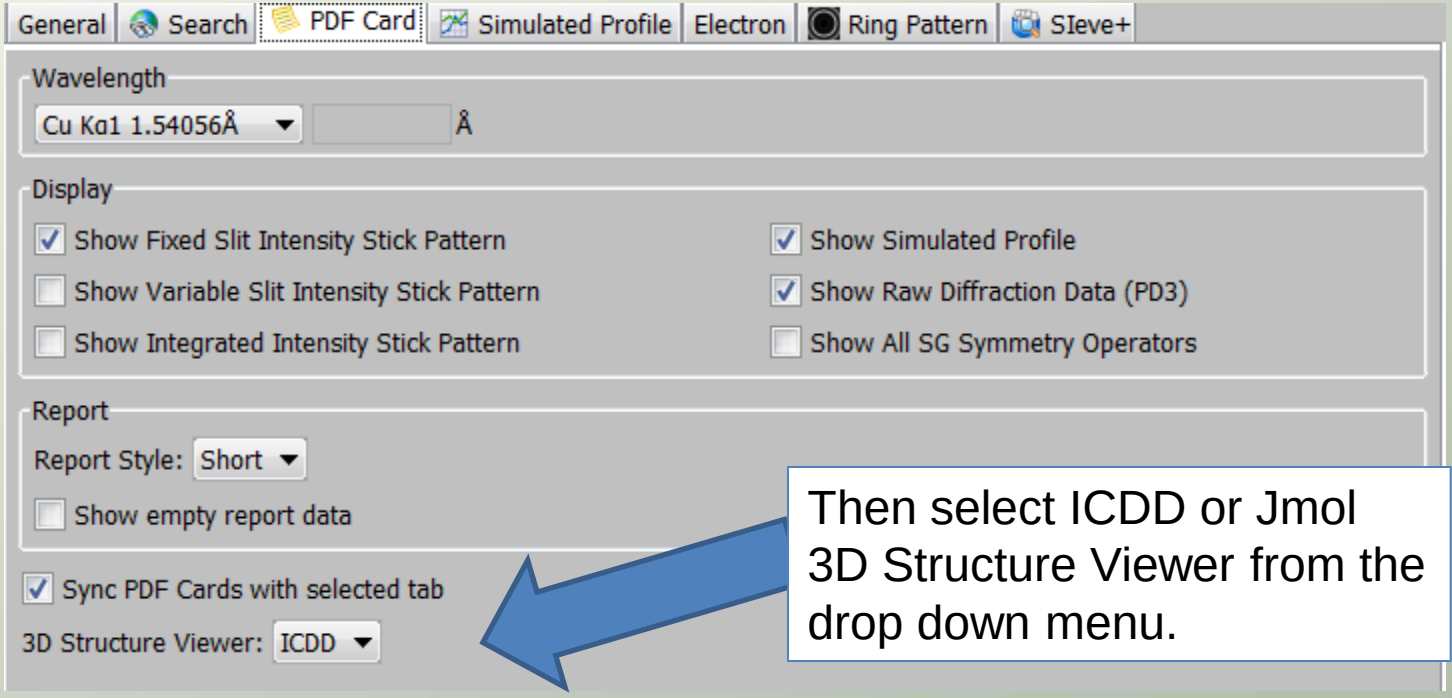
From the previous search we selected Zeolite A, PDF 04-010-2030.

The tool bar at the top of the entry contains several graphics options.

Selecting  results in the molecular graphic menus.

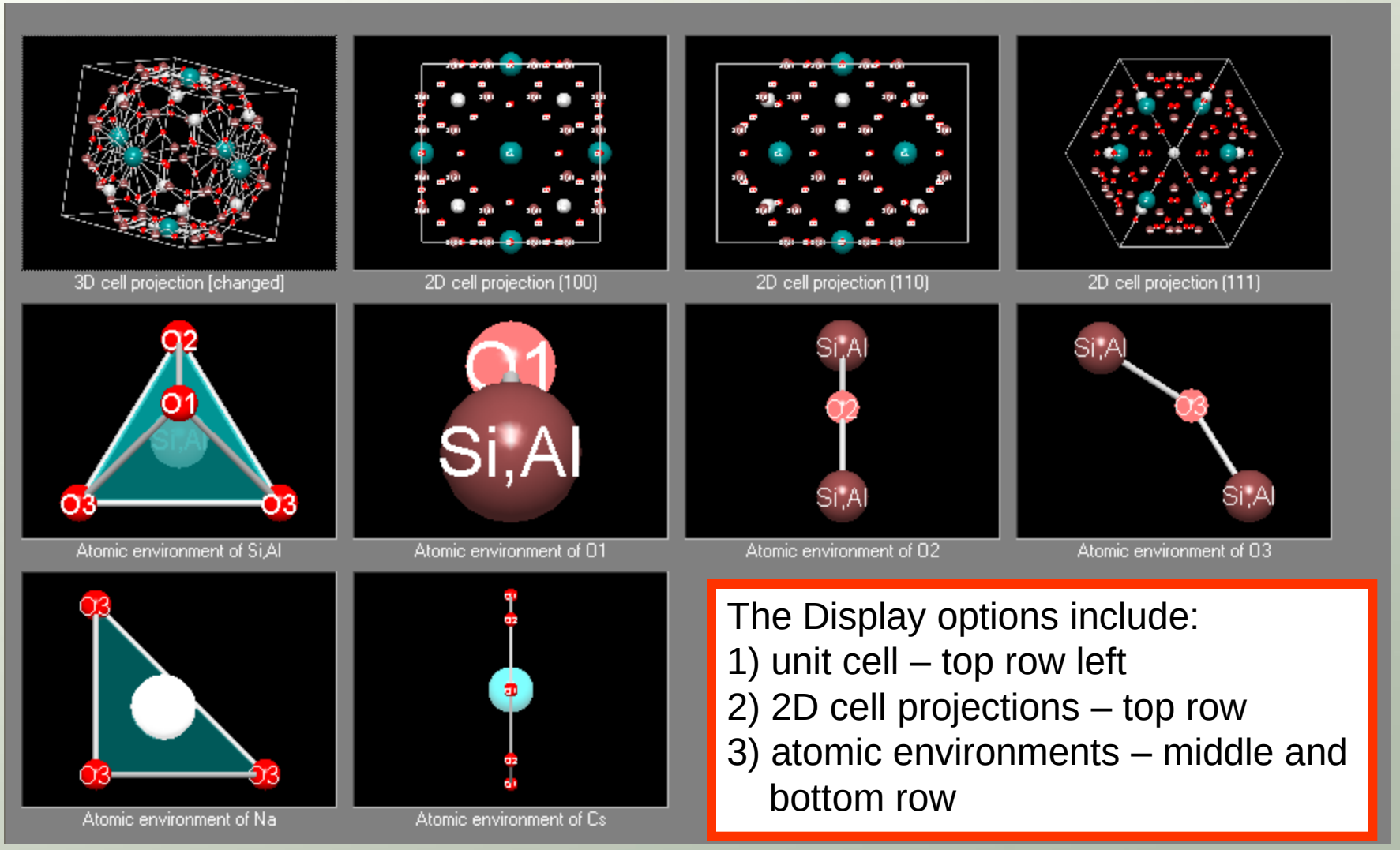
Selection of the Graphics Program

The automatic molecular graphics default program is Jmol. To select another program, click the preferences menu on any entry. 



Display Options

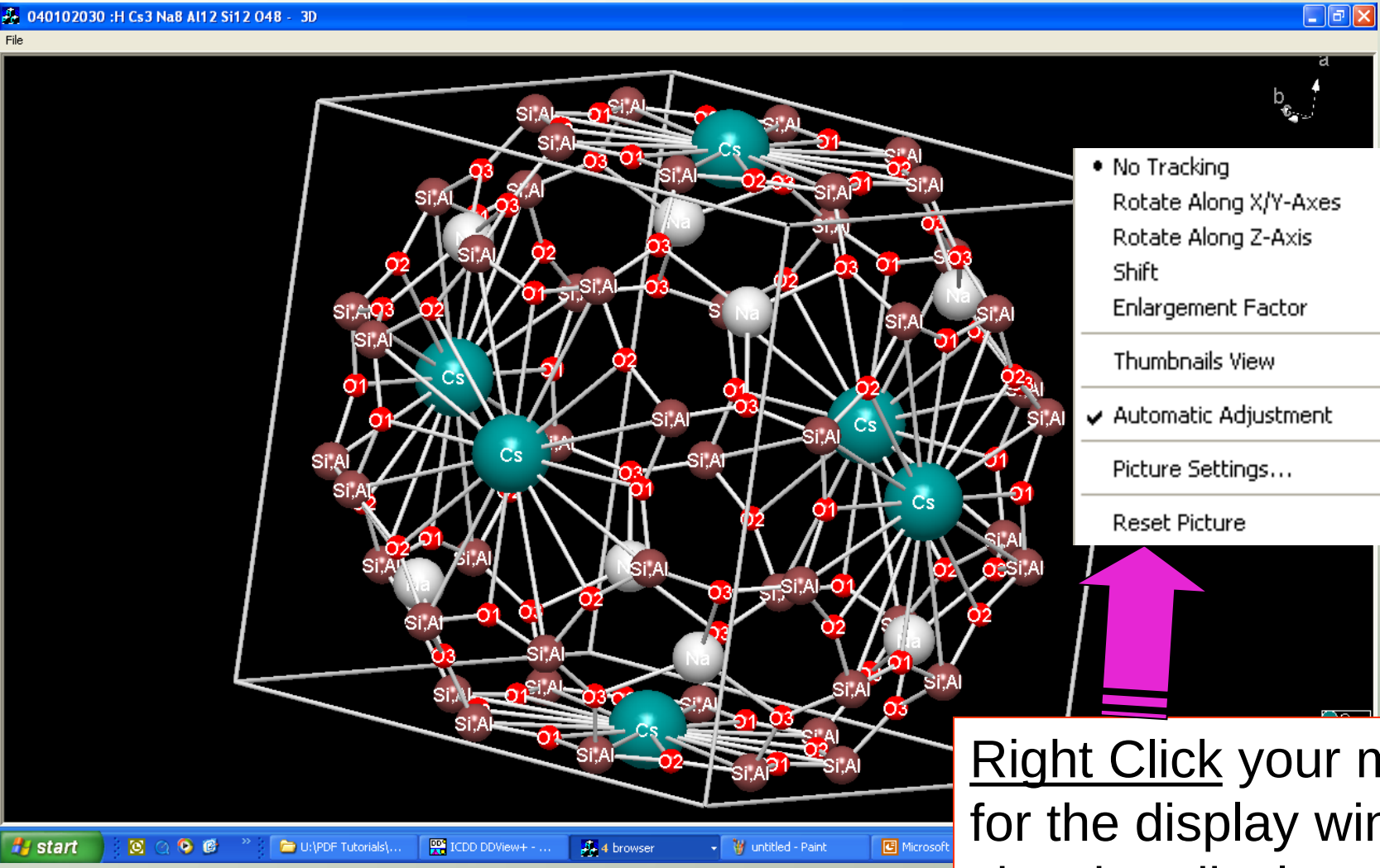
thumbnails – in the product, double click for full scale



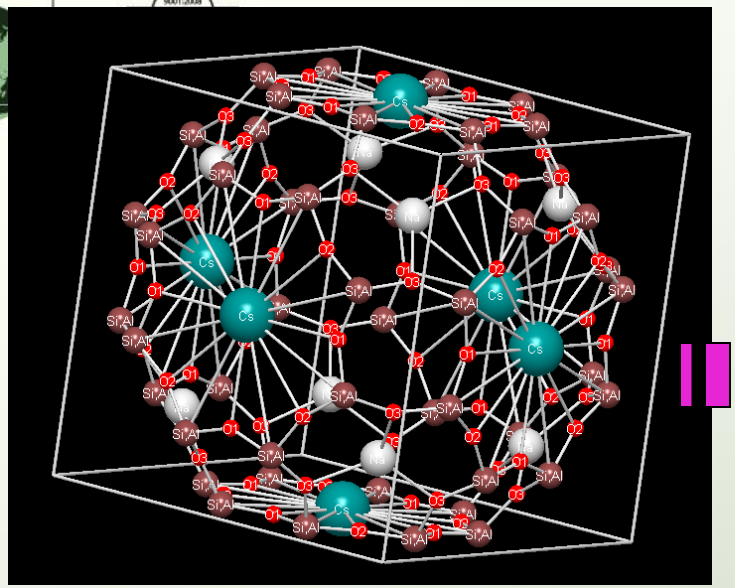
The Display options include:

1) unit cell – top row left
2) 2D cell projections – top row
3) atomic environments – middle and bottom row

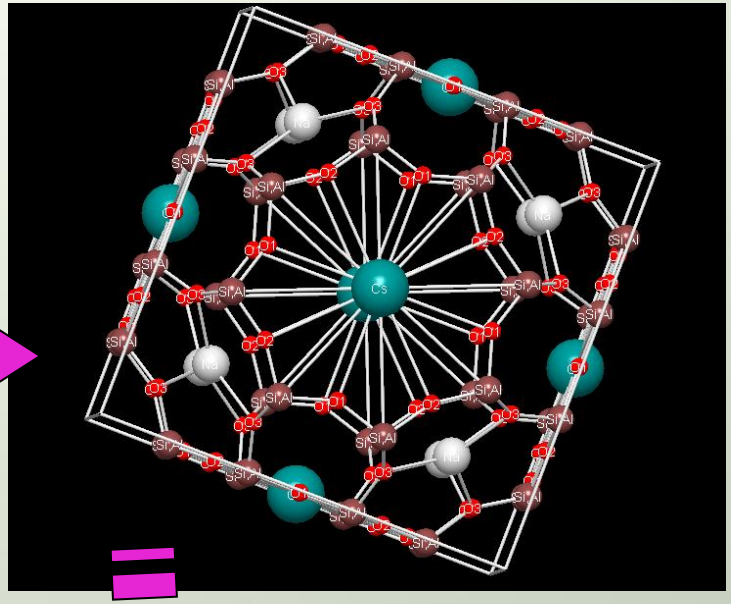
Molecular Display



Right Click your mouse for the display window showing display options.

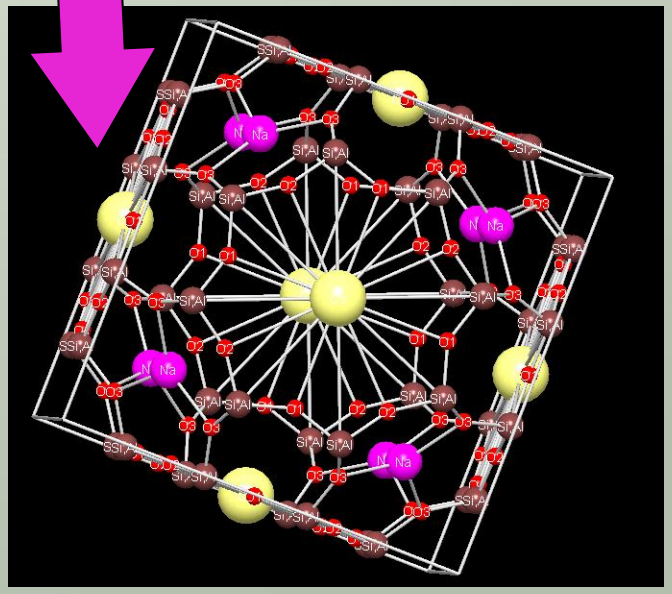


Rotate
x, y or z

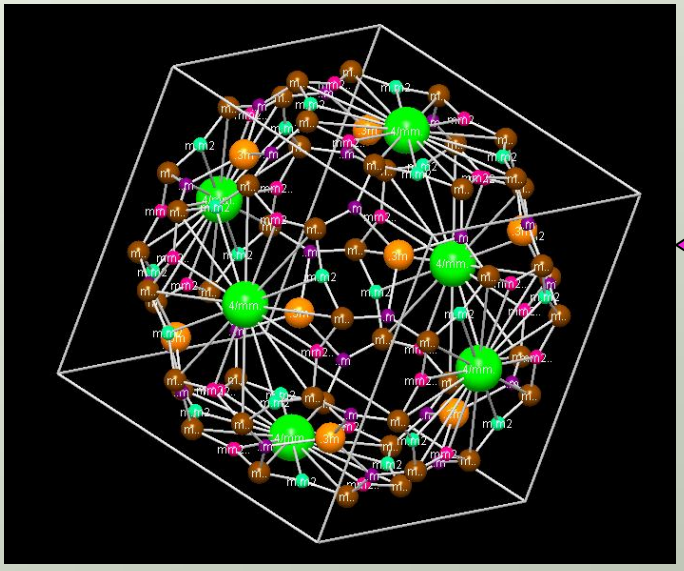


Zeolite A – Different viewing options

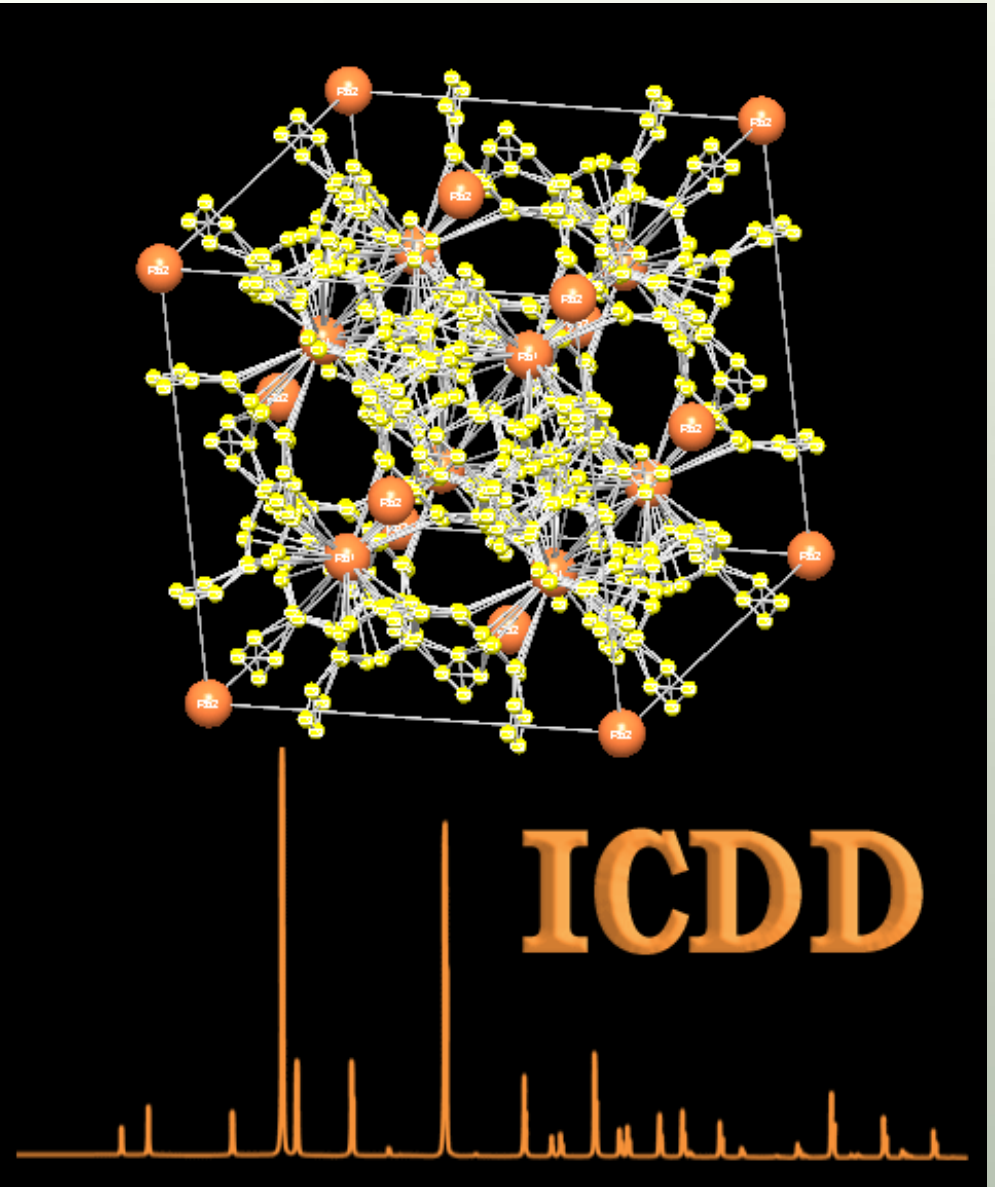
Change atom colors



Replace atom
labels with
Wyckoff labels
and color codes



Export and Import



This rotating display was made by exporting molecular graphics, taken at various rotation angles (shown in the previous slides), and importing the data into Adobe® Photoshop®.

Distributor Software

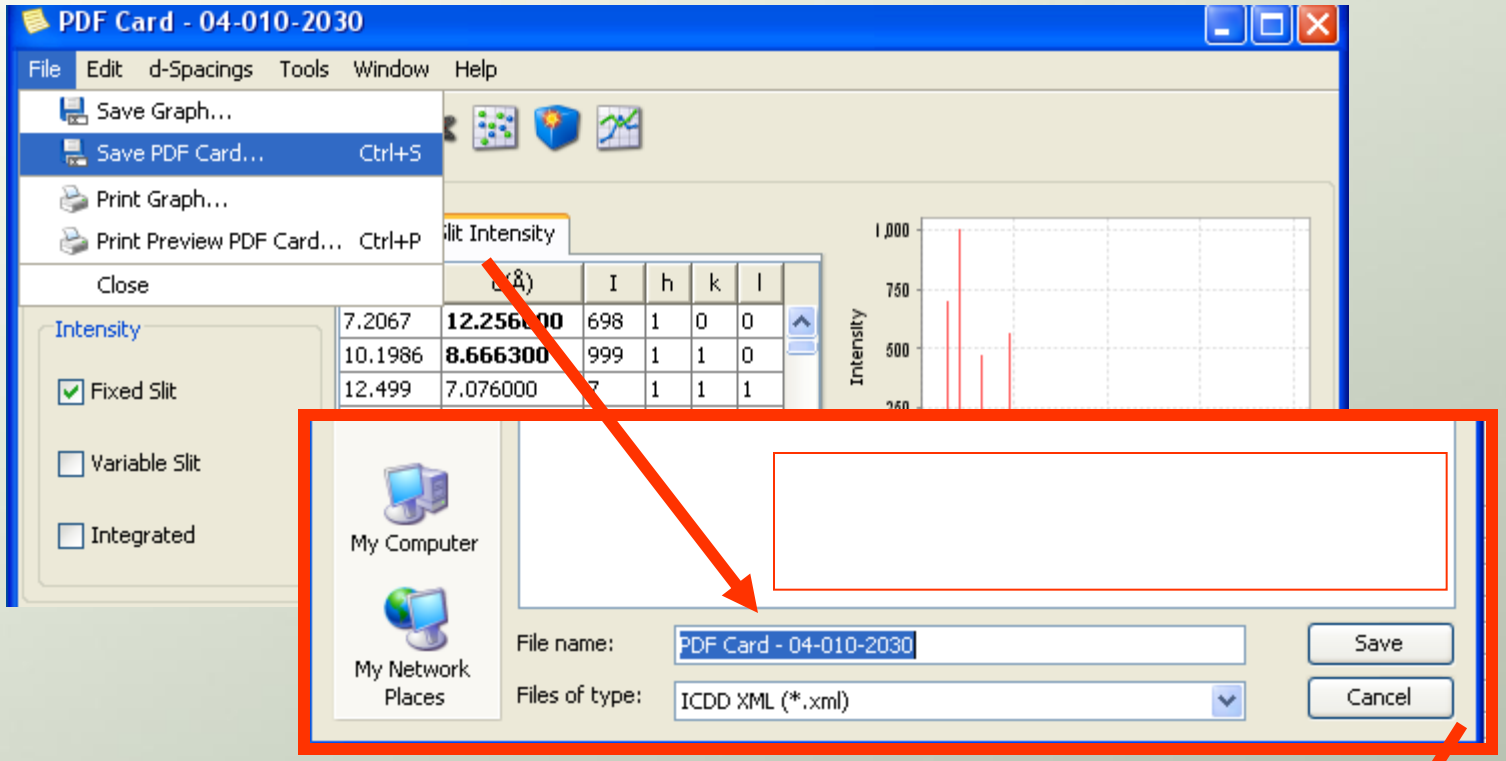
ICDD works with software distributors of many of the worlds' molecular graphics programs to provide enhanced molecular displays.

The distributors work with data tables of atomic coordinates, unit cell parameters, temperature factors, space groups and symmetry operators contained within the PDF-4 so that data are *automatically* entered into their molecular display programs.

The ICDD also works with many software developers and instrument manufacturers who produce molecular refinement programs (i.e., Rietveld Analyses). These programs export atomic coordinates for both refinement and molecular display.

In general, these programs offer tremendous convenience and speed since the user does not have to provide export/import.

How to Export – xml Files



Atomic Coordinates

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	ITF	AET
O	1	24m	..m	0.1119	0.1119	0.3393	1.0		2#a
O	2	12i	m.m2	0.0	0.2944	0.2944	1.0		2#a
Si	3	24k	m..	0.0	0.1832	0.371	0.5		4-a
O	4	12h	mm2..	0.0	0.2228	0.5	1.0		2#a
Na	5	8g	.3m	0.2025	0.2025	0.2025	1.0		3#a
Cs	6	3c	4/mm.	0.0	0.5	0.5	1.0		8#n
Al	7	24k	m..	0.0	0.1832	0.371	0.5		4-a

xml Files

PDF Number	04-010-2030	**Status**	Primary	**Quality Mark**	Star (S)
Pressure/Temperature	Ambient				
Chemical Formula	H Cs3 Na8 Al12 Si12 O48				
Weight %	Al16.09 Cs19.81 H0.05 Na9.14 O38.16 Si16.75				
Atomic %	Al14.29 Cs3.57 H1.19 Na9.52 O57.14 Si14.29				
Compound Name	Hydrogen Cesium Sodium Aluminum Silicon Oxide				
ANX					
Mineral Name					
Also Called	Zeolite A, (Na,Cs,H)				

Experimental

Rad	λ	Filter	d-Spacing	Cutoff	Intensity	I/Ic
CuKα1	1.5406		Calculated		Calculated	4.01

Camera Diameter	Reference
	"Crystal Structures of Encapsulates within Zeolites. 1. Krypton in Zeolite A". Heo N.H., Cho K.H., Kim J.T., Seff K. J. Phys. Chem. 98, 13328 (1994). Calculated from LPF using POWD-12++.

Anisotropic Temperature Factors

Atom	Num	ATF11	ATF22	ATF33	ATF12	ATF13	ATF23
O	1	2.28326	2.28326	2.22318	0.270386	0.090129	0.090129
O	2	4.14593	1.44206	1.44206	0.0	0.0	0.841205
Si	3	1.32189	1.14163	0.721031	0.0	0.0	0.210301
O	4	3.48498	3.06438	1.14163	0.0	0.0	0.0
Na	5	3.54507	3.54507	3.54507	2.07296	2.07296	2.07296
Cs	6	6.72962	4.98713	4.98713	0.0	0.0	0.0

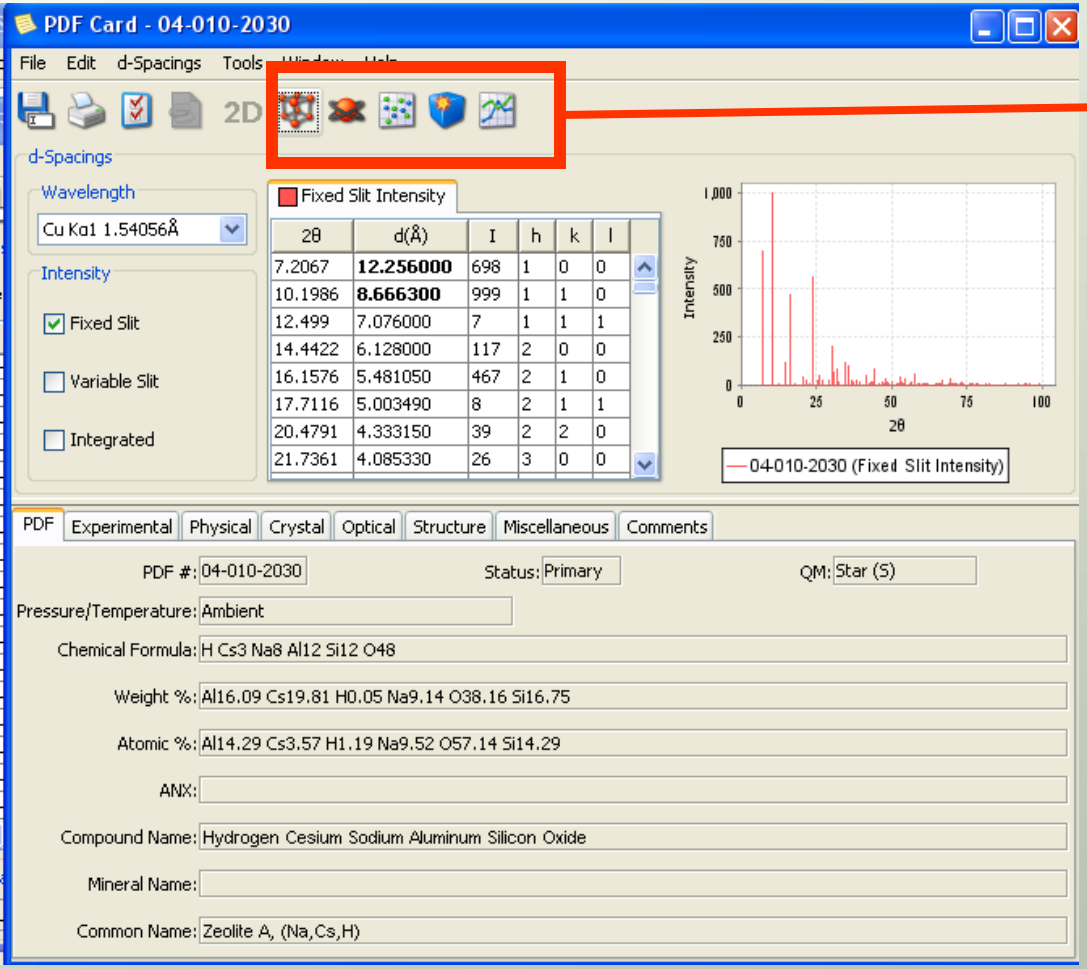
Atomic Coordinates

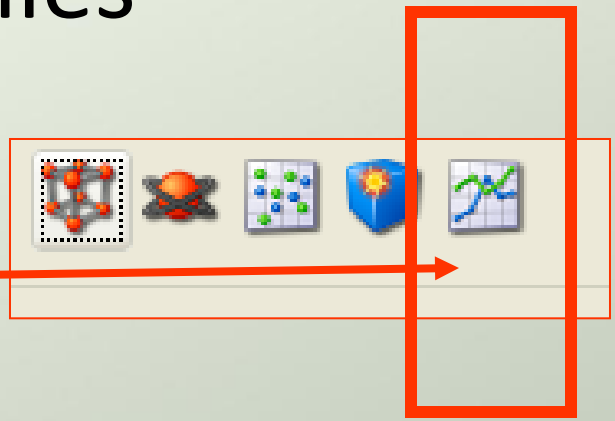
Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	ITF	AET
O	1	24m	..m	0.1119	0.1119	0.3393	1.0		2#a
O	2	12i	m.m2	0.0	0.2944	0.2944	1.0		2#a
Si	3	24k	m..	0.0	0.1832	0.371	0.5		4-a
O	4	12h	mm2..	0.0	0.2228	0.5	1.0		2#a
Na	5	8g	.3m	0.2025	0.2025	0.2025	1.0		3#a
Cs	6	3c	4/mm.	0.0	0.5	0.5	1.0		8#n
Al	7	24k	m..	0.0	0.1832	0.371	0.5		4-a

In the xml "card" format, all data are exported. This includes formula, nomenclature, atomic coordinates, anisotropic temperature factors, references, comments, etc., as shown in the boxes on the left.

It also displays a fully indexed diffraction pattern (not shown).

How to Export – CIF, JPG, CSV Files



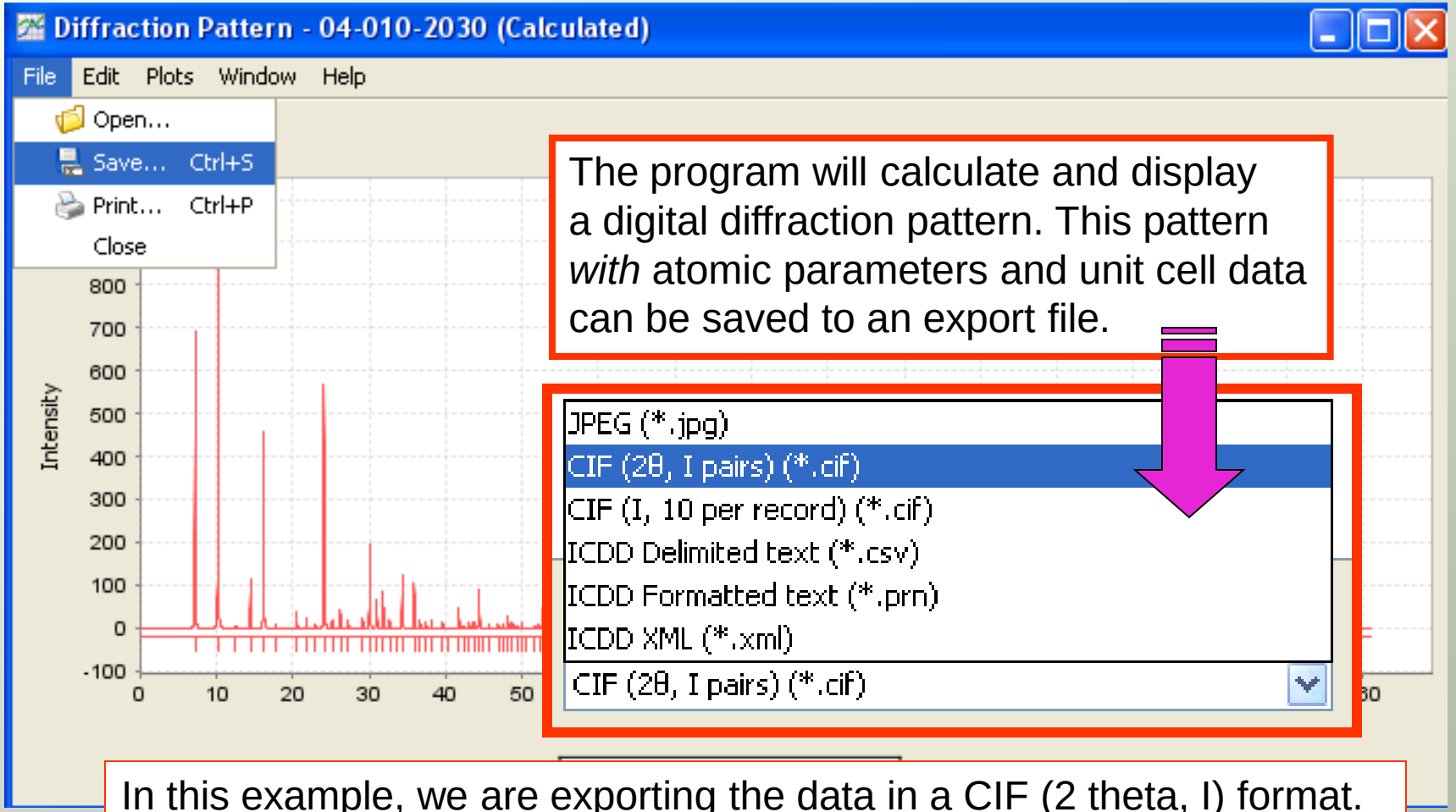


Same Zeolite A entry displayed on earlier slides.

Go to the Toolbar

Click on Diffraction Pattern

How to Export – CIF, JPG, CSV Files



In this example, we are exporting the data in a CIF (2 theta, I) format. The CIF format is used by a wide variety of software programs.

Export/Import

The next three slides are meant to demonstrate how PDF-4+ data can be imported into common molecular visualization programs.

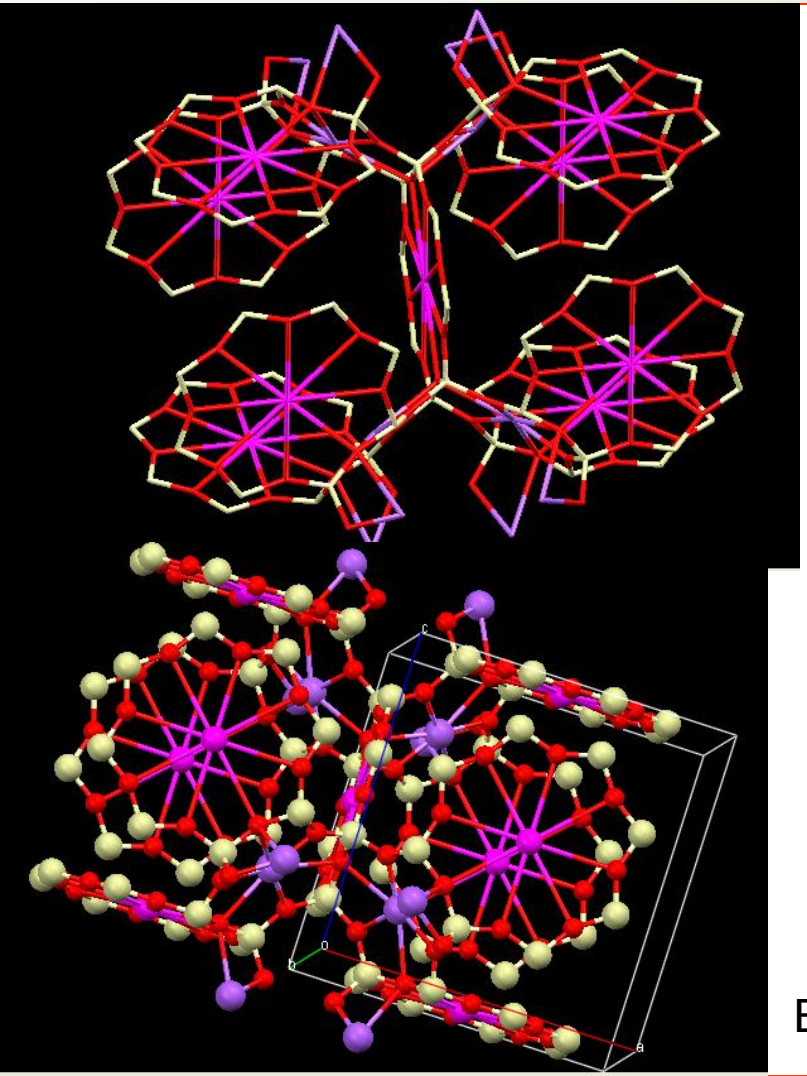
The programs selected are the proprietary software products of ICDD's database partners. Examples are shown to display a few select capabilities, each program has a large number of display options.

	Program
Cambridge Crystallographic Data Centre (CCDC)	Mercury
Fachinformationszentrum Karlsruhe (FIZ)	Visualize
Material Phases Data System	Pearson's Crystal Data

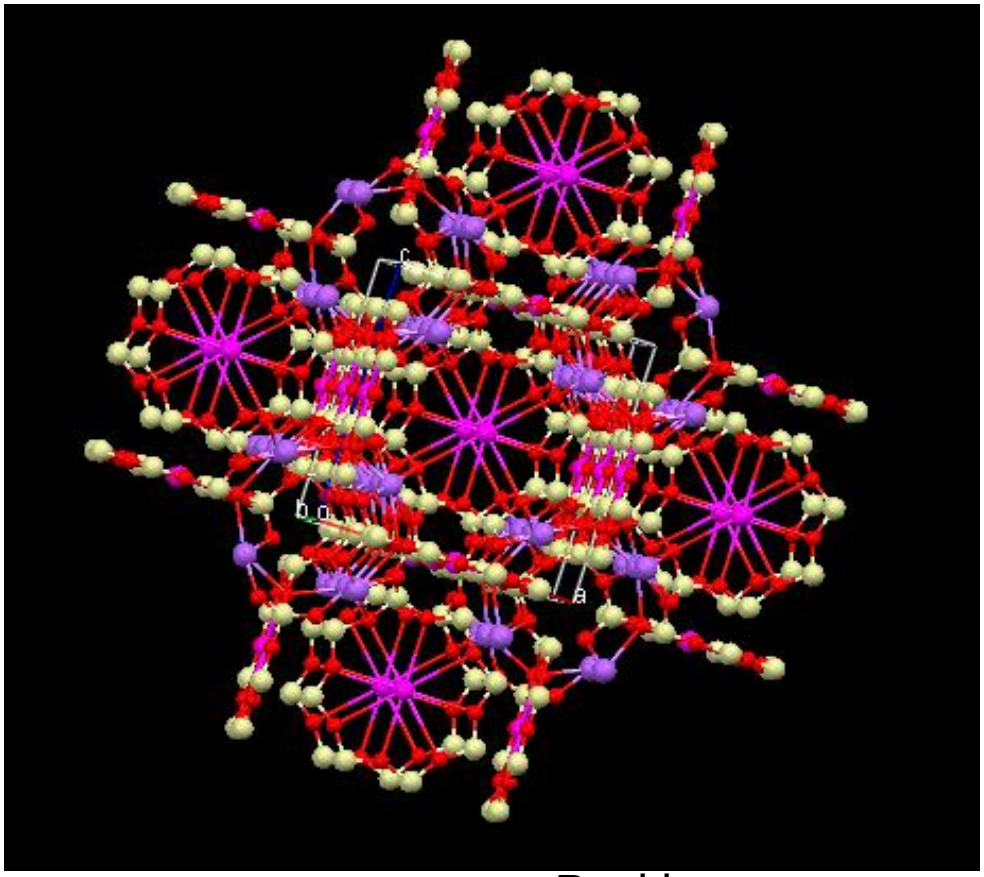
Importing CIF Files

PDF-4+ data file imported into Mercury. Mercury is a freeware program produced by the CCDC, and used with the CSD.

http://www.ccdc.cam.ac.uk/products/mercury



Wireframe



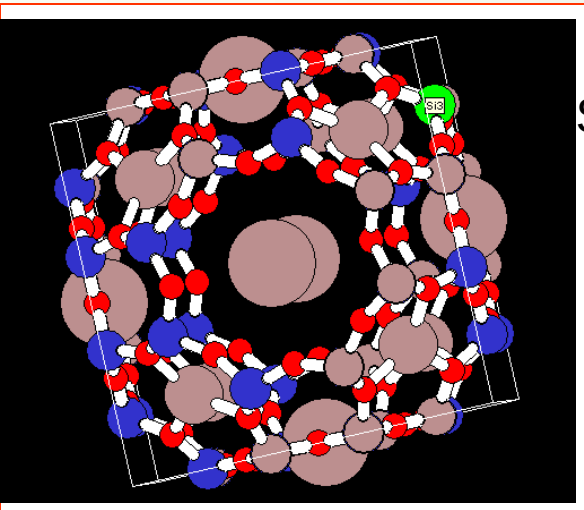
Ball and Stick

Zeolite A

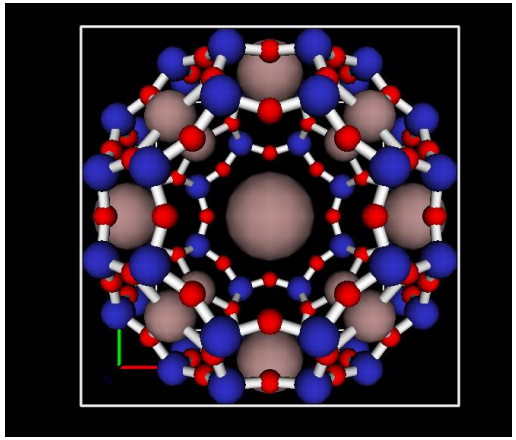
Packing
Multiple Unit Cells

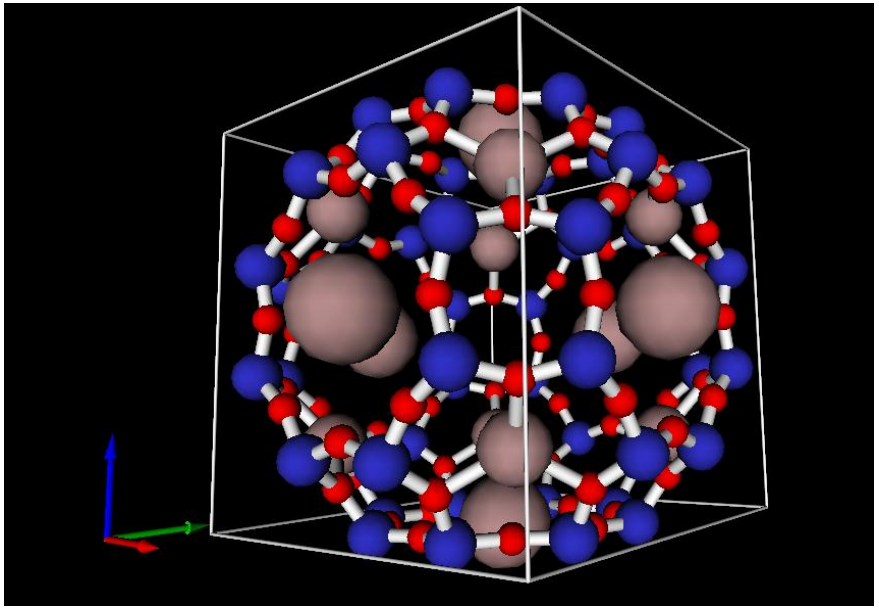
Importing CIF files

PDF-4+ data file imported into Visualize. Visualize is a program produced by FIZ/NIST for the ICSD.



Space Fill Model



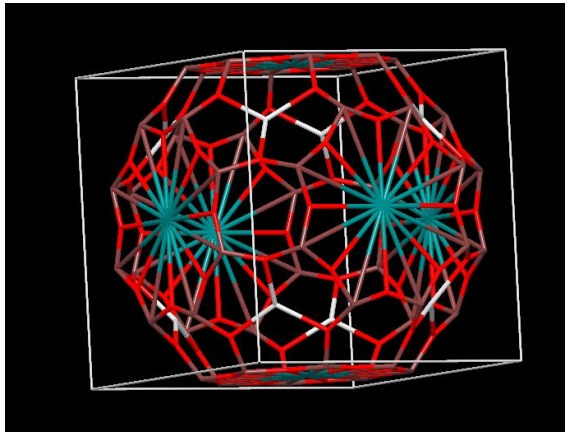


VRML Model

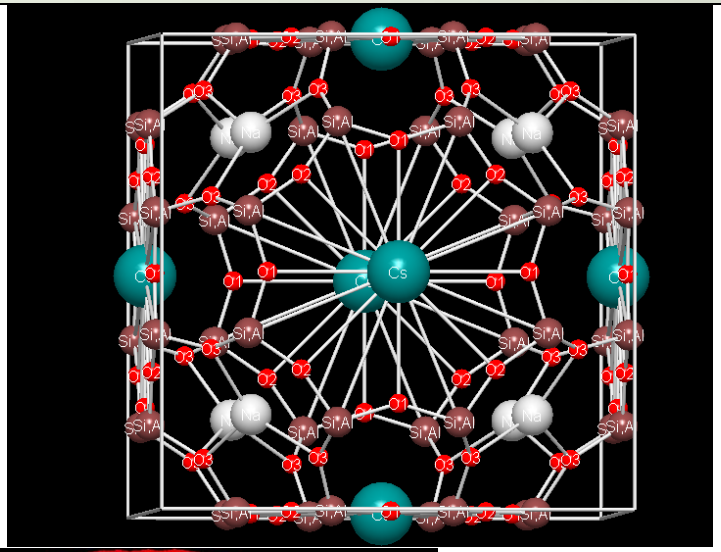
Zeolite A

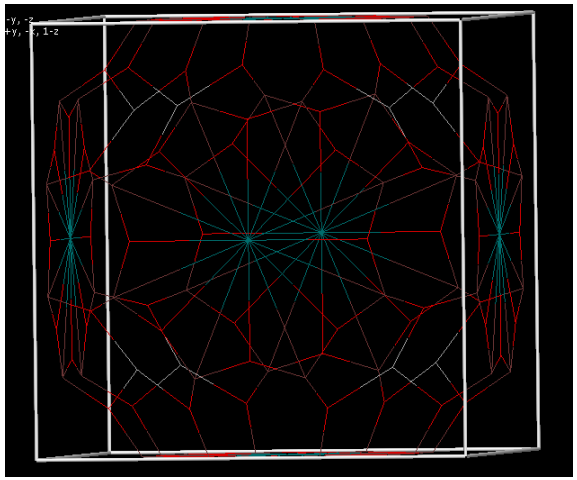
Same Structure Viewed with Pearson's Crystal Data Molecular Visualization Software

Note: This uses the PDF-4+ cross reference.

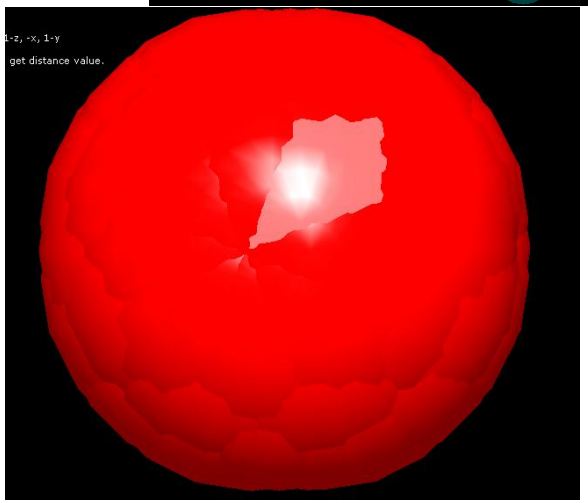


Wireframe





All Wire



Space Filling

Editing and Molecular Visualization

Historically, many databases have faced issues displaying molecular structures. The primary issue has been the lack of uniform conventions and the back-application of recent conventions to historic data.

ICDD Editors:

- Standardize all unit cell settings
- Convert non-standard space groups
- Check and test that the appropriate temperature factors are applied from the literature
- Analyze for correct bond angles and distance
- Check for non-positive temperature factors
- Ensure that the physical properties match the stated chemistry and crystallography
- Apply a quality evaluation system to all entries, including historic data, and publish the results in the comment sections of each entry.

Thank you for viewing our tutorial.

Additional tutorials are available at the ICDD web site (www.icdd.com).

International Centre for Diffraction Data

12 Campus Boulevard

Newtown Square, PA 19073

Phone: 610.325.9814

Toll Free Number in US & Canada: 866.378.0331

Fax: 610.325.9823