

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 (<u>www.jmol.org</u>). 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 Na3AlF6

Atomic Environments (AE)



PDF 04-007-8587



Na (1)







Na (2)



Molecular Graphics

How?





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 [*]
		N /
LPF	Yes, <u>All Data</u>	Yes
ICSD	Select data	Yes
CSD	Select data	Yes
ICDD	Select data	Yes
NIST	Majority	Yes

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

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

Finding Entries with Atomic Coordinates

Search Global Operator Numeric Input Subfiles/Database Filters Period	Help dic Table	Elements Names Reference Structures Discellaneous	Go to the main Search page		-
Not ICDD (00) ICSD-FIZ (01) Cambridge (02) NIST (03) LPF (04)		Not Primary Alternate Deleted Click on the Structure tab	ent) (Non-ambient)		Click Search on the toolbar
Not Star (S) Indexed (I) Blank (B) Low-Precision (O) Calculated (C) Prototyping (P) Rietveld (R)) Or	Global Operator Numeric Input Help Subfiles/Database Filters Periodic Table Elements Names References Structures M Pearson Symbol Code Author's Cell Crystal Data Reduced Cell Pearson Symbol Code (Pearson) Not © Contains © Exartly		←Has Atomic Coordinate	s 🗌 Yes 🛄 No
Hypothetical (H)		Construct Pearson Symbol Code Crystal Symmetry Orthornbic Atom Count: to W/H W/O H Author-Defined Space Group (SPGR) In	Lattice Centering Or Primitive End-Centered Body-Centered Face-Centered Rhombohedral ternational Space Group Number (SG #)		Use the "Has Atomic Coordinates" search
	ĝ Sea	Not ⊙ Contains ○ Exactly 3 Author-Defined Aspect Symbol Cr Not ⊙ Contains ○ Exactly 3 Prototype Structure Not ⊙ Contains Elements ○ Contains Phrase 3 LPF Prototype Structure Not ⊙ Contains Elements ○ Contains Phrase 3 LVFF Prototype Structure 3 3 Not ⊙ Contains Elements ○ Contains Phrase 3 3 Q Search ✓ Show Results © Undock Page	Not ● Exactly ystal (Symmetry Allowed) Not Centrosymmetric ● And ● -Non-centrosymmetric or as Atomic Coordinates Yes No Reset Page Reset All	This sea combine other se	arch can be ed with any earch.



Finding Entries with Atomic Coordinates





Finding Entries with Atomic Coordinates

Has Atomic Coordinates	Has Atomic Coordinates (Coords)
Ves 🗌 No	✓ Yes ✓ Include Cross-Referenced Entries
,	No

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

🛸 PDF Card - 04-010-2030)							
File Edit d-Spacings Tools W	Window Help							
🖶 🍛 🕑 🕘 2D 🕻	\$ 🕺 🗱 🖗	2						
Wavelength Cu Ka1 1.54056Å	Fixed Slit Intensity	I h	1,000 -					
Intensity 7.3	.2067 12.256000 0.1986 8.666300	698 1 999 1						
Fixed Slit 12	2.499 7.076000 4.4422 6.128000	7 1 117 2	1 1 0 0					
Variable Slit 16	6.1576 5.481050 7.7116 5.003490	467 2 8 2		25 50 75 100				
Integrated 20	0.4791 4.333150 1.7361 4.085330	39 2 26 3		+010-2030 (Fixed Slit Intensity)				
PDF Experimental Physical Cry	ystal Optical Structu	re Miscella	aneous Comments					
PDF #: 04-010-203	30	Status: Pi	rimary	QM: Star (S)				
Pressure/Temperature: Ambient								
Chemical Formula: H Cs3 Na8 A	AI12 5I12 048							
Weight %: Al16.09 Cs1	19.81 H0.05 Na9.14 O3	8.16 Si16.7	75					
Atomic %: Al14.29 Cs3	3.57 H1.19 Na9.52 O57	.14 Si14.29)					
ANX:								
Compound Name: Hydrogen C	Cesium Sodium Aluminu	m Silicon O	xide					
Mineral Name:								
Common Name: Zeolite A, (N	Na,Cs,H)							



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.



General 🚷 Search 🛸 PDF Card 🌌 Simulated Profile Electron	🔘 Ring Pattern 🔯 SIeve+
Wavelength Cu Ka1 1.54056Å ▼ Å	
Display	
Show Fixed Slit Intensity Stick Pattern	Show Simulated Profile
Show Variable Slit Intensity Stick Pattern	Show Raw Diffraction Data (PD3)
Show Integrated Intensity Stick Pattern	Show All SG Symmetry Operators
Report	
Report Style: Short 🔻	
Show empty report data	Then select ICDD or Jmol
Sync PDE Cards with selected tab	3D Structure Viewer from the
3D Structure Viewer: ICDD ▼	drop down menu.



Display Options



thumbnails – in the product, double click for full scale





👫 040102030 :H Cs3 Na8 Al12 Si12 048 - 3D

Molecular Display



File No Tracking Rotate Along X/Y-Axes Rotate Along Z-Axis Shift Enlargement Factor Thumbnails View Automatic Adjustment Picture Settings... SI,SI,AI C Microsof 🦺 4 browser 🗸 🦙 untitled - Paint 🛃 start C 🕑 😰 🛅 U:\PDF Tutorials\. ICDD DDView+ - ...

_ 7 🗙

Reset Picture Right Click your mouse for the display window

showing display options.





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 <u>automatically</u> 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

PDF Car	d - 04-01	0-20)30											
File Edit d	-Spacings	Tools	s Window	Help										
🛃 Save G	Graph			e 👬	9	24								
🛛 🔜 Save P	DF Card		Ctrl+S	-										
踚 Print G	raph				_									
踚 Print Pi	review PDF	Card.	Ctrl+P	ilit Intens	sity			- 000, 1						
Close				(Å)	I h l	< 1	750						
Intensity			7.2067	12.256	.00 é	98 1 0	0	usity						
E Fixed S	126		10.1986	8.6663	00 9	999 1 1	0	Intel Intel						
rixed S	iic.		12,777	7.07000			1	260						
Variable	e Slit													
📃 Integra	ited		My Comp	uter										
		_	-											
					ile nam			0.0000					ſ	Saua
			My Netwo	ork	lie Halli		- Card - 04-01	0-2030						Jave
			Places	; F	iles of t	:ype: ICD	D XML (*.×ml)				*		Cancel
				Atom	Num	Wyckoff	Symmetry	х	у	z	SOF	ITF	AET	
				0	1	24m	m	0.1119	0.1119	0.3393	1.0		2#a	
				0	2	12i	m.m2	0.0	0.2944	0.2944	1.0		2#a	
		Atomic		Si	3	24k	m	0.0	0.1832	0.371	0.5		4-a	
	Coordinates		0	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	
				Ce	6	30	1/mm	0.2025	0.2025	0.2025	1.0		8#n	
				A1	7	244	4/11111.	0.0	0.5	0.3	1.0		4.0	
				AI		24K	III	0.0	0.1832	0.3/1	0.5		4-a	



xml Files

DF Number	(04-010-2	2030			Status	tatus Primary				Quality Mark				ar (S)		
ressure/Temperat	ure A	Ambient															
hemical Formula	I	H Cs3 N	Cs3 Na8 Al12 Si12 O48														
/eight %	A	A116.09	5.09 Cs19.81 H0.05 Na9.14 O38.16 Si16.75														
tomic %	ł	A114.29	1.29 Cs3.57 H1.19 Na9.52 O57.14 Si14.29														
ompound Name	ŀ	Hydroge	en Cesit	um Sodi	ium /	Aluminu	im S	Silicon O	kide								
NX																	
Iineral Name																	
lso Called	Z	Zeolite	A, (Na,C	s,H)													
	I	Rad		λ		Filter		d -9	Spac	ing		Cuto	ff I	intensity	· I /I	I/Ic	
	0	Cu K α1		1.5406				Ca	ilcula	ted			(Calculate	d 4.	01	
xperimental	0	Camera Diamete	er	Referen	ice												
				"Crystal K.H., Ki 12++.	Struc in J.T	tures of E I., Seff K	incar J. I	osulates wi Phys. Cher	ithin 2 n. 98	Zeolites. , 13328	1. Kryj (1994)	pton :). Cal	in Zeolite A lculated fro	A". Heo I m LPF u	N.H., C sing PC	'ho)WD	
		Aton	n Num	ATF	11	ATF2	22	ATF33	3	ATF	12	AT	F13	ATF2	3		
		0	1	2.283	326	2.283	26	2.2231	18	0.270)386	0.0	90129	0.090	129		
		0	2	4.14	593	1.442	06	1.4420)6	0.0		0.0)	0.841	205		
Anisotropic		Si	3	1.32	189	1.141	63	0.7210	031	0.0		0.0)	0.210	301		
Femperature		0	4	3.484	198	3.064	38	1.1416	53	0.0		0.0)	0.0			
ractors		Na	5	3.54	507	3.545	07	3.5450)7	2.072	296	2.0	7296	2.072	96		
		Cs	6	6.729	962	4.987	13	4.9871	13	0.0		0.0)	0.0			
			Atom	Num	Wy	ckoff	Sv	mmetr	v x		v		z	SOF	ITF	AF	
			0	1	24	m	n	1	0.	1119	0.11	19	0.3393	3 1.0		2#	
			0	2	12	i	m.	m2	0.	0	0.29	944	0.2944	4 1.0		2#	
Atomic			Si	3	24	k	m.		0.	0	0.1832		0.371	0.5		4-8	
Coord	lina	tes	0	4	12	h	mr	n2	0.	0	0.22	228	0.5	1.0		2#	
Coordinat			Na	5	8g		.3r	n	0.	2025	0.20)25	0.2025	5 1.0		3#	
			Cs	6	3c		4/1	nm.	0.	0	0.5		0.5	1.0		8#	
			Al	7	24	k	m.		0.	0	0.18	332	0.371	0.5		4-8	

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

PPF Card - 04-010-2030 File Edit d-Spacings Tools Image: Spacings <					
File Edit d-Spacings Tools Tools <td< td=""><td>🛸 PDF Card - 04-010-2030</td><td></td><td></td><td>1 🕅 🐭 🐼 🛐</td><td>14</td></td<>	🛸 PDF Card - 04-010-2030			1 🕅 🐭 🐼 🛐	14
Por f:// Curve / Status: Primary Pressure / Temperature: Ambient Por f:// Curve / Temperature: Ambient Por f:// Curve / Temperature: Ambient Por f:// Curve / Temperature: Ambient	File Edit d-Spacings Tools Window				<u></u>
d-Spacings Wavelength Cu Kat 1 1.54056Å 28 d(Å) 2.067 12.256000 10.1986 8.666300 10.1986 8.666300 11.4.4422 6.128000 11.4.4422 6.128000 11.4.4422 6.128000 11.4.4422 6.128000 11.7.115 5.003490 12.7.261 4.085330 20.4791 4.333150 21.7.361 4.085330 21.7.361 4.085330 26 3 0-4010-2030 Fixed Sit PDF #: (0+010-2030 Status: Primary PDF #: (0+010-2030 Status: Primary Pressure/Temperature: Ambient Constant	🖶 چ 💆 🕘 2D 🐯 🕿	K 🐹 🝞 🎢 🚽			
Wavelength Fixed Slit Intensity 100 28 d(Å) 1 h 1 7.0067 12.256000 698 1 0 10.1966 8.666500 999 1 0 12.499 7.076000 7 1 1 14.4422 6.128000 17 2 0 11.1966 8.666500 999 1 0 12.499 7.076000 7 1 1 14.4422 6.128000 17 2 0 11.14422 6.128000 17 0 0 28 11.11 11.4432 6.128000 10 28 0 0 11.1540.6330 26 3 0 0 28 0	∼d-Spacings				
Cu Kat 1.54056Å 28 d(Å) 1 h k 1 Intensity 7.2067 12.256000 698 1 0 1 1 1 Veriable Silt 12.499 7.076000 7 1	Wavelength Fixed S	ilit Intensity	000,1		
Intensity 7.2067 12.256000 698 1 0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1 0 0 1 1 0 1 1 0 1 1 0 1 </td <td>Cu Ka1 1.54056Å 💙28</td> <td>d(Å) I h k l</td> <td>750</td> <td>la de la companya de</td> <td></td>	Cu Ka1 1.54056Å 💙28	d(Å) I h k l	750	la de la companya de	
Fixed Slit 12.499 14.4422 6.128000 117 0 16.1576 5.481050 17.7116 5.003490 8 17.7116 5.003490 8 1 20.4791 4.333150 39 2 04010-2030 (Fixed Slit Intensity) PDF Experimental Physical Crystal Optical Structure Miscellaneous Comments PDF #: 04-010-2030 Status: Primary QM: Star (5) PDF #: 04-010-2030 Status: Primary QM: Star (5) PDF #: 04-010-2030 Status: Primary PDF Status: Primary PDF Status: Primary PDF PI	Intensity 7.2067 10.1986	12.256000 698 1 0 0 1 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	500		
Image: Nariable Slit 14.4422 6.128000 117 2 0 0 Image: Nariable Slit 16.1576 5.481050 467 2 1 0 25 60 75 100 20.4791 4.333150 39 2 2 0 0 20 0 0 20 PDF Experimental Physical Crystal Optical Structure Miscellaneous Comments PDF #: 04-010-2030 Status: Primary QM: Star (5) QM: Star (5) Go to the Toolbar Go to the Toolbar	Fixed Slit 12.499	7.076000 7 1 1 1	250		
Integrated Integrated <td>14.4422 16.1576</td> <td>6.128000 117 2 0 0 5.481050 467 2 1 0</td> <td>- I haddan</td> <td></td> <td></td>	14.4422 16.1576	6.128000 117 2 0 0 5.481050 467 2 1 0	- I haddan		
Integrated 20.4791 4.333150 39 2 20 21.7361 4.085330 26 3 0 Image: Commental Physical Crystal Optical Structure Miscellaneous Comments PDF #: 04-010-2030 Status: Primary QM: Star (5) Go to the Toolbar	17.7116	5.003490 8 2 1 1		Same Zeolite A entry	
PDF Experimental Physical Crystal Optical Structure Miscellaneous Comments PDF #: 04-010-2030 Status: Primary QM: Star (5) Pressure/Temperature: Ambient Go to the Toolbar	Integrated 20.4791 21.7361	4.333150 39 2 2 0 4.085330 26 3 0 0	20 04.040.2020 (Sixed Slithsteerite)	diaplayed an aprilar alida	_
PDF Experimental Physical Crystal Optical Structure Miscellaneous Comments PDF #: 04-010-2030 Status: Primary QM: Star (S) Go to the Toolbar Pressure/Temperature: Ambient Comments Comments				displayed on earlier slides	5 .
PDF #: 04-010-2030 Status: Primary QM: Star (S) Go to the Toolbar	PDF Experimental Physical Crystal O	ptical Structure Miscellaneous Comments	s		
Pressure/Temperature: Ambient	PDF #: 04-010-2030	Status: Primary	QM: Star (S)	Go to the Toolbar	
	Pressure/Temperature: Ambient				1
Chemical Formula: H Cs3 Na8 Al12 Si12 O48	Chemical Formula: H Cs3 Na8 Al12 Si12	2 048			
Weight %: Al16.09 Cs19.81 H0.05 Na9.14 O38.16 Si16.75	Weight %: Al16.09 Cs19.81 H0	.05 Na9.14 O38.16 Si16.75		Click on Diffraction Patter	n
Atomic %: Al14.29 Cs3.57 H1.19 Na9.52 O57.14 Si14.29	Atomic %: Al14.29 Cs3.57 H1.1	19 Na9.52 O57.14 Si14.29			
ANX	ANX:				
Compound Name: Hydrogen Cesium Sodium Aluminum Silicon Oxide	Compound Name: Hydrogen Cesium S	odium Aluminum Silicon Oxide			
Mineral Name:	Mineral Name:				
Common Name: Zeolite A, (Na,Cs,H)	Common Name: Zeolite A, (Na,Cs,H))			



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.

Cambridge Crystallographic	Program						
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





Same Structure Viewed with Pearson's Crystal Data Molecular Visualization Software Note: This uses the PDF-4+ cross reference.





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 (<u>www.icdd.com</u>).

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