

BGMN/Profex User Meeting 2019

Importing CIF files in Profex

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Search / Match Results

Full-profile Search/Match:
Only searches among existing *.str files

Search/Match Phases

Database Controls Results

Score List

File	FoM
Calcite.str	0.096061
Dolomite.str	0.045640
Corundum.str	0.044943
Arcanite.str	0.041963
Troemelite.str	0.035226
Periclase.str	0.034704
Fluorite.str	0.027076
Turmaline-Schorl.str	0.026858
Gyrolite.str	0.026599
Muscovite2M1.str	0.025750
Wollastonite1A.str	0.025408
Graphite-3r.str	0.023557
Shlykovite.str	0.023391
Newberyite.str	0.022614
Kaolinite1A.str	0.022334

Pinned Phases

File	Source

External Software search COD or PDF databases

Matching phases may not be available
in BGMN *.str format

Qualtrix (D:\1519_2007\Profile-search-match\QC_MC.rtg)

Exp-2th, Exp-1, P1,2th, P1,1

Intensity vs 2-theta plot showing experimental pattern (QC_MC.rtg) and reference patterns for Calcite, Corundum, and Dolomite.

Phase	Counts	2-theta	Z-theta	Chemical Formula	Weight	Intensity	Scale	FoM	S-Quot
P.1	10 900 0960	29.8	2.489	CaCO ₃	0.9607	0.9530	0.9949	0.9304	46.51
P.2	10 900 0960	38.1	2.113	Al ₂ O ₃	0.0392	0.7484	0.7068	0.1993	11.86
P.3	10 900 0920	38.1	2.113	CaCO ₃ (Mg)	0.0392	0.6441	0.4196	0.0914	41.72
P.4	10 900 0920	38.1	2.113	SiO ₂	0.0392	0.0005	0.0003	0.1420	4.70
P.5	10 900 0920	38.1	2.113	SiO ₂	0.0392	0.5007	0.7426	0.1700	4.50
P.6	10 900 0920	38.1	2.113	SiO ₂	0.0392	0.5630	0.2007	0.1495	4.45
P.7	10 900 0920	38.1	2.113	SiO ₂	0.0392	0.5707	0.7426	0.1700	4.41
P.8	10 900 0920	38.1	2.113	SiO ₂	0.0392	0.6124	0.2435	0.1700	15.23

Matched POW COD: 10 900 0920 00-230-0370 02 Si

Search Results Table:

Color	Qual	Entry	Formula	Candidate phase	P2(theta)	P3(theta)	I scale	Est. I	LC	Inst.	Matched phase	Quant (%)
1	01-002-4965	Si	SiO ₂	Titanium Oxide (Calcium, van)	0.6807	0.8306	0.0711	4.08	0.912	0.912	01-002-4965	47.9
1	01-002-4969	SiO ₂	Hydrogen Oxide	Hydrogen Oxide	0.9303	0.8989	0.0014	3.06	0.424	0.424	01-002-4969	31.9
1	01-089-0023	Pcs 942 D	Iron Oxide	Iron Oxide	0.5473	0.9978	0.0468	4.75	0.406	0.406	01-089-0023	20.1
1	04-021-0221	Pcs 29462 3AR	Aluminum Iron Nickel (Dianhydrite)	Aluminum Iron Nickel (Dianhydrite)	0.5345	0.9902	0.0013	7.87	0.410	0.410	04-021-0221	20.1
1	01-083-0239	Si O2	Silicon Oxide (Quartz, var)	Silicon Oxide (Quartz, var)	0.5278	0.8788	0.0549	3.07	0.412	0.412	01-083-0239	20.1
1	04-030-2364	SiO2	Silicon Oxide (Quartz)	Silicon Oxide (Quartz)	0.5261	0.9780	0.0014	3.26	0.409	0.409	04-030-2364	20.1
1	04-030-2394	SiO2	Silicon Oxide (Quartz)	Silicon Oxide (Quartz)	0.4879	0.8644	0.0596	3.43	0.426	0.426	04-030-2394	20.1
1	01-070-2217	Si O2	Silicon Oxide (Quartz)	Silicon Oxide (Quartz)	0.5139	0.8937	0.0494	3.03	0.404	0.404	01-070-2217	20.1



Import of crystal structure files from external sources in Profex

- ▶ Supported formats:
 - ▶ CIF (Crystallographic Information File)
 - ▶ ICDD XML (Proprietary format)
- ▶ Semi-automatic conversion to *.str format
 - ▶ Complete CIF files: fully automatic import
 - ▶ Incomplete CIF files: semi-automatic import
- ▶ Many CIF files require manual intervention due to:
 - ▶ Missing information
 - ▶ Ambiguous space group symbols (short notation)
 - ▶ Non-standard atomic settings
- ▶ Profex import is constantly improving



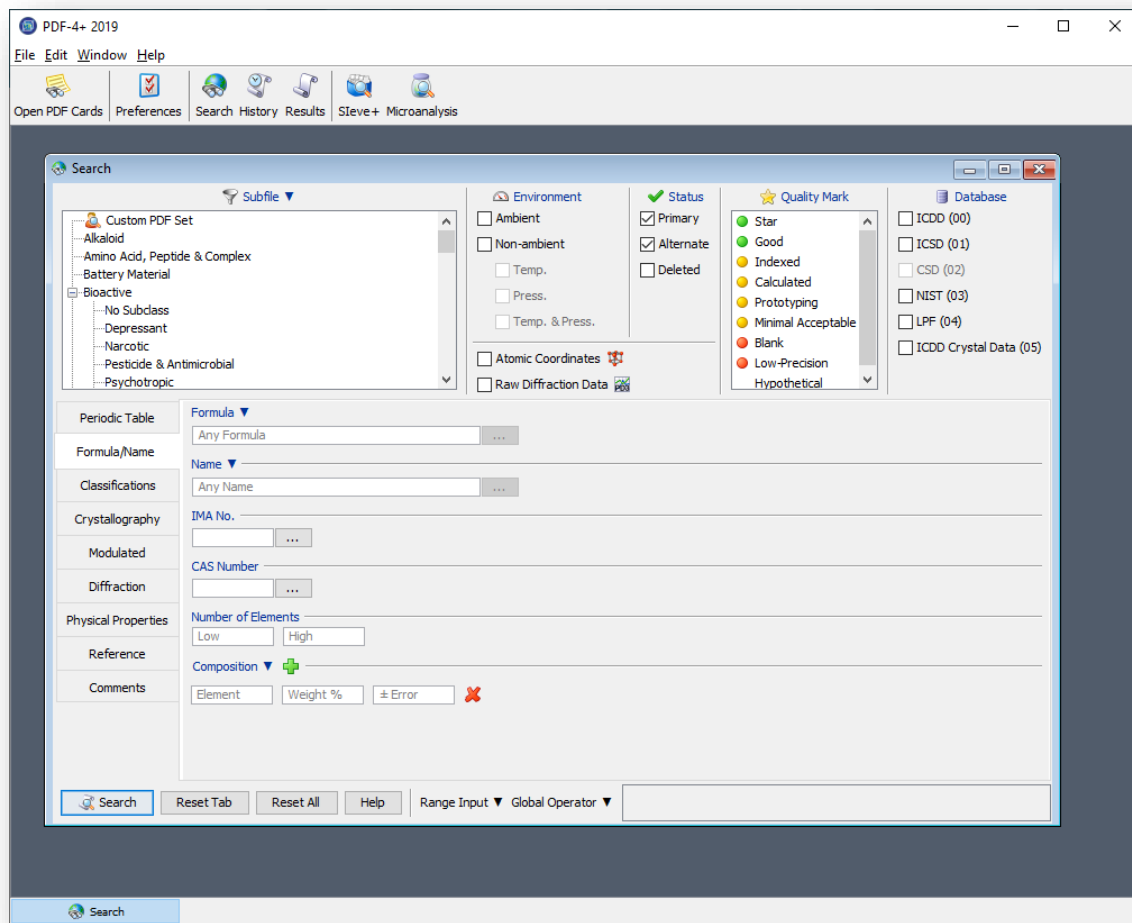
ICDD PDF-4+

Exported XML structure files are often more complete than CIF files obtained from other sources.

Recommendation

If possible, export structures from PDF-4+ in XML format.

Note: PDF-2 database does **not** contain complete structural information.



Example: Export Hydroxylapatite structure from PDF-4+ database

The screenshot shows the search interface with the following search parameters:

- Environment:** Ambient, Non-ambient
- Atomic Coordinates:** Atomic Coordinates
- Quality Mark:** Star (selected)
- Name:** hydroxylapatite

The search criteria at the bottom of the window are: [Environment (Ambient)] And [Has Atomic Coordinates] And [Quality Mark (Star Or Good Or Indexed)] And [Any Name Contains Fragments]

Search parameters:

Name: Calcite
 Environment: Ambient only
 Atomic coordinates: Yes*
 Quality Mark: Star
 Good
 Indexed
 Number of Elements: 0 - 4**

*Required for Rietveld refinement
 ** Stoichiometric Apatite-OH

ICDD XML Format

Results - 79 of 412,083

File Fields Tools Help

Open PDF Card Simulated Profile My Defaults

PDF #	QM	Chemical Formula	SYS	XtlCell a (Å)	XtlCell c (Å)	XtlCell Vol (Å ³)	Phase	Mineral Name	Author - PR	Year - PR
01-070-7716	I	Ca _{4.76} (PO ₄) _{2.91} O _{0.36} (OH)	H	9.396	6.895	527.16		Hydroxylapatite, deuterated, syn	Leventouri, T., Chakoumakos, B.C., ...	2001
01-070-7717	I	Ca _{4.9} (PO ₄) _{2.82} O _{0.72} (OH)	H	9.393	6.898	527.07		Hydroxylapatite, deuterated, syn	Leventouri, T., Chakoumakos, B.C., ...	2001
01-071-5048	S	Ca ₅ (PO ₄) ₃ (OH)	H	9.425	6.884	529.56		Hydroxylapatite	Saenger, A.T., Kuhs, W.F.	1992
01-073-0293	I	Ca ₅ (PO ₄) ₃ (OH)	H	9.432	6.881	530.14		Hydroxylapatite	Kay, M.I., Young, R.A., Posner, A.S.	1964
01-073-1791	I	Ca ₅ (PO ₄) ₃ (OH)	H	9.400	6.930	530.30		Hydroxylapatite	Hendricks, S.B., Jefferson, M.E., M...	1992
01-073-2653	I	Ca _{9.62} (PO ₄) _{5.8} (OH) _{2.35} (...)	H	9.475	6.886	535.39			Wilson, R.M., Elliott, J.C., Dowker, ...	2003
01-073-2634	I	Ca _{9.59} (PO ₄) _{5.75} (OH) _{2.29} (...)	H	9.472	6.886	534.96			Wilson, R.M., Elliott, J.C., Dowker, ...	2003
01-073-2655	I	Ca _{9.56} (PO ₄) _{5.65} (OH) _{2.32} (...)	H	9.474	6.886	535.24			Wilson, R.M., Elliott, J.C., Dowker, ...	2003
01-073-2656	I	Ca _{9.61} (PO ₄) _{5.77} (OH) _{2.29} (...)	H	9.474	6.886	535.25			Wilson, R.M., Elliott, J.C., Dowker, ...	2003
01-073-2657	I	Ca _{9.63} (PO ₄) _{5.78} (OH) _{2.36} (...)	H	9.470	6.884	534.67			Wilson, R.M., Elliott, J.C., Dowker, ...	2003
01-073-6113	I	Ca ₅ (PO ₄) ₃ (OH)	H	9.432	6.881	530.14		Hydroxylapatite	Kay, M.I., Young, R.A., Posner, A.S.	1964
01-073-8418	S	Ca ₅ (PO ₄) ₃ (OH)	H	9.424	6.885	529.59		Hydroxylapatite	Saenger, A.T., Kuhs, W.F.	1992
01-080-7087	I	Ca ₅ (PO ₄) ₃ (OH)	H	9.500	6.560	512.72		Hydroxylapatite, syn	Elayaraja, K., Rajesh, P., Ahymah J...	2012
01-082-1943	I	Ca _{8.86} (PO ₄) ₆ (H ₂ O) ₂	H	9.460	6.888	533.21		Hydroxylapatite, syn	Jeanjean, J., Vincent, U., Fedorov, ...	1994
01-082-2956	S	Ca ₅ (PO ₄) ₃ (OH)	H	9.415	6.879	528.14		Hydroxylapatite, syn	Pogosova, M.A., Kasin, P.E., Trety...	2013
01-084-1998	I	Ca ₅ (PO ₄) ₃ (OH)	H	9.417	6.874	527.91		Hydroxylapatite	Hughes, J.M., Cameron, M., Crowle...	1989
01-085-3476	S	Ca ₁₀ (PO ₄) ₆ (OH) ₂	H	9.415	6.879	528.06		Hydroxylapatite	Kazin, Pavel E., Pogosova, Mariam ...	2016
01-086-0740	I	Ca ₅ (PO ₄) ₃ (OH)	H	9.352	6.882	521.26		Hydroxylapatite	Tomita, K., Kawano, M., Shiraki, K., ...	1996
01-089-4405	S	Ca ₅ (PO ₄) ₃ (OH)	M	16.335	9.426	1060.40		Hydroxylapatite, syn	Ikoma, T., Yamazaki, A., Nakamura...	1999

[Environment (Ambient)] And [Has Atomic Coordinates] And [Quality Mark (Star Or Good Or Indexed)] And [Any Name Contains Fragments 'hydroxylapatite'] And [Number of Elements Between 4 - 4] And [Status (Primary, Alternate)]

Personal preference:

- Skip **old** entries (e.g. < 1980)
- Skip unofficial sources (personal communications etc.)
- Skip **non-stoichiometric** compositions

ICDD XML Format

Ca₅ (P O₄)₃ (O H) - 01-084-1998

File Plots Help

Export Print Temperature Series Toolbox Property Sheet 2D 3D Bonds SAED EBSD Ring Simulated Profile Raw Diffraction Data

To Crystallographic Information File (*.cif)...
To Bruker TOPAS File (*.str)
To ICDD XML File (*.xml)

Electron Diffraction

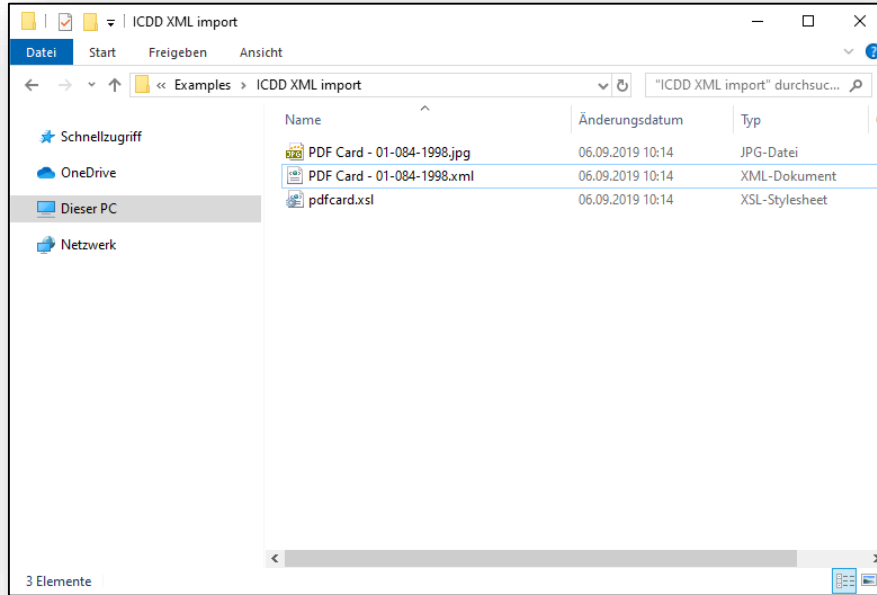
2θ (°)	d (Å)	I	h	k	l	*
10.83988	8.155010	140	1	0	0	
16.85400	5.256120	40	1	0	1	
18.83188	4.708300	21	1	1	0	
21.77829	4.077510	59	2	0	0	
22.87428	3.884560	57	1	1	1	
25.37579	3.507010	23	2	0	1	
25.89966	3.437250	348	0	0	2	
28.14070	3.167400	86	1	0	2	

Intensity

2θ (°)

PDF Status: Alternate Quality Mark: Indexed
Experimental Environment: Ambient Temperature: 298.0 K (Assigned by ICDD editor) Pressure: -
Physical Phase: -
Crystal Chemical Formula: Ca₅(P O₄)₃(O H)
Structure Structural Formula: -
Classifications Empirical Formula: Ca₅H O₁₃ P₃
Cross-references Weight %: Ca39.90 H0.20 O41.41 P18.50
Atomic %: Ca22.73 H4.55 O59.09 P13.64
References Compound Name: Calcium Phosphate Hydroxide
Comments Mineral Name: Hydroxylapatite | IMA No: -
Alternate Name: -
CAS Number: 1306-06-5
Entry Date: 09/01/1998
Modification Date: 09/01/2016 | Modifications: Quality

ICDD XML Format

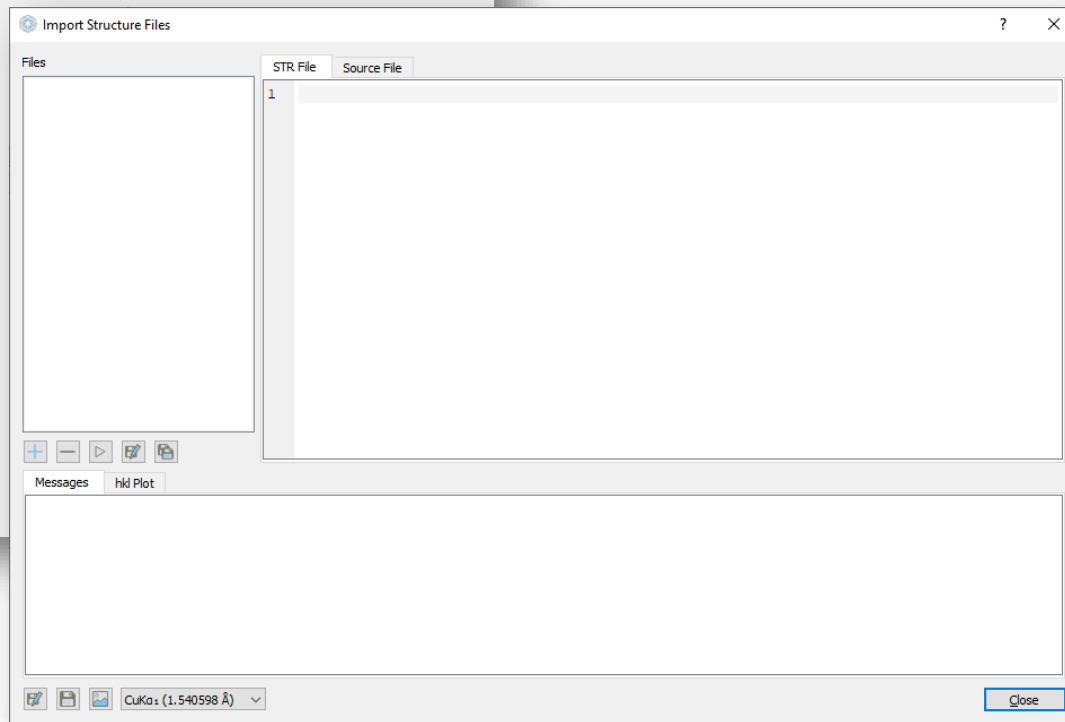
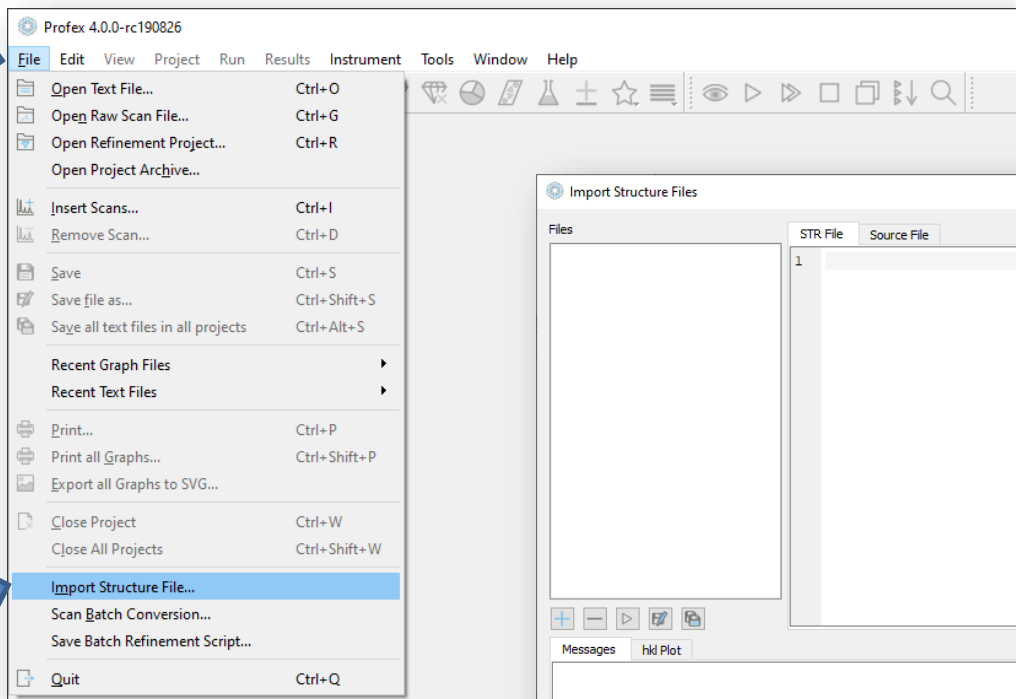


XML file can be viewed in Microsoft Edge →

PDF Card

PDF Number	01-084-1998	Status		Alternate		Quality Mark		Index	
Environment	Ambient								
Temperature	298.0								
Pressure									
Phase									
Chemical Formula	Ca ₅ (P O ₄) ₃ (OH)								
Structural Formula									
Empirical Formula	Ca ₅ H O ₁₃ P ₃								
Weight %	Ca39.90 H0.20 O41.41 P18.50								
Atomic %	Ca22.73 H4.55 O59.09 P13.64								
Compound Name	Calcium Phosphate Hydroxide								
Mineral Name	Hydroxylapatite								
IMA No.									
Alternate Name									
CAS Number	1306-06-5								
Entry Date	09/01/1998								
Modification Date	09/01/2016								
Modifications	Quality								
Experimental	Rad	λ	Filter	d-Spacing	Cutoff	Intensity	I/Ic		
	CuKα1	1.5406		Calculated		Calculated - Peak	1.05		
	I/Ic - ND	Camera Diameter	Internal Standard						
	0.22								
	SYS	Space Group	Aspect	Modulation Wave Vectors					

ICDD XML Format



The image shows two overlapping windows from a software application. The background window is titled "Import Structure Files" and has a "Files" section with a large empty list box. Below the list box is a toolbar with a "+" button, a "-" button, a play button, a refresh button, and a save button. A blue arrow labeled "1" points to the "+" button. Below the toolbar are "Messages" and "hkd Plot" tabs, and a large empty text area. At the bottom of this window, there is a "CuKα₁ (1.540598 Å)" dropdown menu and a "Close" button.

The foreground window is titled "Open crystal structure data files" and shows a file explorer view. The address bar indicates the current location is "Examples > ICDD XML import". The search bar contains the text "ICDD XML import" followed by "durchsuc...". The file list shows a single file:

Name	Änderungsdatum	Typ	Größe
PDF Card - 01-084-1998.xml	06.09.2019 10:14	XML-Dokument	26 KB

A blue arrow labeled "3" points to this file. At the bottom of the file explorer, the "Dateiname:" field is empty, and the file type dropdown is set to "ICDD XML Files (*.xml *.XML)". A blue arrow labeled "2" points to this dropdown. Below the dropdown are "Öffnen" and "Abbrechen" buttons.

Import Structure Files

Files

PDF Card - 01-084-1998.xml

STR File Source File

```

1 PHASE=Hydroxylapatite // 01-084-1998
2 Reference=01-084-1998 //
3 Formula=Ca5_(P_O4)_3_(O_H) //
4 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
5 PARAM=A=0.941660_0.932243^0.951077 PARAM=B=0.941660_0.932243^0.951077
  PARAM=C=0.687450_0.680575^0.694325 //
6 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
7 GOAL:Hydroxylapatite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
8 E=CA Wyckoff=f x=0.333330 y=0.666660 z=0.000700 TDS=0.000000
9 E=CA Wyckoff=h x=0.242600 y=0.990400 z=0.250000 TDS=0.000000
10 E=P Wyckoff=h x=0.394800 y=0.365700 z=0.250000 TDS=0.000000
11 E=O Wyckoff=h x=0.327000 y=0.484900 z=0.250000 TDS=0.000000
12 E=O Wyckoff=h x=0.579100 y=0.461800 z=0.250000 TDS=0.000000
13 E=O Wyckoff=i x=0.341700 y=0.257800 z=0.071100 TDS=0.000000
14 E=O(0.4650) Wyckoff=e x=0.000000 y=0.000000 z=0.183700 TDS=0.000000
15 E=H(0.0800) Wyckoff=e x=0.000000 y=0.000000 z=0.060800 TDS=0.000000
16

```

Messages hkl Plot

Intensity [%]

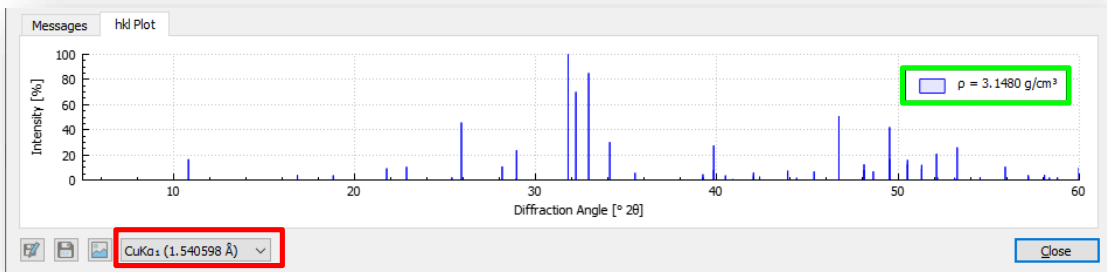
Diffraction Angle [° 2θ]

ρ = 3.1480 g/cm³

CuKα₁ (1.540598 Å)

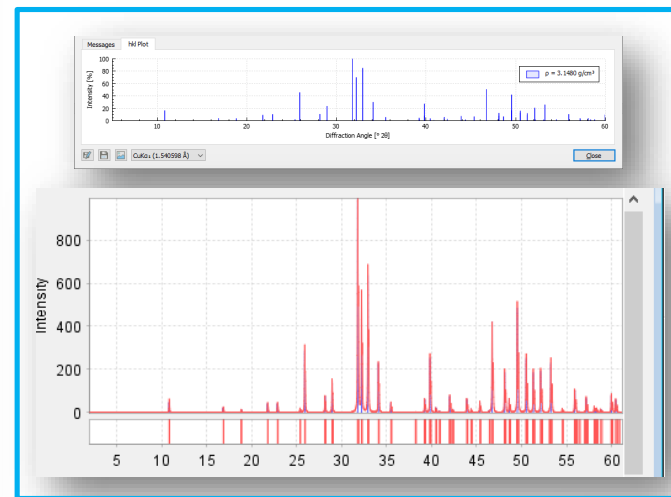
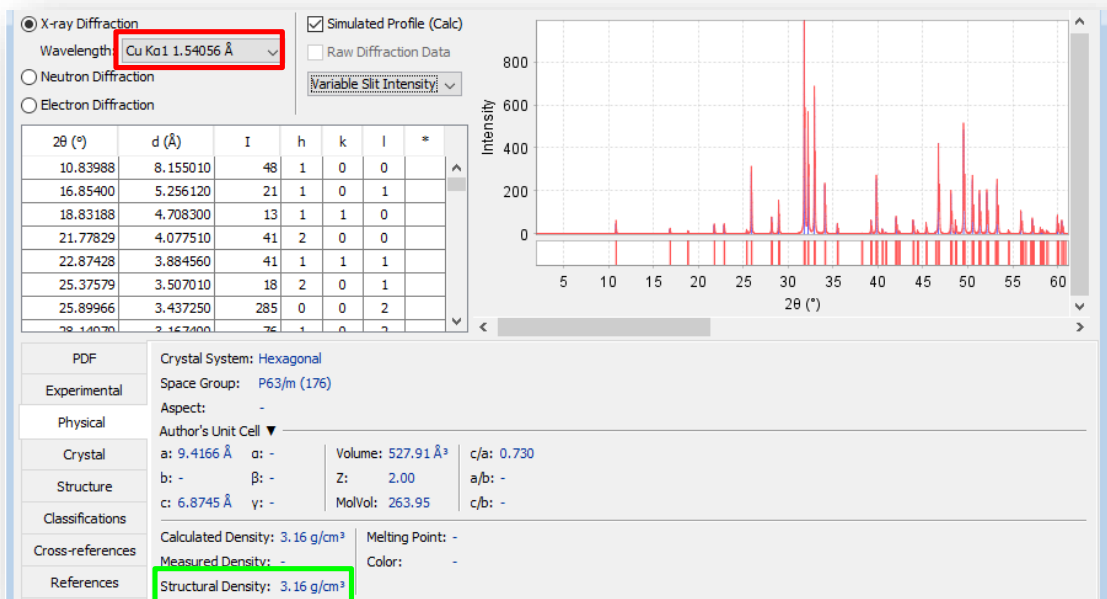
Close

ICDD XML Format



Quick check with PDF card

- Set to the same wavelength
- Check density
- Check hkl plot



The screenshot displays two overlapping windows from a software application. The background window is titled "Import Structure Files" and shows a list of files on the left, including "PDF Card - 01-084-1998.xml". The main area contains a text editor with the following content:

```
1 PHASE=Hydroxylapatite // 01-084-1998
2 Reference=01-084-1998 //
3 Formula=Ca5_(P_O4)_3_(O_H_) //
4 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
5 PARAM=A=0.941660_0.932243^0.95
6 PARAM=C=0.687450_0.680575^0.69
7 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.
8 GOAL:Hydroxylapatite=GEWICHT*i
9 E=CA Wyckoff=f x=0.333330 y=0.
10 E=CA Wyckoff=h x=0.242600 y=0.
11 E=P Wyckoff=h x=0.394800 y=0.3
12 E=O Wyckoff=h x=0.327000 y=0.4
13 E=O Wyckoff=h x=0.579100 y=0.4
14 E=O(0.4650) Wyckoff=e x=0.0000
15 E=H(0.0800) Wyckoff=e x=0.0000
16
```

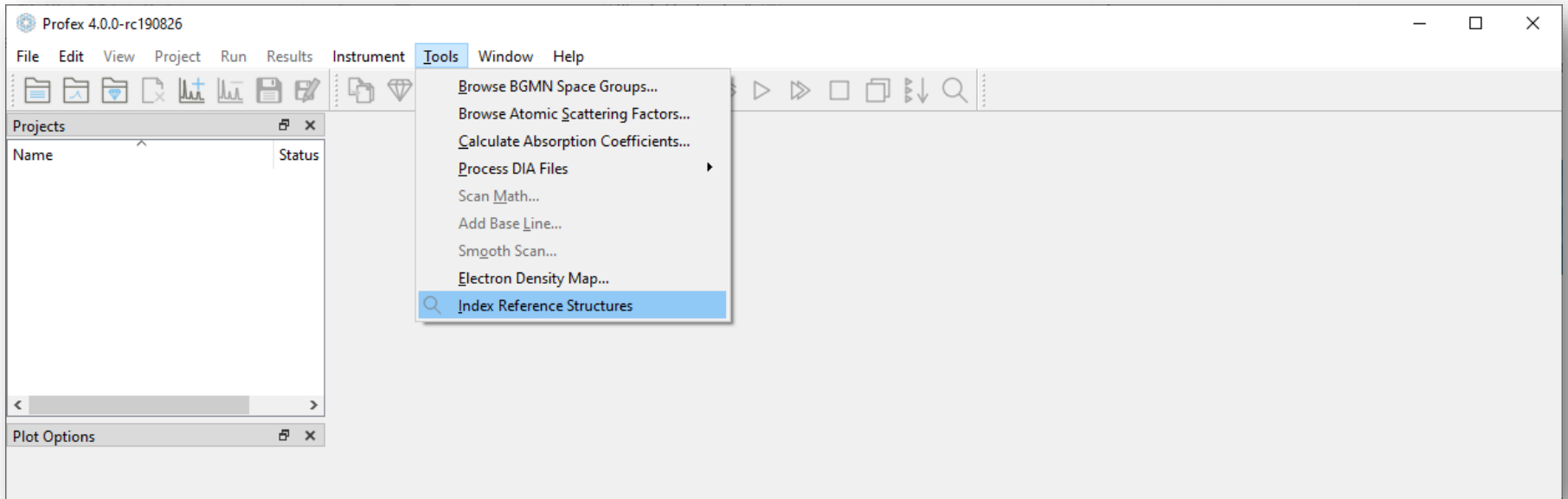
The foreground window is titled "Save STR File" and shows a file explorer view of a directory named "Phosphate". The file list includes:

Name	Änderungsdatum	Typ
AIPO4.str	29.08.2019 08:52	STR-Dat
AIPO4-1Hydrate.str	29.08.2019 08:52	STR-Dat
Apatite-Cl.str	29.08.2019 08:52	STR-Dat
Apatite-CO3-A.str	29.08.2019 08:52	STR-Dat
Apatite-CO3-B.str	29.08.2019 08:52	STR-Dat
Apatite-F.str	29.08.2019 08:52	STR-Dat
Apatite-F-Mn.str	29.08.2019 08:52	STR-Dat
Apatite-F-Sr.str	29.08.2019 08:52	STR-Dat
Apatite-O.str	29.08.2019 08:52	STR-Dat

The "Save STR File" dialog shows the filename "Apatite-OH-Workshop.str" and the file type "BGMN Structure Files (*.str *.STR)". A blue arrow points to the save icon in the "Import Structure Files" window.

Save in Profex STR-file repository

In Profex main window: Index the new reference structure



Structure Import

Profex 4.0.0-rc190826

File Edit View Project Run Results Instrument Tools Window Help

180131-06.raw 180131-06.sav 180131-06.lst

D18_0001 01-00-00c 180131-06.raw

Intensity [counts]

5000
4000
3000
2000
1000
0

5.00 45.00 50.00 55.00 60.00

Plot Options

Scan	Scaling	Vertical
<input checked="" type="checkbox"/> D18_0001 01-00-00c	1.00	0.00

Refinement Protocol

Refined Parameters

Parameter	Value	ESD
> Statistics		
> Global GOALS		
QHydroxyapatite	1.0000	
> Local GOALS		

C:\xrd\S19_0007\Profex-first-start\180131-06.raw

1 Project $\lambda = 1.5406 \text{ \AA}$ $2\theta = 0.000^\circ$ $I = 0.000 \text{ cts}$ $d = 0.000 \text{ \AA}$

Free structure databases

Crystallography Open Database (COD)

<http://www.crystallography.net>

American Mineralogist Structure Database

<http://rruff.geo.arizona.edu/AMS/amcsd.php>

American Mineralogist Crystal Structure Database

This site is an interface to a crystal structure database that includes every structure published in the American Mineralogist, The Canadian Mineralogist, European Journal of Mineralogy and Physics and Chemistry of Minerals, as well as selected datasets from other journals. The database is maintained under the care of the Mineralogical Society of America and the Mineralogical Association of Canada, and financed by the National Science Foundation.

<input type="text" value="apatite"/>	Mineral
<input type="text" value="hughes"/>	Author
<input type="text"/>	Chemistry Search
<input type="text"/>	Cell Parameters and Symmetry
<input type="text"/>	Diffraction Search
<input type="text"/>	General Search
	Search Tips

Logic interface AND OR

Viewing (About [File Formats](#)) amc long form amc short form cf

Download amc cf diffraction data

Crystallography Open Database

COD Home
[Home](#)
[What's new?](#)

Accessing COD Data
[Browse](#)
[Search](#)
[Search by structural formula](#)

Add Your Data
[Deposit your data](#)
[Manage depositions](#)
[Manage/release prepublications](#)

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[COD Wiki](#)
[Obtaining COD](#)
[Querying COD](#)
[Citing COD](#)
[COD Mirrors](#)
[Advice to donors](#)
[Useful links](#)

Search

(For more information on search see the [hints and tips](#))

Search by COD ID:


[OpenBabel FastSearch:](#) Enter [SMILES:](#)


Note: substructure search by SMILES is currently available in a subset of COD containing 180100 structures.

text (1 or 2 words)	<input style="width: 100px;" type="text" value="apatite"/>
journal	<input style="width: 100px;" type="text"/>
year	<input style="width: 100px;" type="text"/>
volume	<input style="width: 100px;" type="text"/>
issue	<input style="width: 100px;" type="text"/>
DOI	<input style="width: 100px;" type="text"/>
Z (min, max)	<input style="width: 50px;" type="text"/> <input style="width: 50px;" type="text"/>
Z' (min, max)	<input style="width: 50px;" type="text"/> <input style="width: 50px;" type="text"/>
chemical formula (in Hill notation)	<input style="width: 100px;" type="text"/>
1 to 8 elements	Ca <input style="width: 20px;" type="text"/> P <input style="width: 20px;" type="text"/> O <input style="width: 20px;" type="text"/> H <input style="width: 20px;" type="text"/>
NOT these elements	<input style="width: 100px;" type="text"/>
volume min and max	<input style="width: 50px;" type="text"/> <input style="width: 50px;" type="text"/>
number of distinct elements min and max	<input style="width: 20px;" type="text"/> <input style="width: 20px;" type="text" value="4"/>
filters	<input type="checkbox"/> has F _{obs} <input type="checkbox"/> include duplicate entries <input type="checkbox"/> include entries with errors <input type="checkbox"/> include theoretical structures

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
9001233	CIF	Ca ₅ H O ₁₃ P ₃	P 63/m	9.4166; 9.4166; 6.8745 90; 90; 120	527.91	Hughes J M; Cameron M; Crowley K D Structural variations in natural F, OH, and Cl apatites Locality: Holly Springs, Georgia, USA American Mineralogist , 1989 , 74 , 870-876

Apatite-(CaOH)

 Hughes J M, Cameron M, Crowley K D

 [American Mineralogist 74 \(1989\) 870-876](#)

Structural variations in natural F, OH, and Cl apatites
Locality: Holly Springs, Georgia, USA

_database_code_amcsd 0001260

9.4166 9.4166 6.8745 90 90 120 P6_3/m

atom	x	y	z	occ	Biso	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
Ca1	2/3	1/3	.00144			.00408	.00408	0.0033	.00204	0	0
Ca2	-.00657	.24706	.25			.00308	.00353	.00417	.00156	0	0
P	.36860	.39866	.25			.00223	.00250	.00034	.00127	0	0
O1	.4850	.3289	.25			0.0036	0.0044	0.0059	.0027	0	0
O2	.4649	.5871	.25			0.0035	0.0031	0.0105	.0016	0	0
O3	.2580	.3435	.0703			0.0050	0.0096	0.0070	.00505	-.0025	-.0041
O(H)	0	0	.1979	.5		0.0030	0.0030	0.012	.0015	0	0
H	0	0	.04	.5	3.3						

[Download AMC data \(View Text File\)](#)

[Download CIF data \(View Text File\)](#)

[Download diffraction data \(View Text File\)](#)

[View JMOL 3-D Structure \(permalink\)](#)

Saved in «Examples → CIF Import»

The image shows a software interface for importing crystal structure files. The main window, titled "Import Structure Files", has a "Files" pane on the left containing "PDF Card - 01-084-1998.xml". The main area displays a "STR File" with the following content:

```
1 PHASE=Hydroxylapatite // 01-084-1998
2 Reference=01-084-1998 //
3 Formula=Ca5_(P_O4)_3_(O_H_) //
4 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
5 PARAM=A=0.941660_0.9
  PARAM=C=0.687450_0.6
6 RP=4 k1=0 k2=0 PARAM
7 GOAL:Hydroxylapatite
8 E=CA Wyckoff=f x=0.3
9 E=CA Wyckoff=h x=0.2
10 E=P Wyckoff=h x=0.39
11 E=O Wyckoff=h x=0.32
12 E=O Wyckoff=h x=0.57
13 E=O Wyckoff=i x=0.4
14 E=O(0.4650) Wyck
15 E=H(0.0800)
16
```

An "Open crystal structure data files" dialog is overlaid on the main window. It shows a file explorer view of "Examples > CIF Import" with the following table:

Name	Änderungsdatum	Typ	Größe
9001233-COD.cif	06.09.2019 10:56	CIF-Datei	3 KB
Apatite-OH-Hughes-AMS.cif	06.09.2019 10:56	CIF-Datei	2 KB

Three blue arrows indicate the workflow: Arrow 1 points to the "+" button in the "Files" pane; Arrow 2 points to the "Öffnen" button in the file dialog; Arrow 3 points to the "Apatite-OH-Hughes-AMS.cif" file in the file dialog.

Files

- PDF Card - 01-084-1998.xml
- *9001233-COD.cif
- *Apatite-OH-Hughes-AMS.cif

STR File

```

1 PHASE=Hydroxylapatite //
2 Formula=Ca5_H_O13_P3 //
3 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
4 PARAM=A=0.941660_0.932243^0.951077 PARAM=B=0.941660_0.932243^0.951077
  PARAM=C=0.687450_0.680575^0.694325 //
5 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
6 GOAL:Hydroxylapatite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
7 *E=CA Wyckoff= x=0.666670 y=0.333330 z=0.001440 TDS=0.009319
8 *E=CA Wyckoff= x=0.993430 y=0.247060 z=0.250000 TDS=0.008596
9 *E=P Wyckoff= x=0.368600 y=0.398660 z=0.250000 TDS=0.006231
10 *E=O Wyckoff= x=0.485000 y=0.328900 z=0.250000 TDS=0.009983
11 *E=O Wyckoff= x=0.464900 y=0.587100 z=0.250000 TDS=0.012526
12 *E=O Wyckoff= x=0.258000 y=0.343500 z=0.070300 TDS=0.015704
13 *E=O(0.5000) Wyckoff= x=0.000000 y=0.000000 z=0.197900 TDS=0.012885
14 *E=H(0.5000) Wyckoff= x=0.000000 y=0.000000 z=0.040000 TDS=0.032996
  
```

Messages | hkl Plot

```

Line 7 (CA): No Wyckoff symbol found
Line 8 (CA): No Wyckoff symbol found
Line 9 (P): No Wyckoff symbol found
Line 10 (O): No Wyckoff symbol found
Line 11 (O): No Wyckoff symbol found
Line 12 (O): No Wyckoff symbol found
Line 13 (O): No Wyckoff symbol found
Line 14 (H): No Wyckoff symbol found
  
```

Annotations:

- Errors highlighted
- * = verification failed
- Error Messages

Footer: CuKα₁ (1.540598 Å) | Close

CIF Import – Wyckoff Symbols

Profex 4.0.0-rc190826

File Edit View Project Run Results Instrument Tools Window Help

Projects

Name	Status

Tools menu:

- Browse BGMN Space Groups...
- Browse Atomic Scattering Factors...
- Calculate Absorption Coefficients...
- Process DIA Files
- Scan Math...
- Add Base Line...

Space Group Settings

Spacegroup Number	Hermann Mauguin	Wyckoff	Symmetry
170	P6_3/m	i (N=12)	0 0 1/4
171		h (N=6)	0 0 3/4
172		g (N=6)	
173		f (N=4)	
174		e (N=4)	
175		d (N=2)	
176		c (N=2)	
177		b (N=2)	
178		a (N=2)	
179			
180			
181			
182			

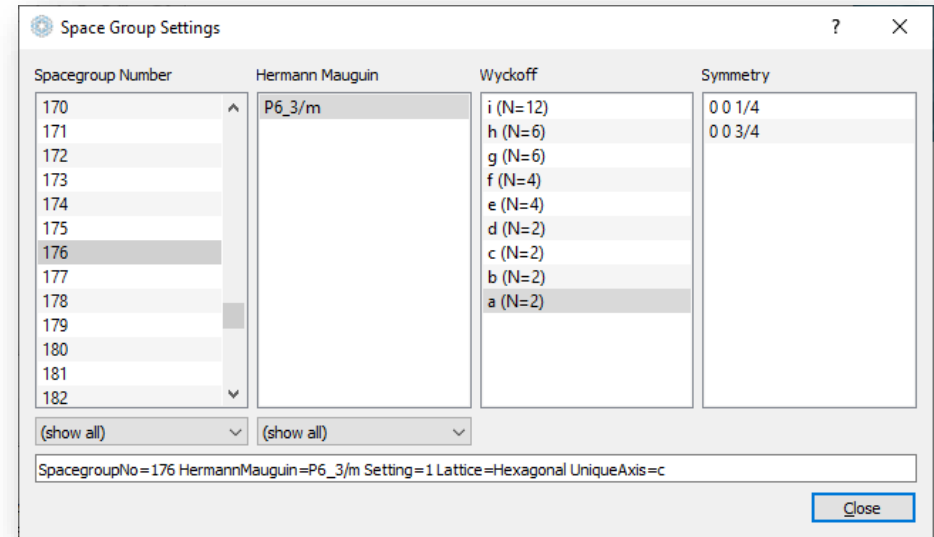
(show all) (show all)

SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 Lattice=Hexagonal UniqueAxis=c

Close

Identifying the Wyckoff symbol:

- ▶ Try to identify special coordinates
 - ▶ Special = 0.0, $\frac{1}{2}$, $\frac{1}{3}$, $\frac{1}{4}$, $\frac{1}{8}$, $\frac{2}{3}$, $\frac{3}{8}$, $\frac{5}{8}$, $\frac{7}{8}$
 - ▶ General coordinates («non-special») = x, y, z
- ▶ Write coordinate in abstract form
- ▶ Search matching Wyckoff Symbol in Profex dialog



```
E=CA Wyckoff= x=0.666670 y=0.333330 z=0.001440 TDS=0.009319
E=CA Wyckoff= x=0.993430 y=0.247060 z=0.250000 TDS=0.008596
E=P Wyckoff= x=0.368600 y=0.398660 z=0.250000 TDS=0.006231
E=O Wyckoff= x=0.485000 y=0.328900 z=0.250000 TDS=0.009983
E=O Wyckoff= x=0.464900 y=0.587100 z=0.250000 TDS=0.012526
E=O Wyckoff= x=0.258000 y=0.343500 z=0.070300 TDS=0.015704
E=O(0.5000) Wyckoff= x=0.000000 y=0.000000 z=0.197900 TDS=0.012885
E=H(0.5000) Wyckoff= x=0.000000 y=0.000000 z=0.040000 TDS=0.032996
```

CIF Import – Wyckoff Symbols

Import Structure Files

Files

- PDF Card - 01-084-1998.xml
- *9001233-COD.cif
- *Apatite-OH-Hughes-AMS.cif

STR File Source File

```
1 PHASE=Hydroxylapatite //
2 Formula=Ca5_H_O13_P3 //
3 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
4 PARAM=A=0.941660_0.932243^0.951077 PARAM=B=0.941660_0.932243^0.951077
PARAM=C=0.687450_0.680575^0.694325 //
5 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
6 GOAL:Hydroxylapatite=GEWICHT*ifthenelse (ifdef(d), exp(my*d*3/4), 1) //
7 E=CA Wyckoff= x=0.666670 y=0.333330 z=0.001440 TDS=0.009319
8 E=CA Wyckoff= x=0.993430 y=0.247060 z=0.250000 TDS=0.008596
9 E=P Wyckoff= x=0.368600 y=0.398660 z=0.250000 TDS=0.006231
10 E=O Wyckoff= x=0.485000 y=0.328900 z=0.250000 TDS=0.009983
11 E=O Wyckoff= x=0.464900 y=0.587100 z=0.250000 TDS=0.012526
12 E=O Wyckoff= x=0.258000 y=0.343500 z=0.070300 TDS=0.015704
13 E=O(0.5000) Wyckoff= x=0.000000 y=0.000000 z=0.197900 TDS=0.012885
14 E=H(0.5000) Wyckoff= x=0.000000 y=0.000000 z=0.040000 TDS=0.032996
```

Messages hkl Plot

Run verification

Messages hkl Plot

Line 7 (CA): Coordinates 0.666670 0.333330 0.001440 do not match first Wyckoff symmetry for f (1/3 2/3 z).

Line 8 (CA): The following coordinates are redundant, consider removing: z

Line 9 (P): The following coordinates are redundant, consider removing: z

Line 10 (O): The following coordinates are redundant, consider removing: z

Line 11 (O): The following coordinates are redundant, consider removing: z

Line 13 (O): The following coordinates are redundant, consider removing: x y

Line 14 (H): The following coordinates are redundant, consider removing: x y

CuKα₁ (1.540598 Å)

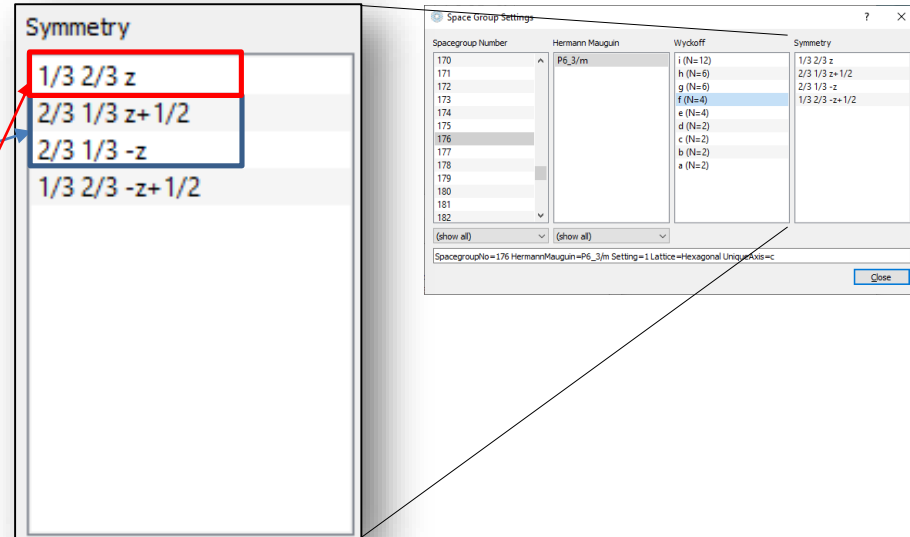
Close

Coordinates:

$x=0.666670$ $y=0.333330$ $z=0.001440$
=
 $2/3$ $1/3$ «general»

Error message:

Line 7 (CA): Coordinates 0.666670
0.333330 0.001440 do not match **first**
Wyckoff symmetry for f ($1/3$ $2/3$ z).



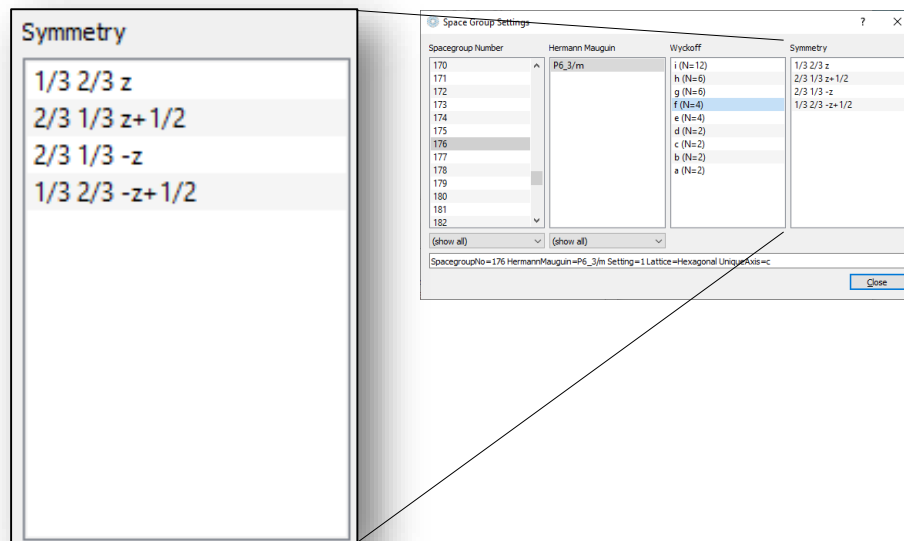
Manually convert coordinates to first symmetry description if necessary

CIF Import – Wyckoff Symbol

Coordinates:

$x=0.666670$ $y=0.333330$ $z=0.001440$

- Set x to $1/3$ (or 0.3333)
- Set y to $2/3$ (or 0.6667)
- Two options for z :
 - Subtract $1/2$
 - Invert the sign



$x=0.666670$
 $y=0.333330$
 $z=0.001440$

$z = z - 1/2$

$x=0.333333$
 $y=0.666667$
 $z=-0.49856$

$z = z + 1$

$x=0.333333$
 $y=0.666667$
 $z=0.501440$

Optional:
 Add +1 to negative
 coordinates

$z = -z$

$x=0.333333$
 $y=0.666667$
 $z=-0.001440$

$z = z + 1$

$x=0.333333$
 $y=0.666667$
 $z=0.998560$

Import Structure Files
? X

Files

PDF Card - 01-084-1998.xml

9001233-COD.cif

*Apatite-OH-Hughes-AMS.cif

STR File
Source File

```

1 PHASE=Hydroxylapatite //
2 Formula=Ca5_H_O13_P3 //
3 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
4 PARAM=A=0.941660_0.932243^0.951077 PARAM=B=0.941660_0.932243^0.951077
PARAM=C=0.687450_0.680575^0.694325 //
5 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
6 GOAL:Hydroxylapatite=GEWICHT*ifthenelse(ifdef(d),exp(my*d*3/4),1) //
7 E=Ca Wyckoff=f x=0.333333 y=0.666667 z=0.9985600 TDS=0.009319
8 E=CA Wyckoff=h x=0.993430 y=0.247060 z=0.250000 TDS=0.008596
9 E=P Wyckoff=h x=0.368600 y=0.398660 z=0.250000 TDS=0.006231
10 E=O Wyckoff=h x=0.485000 y=0.328900 z=0.250000 TDS=0.009983
11 E=O Wyckoff=h x=0.464900 y=0.587100 z=0.250000 TDS=0.012526
12 E=O Wyckoff=i x=0.258000 y=0.343500 z=0.070300 TDS=0.015704
13 E=O(0.5000) Wyckoff=e x=0.000000 y=0.000000 z=0.197900 TDS=0.012885
14 E=H(0.5000) Wyckoff=e x=0.000000 y=0.000000 z=0.040000 TDS=0.032996
                    
```

+ - > ↺ ↻

Messages
hkl Plot

Diffraction Angle [° 2θ]

CuKα₁ (1.540598 Å) ▾
Close

Import Structure Files

Files

- PDF Card - 01-084-1998.xml
- 9001233-COD.cif
- Apatite-OH-Hughes-AMS.cif

STR File | Source File

```


1 PHASE=Hydroxylapatite //
2 Formula=Ca5_H_O13_P3 //
3 SpacegroupNo=176 HermannMauguin=P6_3/m Setting=1 UniqueAxis=c Lattice=Hexagonal //
4 PARAM=A=0.941660_0.932243^0.951077 PARAM=B=0.941660_0.932243^0.951077
  PARAM=C=0.687450_0.680575^0.694325 //
5 RP=4 k1=0 k2=0 PARAM=B1=0_0^0.01 GEWICHT=SPHAR4 //
6 GOAL:Hydroxylapatite=GEWICHT*ifthenelse (ifdef (d),exp(my*d*3/4),1) //
7 E=CA Wyckoff=f x=0.333333 y=0.666667 z=0.9985600 TDS=0.009319
8 E=CA Wyckoff=h x=0.993430 y=0.247060 z=0.250000 TDS=0.008596
9 E=P Wyckoff=h x=0.368600 y=0.398660 z=0.250000 TDS=0.006231
10 E=O Wyckoff=h x=0.485000 y=0.328900 z=0.250000 TDS=0.009983
11 E=O Wyckoff=h x=0.464900 y=0.587100 z=0.250000 TDS=0.012526
12 E=O Wyckoff=i x=0.258000 y=0.343500 z=0.070300 TDS=0.015704
13 E=O(0.5000) Wyckoff=e x=0.000000 y=0.000000 z=0.197900 TDS=0.012885
14 E=H(0.5000) Wyckoff=e x=0.000000 y=0.000000 z=0.040000 TDS=0.032996

```

Messages | hkl Plot

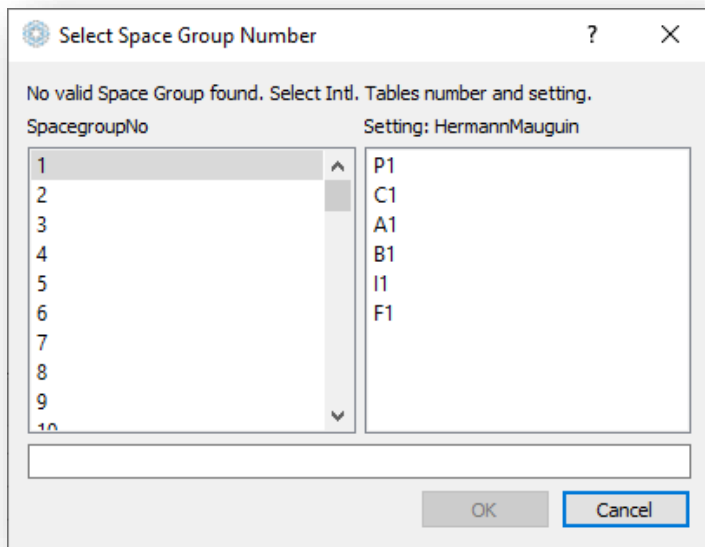
Line 7 (CA): The following coordinates are redundant, consider removing: x y
 Line 8 (CA): The following coordinates are redundant, consider removing: z
 Line 9 (P): The following coordinates are redundant, consider removing: z
 Line 10 (O): The following coordinates are redundant, consider removing: z
 Line 11 (O): The following coordinates are redundant, consider removing: z
 Line 13 (O): The following coordinates are redundant, consider removing: x y
 Line 14 (H): The following coordinates are redundant, consider removing: x y
 Verification successful

CuKα: (1.540598 Å) Close

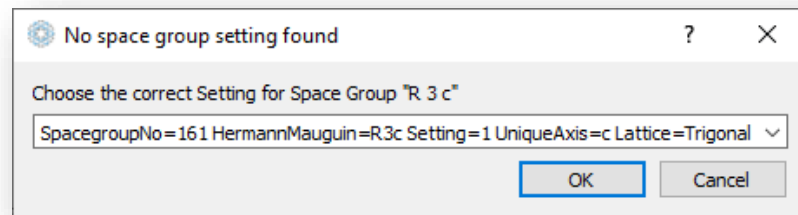


Warnings

Dialogs asking for information missing in the CIF file



Space group number (from intl. Tables) missing



Ambiguous Hermann-Mauguin symbol
(ambiguous short notation)

Other issues in CIF files causing warnings:

- No or illegal values for TDS (or TDS = 0.0)
- Illegal element symbols (e.g. «W» of water oxygens)