RMS

Testing · Research · Consulting

BGMN/Profex User Meeting 2019

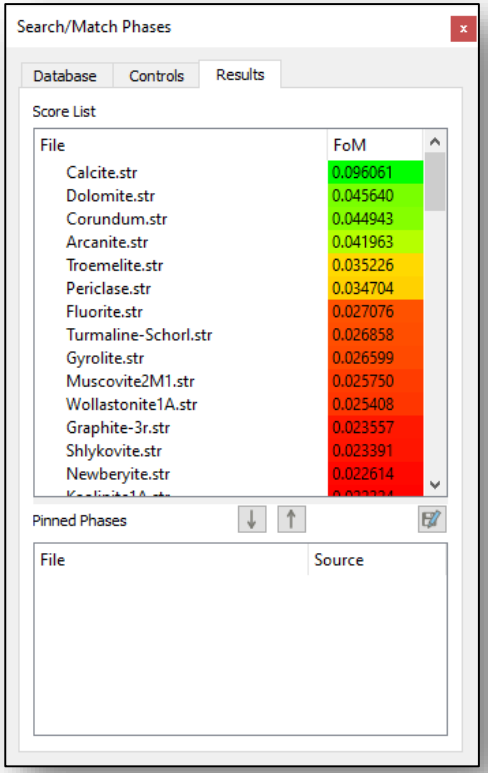
Importing CIF files in Profex

Nicola Döbelin

RMS Foundation, Bettlach, Switzerland

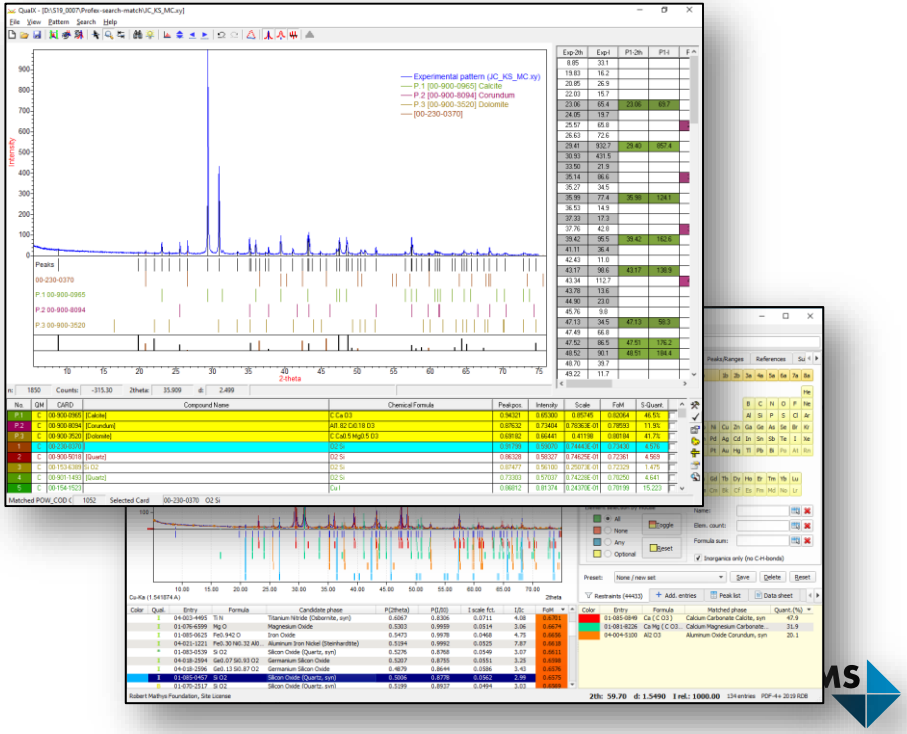
Search / Match Results

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



External Software search COD or PDF databases

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



Importing Crystal Structure Files

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 XML Format

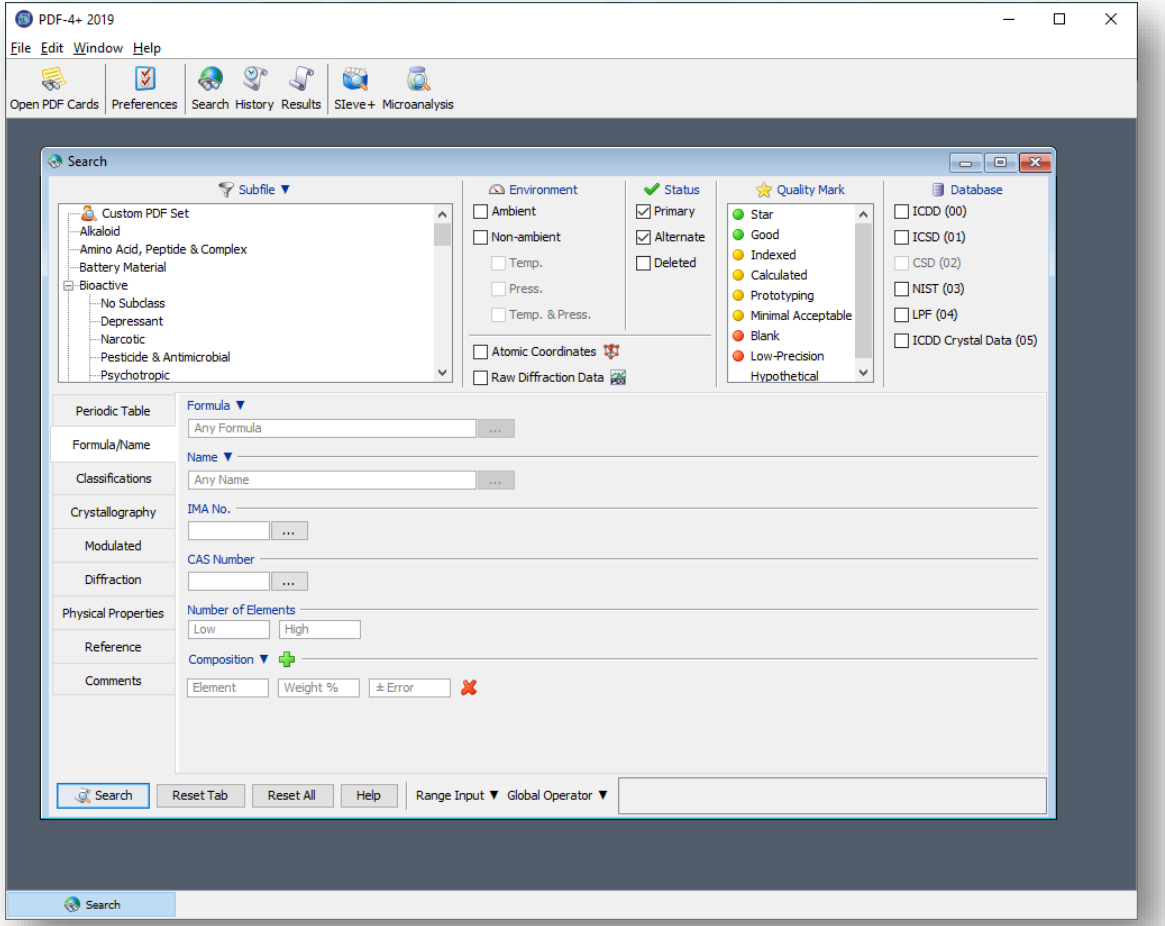
ICDD PDF-4+

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

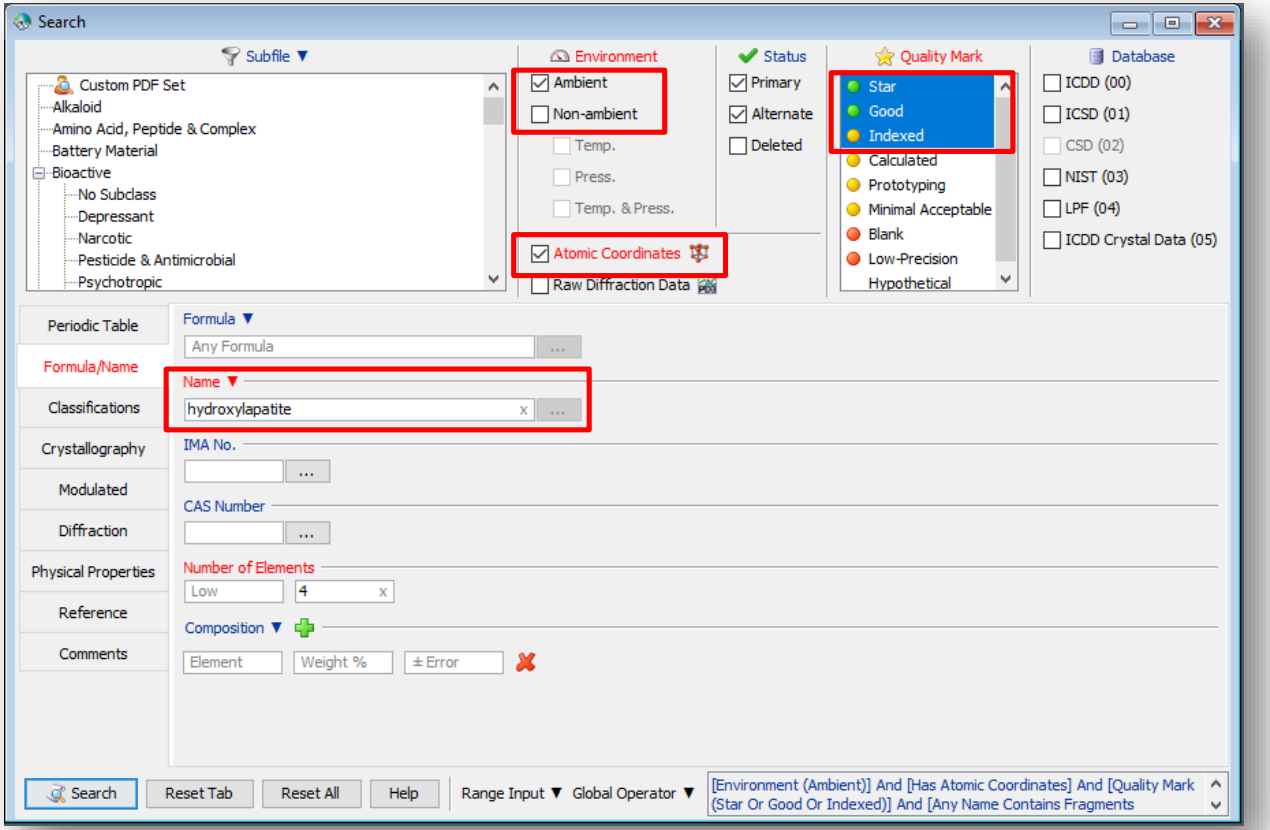
Recommendation

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

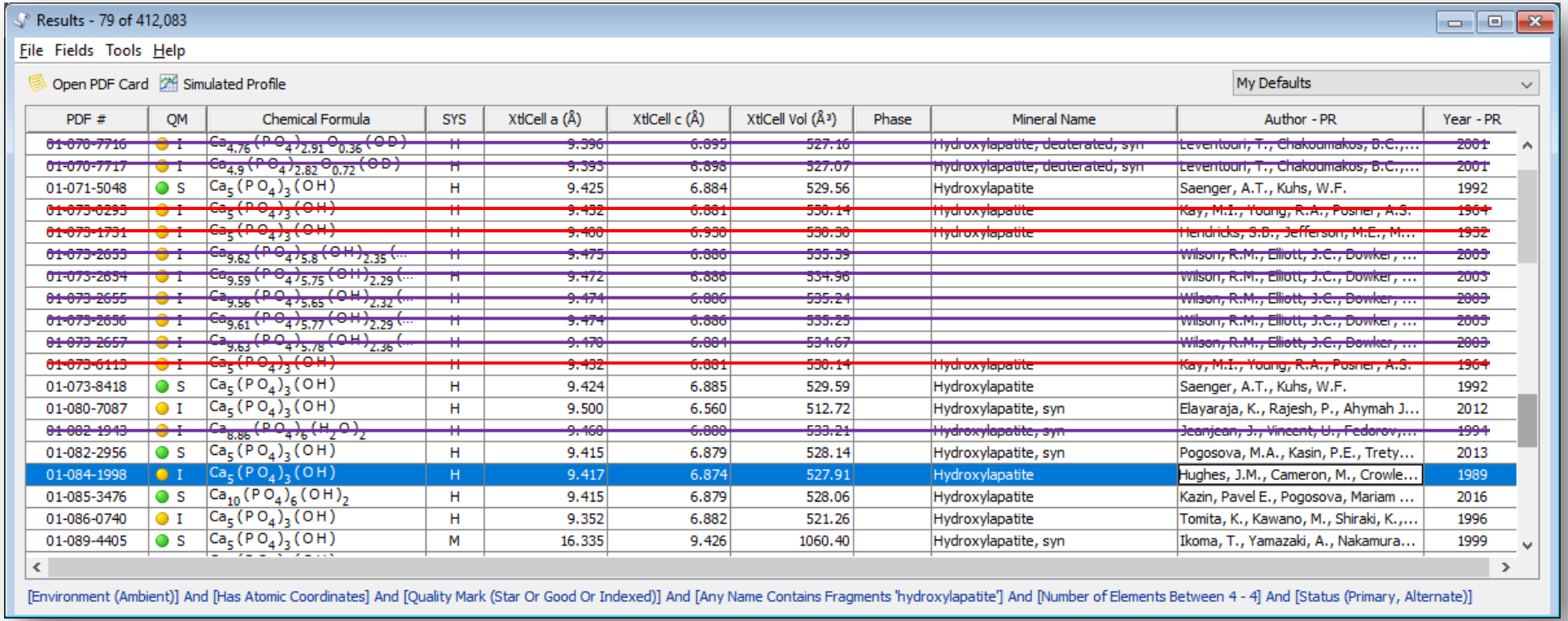


Search parameters:

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

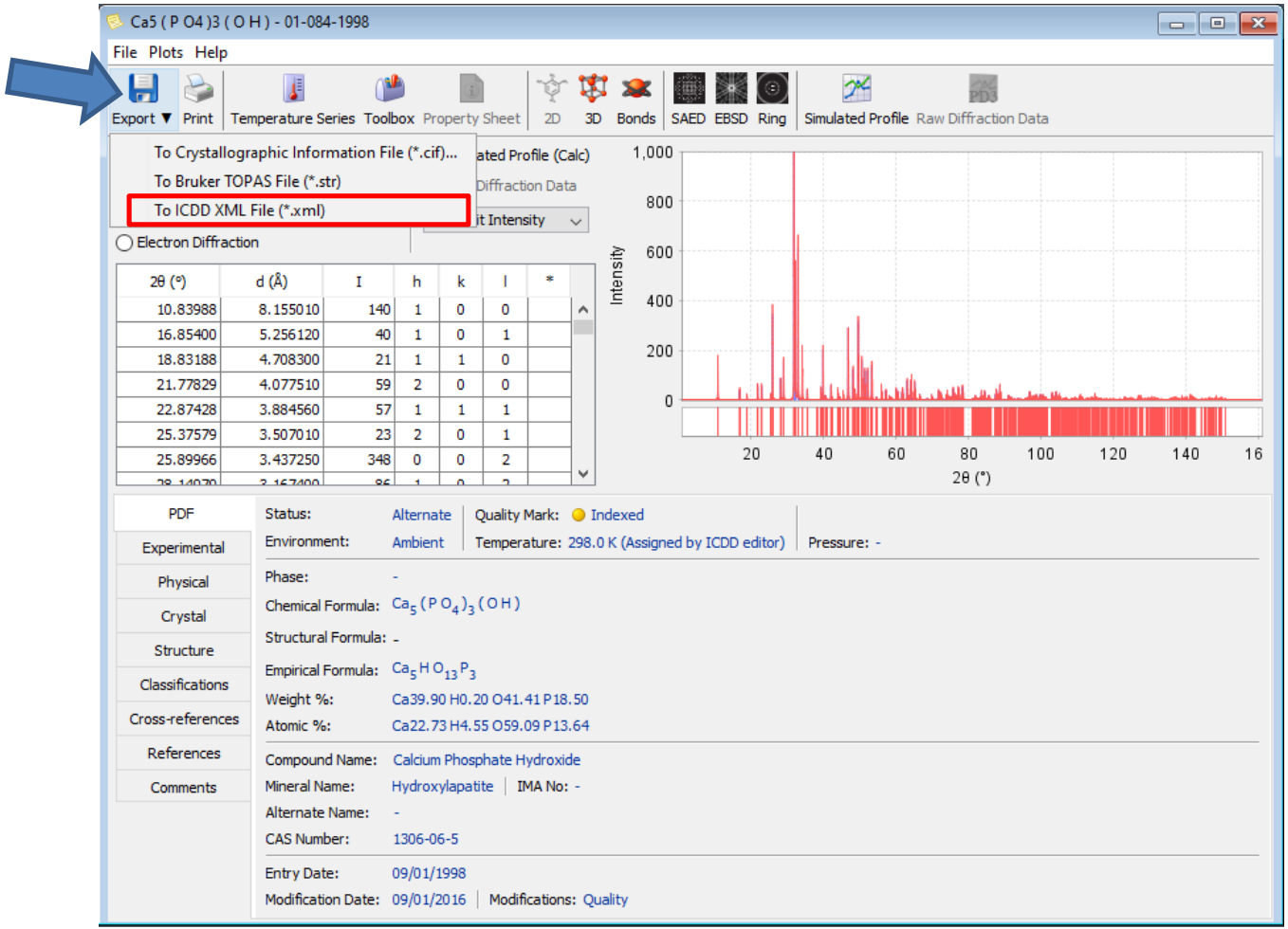
ICDD XML Format



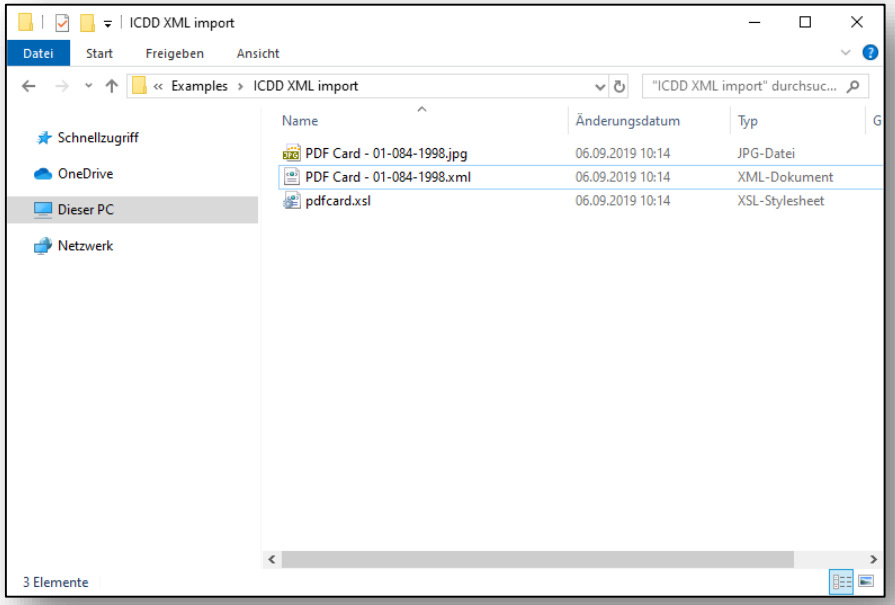
Personnal preference:

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

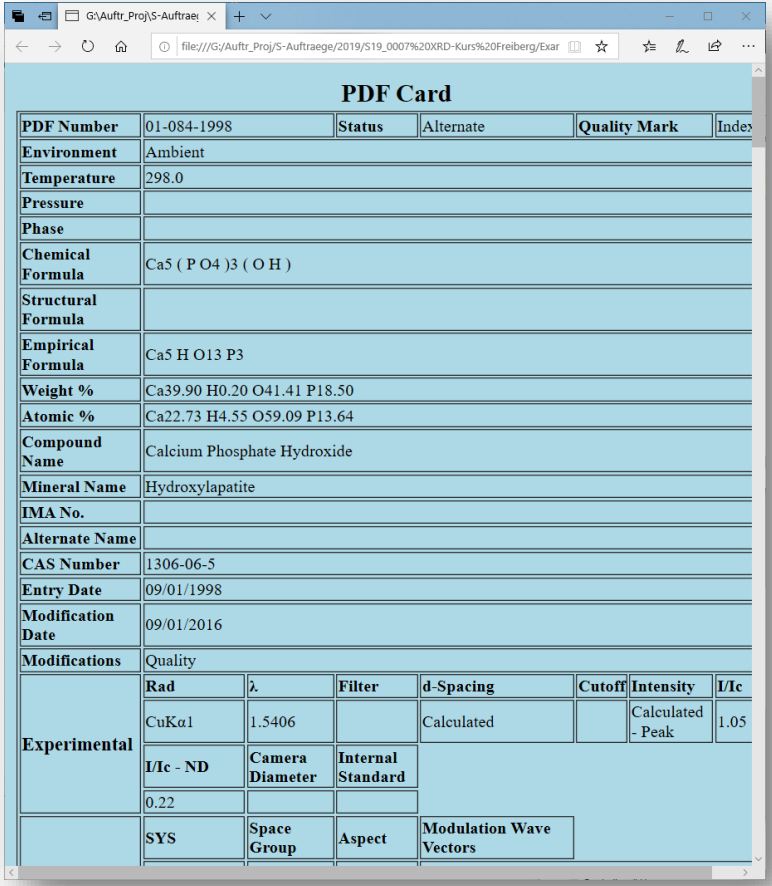
ICDD XML Format



ICDD XML Format



XML file can be viewed in Microsoft Edge →

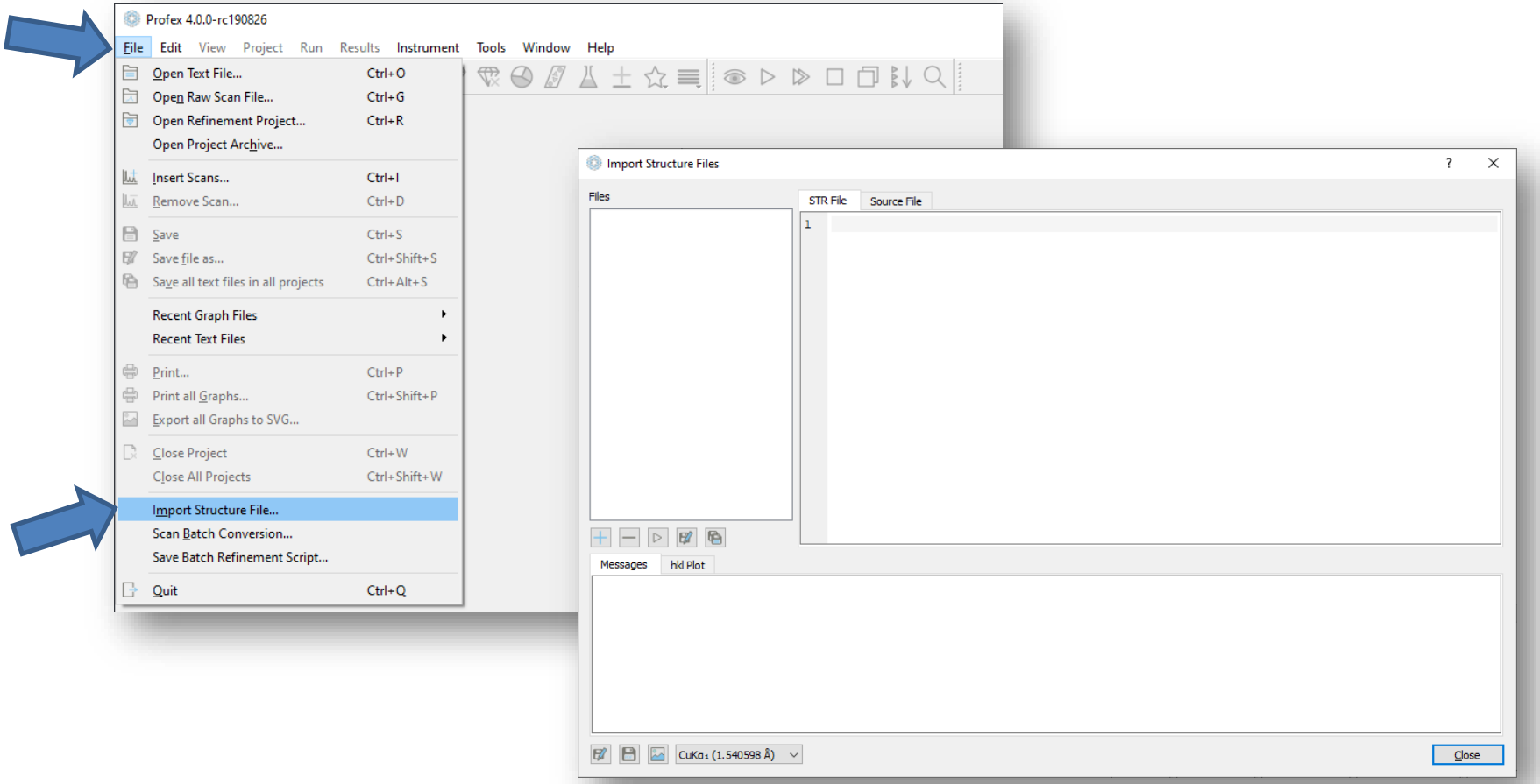


PDF Card

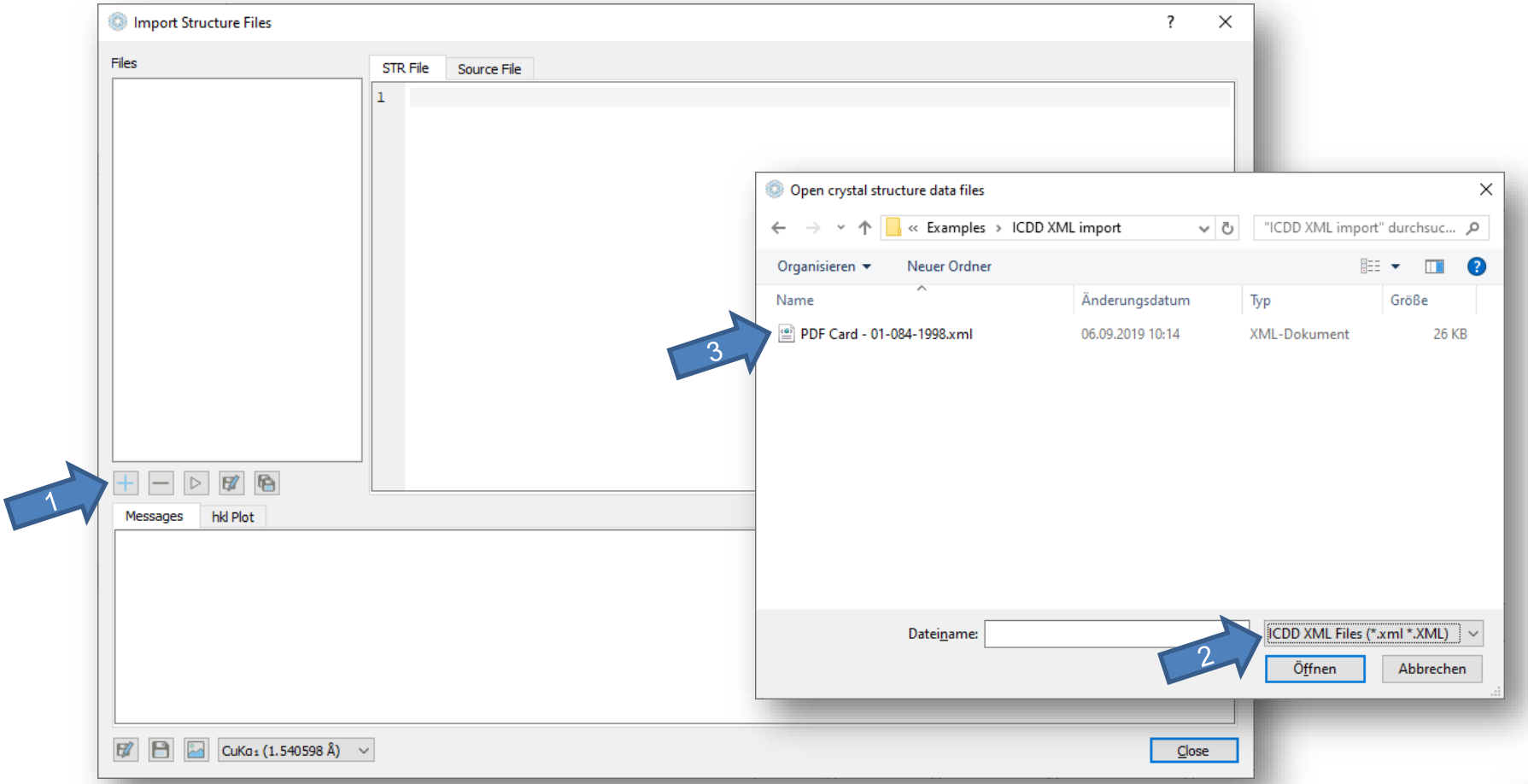
PDF Number	01-084-1998	**Status**	Alternate	**Quality Mark**	Index
Environment	Ambient				
Temperature	298.0				
Pressure					
Phase					
Chemical Formula	Ca5 (P O4)3 (O H)				
Structural Formula					
Empirical Formula	Ca5 H O13 P3				
Weight %	Ca39.90 H0.20 O41.41 P18.50				
Atomic %	Ca22.73 H4.55 O59.09 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**			

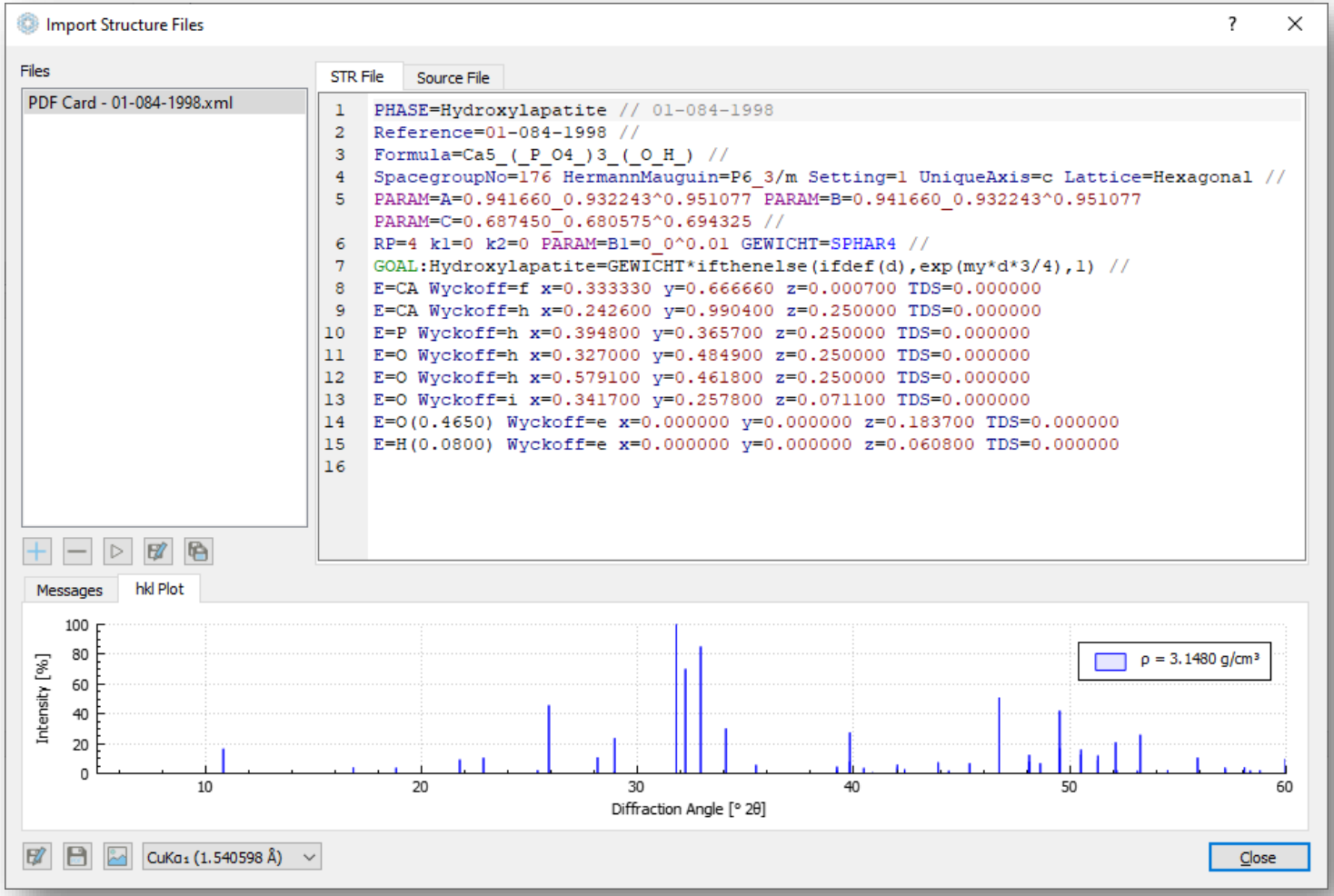
ICDD XML Format



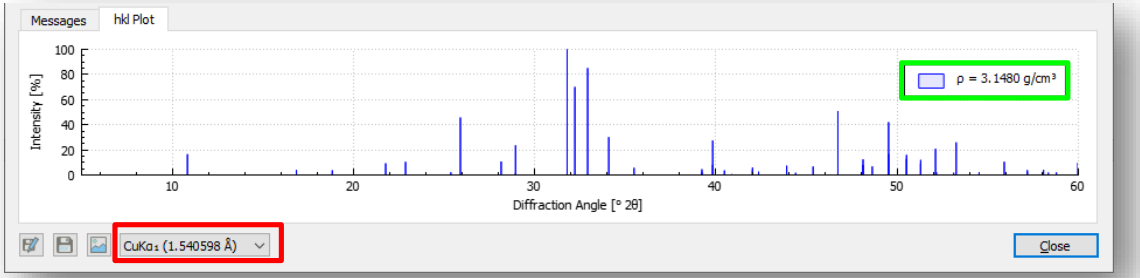
ICDD XML Format



ICDD XML Format

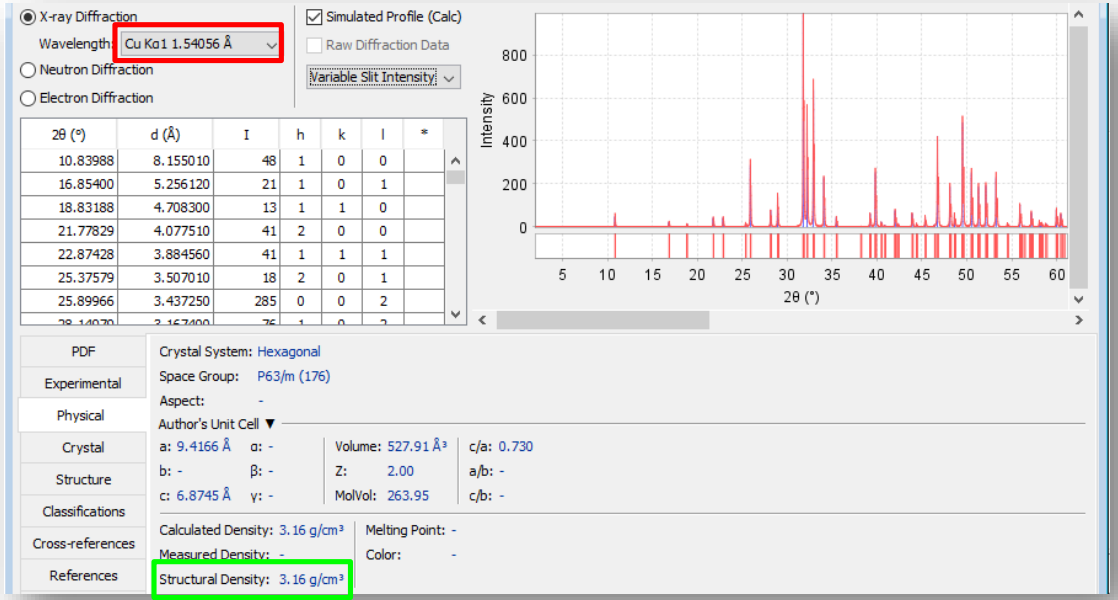


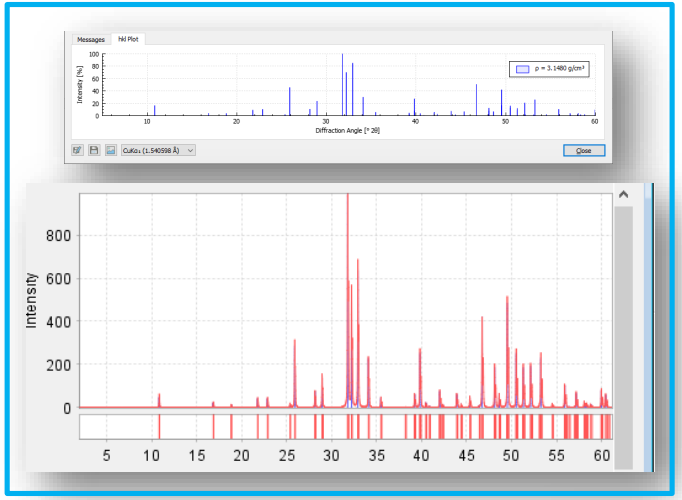
ICDD XML Format



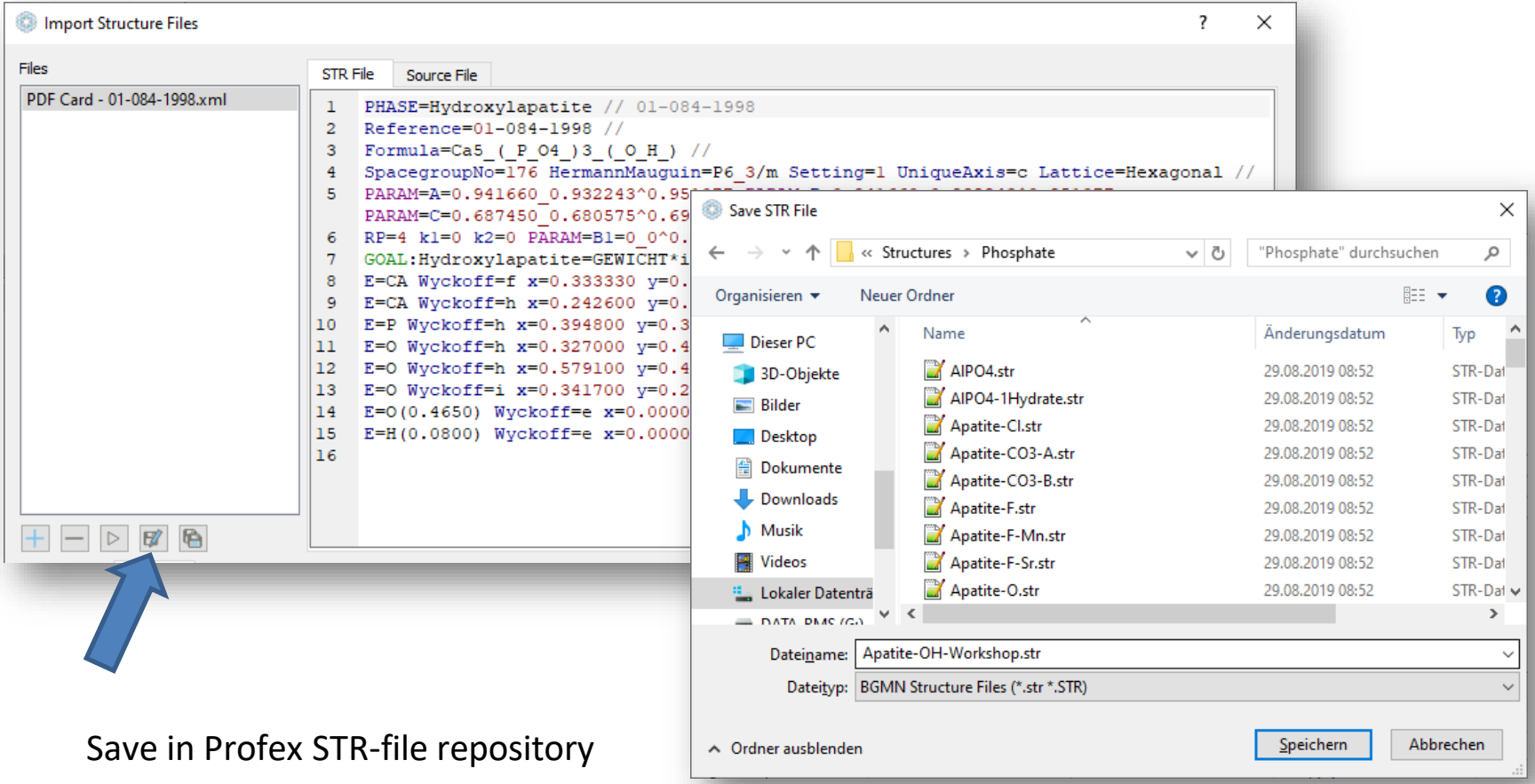
Quick check with PDF card

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



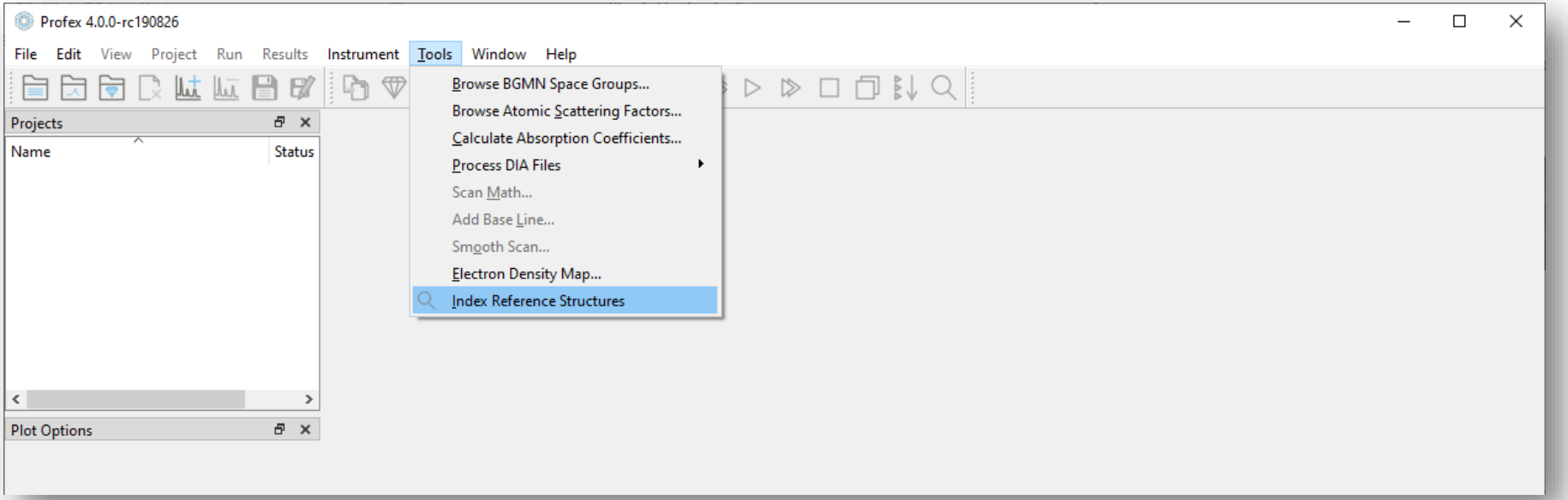


ICDD XML Format

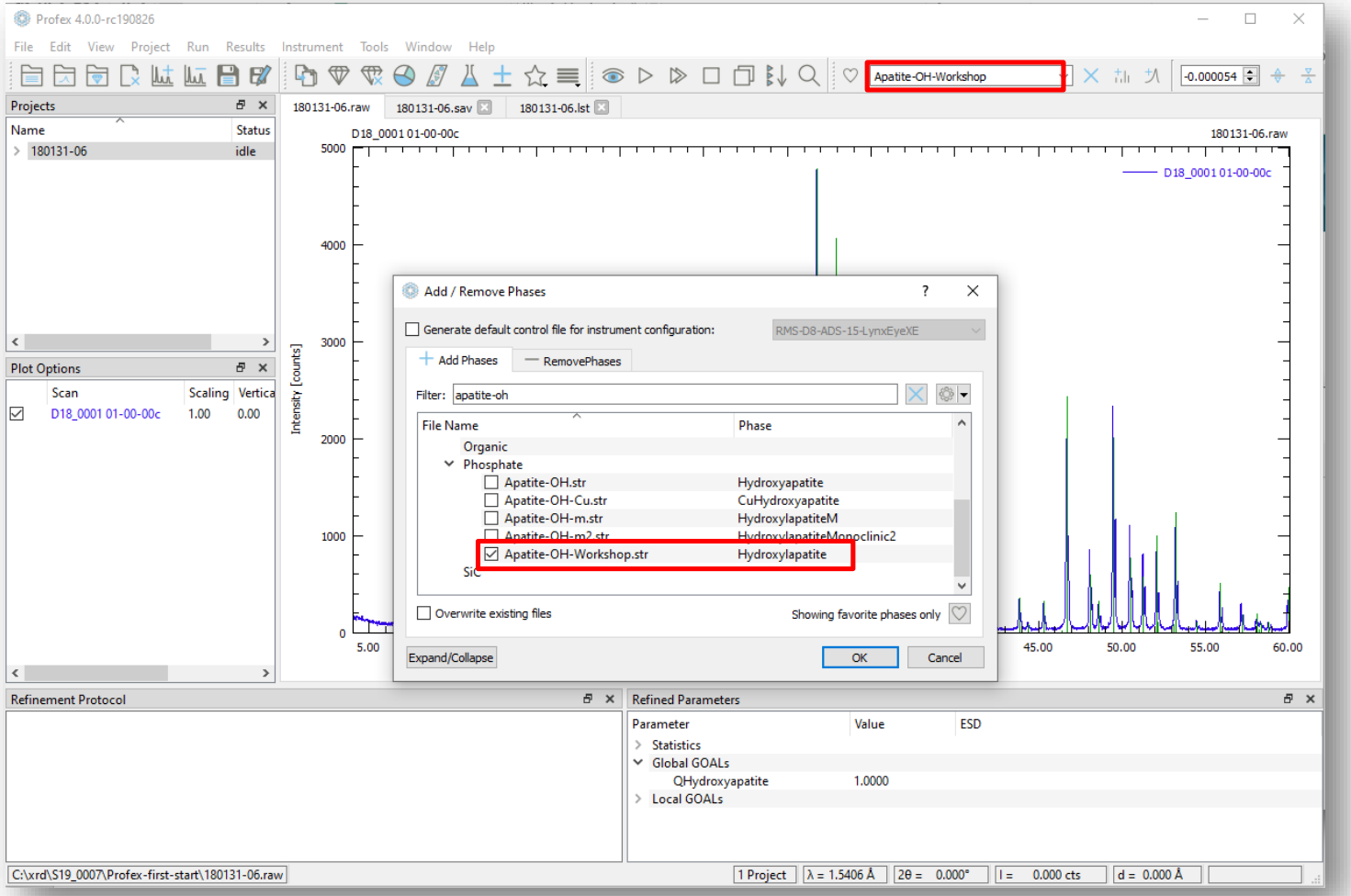


Save in Profex STR-file repository

In Profex main window: Index the new reference structure



Structure Import



CIF Format

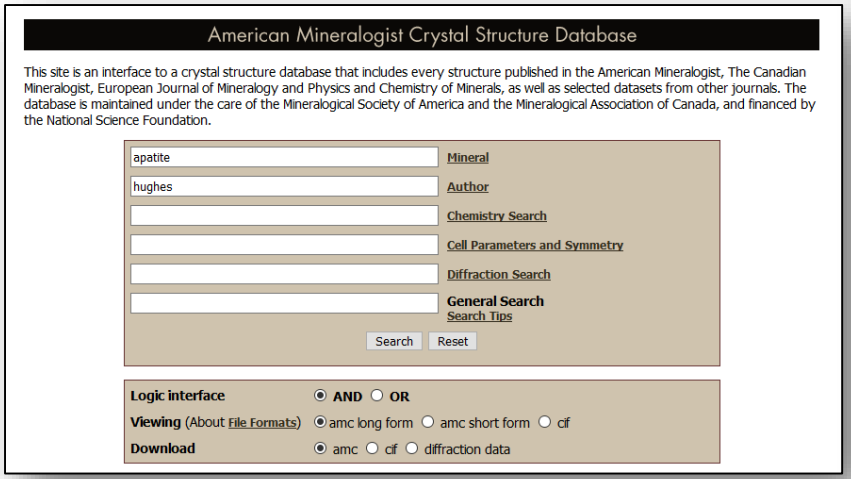
Free structure databases

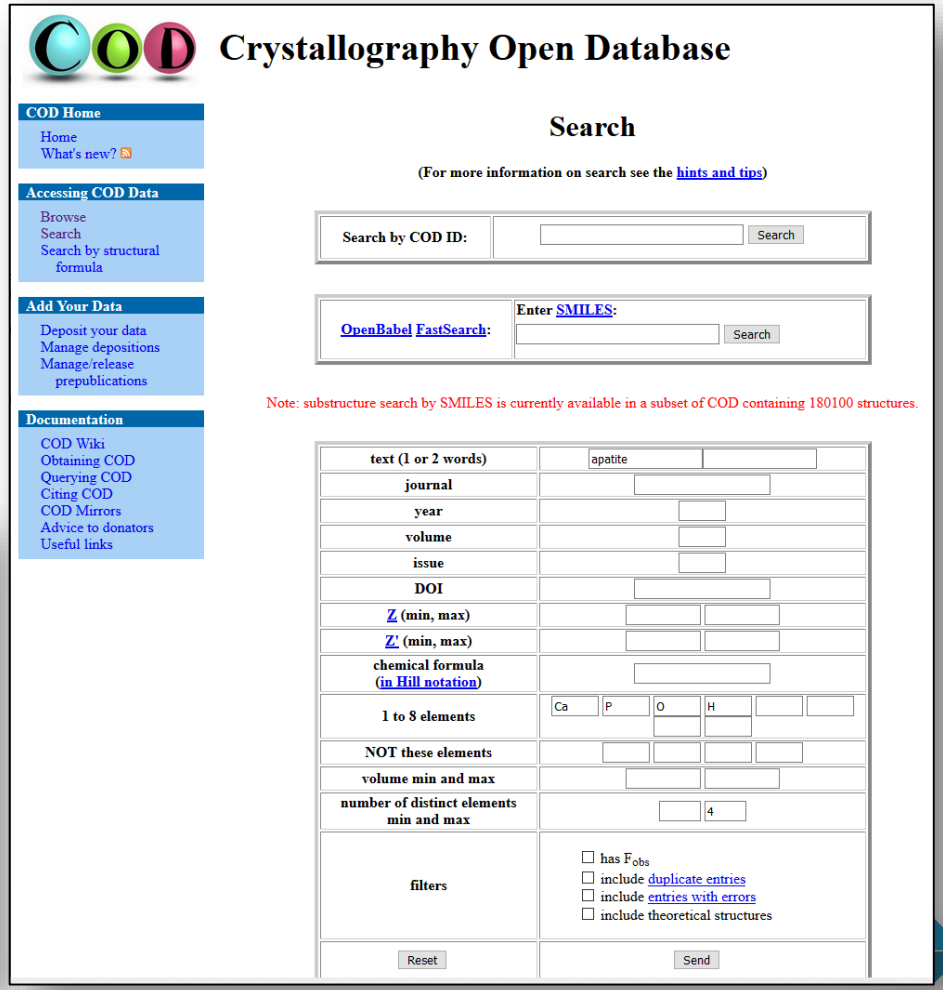
Crystallography Open Database (COD)

http://www.crystallography.net

American Mineralogist Structure Database

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





CIF Format

COD ID ▲	Links	Formula ▲	Space group ▲	Cell parameters	Cell volume ▲	Bibliography
9001233	CIF	Ca5 H O13 P3	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	0.0034	.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)

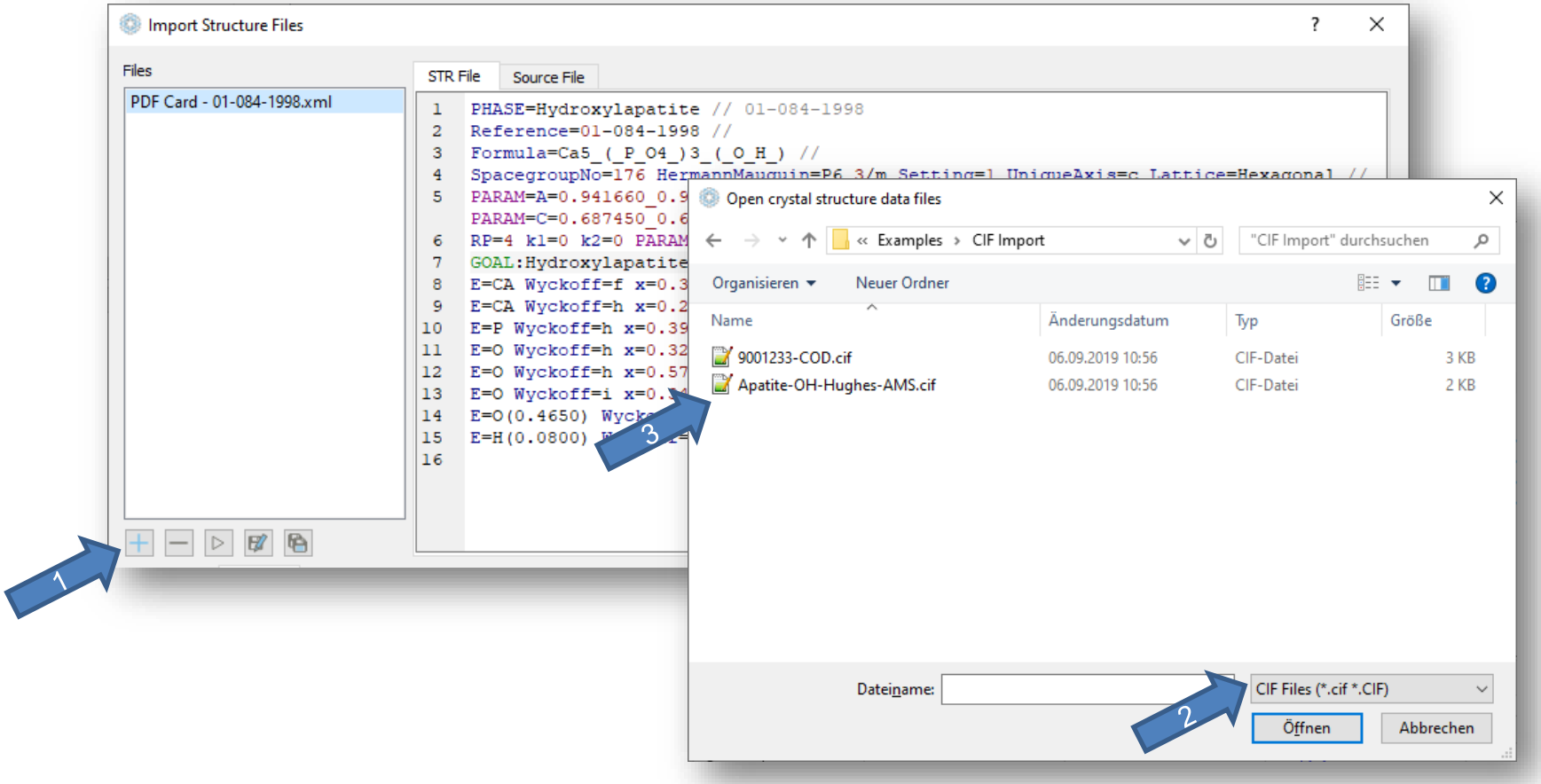
Download CIF data (View Text File)

Download diffraction data (View Text File)

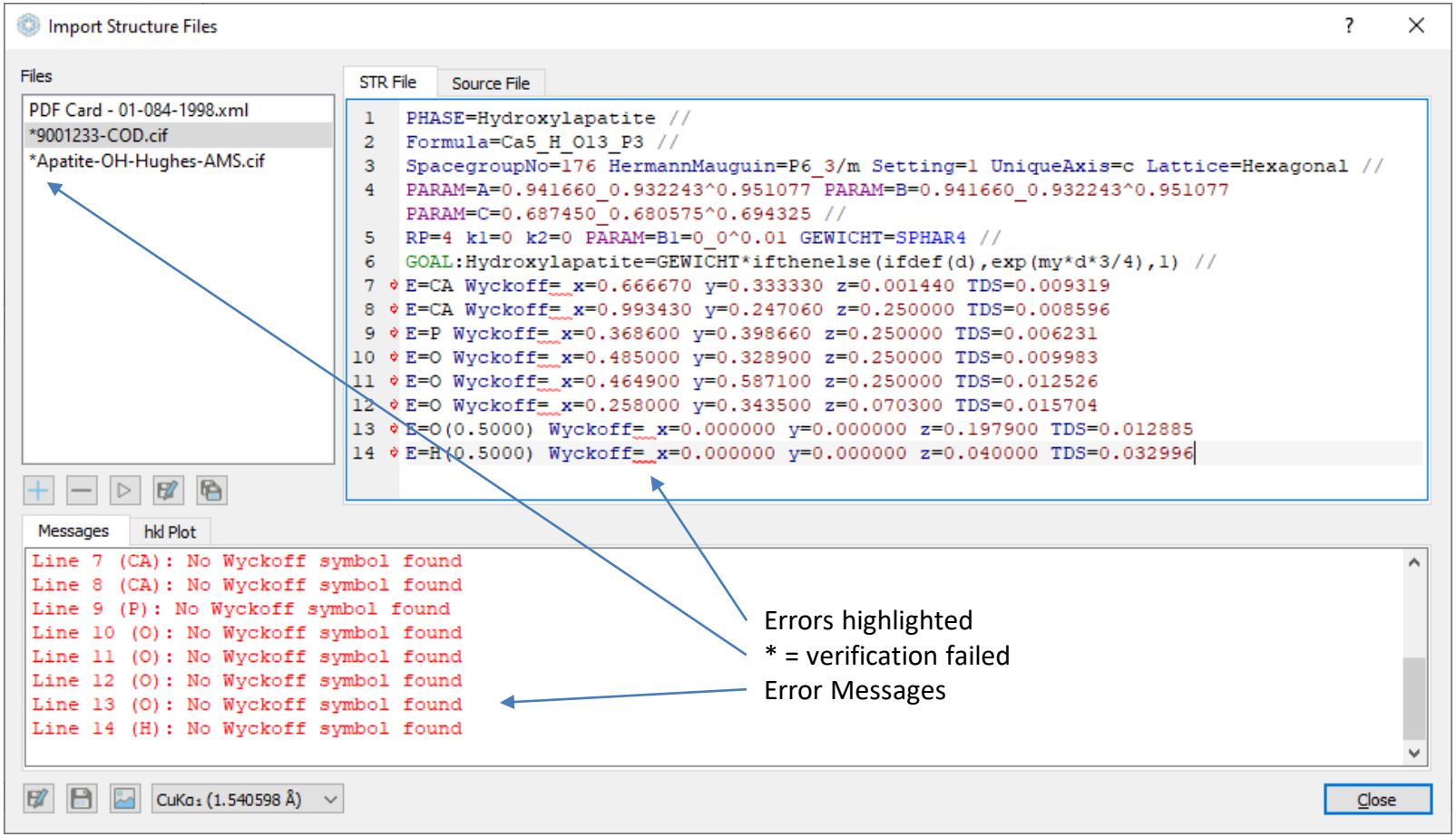
View JMOL 3-D Structure (permalink)

Saved in «Examples → CIF Import»

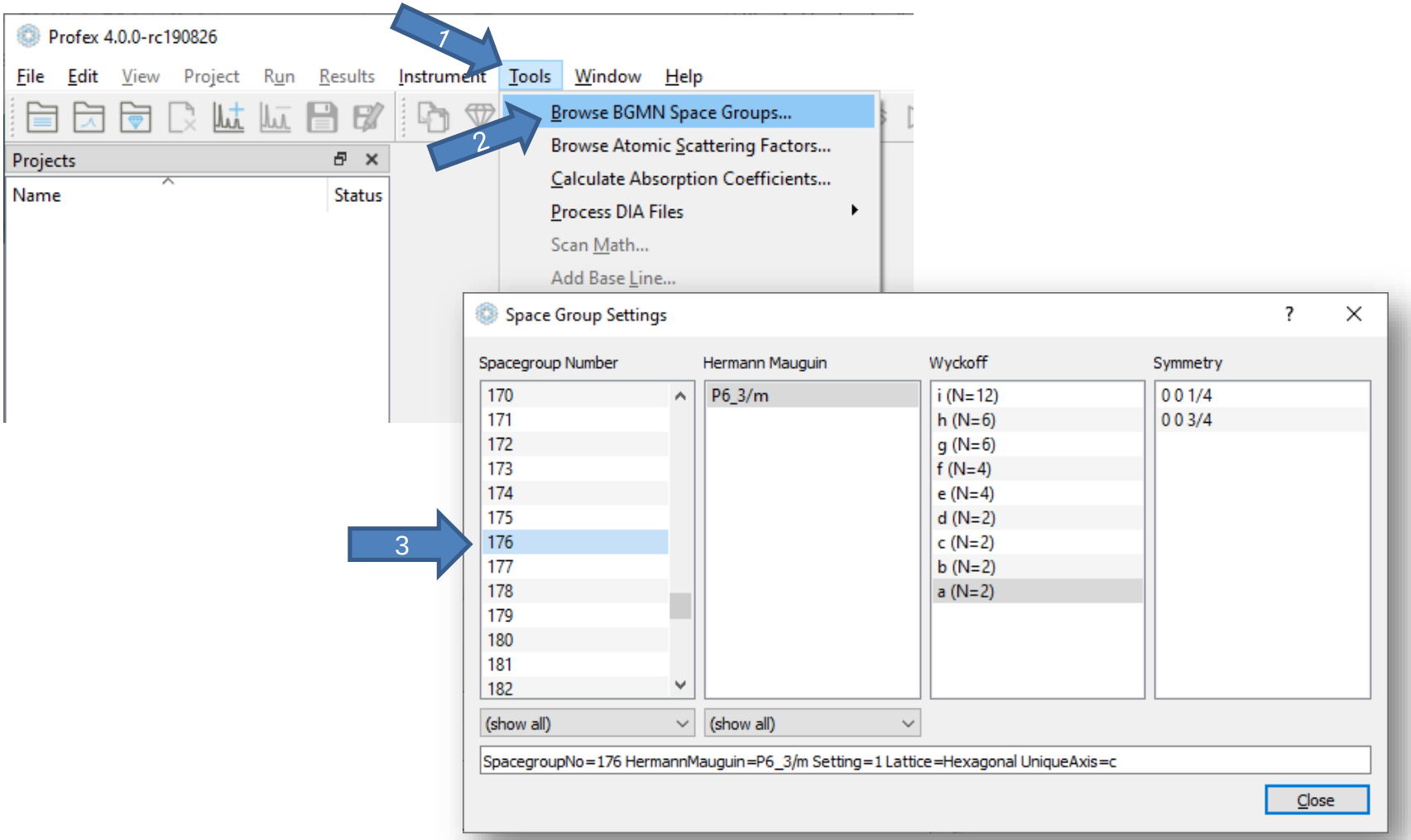
CIF Format


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_0.9
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.
14 E=O(0.4650) Wycko
15 E=H(0.0800)
16
Open crystal structure data files
« Examples › CIF Import
"CIF Import" durchsuchen
Organisieren
Neuer Ordner
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
Dateiname:
CIF Files (*.cif *.CIF)
Öffnen
Abbrechen
1
2
3

CIF Format


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
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
CuKα1 (1.540598 Å)
Close
Errors highlighted
* = verification failed
Error Messages

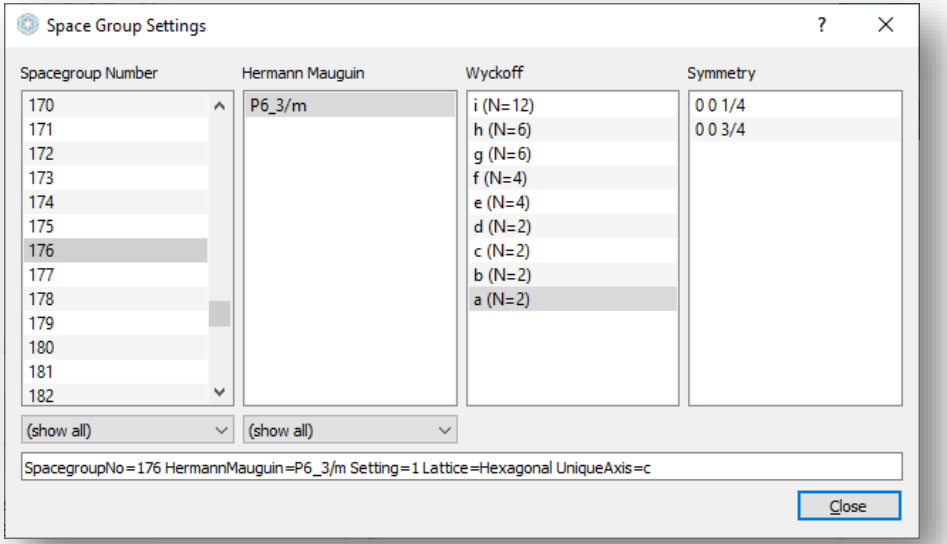
CIF Import – Wyckoff Symbols



CIF Import – Wyckoff Symbols

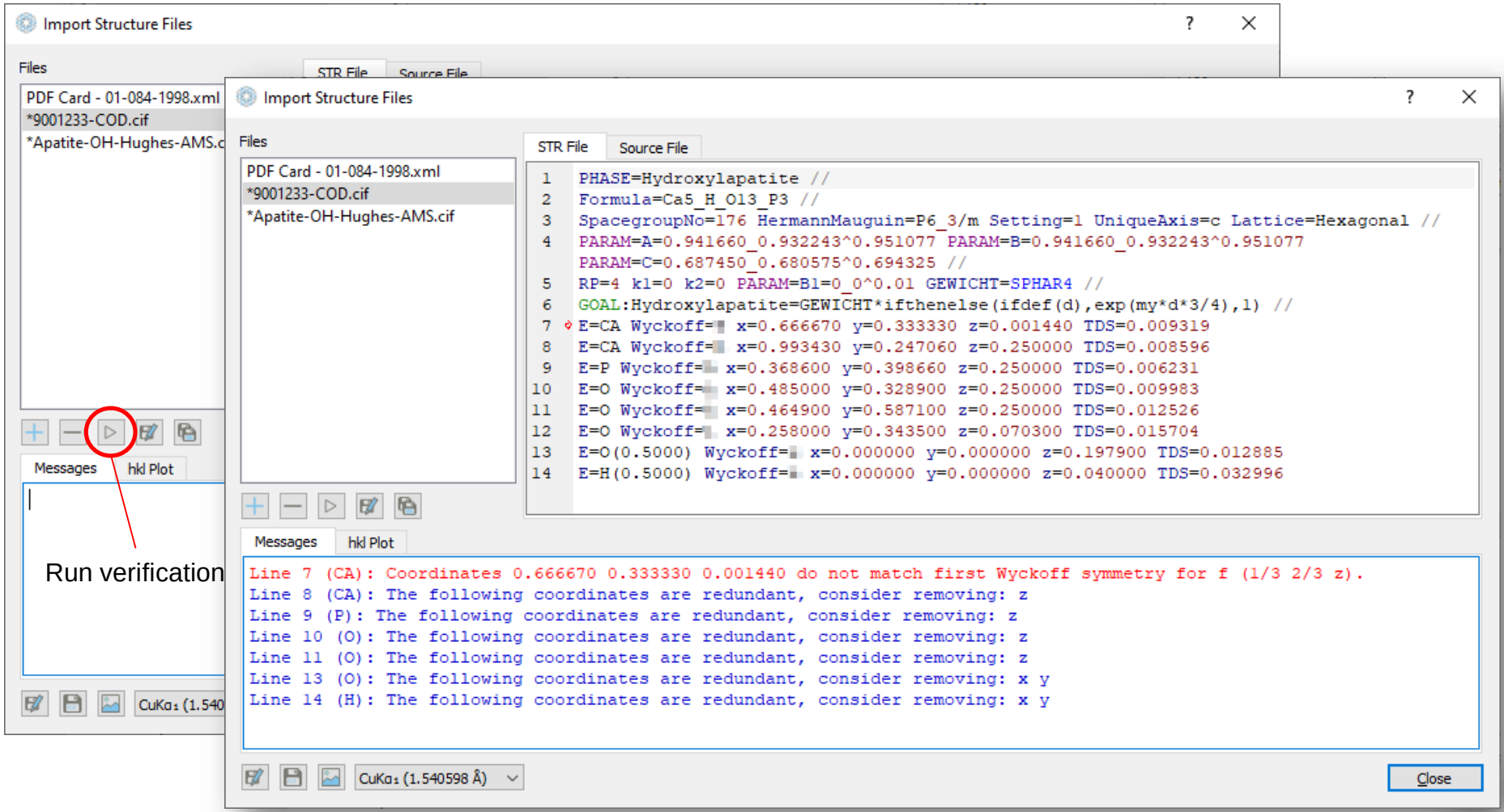
Identifying the Wyckoff symbol:

- Try to identify special coordinates
  - Special = 0.0, ½, 1/3, ¼, 1/8, 2/3, 3/8, 5/8, 7/8
  - General coorinates («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
```

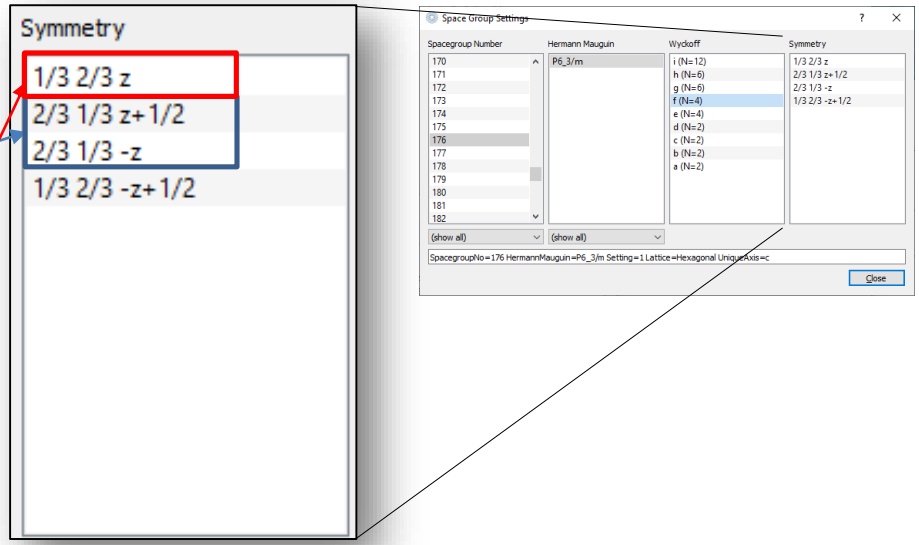
CIF Import – Wyckoff Symbols



CIF Import – Wyckoff Symbol

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).
```

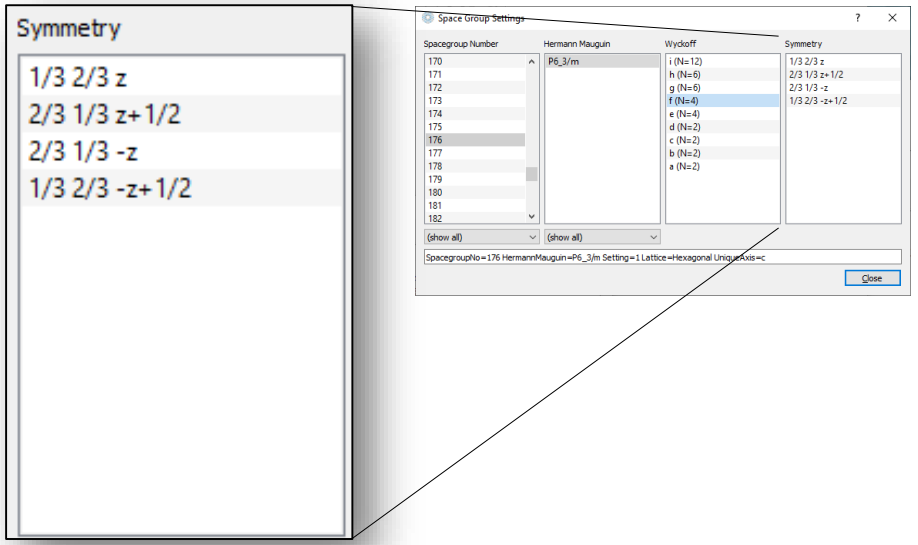
Manualy convert coordinates to first symmetry description if necessary

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 ½
  - 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
```

z = -z

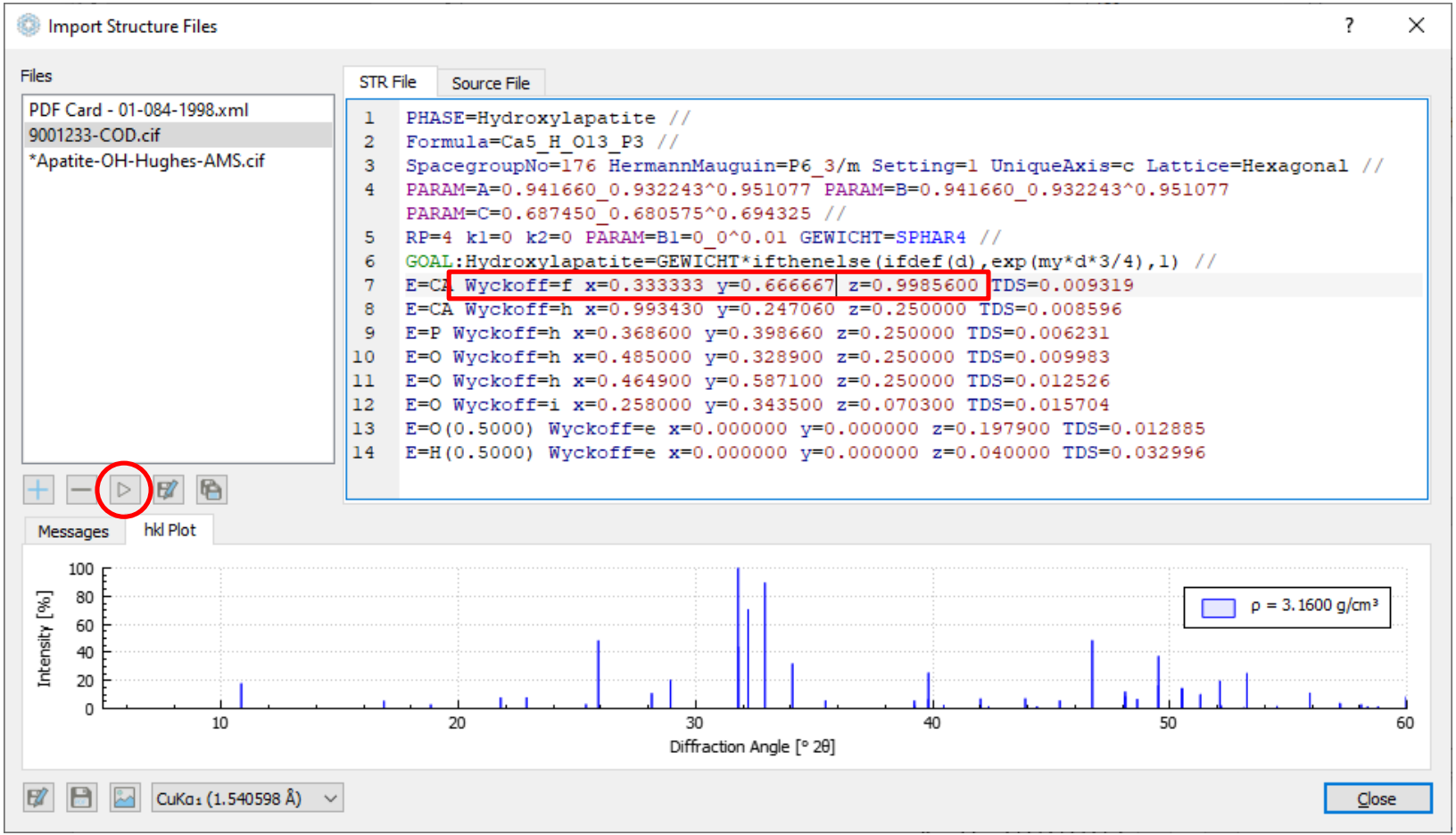
```
x=0.333333
y=0.666667
z=-0.001440
```

z = z + 1

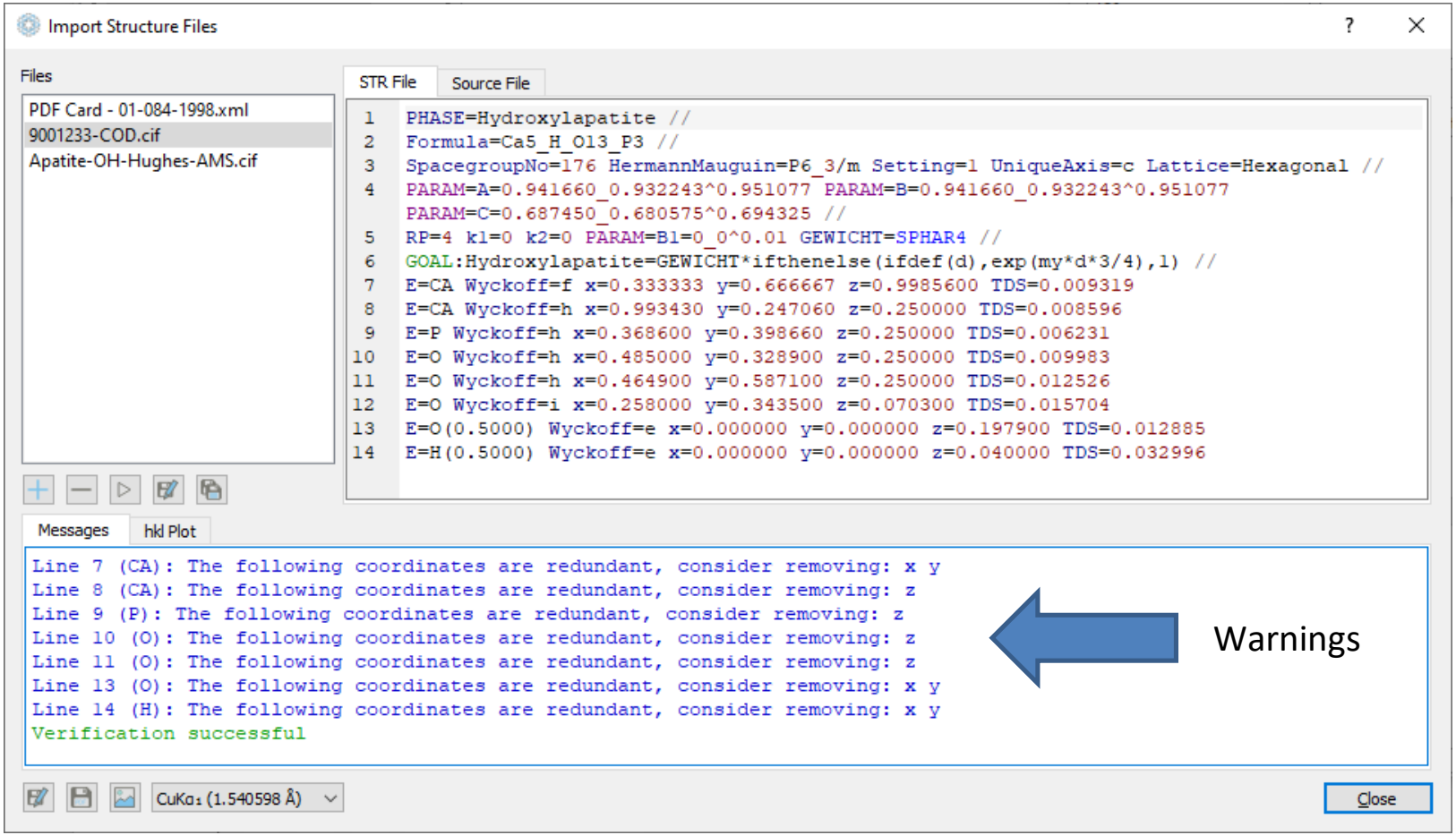
```
x=0.333333
y=0.666667
z=0.998560
```

Optional:
Add +1 to negative coordinates

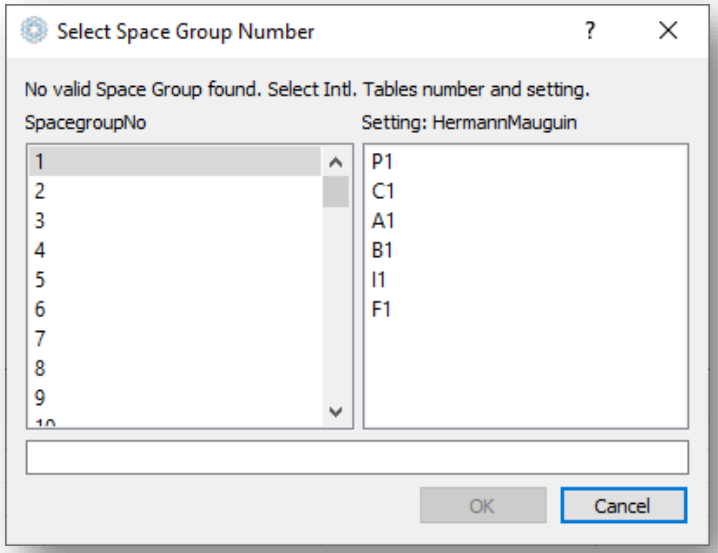
CIF Import


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
Intensity [%]
100
80
60
40
20
0
10
20
30
40
50
60
Diffraction Angle [° 2θ]
ρ = 3.1600 g/cm³
CuKα₁ (1.540598 Å)
Close

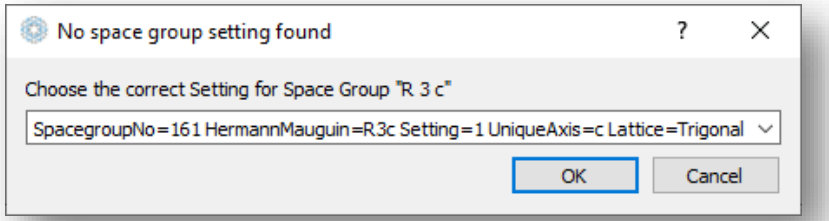
CIF Import


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
CuKα1 (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)