



New Features for Release 2022

New Topology Searches

Topology Volume Search

- The volume (V_{vdw}) of space confined by van der Waals surface of atoms in the unit cell and boundaries of unit cell

Surface Area Search

- The area (S_{vdw}) of van der Waals surface of atoms in the unit cell

Total Porosity Search

- The percent of empty space in a structure

The screenshot shows the ICDD Search application window. The 'Physical Properties' tab is selected on the left sidebar. The main panel contains various search filters and options. A red rectangle highlights the 'Topology' section, which includes three search criteria: 'Topology vdW Volume (Å³)', 'Topology vdW Surface Area (Å²)', and 'Topology Total Porosity (Å)'. Each criterion has a 'Low' and 'High' input field. Above this section, there are checkboxes for 'Measured Density', 'Calculated Density', and 'Structural Density'. The top of the window features a 'Subfile' dropdown, 'Environment' and 'Status' checkboxes, 'Quality Mark' options, and a 'Database' list. The bottom of the window has a 'Range Input' and 'Global Operator' section.

New topology data mining searches located in the Physical Properties tab.

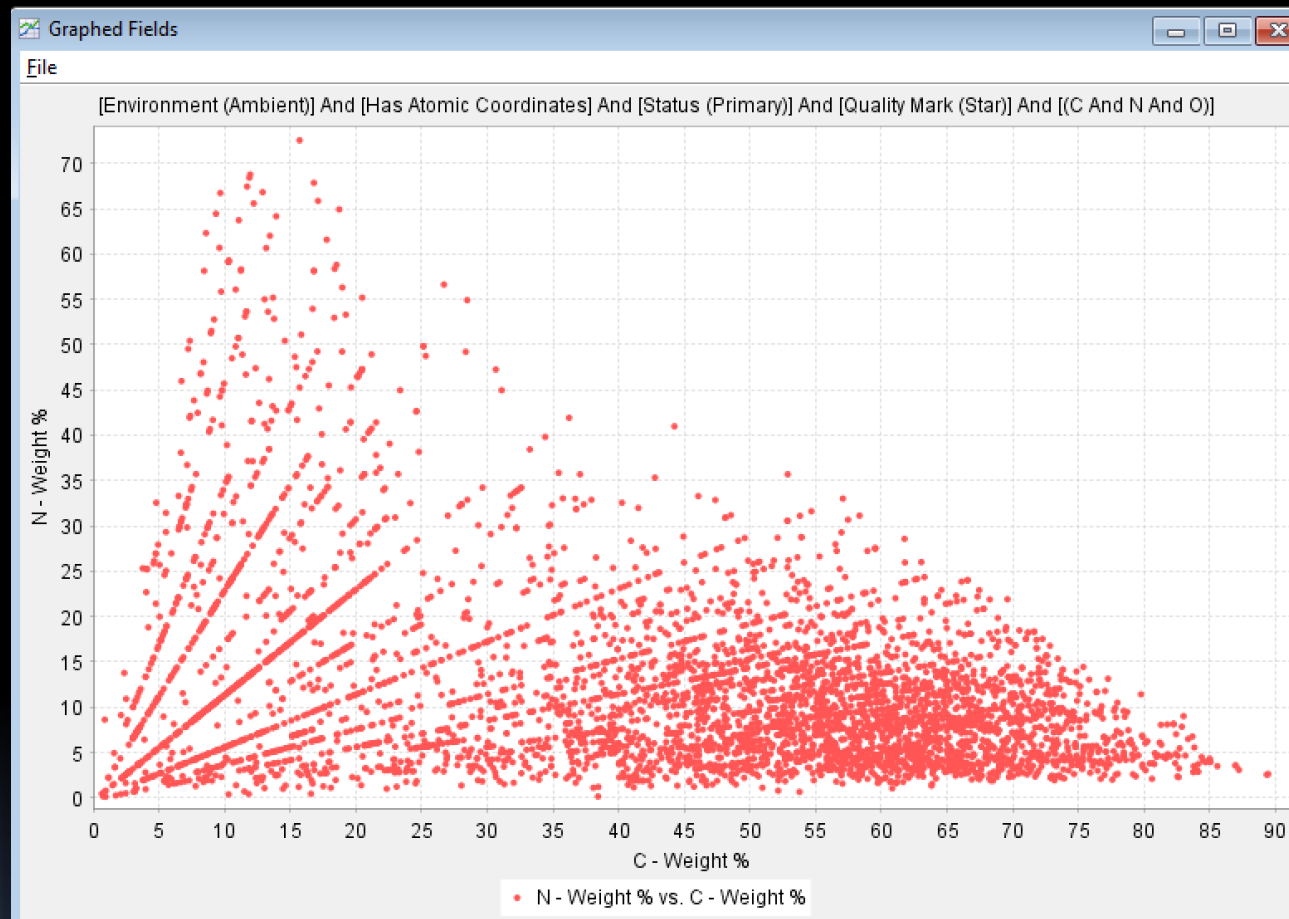
New Features for User-Created Graphs

Weight % and atomic % values can be graphed against themselves

Customize the size of graph data points for publication use

- Small points
- Medium points
- Large points

Export regression coefficients to spreadsheet programs



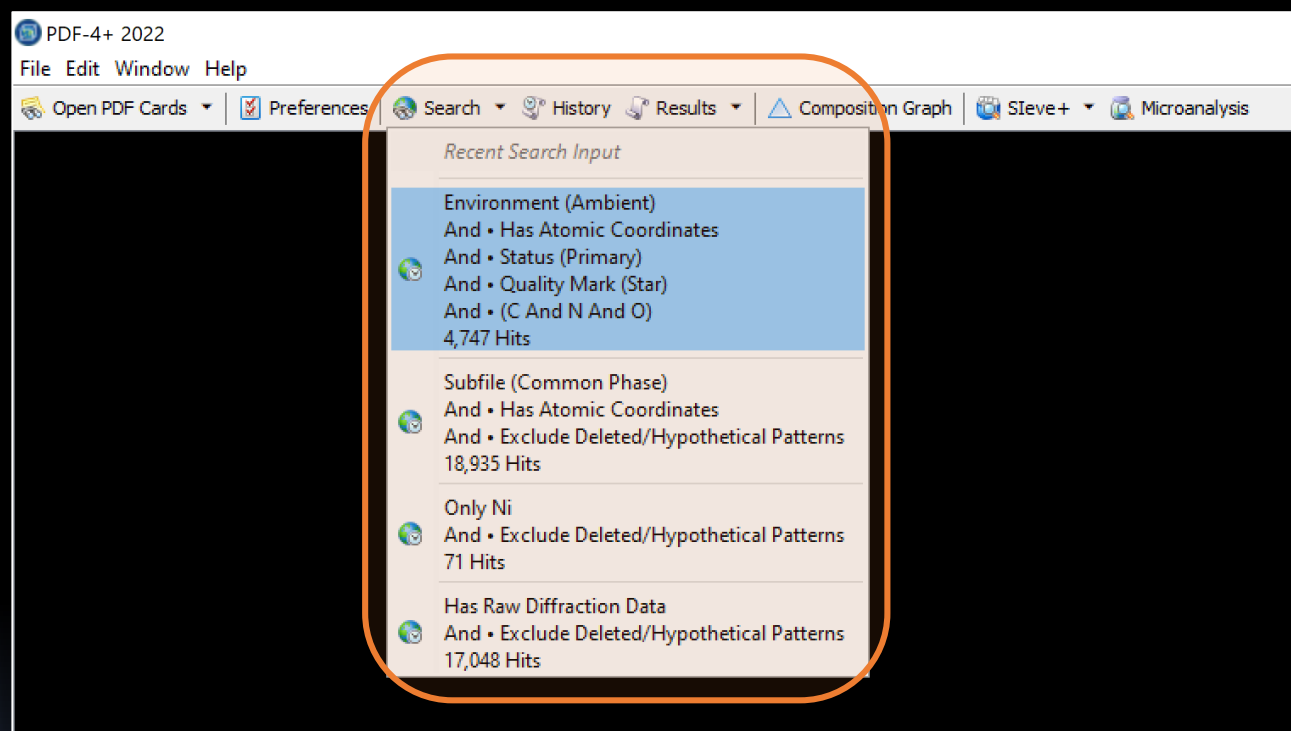
Graph of wt% of carbon vs wt% of nitrogen for PDF entries containing carbon, nitrogen, and oxygen.

Drop-Down Menu of Recent Search Input

Easily re-populate search input from any past search using new drop-down menu

Save time by no longer having to re-enter search input

Drop-down menu contains full search description and number of hits



Drop-down menu of recent data mining search input.

Drop-Down Menu of Recent Search Results

Quickly toggle between previous search results using new drop-down menu

Drop-down menu contains full search description and number of hits

All searches are saved/restored using XML files

The screenshot displays the PDF-4+ 2022 software interface. The main window shows a table of search results with columns for PDF #, QM, Chemical Formula, and a list of search criteria. A drop-down menu is open, showing a list of recent searches with their descriptions and hit counts. The menu is titled "Recent Search Results" and contains several entries, each with a search icon and a description of the search criteria and the number of hits.

PDF #	QM	Chemical Formula
00-014-0694	● S	$\text{Na}_4\text{Fe}(\text{CN})_6 \cdot 10\text{H}_2\text{O}$
00-014-0862	● S	$\text{CH}_6\text{AlN}_3\text{O}_8\text{S}_2 \cdot 6\text{H}_2\text{O}$
00-020-0907	● S	$\text{K}_3\text{MnNO}(\text{CN})_5 \cdot 2\text{H}_2\text{O}$
00-023-1367	● S	$\text{K}_3\text{V}(\text{CN})_5\text{NO} \cdot 2\text{H}_2\text{O}$
00-031-0372	● S	$\text{Cs}_2(\text{Pt}(\text{CN})_4) \cdot \text{H}_2\text{O}$
00-031-1979	● S	$\text{CH}_4\text{N}_2\text{O}$
00-032-1411	● S	$\text{CH}_4\text{F}_3\text{N}_2\text{O Sb}$
00-032-1683	● S	$\text{CH}_4\text{N}_2\text{O}_2\text{S}$
★ 00-033-1271	● S	$\text{Na}_2\text{NOFe}(\text{CN})_5 \cdot 2\text{H}_2\text{O}$
★ 00-034-0302	● S	$\text{Sr}(\text{Hg}(\text{CN})_2\text{SCN})_2 \cdot 4\text{H}_2\text{O}$
★ 00-035-0975	● S	$\text{SrHg}(\text{SCN})_4 \cdot 3\text{H}_2\text{O}$
00-035-0976	● S	$\text{MgHg}(\text{SCN})_4 \cdot 2\text{H}_2\text{O}$
★ 00-035-0977	● S	$\text{CaHg}(\text{SCN})_4 \cdot 3\text{H}_2\text{O}$
★ 00-035-1806	● S	$\text{CH}_6\text{N}_4\text{O}$
★ 00-036-0799	● S	$\text{BaZn}(\text{NCS})_4 \cdot 7\text{H}_2\text{O}$
00-037-0746	● S	$\text{Co}(\text{NH}_3)_6\text{Cr}(\text{CN})_6 \cdot \text{H}_2\text{O}$

Recent Search Results

- Environment (Ambient)
And • Has Atomic Coordinates
And • Status (Primary)
And • Quality Mark (Star)
And • (C And N And O)
4,747 Hits
- Subfile (Common Phase)
And • Has Atomic Coordinates
And • Exclude Deleted/Hypothetical Patterns
18,935 Hits
- Only Ni
And • Exclude Deleted/Hypothetical Patterns
71 Hits
- Has Raw Diffraction Data
And • Exclude Deleted/Hypothetical Patterns
17,048 Hits

Drop-down menu of recent data mining searches.

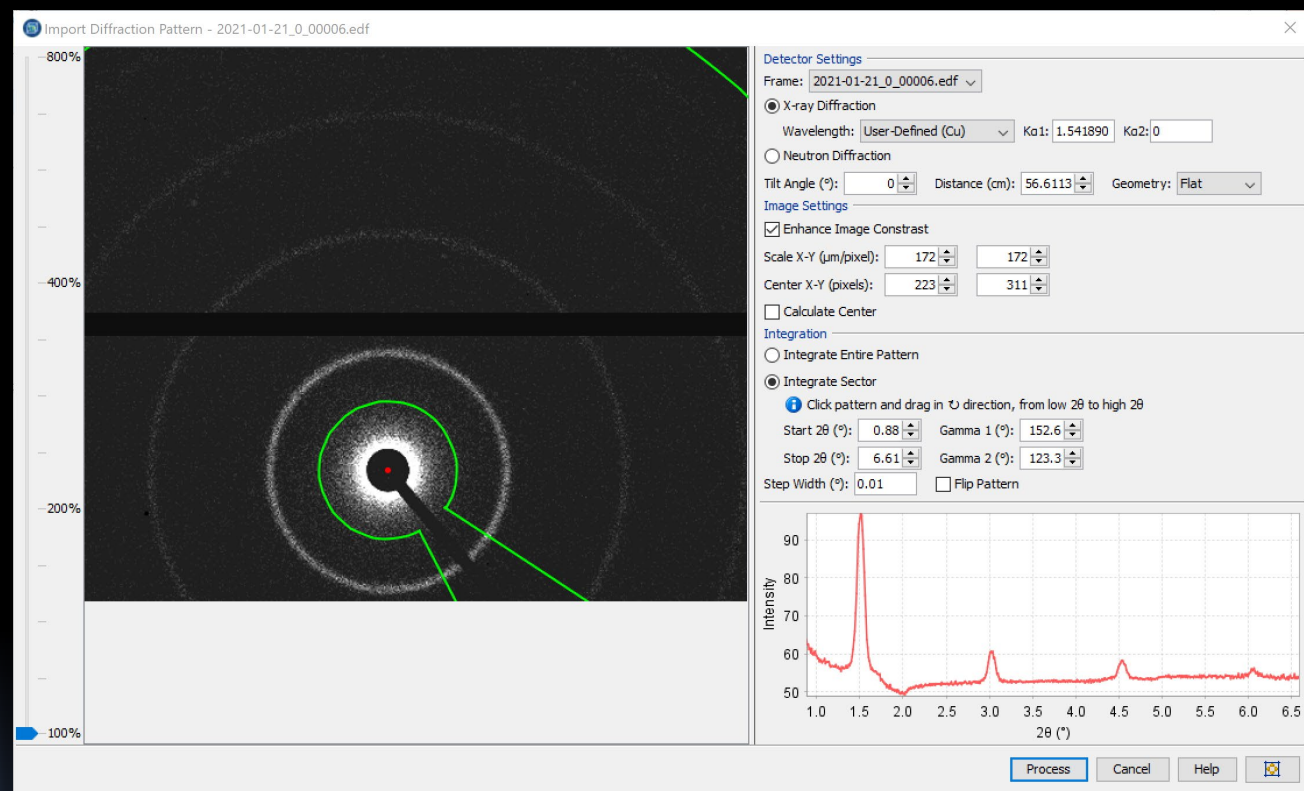
New Features for Importing Diffraction Data

New supported file types

- *.txl files (1D diffraction)
- ESRF *.edf files (2D diffraction)

Enhance the contrast of imported 2D images (*.jpg, *.png, *.tiff)

Optimized importing files over a network



Integration of an ESRF 2D diffraction pattern of silver behenate for phase ID.

New Features for Phase ID (Sleve+)

Customize display fields for the phases table

- Access to 85+ display fields
- Display fields are remembered between program sessions

Prefer mineral name in graph legend

The screenshot shows the Sleve+ software interface with the 'Phases (4)' table selected. The table displays the following data:

1D Diffraction Patterns	Phases (4)	Peaks (47 of 50)								
Compound Name	Mineral Name	Empirical Formula	Auth SPGR	Dcalc (g/cm ³)	QM	Peaks Matched	I Ratio	I %	Est Wt	PDF #
1 Iron Oxide	Hematite, syn	Fe ₂ O ₃	R-3c	5.27	S	11 of 16 (69%)	0.23	15.06	12%	01-080-5405
2 Aluminum Hydroxide	Gibbsite	Al ₂ (OH) ₃	P21/n	2.431	B	33 of 127 (26%)	0.65	43.13	60%	04-016-3819
3 Aluminum Oxide Hydrate	Bohmite	Al ₂ (OH) ₃	Cmcm		I	9 of 16 (56%)	0.25	16.60	16%	00-005-0190
4 Iron Oxide Hydroxide	Goethite	Fe ₂ (OH) ₃	Pbnm	4.257	I	17 of 31 (55%)	0.19	12.87	12%	00-029-0713
s-Triazine		C ₃ H ₃ N ₃	R-3m	1.366	S	8 of 21 (38%)	0.19	12.34		00-031-1954

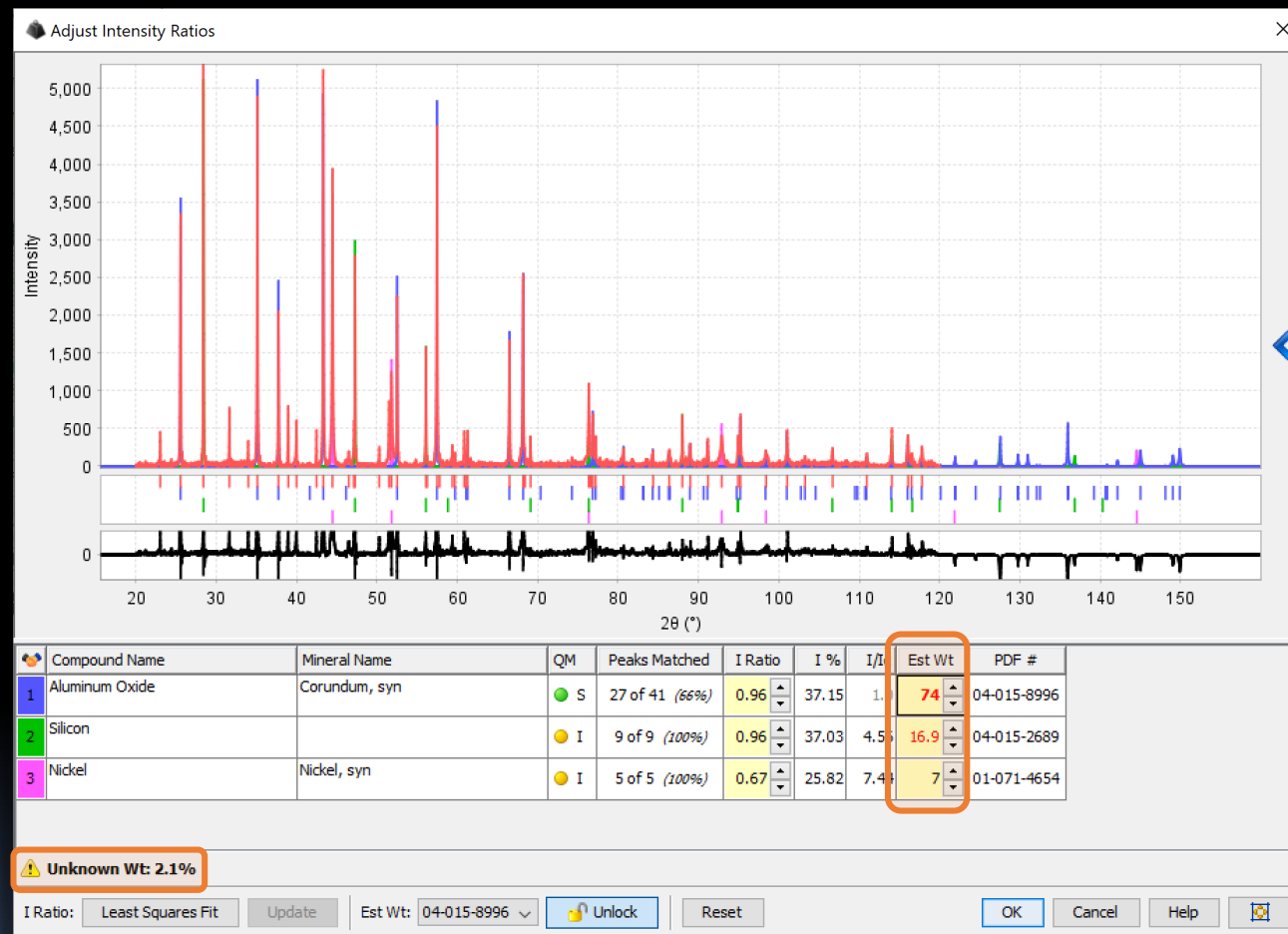
The phases table in Sleve+ with user-defined display fields (empirical formula, space group, and calculated density).

New Features for RIR Quantitative Analysis

Lock the wt% of a specific phase (as an internal standard) for RIR analysis

- Using standard addition or XRF data
- Unknown/amorphous wt% will be calculated and displayed

User-modified values are highlighted in red



The wt% of corundum is designated as an internal standard using XRF data for RIR quantitative analysis.

New Features for Phase ID (Sieve+)

Easily open previous Sieve+ session files and imported data files using new drop-down menu

Drop-down menu displays a preview of the accepted phases and their wt%

All Sieve+ sessions are supported

- X-ray diffraction analysis
- Neutron diffraction analysis
 - Constant wavelength
 - Time-of-flight
- Electron diffraction analysis
- 1D and 2D diffraction patterns

The screenshot shows the PDF-4+ 2022 software interface. The 'Sieve+' menu is open, displaying a list of recent files. The list includes session files (BAUXITE.xml, my session.xml) and data files (Corundum Osci_001.gfrm + 3, LaB6_1333-TOF (bank 3).xye, MnMoO4_Mn2O3.dat). A preview of the accepted phases and their wt% is shown for the selected file.

GOM	Peaks Matched	Chemical Formula	Compound Name	Mineral Name
3660	24 of 194 (12%)	Au Zr	Gold Zirconium	
2973	9 of 31 (29%)	Cu _{0.8} Mn _{0.4} In _{0.8} Se ₂	Copper Manganese Indium Selenide	
2832	46 of 830 (6%)	C ₁₁ H ₈ Fe ₂ N ₁₀ O	Bis(imidazol-1-yl)iron pentacyanonitrosyliron(2-)	
2768	8 of 21 (38%)	C ₃ H ₃ N ₃	s-Triazine	
2760	6 of 18 (33%)	Ge _{0.2} Si _{0.8} O ₂	Germanium Silicate	
2726	14 of 105 (13%)	Cd ₁₃ In ₂₆ Se ₅₄	Cadmium Indium Selenide	
2511	9 of 23 (39%)	Al O (OH) _{0.033} (OD) _{0.967}	Aluminum Oxide Hydroxide Deuteriooxide	Bohmite,
2499	4 of 10 (40%)	Au Br Se	Gold Bromide Selenide	
2474	6 of 19 (32%)	C ₁₂ H ₈ O ₂	2,5-Dimethyl-p-benzoquinone	2,5-dimethylcyclohexa-2,5-dien

Compound Name	Mineral Name	QM	Peaks Matched	I Ratio	I %	I/Ic	Est Wt	PDF #
1 Iron Oxide	Hematite, syn	● S	11 of 16 (69%)	0.23	12.16	3.2	10%	01-080-5405
2 Aluminum Hydroxide	Gibbsite	● B	33 of 127 (26%)	0.65	34.81	1.76	52%	04-016-3819
3 Aluminum Oxide Hydrate	Bohmite	● I	9 of 16 (56%)	0.25	13.40	2.59	14%	00-005-0190
4 Iron Oxide Hydroxide	Goethite	● I	17 of 31 (55%)	0.19	10.39	2.54	11%	00-029-0713
5 Silicon Oxide	Quartz	● I	6 of 18 (33%)	0.19	10.38	2.65	10%	01-086-2237
6 Titanium Oxide	Anatase, syn	● I	5 of 11 (45%)	0.07	3.92	3.6	3%	01-086-1157
Gold Zirconium		● I	24 of 194 (12%)	0.28	14.95	7.79		04-014-3461

Drop-down menu of all recent Sieve+ session files and imported data files.

New System-Wide Features

- Improved user interface for small screens
 - Option to show smaller toolbar
 - Option to hide program taskbar
- 64-bit support
 - Performance increase for multi-threading operations

	32-bit	64-bit
Similarity indexes (928 patterns)	30s	11s
Similarity indexes (2,853 patterns)	1m 50s	51s
2D integration of one Rigaku file	13s	9s
2D integration of four Bruker files	16s	12s