ICDD® POLYMER DIFFRACTION RAW DATA PROJECT – POLYMERS, GLASSES AND "MINERALS"

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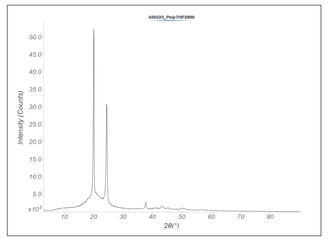
ICDD has been adding polymer diffraction data to the Powder Diffraction File™ (PDF®) with the focus on adding raw data (PD3) diffraction patterns as part of the PDF entry. The inclusion of the raw data diffraction pattern is important in correctly identifying the polymer contribution to a composite material diffraction pattern. A traditional d-spacing/intensity stick pattern or simulated diffraction pattern is not capable of accounting for the full-pattern diffraction profile of polymers since all polymers have some amorphous component. A total of 161 PD3 polymer patterns from this project are in the present PDF-5+ Release 2024 database. In addition to polymer PD3 patterns, the project has expanded to include PD3 patterns for glasses and mineral related phases. Examples of current and upcoming PDF-5+ 2025 PD3 entries from this project will be presented.

Polymers

The ICDD raw data project started with a focus on polymers both amorphous and semicrystalline. The interchain, intrachain and side group microstructure of polymers result in diffraction patterns with broad diffraction profiles that are not defined from conventional d-spacing/intensity lists.

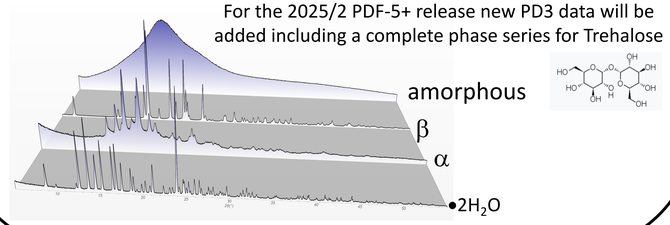
New raw data polymer entries for Release 2025
Butyl methacrylate/isobutyl methacrylate copolymer
Hydroxyethyl cellulose
Poly(1-vinylpyrrolidone-co-vinyl acetate) 0.7/0.3
Poly(4,4'-dipropoxy-2,2'-diphenyl propane fumarate)
Poly(ethyl methacrylate)
Poly(tetrahydrofuran) 250
Poly(tetrahydrofuran) 2900

When the XRD data show a polymer is semicrystalline, the unit cell indexing is evaluated using JADE Pro.



Poly(tetrahydrofuran) 2900
Unit Cell: monoclinic
Space Group: C2/c (15)
Z: 4
a=5.622 Å
b=8.899 Å
c=12.265 Å
β=134.5°
V = 437.83 Å^3

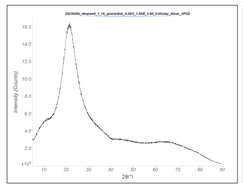
For the 2025/2 PDF-5+ release new PD3 data will be added including a complete phase series for Trehalose

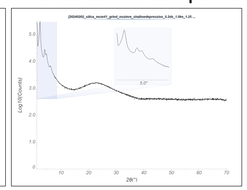


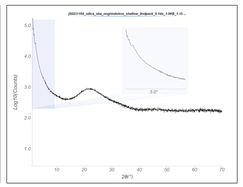
Glasses

Glass can be used as a substrate for deposition of thin films, a protective cover for electronic devices, and amorphous silica is often present in respirable dusts. The ICDD PD3 project has expanded to include raw XRD data for glasses.

In Release 2024 the first glass PD3 data (samples provided by J. Lyza, E.C. Levy Co.) were added to the PDF-5+ database. In Release 2025 amorphous quartz, and two meso-silicates will be added as PDF entries with PD3 patterns.

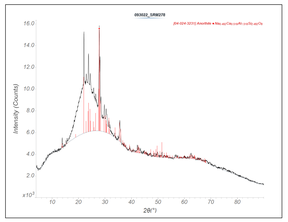

Amorphous quartz


MCM41 meso-silica

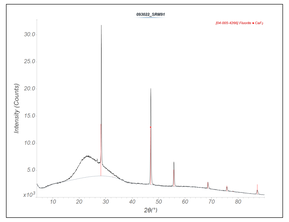

SBA15 meso-silica

Not all glasses are just glass!

Investigation of "glasses" found some samples were comprised of amorphous and crystalline phases. Those samples with crystalline phases are not added to the PDF-5+ database.



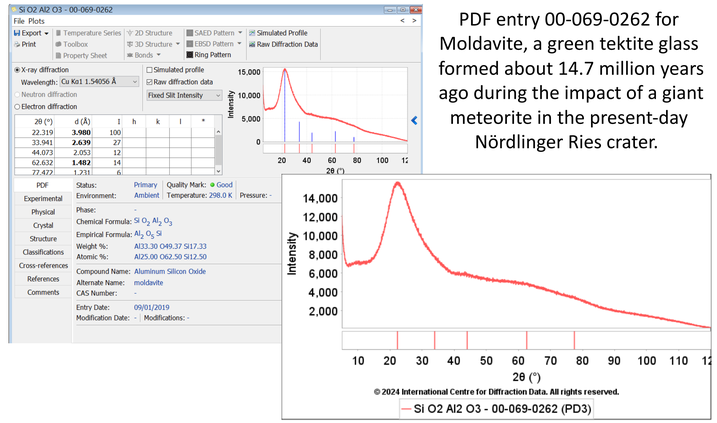
NIST SRM278 Glass has a feldspar $(Ca,Na)(Al_2Si_2O_8)$ anorthite-type phase present



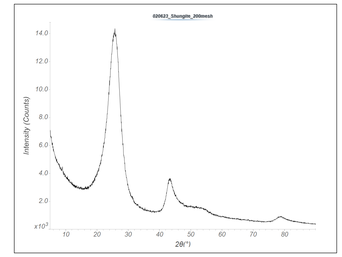
NIST SRM91 Glass has a fluorite CaF_2 phase present

"Minerals"

Though minerals are not typically found to be amorphous (there are a small number that are, i.e. opal), there are phases considered as "mineral related" that do fall into the amorphous category. As sample types are available, they will be added to the PDF-5+ database as part of the raw data project.



PDF entry 00-069-0262 for Moldavite, a green tektite glass formed about 14.7 million years ago during the impact of a giant meteorite in the present-day Nördlinger Ries crater.



Shungite is a carbon-rich metallic black stone, but not approved as a mineral by the IMA. A new entry for PDF-5+ 2025. From the Shunga village, in Karelia.

For the 2025/2 PDF-5+ release, new mineral related PD3 data will be added.


Libyan desert glass


chrysocolla