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QualX2.0: a software for qualitative phase analysis from powder diffraction data

Corriero Nicola

Institute of Crystallography - Cnr - Bari

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Outline of the talk

- Aim and applications of phase identification by X-ray powder diffraction (XRPD) (qualitative analysis);
- A freely available database for qualitative analysis: POW_COD;
- Main features of QUALX2.0, a computer program for qualitative analysis;
- Some applications of QUALX2.0;
- Final remarks;
- QualXWeb.

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Qualitative Analysis

Aim of phase identification by X-ray powder diffraction (qualitative analysis):

To identify the phases of a polycrystalline mixture via a powder diffraction pattern analysis.

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Qualitative Analysis

Aim of phase identification by X-ray powder diffraction (qualitative analysis):

To identify the phases of a polycrystalline mixture via a powder diffraction pattern analysis.

Applications of qualitative analysis:

- Scientific fields: Organic, metallorganic and inorganic Chemistry, Pharmaceutics, Mineralogy, Cultural heritage, Materials science,...
- Industrial fields: quality control of drugs, check of manufacturing process,...

Qualitative Analysis

Some remarks

- Peak intensities (I) contain information on the composition of a crystalline compound (unit cell content)
- Peak positions (2θ), and consequentely, interplanar distances ($d = \lambda/2sin\theta$), contain information on the unit cell parameters of a crystalline compound

Qualitative Analysis

Some remarks

- Peak intensities (I) contain information on the composition of a crystalline compound (unit cell content)
- Peak positions (2θ), and consequentely, interplanar distances ($d = \lambda/2sin\theta$), contain information on the unit cell parameters of a crystalline compound

Basic idea of qualitative analysis

By reducing the powder diffraction pattern of a crystalline compound into a set of *(d, I)* values, the phase identification can be performed by comparing them with the observed (or calculated) *(d, I)* values corresponding to known single-phase crystalline samples, usually belonging to a database.

Qualitative Analysis

Traditional methods

They consist of a three steps procedure

- **Search**, satisfying a guiding criterion;
- **Match** with respect to reference diffraction patterns of known compounds (e.g., belonging to a database);
- **Identification** by assessing the reliability of the match via a figure of merit and/or available prior information and/or experience.

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The success of the phase identification process depends on

- the quality of the experimental data and, consequently, the accuracy of the experimental *(d, I)* values;
- the adopted phase identification method;
- the accuracy of the *(d, I)* values of the reference database of known crystalline phases;
- the completeness of the reference database.

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QUALX2.0 applies the most widely used approach for qualitative analysis

- reducing the experimental powder diffraction pattern into a ‘stick pattern’ [i.e., a set of *(d, I)* values representing the diffraction peaks];
- querying a database of stick patterns of known crystalline compounds to search for the database pattern(s) best matching the experimental one (i.e., search-match step);
- supplying a list of the most plausible database pattern(s) matching the experimental data and ranked according to a Figure of Merit (FoM).

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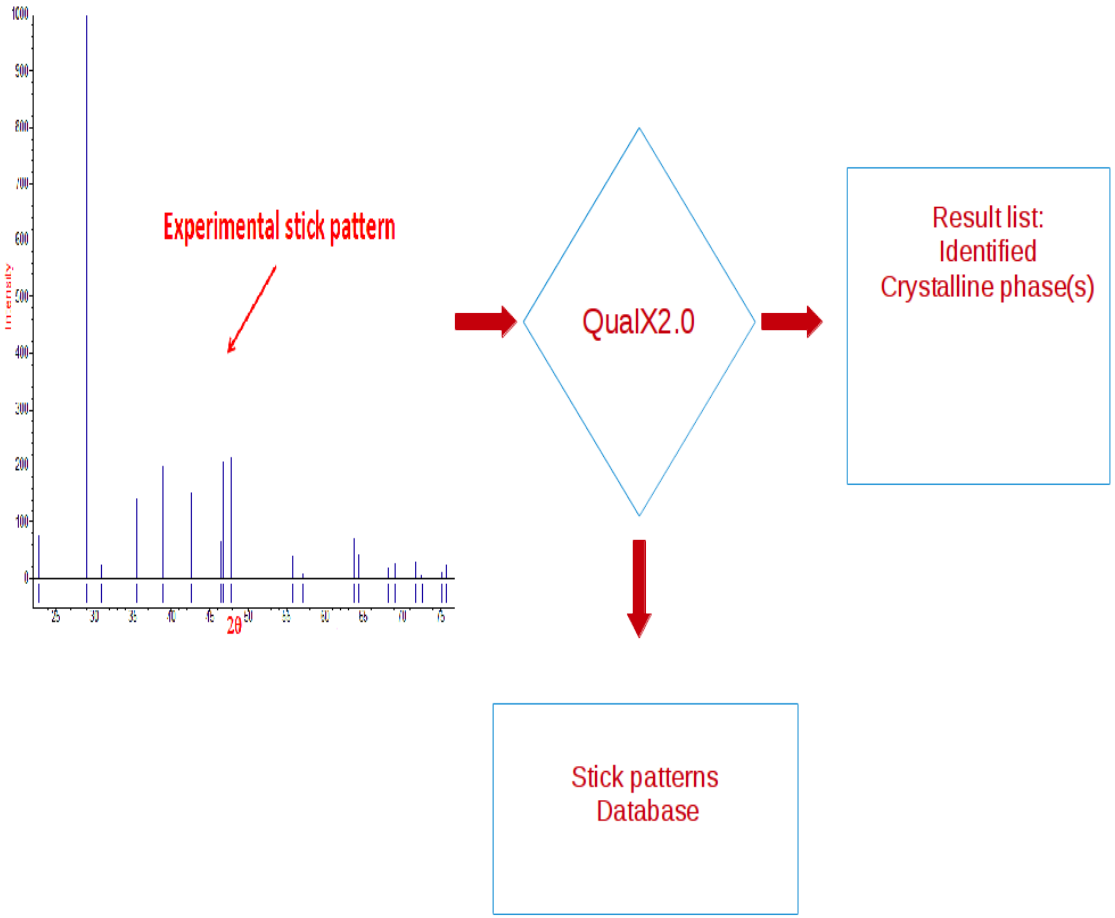
QualX2.0 Approach



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PDF database

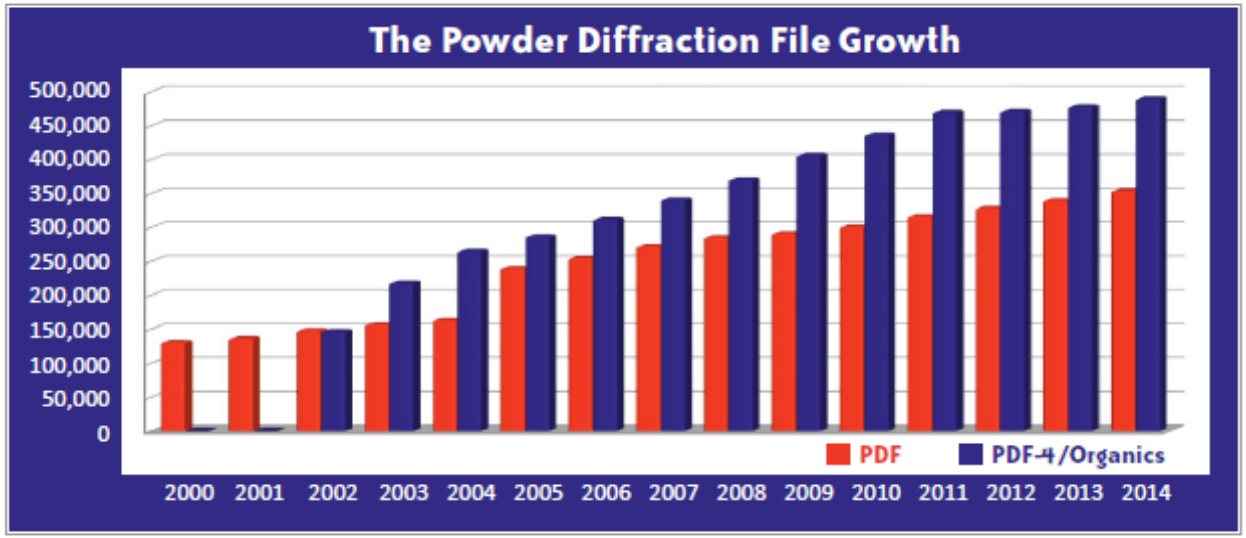
Most of the databases for qualitative analysis are commercial.

Among them, the most complete and widely used is the **Powder Diffraction File (PDF)**, maintained and continually updated by the *International Center of Diffraction Data* (ICDD, www.icdd.com).

PDF involves minerals, inorganic, organic and metallorganic materials, pharmaceuticals,...

PDF database

PDF database: for each compound, main crystallographic, experimental information and data quality are stored in entries.



Data Entry Source	PDF-2 Release 2014	PDF-4+ 2014 WebPDF-4+ 2014	PDF-4/ Minerals 2014	PDF-4/ Organics 2015
00- ICDD	111,864	111,864	11,747	37,753
01- FIZ	152,103	61,376	10,929	10,991
02- CCDC	0	0	0	431,359
03- NIST	10,067	3,018	207	281
04- MPDS	0	177,597	18,518	0
05- ICDD Crystal Data	409	409	22	14,582
Total No. of Data Sets	274,443	354,264	41,423	494,966
New Entries	9,316	19,420	1,253	15,689
No. with atomic coordinates	0	239,568	29,456	59,746
Reference Intensity Ratio - I/I_c	178,318	258,125	30,587	463,710
Experimental Digital Patterns	0	9,029	106	4,869
Calculated Digital Patterns	0	354,264	41,423	494,966

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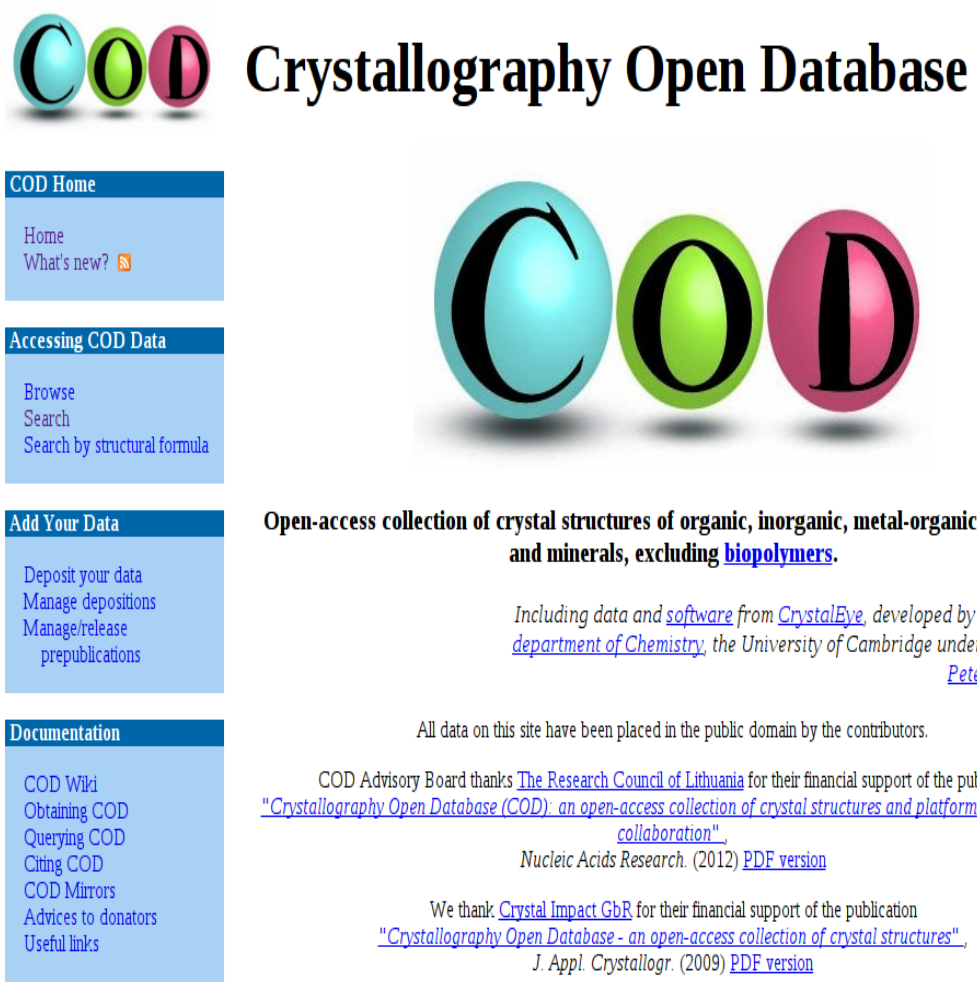
Crystallography Open Database

COD includes entries in CIF format. Currently there are 412558 entries in the COD. Their number is continually growing.



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Crystallography Open Database

Recently, some private companies, which develop crystallographic software and/or X-ray instrumentation, have distributed freely available databases which can be read by their qualitative analysis commercial software.

- **HighScore Plus** (Panalytical, www.panalytical.com)
- **Match!** (Crystal Impact, www.crystalimpact.com)
- **PDXL** (Rigaku, www.rigaku.com)

The freely available databases are built from the crystallografic information contained in the CIF files of the **Crystallographic Open Database** (COD).

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The POW_COD database

POW_COD is a database for qualitative analysis consisting of a collection of entries whose main crystallographic information is generated via **EXPO2014** program from the cell parameters, space group, atomic fractional coordinates and thermal factor supplied by the CIF file of **COD** database.

The CIF files are downloaded via the Subversion tool that enables an open access to **COD** and an easy update of the downloaded set of **COD** CIF files.

Each **POW_COD** entry is identified by the same seven-digit number associated to the corresponding CIF file of the **COD** database.

The POW_COD database

The main information of a POW_COD entry:

- for each reflection, the h,k,l Miller indices, the 2θ value, the interplanar distance d, the multiplicity and the ratio $I = (I_1 / I_{1max}) * 1000$, where I_1 is the reflection intensity and I_{1max} is the maximum value of the intensity calculated for all the generated reflections.
- The **Reference Intensity Ratio (RIR)** value, calculated according to the formula suggested by Hubbard et al. (1976). J. Appl. Cryst. 9, 169-174. **RIR** is useful for semi-quantitative analysis.
- The unit cell parameters, the cell volume, the crystal system, the space group, the chemical formula, the density, the Web address of the corresponding **COD** CIF file,...

The POW_COD structure

The **POW_COD** is a relational database that has been exported in **SQLite3** and can be readable not only by **QUALX2.0** but also by any reading/computing tool.

We preferred to use **SQLite** instead of other more popular software (e.g., MySQL, Oracle,. . .) because **SQLite** does not require any installation by the user.

POW_COD consists of about 10 tables storing all the information associated to each entry and structured so that **QUALX2.0** inquiry is fast and optimized.

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QUALX2.0 is the updated version of **QUALX** [Altomare et al. (2008). J. Appl. Cryst. 41, 815-817], a computer program for qualitative analysis inquiring the **PDF-2** commercial database.

QUALX2.0 retains the main features of **QUALX** searching the crystalline phases contained in both the **PDF-2** commercial database and the free **POW_COD** database.

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QUALX2.0 retains the main features of **QUALX** searching the crystalline phases contained in both the **PDF-2** commercial database and the free **POW_COD** database.
Actually **QUALX2.0** has more than 8000 users

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Main features of QUALX2.0

- It is characterized by a high level of automatism and a user-friendly graphic interface;

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Main features of QUALX2.0

- It is characterized by a high level of automatism and a user-friendly graphic interface;
- it can estimate background contribution and substract it from the experimental pattern;

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Main features of QUALX2.0

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Main features of QUALX2.0

- It is characterized by a high level of automatism and a user-friendly graphic interface;
- it can estimate background contribution and substract it from the experimental pattern;
- it can locate peaks and derive *(d, I)* values;
- it can search for the **PDF-2** or **POW_COD** phases; a graphic interface enables to select one of the two databases;

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- it can actively use suitable restraints;

Main features of QUALX2.0

- It is characterized by a high level of automatism and a user-friendly graphic interface;
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Main features of QUALX2.0

- It is characterized by a high level of automatism and a user-friendly graphic interface;
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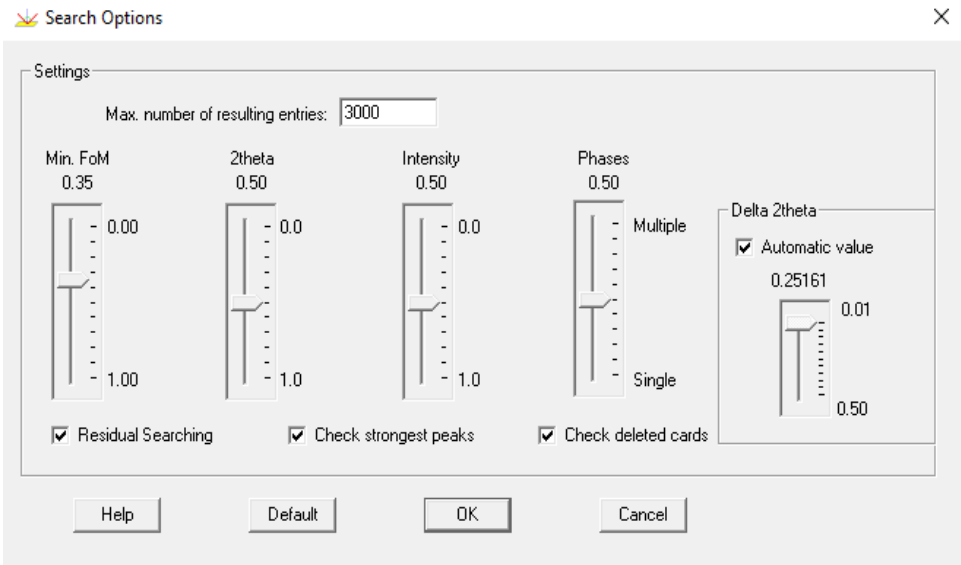
- it can locate peaks and derive *(d, I)* values;
- it can search for the **PDF-2** or **POW_COD** phases; a graphic interface enables to select one of the two databases;
- it can actively use suitable restraints;
- it can perform semi-quantitative analysis.

The main novelty of **QUALX2.0** is the possibility of inquiring the **POW_COD** database.

Search-match by QualX2.0

An **automatic search-match** is carried out using the Bragg reflections by seeking through enormous arrays of data, which a typical database contains.



Search-match by QualX2.0

The number of strongest reflections of a database entry to be matched.

Tolerance on 2θ position: a difference between the observed and database positions of peaks.

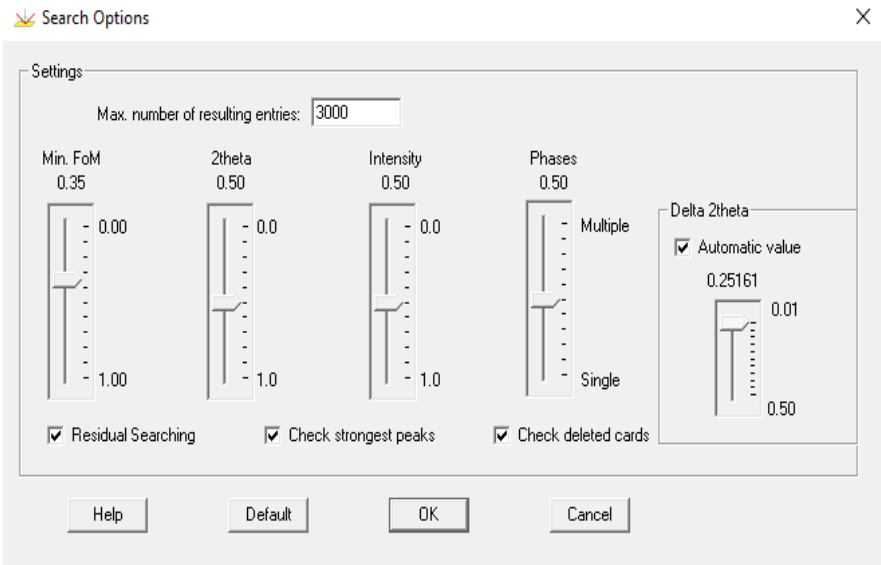


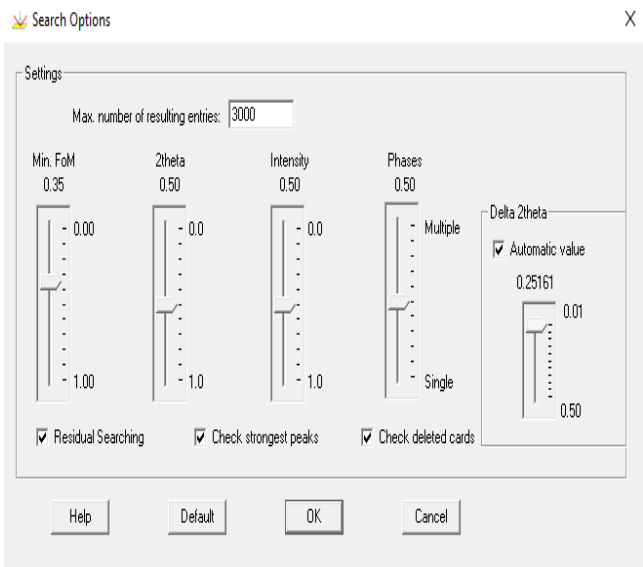
Figure of merit (FoM)

The right solution should be selected by visual comparison between similar patterns sorted in function of a figure of merit (FoM)

FoM includes information on the matched peaks:

- average difference in peak positions;
- number of matched reflections;
- relative intensities.

The weighting factors on the contributions to the FoM can be adjusted directly by the user by using the graphical interface



Restraints

on the elemental composition

Search with restraints options

- inclusive OR
- inclusive AND
- exclusive OR (just)
- exclusive AND (only)

Restraints

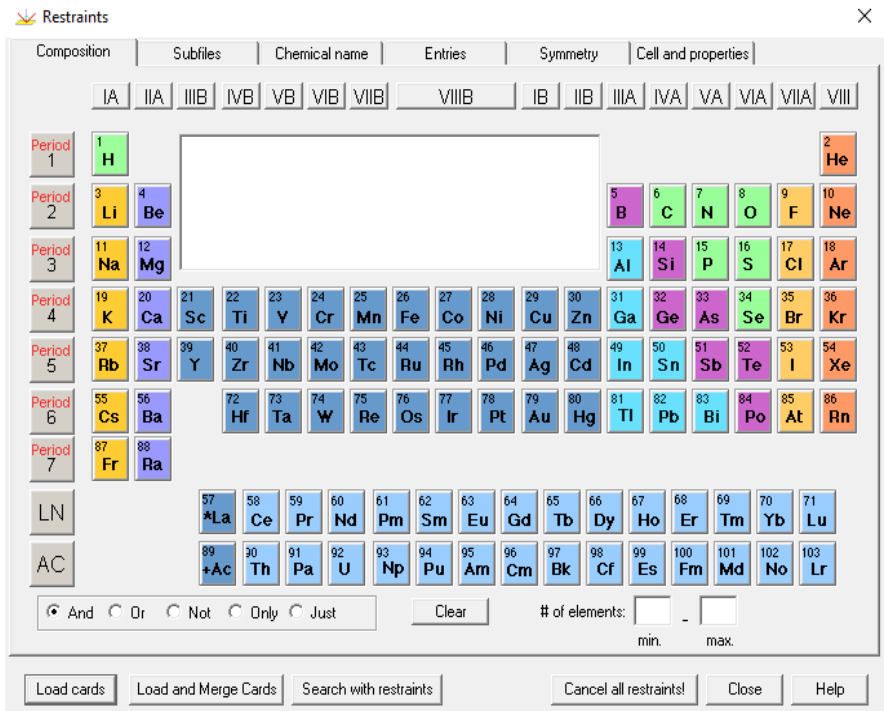
on the elemental composition

Search with restraints options

- inclusive OR
- inclusive AND
- exclusive OR (just)
- exclusive AND (only)

Other constraints

- organic or inorganic
- space-groups
- subfiles
- density
- color
- cell dimensions



Steps of phase identification

using QualX2.0

1. **File** > *Import diffraction data* and select the wavelength
2. **Pattern** > *Create Background* to estimate automatically the background. The background can be modified manually selecting **Pattern** > *Background Options*
3. **Pattern** > *Subtract Background* to subtract the background contribution from the experimental pattern
4. **Pattern** > *Peak Search* to activate the search of peaks in the pattern. To modify the default peak search approach press **Pattern** > *Peak Search Options*
5. **Search** > *Search-Match* enables the search of database reference patterns best matching the experimental powder diffraction data.

Otherwise you can select step 5 just after step 1 to perform ***automatic data reduction*** (steps 2,3,4 will be automatically performed)

The problem is far from trivial

Automatic search may generate a massive number of matches

- Your diffraction pattern contains a large number of peaks. Inspect the peaks carefully one by one, and delete those peaks that you are not really sure about. Afterwards, run the search-match again;
- The current value of the tolerance on the 2θ position may be too large. Its modifications can be useful.

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QUALX2.0 in action

At the end of the search-match procedure a set of plausible crystalline phases is provided.

The plausible database phases are ranked according to decreasing values of the **figure of merit (FoM)** taking into account the number of matched peaks and the agreement between the *(d, I)* values of database phases and those ones of the unknown compound.

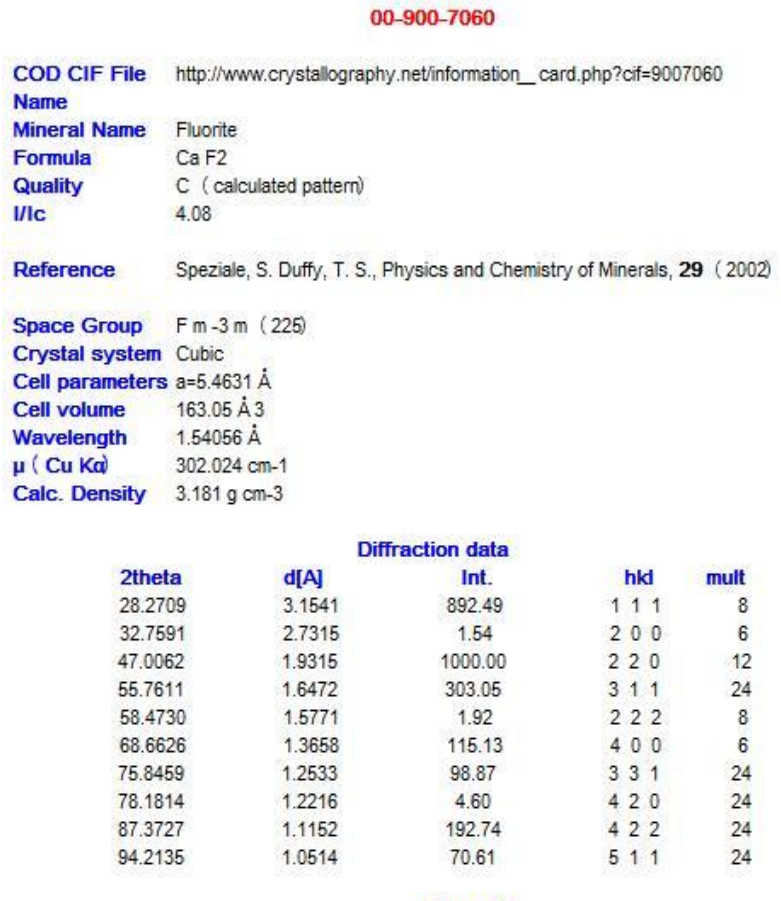
When a possible database phase (i.e., *entry*) is graphically accepted, its contribution is subtracted from the list of experimental *(d, I)* values obtaining an updated set of *(d, I)* values. The figure of merit is calculated again by taking into account the updated *(d, I)* values (*residual searching* option, default choice of **QUALX2.0**).

QUALX2.0 in action

QUALX2.0 enables to visualize the main crystallographic information of each database entry by graphic interface. In the case of a **POW_COD** database entry:

Main features

- Web address of the source CIF file of **COD** database
- Entry number (the same of the source **COD** CIF file)
- The 2θ values are calculated by taking into account the wavelength value supplied by the user



00-900-7060

COD CIF File Name	http://www.crystallography.net/information_card.php?cif=9007060
Mineral Name	Fluorite
Formula	Ca F2
Quality	C (calculated pattern)
I/Ic	4.08
Reference	Speziale, S. Duffy, T. S., Physics and Chemistry of Minerals, **29** (2002)
Space Group	F m -3 m (225)
Crystal system	Cubic
Cell parameters	a=5.4631 Å
Cell volume	163.05 Å3
Wavelength	1.54056 Å
μ (Cu Kα)	302.024 cm-1
Calc. Density	3.181 g cm-3

Diffraction data

2theta	d[A]	Int.	hkl	mult
28.2709	3.1541	892.49	1 1 1	8
32.7591	2.7315	1.54	2 0 0	6
47.0062	1.9315	1000.00	2 2 0	12
55.7611	1.6472	303.05	3 1 1	24
58.4730	1.5771	1.92	2 2 2	8
68.6626	1.3658	115.13	4 0 0	6
75.8459	1.2533	98.87	3 3 1	24
78.1814	1.2216	4.60	4 2 0	24
87.3727	1.1152	192.74	4 2 2	24
94.2135	1.0514	70.61	5 1 1	24

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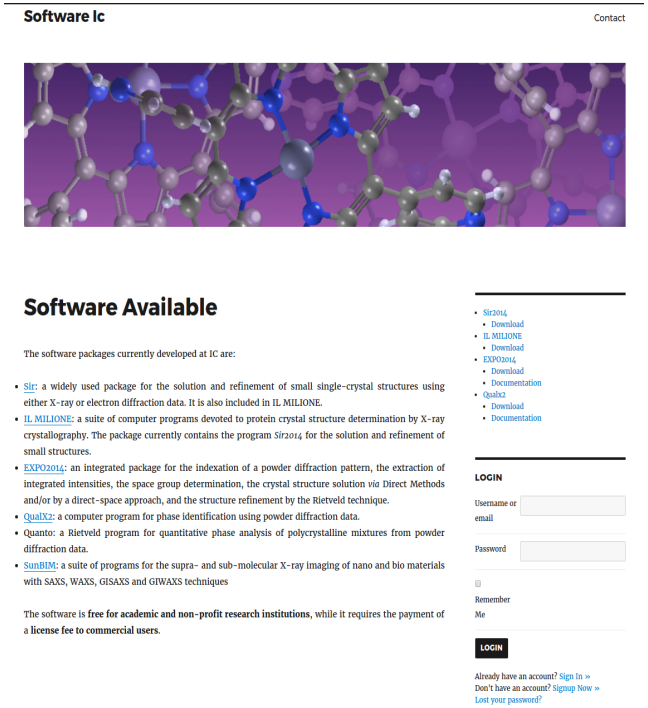
- Connect to *http://www.ba.ic.cnr.it/softwareic*
- Click on ***Register*** and enter your personal data

After your registration, you will receive an e-mail message of confirmation and you will be allowed to download QUALX2.0.



How to download QualX2.0

After registration, free download by connecting to *http://www.ba.ic.cnr.it/softwareic/qualx/*

QualX2 download

QualX2 software is distributed free of charge for academic, scientific, educational, noncommercial users and not-for-profit use.
It is required the payment of a license fee to commercial users.

For information about the distribution of QualX2, please, contact caterina.chiarella@ic.cnr.it.

The QualX2 team thanks you very much for your availability in the compilation of the following survey.

QualX User Experience Survey

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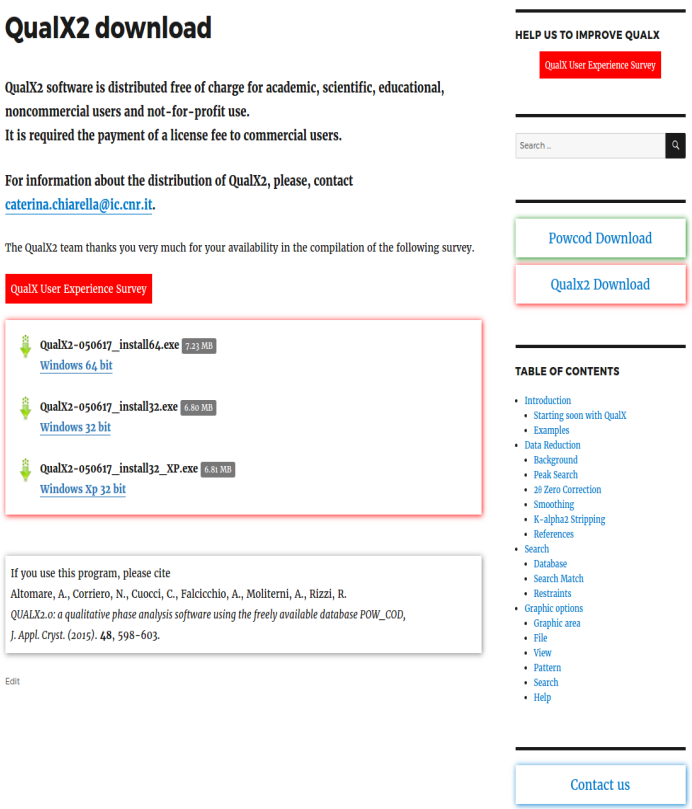

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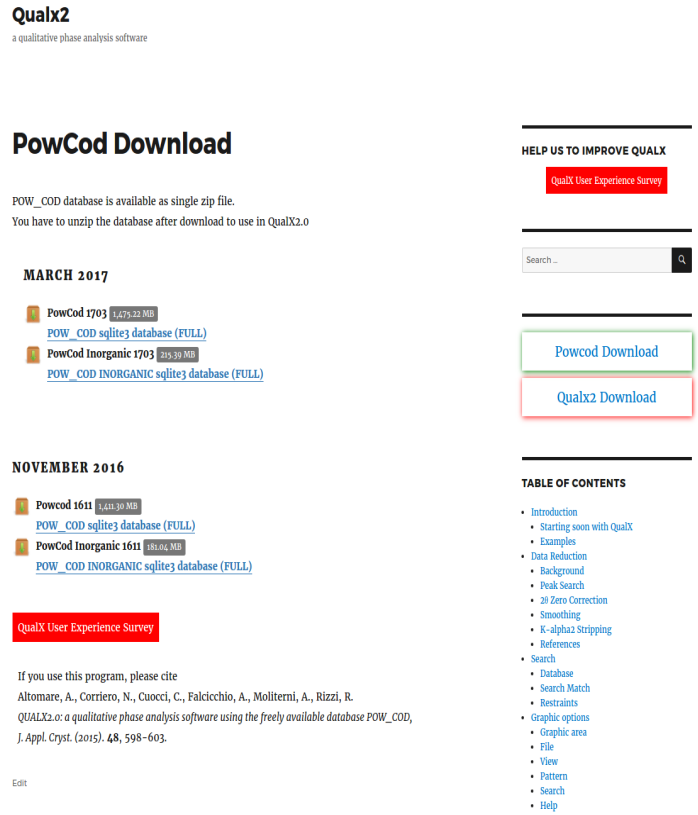

Qualx2

a qualitative phase analysis software

PowCod Download

POW_COD database is available as single zip file.
You have to unzip the database after download to use in QualX2.0

MARCH 2017

PowCod 1703 1,475.22 MB
POW_COD sqlite3 database (FULL)
PowCod Inorganic 1703 215.39 MB
POW_COD INORGANIC sqlite3 database (FULL)

NOVEMBER 2016

Powcod 1611 1,411.30 MB
POW_COD sqlite3 database (FULL)
PowCod Inorganic 1611 181.04 MB
POW_COD INORGANIC sqlite3 database (FULL)

QualX User Experience Survey

If you use this program, please cite
Altomare, A., Corriero, N., Cuocci, C., Falcicchio, A., Moliterni, A., Rizzi, R.
QUALX2.0: a qualitative phase analysis software using the freely available database POW_COD,
J. Appl. Cryst. (2015). **48**, 598-603.

Edit

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QualX User Experience Survey

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Outline of the talk

Qualitative Analysis

Main aim

Remarks

Success

Databases

PDF

COD

The POW_COD database

QualX2.0

Features

Card

Download QualX2.0

Examples

QualXWeb

Research Group

Example 1: CPD2

(laboratory data - Philips X'Pert X-ray diffractometer, CuKα1,2 radiation)

CPD2 is a four-phase crystalline mixture belonging to a set of test mixtures prepared for a round robin on quantitative phase analysis (QPA) organized by the International Union of Crystallography (IUCr) Commission on Powder Diffraction (CPD).

Example 1: CPD2

(laboratory data - Philips X'Pert X-ray diffractometer, CuKα1,2 radiation)

CPD2 is a four-phase crystalline mixture belonging to a set of test mixtures prepared for a round robin on quantitative phase analysis (QPA) organized by the International Union of Crystallography (IUCr) Commission on Powder Diffraction (CPD).

Phase	**True w_T (%)**
corundum (Al_2O_3)	21.27
fluorite (CaF_2)	22.53
zincite (ZnO)	19.94
brucite [$Mg(OH)_2$]	36.26

Example 2: MIXT6.dat

MIXT_6.dat *(laboratory data, CuKα1 radiation)*. It is an example of a laboratory-prepared six-phase mixture. Its composition is: corundum, lanthanum hexaboride, zincite, calcite, potassium chloride, silicon.
The true weight fraction of each phase is equal to 16.67%.

Example 2: MIXT6.dat

MIXT_6.dat *(laboratory data, CuKα1 radiation)*. It is an example of a laboratory-prepared six-phase mixture. Its composition is: corundum, lanthanum hexaboride, zincite, calcite, potassium chloride, silicon.
The true weight fraction of each phase is equal to 16.67%.

Phase

corundum

lanthanum hexaboride

zincite

calcite

potassium chloride

silicon

Example 3: Pompei

Identification of crystalline phases in the case of materials of cultural heritage interest.

Casa della fontana grande - Pompei

(In cooperation with Dr. Fabio Galeandro,Soprintendenza di Pompei)

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Identification of crystalline phases in the case of materials of cultural heritage interest.

Casa della fontana grande - Pompei

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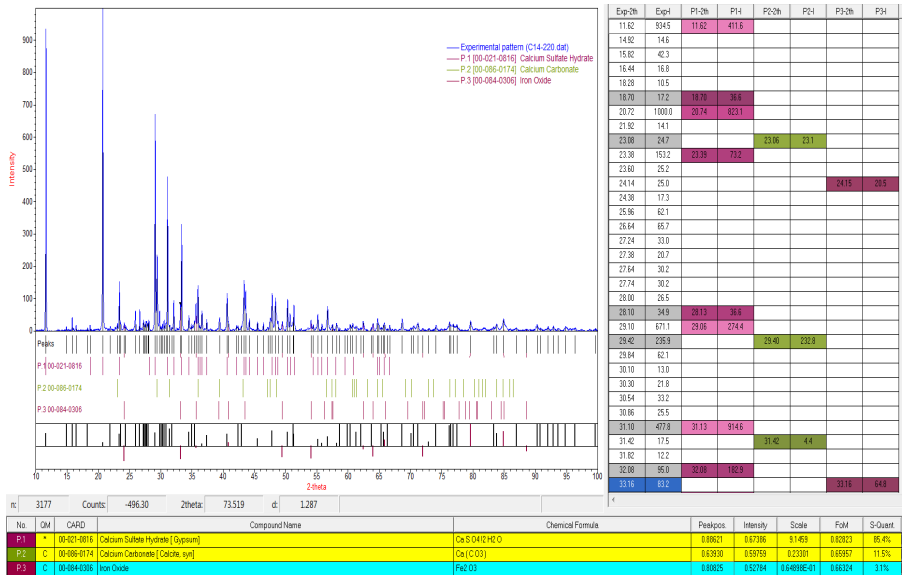
Phase

Gypsum
Calcite
Hematite
+minority phases



Final remarks

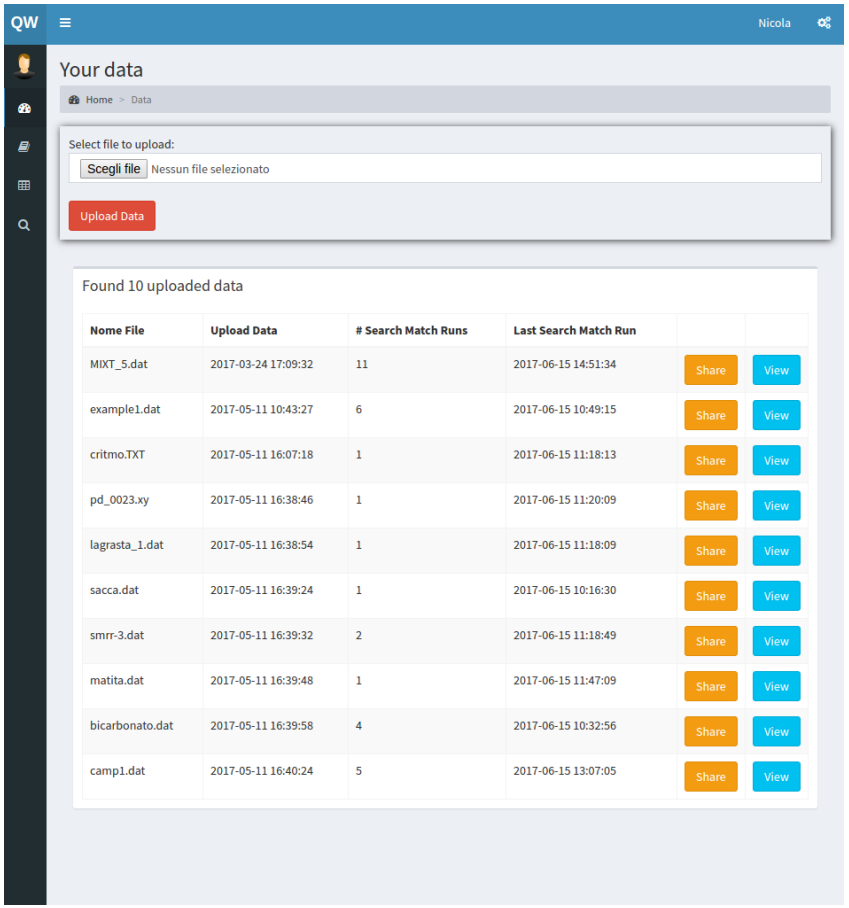
- X-ray powder diffraction is widely applied for phase identification of crystalline compounds;
- The success of phase identification can be strongly influenced by the quality of the experimental diffraction data and the completeness of the qualitative analysis database;
- **POW_COD** is a freely available database for qualitative analysis built from the crystallographic information supplied by the **COD** database CIF files;
- **QUALX2.0**, the updated version of **QUALX**, is the only software, in the panorama of qualitative analysis computer programs, to be freely available and able to inquire a freely available database (**POW_COD**).

QualXWeb

Features

User can:

- upload data on web server;
- perform search-match;
- share data with other people;
- carried out search with restraints.

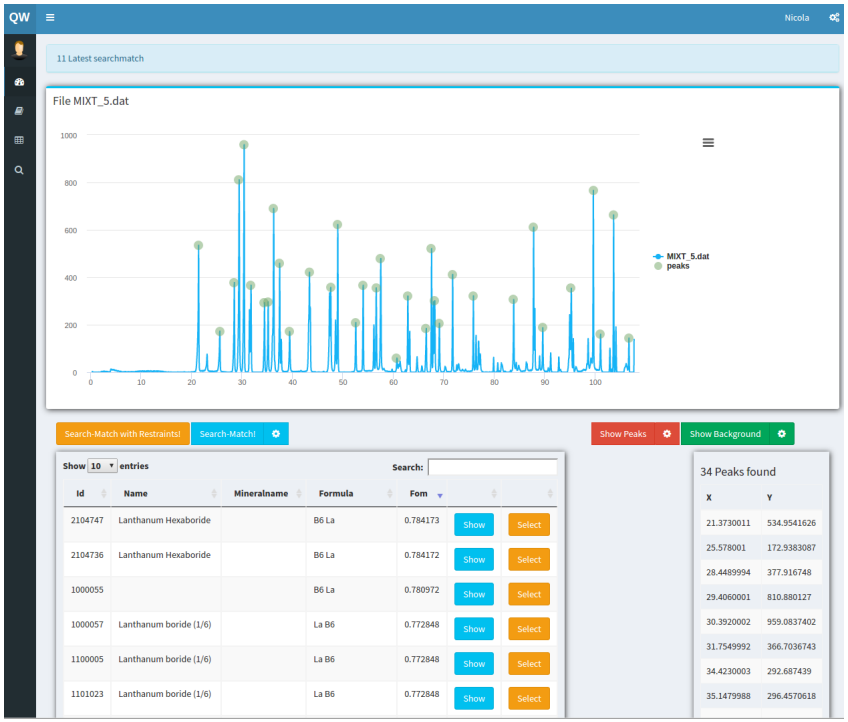


QualXWeb

Search-match results

User can:

- manage background refinement;
- perform peaks search;
- launch search-match;
- reload old search-match results.

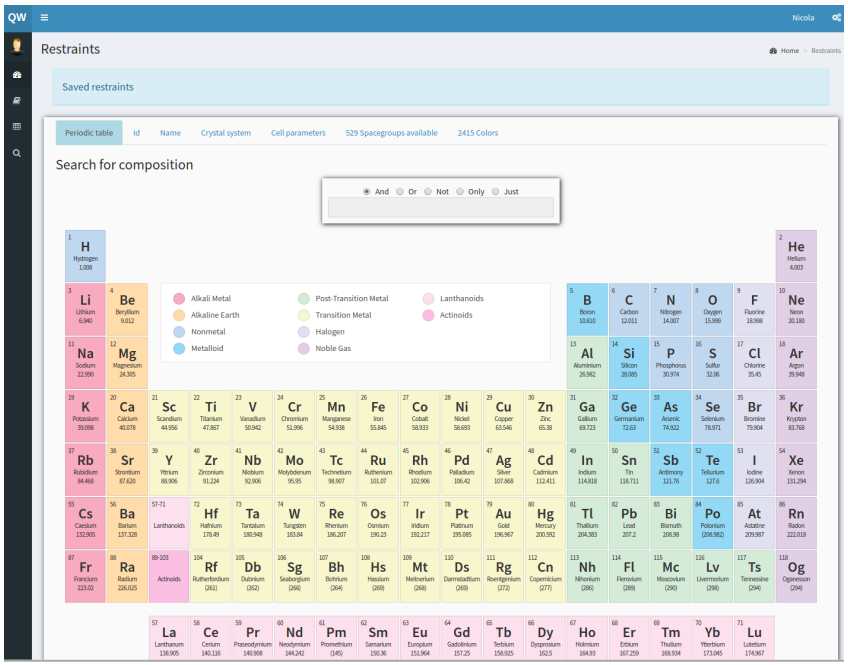


QualXWeb

Restraints

User can filter cards according to:

- chemical composition;
- card id;
- card name;
- crystal system;
- cell parameters;
- space group.



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