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CONCEPT OF STRUCTURAL TYPES IN THE INORGANIC CRYSTAL STRUCTURE DATABASE (ICSD)

F. Laufek

Czech Geological Survey, Geologická 6, 152 00 Praha 5
Institute of Physics of the AS CR, v.v.i., Na Slovance 2, 182 21, Praha 8, Czech Republic
frantisek.laufek@geology.cz

The Inorganic Crystal Structure Database (ICSD)

The Inorganic Crystal Structure Database (ICSD) is the world's largest database for completely determined inorganic crystal structures. It is developed and maintained by Fachinformationszentrum Karlsruhe (FIZ), Germany. The database offers an extensive collection of known inorganic crystal structures published since 1913 including their atomic coordinates [1]. A typical entry includes the chemical name, formula, unit cell, space group, complete atomic parameters, atomic displacement parameters, site occupation factors and complete literature citation. In addition to the structural data of inorganic compounds, the database also provides information on useful structural descriptors (e.g. Pearson symbol, ANX formula, Wyckoff sequences, mineral name) and synthesis conditions. The atomic coordinates of all structures contained in ICSD have been fully determined or were derived from the corresponding structure types. The current release (2015/1) contains 177 373 crystal structures [1]. The structural data are extracted by regular scanning of scientific journals, bibliographic databases and internet publications. The database is updated twice a year; each time is added approximately 3 500 new entries. The entries are tested for formal errors, plausibility and logical consistency. The ICSD database is offered with two different retrieval interfaces: the off-line *FindIt* interface and the stand-alone web portal (ICSD web).

Different degrees of similarity between inorganic structures

The theoretical concepts for definition of a structural type and different degrees of similarities between inorganic structures were defined in the report of the IUCr Commission on Crystallographic Nomenclature [2]. The report defines two most important terms, which define different degree of similarity between inorganic structures – *isopotential* and *isoconfigurational* structures. According to the report [2], two structures are *isopotential* if:

- they have the same space group or belong to a pair of enantiomorphic space groups;
- the atomic positions, occupied either fully or partially at random, are the same in the two structures, i.e. the complete sequence of the occupied Wyckoff positions is the same for the two structures when the structural data have been standardized.

The group of isoconfigurational structures can be viewed as a subgroup of isopotential structures. Two structures are *isoconfigurational* if [2]:

- they are isopotential
- for all corresponding Wyckoff positions, both the crystallographic point configurations and their geometrical interrelationships are similar.

These conditions require the entire configuration of the two isoconfigurational structures to be similar. Consequently, all geometrical properties, such as axial ratios, angles between crystallographic axes, values of corresponding adjustable positional parameters (x , y , z) and coordinations of corresponding atoms are similar.

The introduction of the structure types into the ICSD database

Since 2005, FIZ Karlsruhe began to introduce structure types into the ICSD database [3]. In the ICSD database, two crystal structures are regarded as *isostructural* (i.e. they belong to the same structure type) if they are *isoconfigurational*. For zeolite crystal structures, only the framework atoms are taken into account in the determination of isoconfigurational structures. Hence, the determination of the isoconfigurational structures in the ICSD database consists of two steps [3]:

1. Determination of isopotential structures
2. Subdivision of isopotential structures into the different structural types by means of additional structural descriptors.

For this subdivision, the following criteria are used:

- (i) crystallographic composition type (ANX formula);
- (ii) range of c/a ratio;
- (iii) beta range;
- (iv) necessary elements (combined by “and” or “or”);
- (v) forbidden elements (combined by “and” or “or”);
- (vi) atomic coordinates.

The criteria (iv) and (v) take into consideration the crystal chemistry: same elements occur in representative of a given type (e.g. O in oxide structures or F, Cl, Br, I in halides), whereas O in intermetallics is the forbidden element [3]. The criteria i-v are sufficient for separation and assignment of most structure types. Only in a few cases, the atomic coordinates must be checked as an additional criterion (vi). A final criterion that must be fulfilled before a new structure type is introduced into the ICSD database is that it must represent the structures of at least three different compounds with the same given structure [3]. The prototype of the structure type is an arbitrary chosen representative of this structure type, mostly one of the early published structures. The current release of the ICSD database (2015/1) contains 177 373 structures. More than

143 500 ICSD entries have now been assigned to 9 136 distinct structure types. The most frequent are spinel (Al_2MgO_4), halite (NaCl) and perovskites (CaTiO_3 and GdFeO_3).

1. http://www.fiz-karlsruhe.de/icsd_home.html
2. J. Lima-de-Faria, E. Hellner, F. Libeau, E. Makovicky, E. Parthé, *Acta Cryst.*, **A46**, (1990), 1.
3. R. Allman & R. Hinek, *Acta Cryst.*, **A63**, (2007), 412.

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USE OF POWDER DIFFRACTION FILE – PDF- 4+, OPEN STRUCTURAL DATABASES

R. Kužel

Charles University in Prague, Faculty of Mathematics and Physics, Ke Karlovu 5, 121 16 Praha 2

Inorganic structural databases and related databases were described for example in [1]. However, the text needs some updates.

Powder Diffraction File - PDF

The database has already long history. It was started in a form of card sets – ASTM in Fifties, later on as JCPDS and in last decades it is called PDF. It is developed, edited and maintained by the ICDD - the International Centre for Diffraction Data [2] and it is now offered in several versions declared as follows.

Table 1. PDF versions available.

Version	Brief characterization	Entries in 2014
PDF-4+	the most comprehensive database designed for phase identification and quantitative analysis of inorganic materials	354 264
WebPDF-4+	provides portability of the PDF-4+ database via the Internet	354 264
PDF-2	is designed for phase identification of inorganic materials	274 443
PDF-4+/Organics	is a comprehensive database for phase identification combining both single crystal and powder diffraction data for organics and organometallics	494 966
PDF-4+/Minerals	is the most comprehensive collection of mineral data with nearly 97% of all known mineral types	41 423

Single license of the first four versions for one year is 8 660 USD (5 775 USD for Academics), one year renewal for 1 760 USD (1 150 USD). See icdd.com for 3-year, 5-year or site licenses.

In the following paragraphs some text from the website (icdd.com) is used.

Release 2014 of the Powder Diffraction File (PDF) contains 799,700+ unique material data sets. Each data set contains diffraction, crystallographic and bibliographic data, as well as experimental, instrument and sampling conditions, and select physical properties in a common standardized format.

Traditional form of the database is **PDF-2** and it is a collaborative product between ICDD, FIZ (Karlsruhe) and NIST (National Institute of Standards). It is designed for inorganic materials analyses. Many common organic materials from ICDD are added to this database to facilitate rapid material identification. It must be take into account that quite often more records correspond to single phase. Each record contains table of interplanar spacings (d), relative intensities (I) and often also diffraction indices (hkl). In addition, chemical formula, chemical name, mineral name for minerals, crystal system, some physical characteristics, experimental parameters, bibliographic information and mark of data quality. The PDF-2 licence is lifetime, of course, without updates.

Preferred form of database distribution is now **PDF-4+**. It is designed for both phase identification and quantitative analysis. It contains the data from both the PDF-2 and ICDD's collaboration with MPDS. This database has comprehensive material coverage for inorganic materials and it contains numerous additional features such as digitized patterns, molecular graphics, and atomic parameters. Some features were included to enhance the ability to do quantitative analysis using third party software by any of three methods: Rietveld Analysis, Reference Intensity Ratio (RIR) Method or Total Pattern Analysis. In latest version, the ICDD added modulated entries with atomic coordinates. In 2015, new molecular graphics that visualize various modulations will be included. These entries are part of the new data source, designated '05', which contains crystal structures abstracted and quality checked by ICDD.

The database has the following features (2014)

- All 354,264 entries have digital patterns for use in total pattern analysis
- 258,125 entries have I/I_c values for quantitative analysis by Reference Intensity Ratio (RIR)
- 239,568 entries with atomic coordinates for quantitative analysis by the Rietveld method

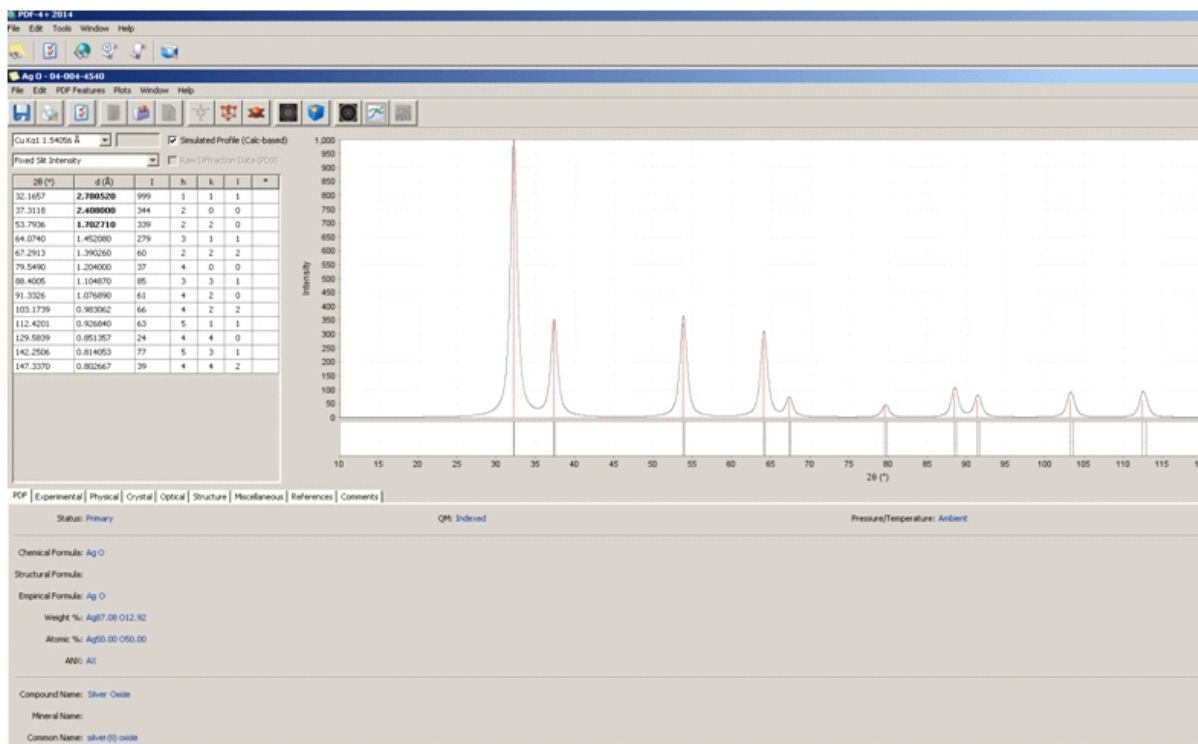


Figure 1. Example of search output for one phase with *d*-spacings, intensities, *hkl* indices and simulated powder pattern.

- Experimental digital reference patterns for non-crystalline materials

The PDF-4 license is strictly limited to a single computer (for single license) and also time limited. If expired, nothing works.

WebPDF-4+ provides the needed portability for accessing the PDF-4+ database via the internet. It enables full functionality of the PDF-4+ database using a high-speed internet connection. WebPDF-4+ is delivered as a USB compatible dongle.

PDF-4/Organics is a highly targeted database with the world’s largest collection of pharmaceutical excipients and polymer materials. It is designed for a multitude of applications in pharmaceutical, regulatory, specialty chemical, biomaterial, and forensic fields. The product has all of the display software and data mining capabilities contained in the PDF-4 family of products.

Comparison of database features can be found at <http://www.icdd.com/products/pdf4-2-comparison.htm>

The ICDD and the collaborating database organizations each have editorial mechanisms for updating historic data. Updates are frequently made by authors. Corrections in the

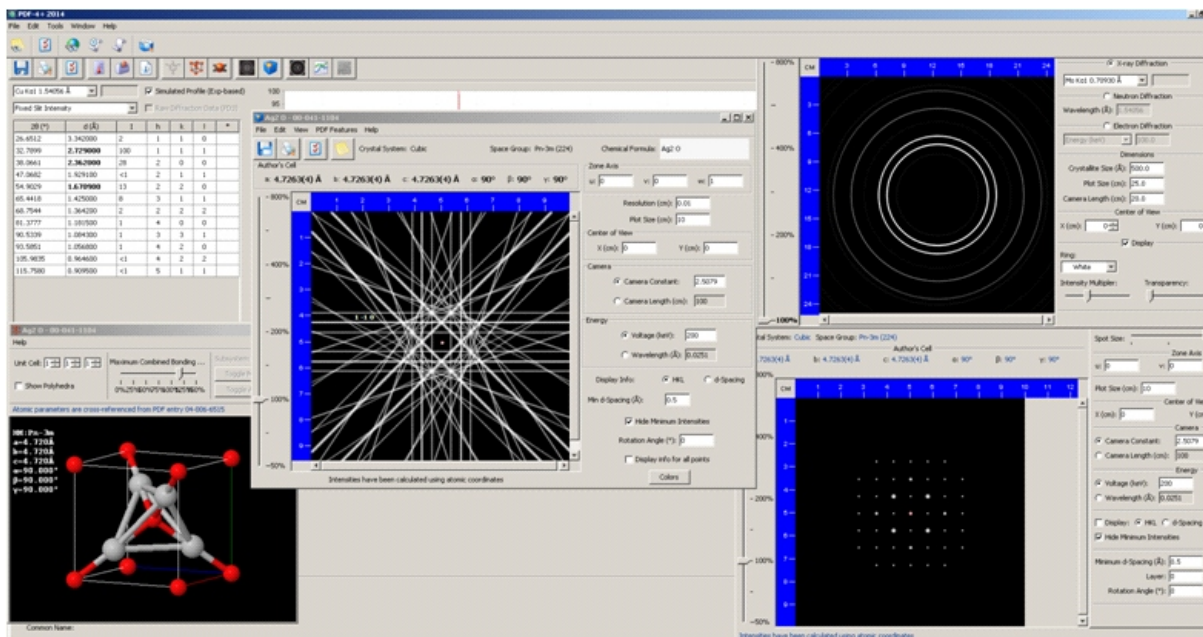


Figure 2. Example of search output for one phase. If structure is known (atomic coordinates), the structure can be visualized, Kikuchi lines, 2D diffraction pattern (back-reflection) and electron diffraction can be calculated.

data are made by users of the database or editorial reviewers. Typically, tens of thousands of historical entries are updated each year.

ICDD's search indexing programs, **SIeve** for PDF-2 and **SIeve+** for PDF-4, are designed to search and identify unknown materials. SIeve and SIeve+ are integrated into the ICDD databases to allow the use of the extensive data mining interfaces, searches, and sorts available to improve accuracy and precision of the identification process. For example, users can utilize the extensive permutable searches in each database, then define their own search subfile or use any of the "application or expert-defined" subfiles and subclasses to increase the accuracy of their phase identification. In many cases, this provides a unique capability to analyze the most difficult problems.

SIeve and SIeve+ offer a variety of algorithms and options that allow users to optimize results for particular chemistries and both standard and non-standard diffraction systems. SIeve and SIeve+ features automatic rotation of the eight strongest lines (Hanawalt) or the eight longest of the strongest lines (Fink) or the eight longest lines (Long8) to look for entries that exhibit the best Goodness of Match (GOM). In the last few years, new algorithms have been added to identify non-crystalline materials and complex multi-phase specimens. Most of the algorithms were developed and optimized for a particular type of analysis and the selection options provide the user with a wide breadth of analytical capability. Since the fundamental algorithms used by SIeve/SIeve+ are different than those used by most commercial software programs, they can be strongly complimentary.

Several useful presentations on the use of PDF can be downloaded from

<http://www.icdd.com/resources/tutorials/index.htm>

Some of them will be used during the presentation which will be focussed on new features and possibilities like to plot different graphs – dependencies in the database (for example, lattice parameters vs. stoichiometry, temperature etc.), using the approximate fields, multiple space group search, more powder diffraction pattern simulation options, experimental data corrections etc.

Open structural and related databases

A list of primary and secondary crystallographic databases can be found at <http://www.iucr.org/resources/data>. However, one is still missing there and it is the COD – Crystallography Open Database [3] that is - *Open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers* [4]. Currently (June 2015) there are 315 590 entries in the database which is fully open access as it has been constructed this way from the very beginning. Only simple search is available including basically text, up to 8 elements chemical search (Boolean logics), cell volume limits, journal, year, volume, issue, Z-limits, lattice parameters limits. However, then CIF files are available containing all necessary structural information as well as JSmol structure preview.

Mineralogical databases are essentially also open.

American Mineralogist Crystal Structure Database [5] 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. The interface offers chemistry, diffraction, lattice, author and mineral searches.

Mineralogy Database [6] contains 4714 minerals with a links and a comprehensive image library. Each mineral has a page linked to tables devoted to crystallography, crystal structures, X-Ray powder diffraction, chemical composition, physical and optical properties, Dana's New classification, Strunz classification, mineral specimen images, and alphabetical listings of mineral species. There also are extensive links to other external sources of mineral data and information. Structures can be visualized in Jmol applets.

Mincrust [7] the Russian database (Institute of Experimental Mineralogy, Moscow) was created in 1997 and it is called "Crystallographic and Crystallochemical Database for Mineral and their Structural Analogues" and can be entered via English or Russian gate. Currently it contains 9016 entries. It is a combination of structural database, theoretical powder patterns and software. Each entry has a mineral name, chemical formula, space group, lattice parameters, atomic coordinates, temperature factors, occupation and bibliographic information. Software package includes calculation of powder pattern or mixture of phases, standardless phase analysis, structure visualization etc.

Specia databases for zeolites can be found at [8].

Crystallographic server in Bilbao [9] provides information on space groups (e.g. generators of positions in individual space groups, subgroups etc.) similar to the information in International Tables for Crystallography vol. 1. It is continuously developed and it is also a base for theoretical crystallography.

Data of general interest like periodic element tables can be found at [10-12]. The last one [20] is focused on X-ray characteristics.

Pearson's Crystal Data

In the end one commercial database should be mentioned and this is Pearson's Crystal Data – crystal structure database for inorganic compounds [13]. The database is published by [ASM International](#) (Materials Park, Ohio, USA), edited by Pierre Villars and Karin Cenzual. It contains crystal structures of a large variety of inorganic materials and compounds. The "PCD" (as it is typically abbreviated) is a collaboration between ASM International and [Material Phases Data System](#), Vitznau, Switzerland (MPDS), aiming to create and maintain the world's largest critically evaluated "Non-organic database". The current release contains nearly 258,500 structural data sets (including atom coordinates and displacement parameters, when determined) for about 150,000 different chemical formulas, roughly 16,800 experimental powder diffraction patterns and about 232,000 calculated patterns (interplanar spacings, intensities, Miller indices).

Main advantage is very user –friendly software with many features which allows really easy work. It all structural information, list of distances, structure 3D visualization, powder pattern simulation, selection criteria, entry



data sheet etc. from a single page. It includes the so-called perpetual restraining giving estimation of results during defining search criteria. We have an experience that users in our lab and newcomers usually select primarily this database for their work.

1. R. Kužel, S. Daniš, *Materials Structure*, **14** (2007) 89-96.
2. International Centre for Diffraction Data – <http://icdd.com>
3. <http://www.crystallography.net/>
4. S. Grazulsi et. al. *J. Appl. Cryst.* **42** (2009) 726-729. [Open access](#)
5. <http://ruff.geo.arizona.edu/AMS/amcsd.php>
6. <http://webmineral.com/>
7. <http://database.iem.ac.ru/minicryst/>
8. <http://www.iza-structure.org/databases/>
9. <http://www.cryst.ehu.es>
10. <http://www.webelements.com/>
11. <http://www.physics.nist.gov/PhysRefData/Elements/cover.html>
12. <http://www.csrii.iit.edu/periodic-table.html>
13. <http://www.crystalimpact.com/pcd/>

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ŘEŠENÍ STRUKTUR Z LABORATORNÍCH PRÁŠKOVÝCH DIFRAKČNÍCH DAT - TRENDY, MOŽNOSTI, PŘÍKLADY

Jan Rohlíček

Fyzikální ústav AV ČR, v. v. i. Na Slovance 1999/2, 182 21 Praha 8

Řešení struktur z laboratorních RTG práškových difrakčních dat již nějakou dobu není nic neobvyklého. Dnes lze s lehkým srdcem říci, že pro jednoduché a dobře difrakující látky je řešení její krystalové struktury spíše rutinní záležitostí. Instrumentální rozšíření reflexí je u laboratorních přístrojů přibližně o řád vyšší, než u difraktometru na synchrotronu. Ani intenzita a kvalita záření laboratorního přístroje zdaleka nedosahuje takové úrovně jako synchrotronové záření. I přes tyto nedostatky jsou laboratorní přístroje dobrou konkurencí synchrotronovým zdrojům, zejména kvůli jejich dostupnosti. Svědčí o tom i následující statistika: z celkového počtu 3049 vyřešených struktur z práškových dat v CSD databázi obsahujících 3D souřadnice atomů (ver. 5.36, update 1) je přibližně jen asi 31% z nich označena jako synchrotronová data.

Existují tři obecné skupiny metod pro řešení struktur z difrakčních dat – (i) metody přímé (metody recipročního prostoru), (ii) metody přímého prostoru a (iii) metody „dual-space“. Zatímco metody přímého prostoru (ii) byly a jsou výhradně používány pro řešení struktur z práškových dat, zbylé metody (i) a (iii) byly původně vyvinuty pro řešení struktur z monokrystalových dat a pak následně byly upravovány pro prášková data tak, aby dosahovaly vyšší úspěšnosti.

Pro použití přímých metod je potřeba naměřit kvalitní práškový difrakční záznam nejlépe alespoň do atomárního rozlišení (<1.0, někdy dokonce jen <1.2 Å) a s úzkými profily reflexí, aby nedocházelo k výraznému překryvu reflexí. V současné době asi nejznámějším programem, který používá přímé metody pro řešení struktur z práškových dat, je program EXPO (Altomare *et al.*, 2013).

Zástupce dual-space metod je algoritmus charge-flipping (Osžlányi a Suto, 2004). Pro prášková data je zajímavá jeho kombinace s metodou histogram matching (Baerlocher *et al.*, 2007). V tomto případě jsou překryté intenzity, které bývají obvykle zatíženy značnou chybou, upravovány na základě histogramu zadané elektronové hustoty, např. podobné látky. Tato kombinace umožňuje řešit i struktury čistě organických látek (Sisak *et al.*, 2014).

Asi nepoužívanějšími metodami pro řešení krystalové struktury z práškových difrakčních dat jsou metody přímého prostoru, též nazývané jako metody globální optimalizace. Tyto metody byly vyvinuty právě pro řešení struktur z práškových dat v 90. letech a jejich vývoj bouřlivě pokračoval s rostoucím výkonem počítačů zejména mezi léty 2000 až 2010 (Shankland *et al.* 2013; Černý a Favre-Nicolin, 2007). Metody přímého prostoru se nesnaží vyřešit strukturu ze separovaných intenzit jednotlivých reflexí, ale pokoušejí se modifikovat zadaný počáteční model tak, aby jeho teoretický difrakční záznam vysvětloval změřená data. Tyto metody lze teoreticky použít všude tam, kde známe přesné složení zkoumané látky. V praxi jsme ovšem omezeni časem potřebným k nalezení řešení, jinými slovy složitostí řešeného problému.

Obecně nelze říci, která metoda je nejlepší, záleží vždy na okolnostech, zejména na kvalitě dat a složitosti struktury. Máme-li ovšem jednoduchou krystalovou strukturu, která dobře difraktuje i do vyšších úhlů, s velkou pravděpodobností nebude nalezení pozic atomů problémem pro žádnou ze současných metod. V případě složitějších krystalových struktur naopak nemusí pomoci ani jedna metoda. V současné době mají nejsložitější struktury, které byly vyřešeny z prášku, obvykle více jak 30 nevodíkových atomů v asymetrické části buňky nebo o málo více než 30 stupňů volnosti. Na ukázkách postupu řešení takových struktur lze nastínit možný budoucí vývoj v práškové difrakci, jelikož pro jejich vyřešení je třeba používat dnes nestandardní postupy. Jedna z možností je kombinace několika stávajících metod, kdy se část vyřeší jednou metodou a tato informace se použije k dohledání zbylé struktury (Rivera *et al.*, 2014). Další ze zajímavých možností, jak získat více informací z naměřených dat, je využití anizotropní teplotní roztažnosti k separaci reflexí (Brunelli *et al.*, 2003). Nebo je možné modifikovat stávající algoritmy nebo zkoušet úplně nové (Shankland *et al.* 2010, Habermehl *et al.*, 2014). Někdy „stačí“ nad řešením dlouho přemýšlet a využít pak všechny známé

nebo nejvíce pravděpodobné hodnoty neznámých proměnných, pak lze vyřešit i takovou krystalovou strukturu, která má 36 nevodíkových atomů v asymetrické části buňky a 45! stupňů volnosti (Rukiah et al., 2004).

Altomare A., Cuocci C., Giacobozzo C., Moliterni A., Rizzi R., Corriero N., Falcicchio A. (2013). *J. Appl. Cryst.* **46**, 1231-1235.

Baerlocher Ch., McCusker L. B., Palatinus L. (2007). *Z. Kristallogr.* **222**(2), 47-53.

Cerny R., Favre-Nicolin V. (2007). *Z. Kristallogr.* **222** 105-113.

Habermehl S., Morschel P., Eisenbrandt P., Hammer S.M., Schmidt M.U. (2014). *Acta Cryst.* **B70**, 347-359.

Oszlányi, G. & Suto, A. (2004). *Acta Cryst.* **A60**, 134-141.

Rukiah M., Lefebvre J., Hernandez O., van Beeke W., Serpelloni M. (2004). *J. Appl. Cryst.* **37**, 766-772.

Rivera A., Rohlíček J., Sadat-Bernal J., Ríos-Motta J., Dušek M. (2014). *Z. Kristallogr.* **229**(4), 319-327.

Sisak D., Baerlocher Ch., McCusker L.B., Yoshinari T., Seebach D. (2014) *J. Appl. Crystallogr.* **47**, 1569-1576.

Shankland K., Spillman M.J., Kabova E.A., Edgeleya D.S., Shankland N. (2013). *Acta Cryst.* **C69**, 1251-1259.

Shankland K., Markvardsen A.J., Rowlatt C., Shankland N., David W.I.F. (2010). *J. Appl. Cryst.* **43**, 401-406.

Session VIII, Thursday, June 25

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DIVERSITY AND SYSTEMATICS OF STRUCTURES OF BINARY MIXTURES OF ORGANIC SEMICONDUCTORS

J. Novák¹, A. Hinderhofer², K. Broch², A. Gerlach², A. Aufderheide², R. Banerjee², J. Dieterle², C. Frank², S. Kowarik³, F. Schreiber²

¹CEITEC Masaryk University, Group of Functional Properties of Nanostructures, Kotlářská 2, bldg. 9, CZ-611 37 Brno, Czech Republic

²Inst. Für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen, Germany

³Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany
frank.schreiber@uni-tuebingen.de

In the past decades, organic semiconductors (OSC) have attracted interest of researchers for their possible applications in organic field effect transistors, organic photovoltaic (OPV), and organic light emitting diodes (OLEDs) [1, 2]. In many of these applications, several molecular components, typically donor-acceptor (D/A) combinations, are needed and their mixing behaviour plays a key role for the performance of the devices. As an example, in OPV devices, the size of the D/A domains for partially mixing OSCs has to be comparable to the effective charge carrier diffusion length for the effective charge carriers separation and their withdrawal towards electrodes. Recent research on OSCs mixing, stimulated by the device related importance of the topic, has also shown some new and unexpected results at the fundamental level.

The presentation will review recent findings in the field of OSCs mixing behaviour. We will focus on blends of small OSCs molecules in thin films prepared by co-evaporation on weakly interacting silicon substrates. At the very beginning, we shortly introduce some most studied OSCs and highlight the importance of the OSCs blends for device applications. Thereafter, we will mention the process of OSM thin film growth via organic molecular beam deposition and the X-ray scattering techniques employed in the structural studies on them, including X-ray specular reflectivity and grazing incidence X-ray diffraction [3].

The main part of the presentation will deal with crystal structure of binary mixtures of OSCs and how it is influenced by molecular interactions. Some structures of OSC blends find direct counterparts in the well explored ele-

mental systems, such as binary alloys, while other mixing scenarios are completely new and surprising. Similar to the elemental systems, phase separation, statistical mixing of molecular components, and formation of a new molecular compound phase, respectively, are observed for OSC mixtures [4]. However, in contrast to the elemental blends, not only interaction between molecular components of mixtures determines the realized mixing scenario but also the steric, i.e. shape, compatibility of the molecules plays an important role [4, 5]. Additionally, anisotropy of the shape and of the interaction potential of the OSC molecules can lead to an ordering anisotropy, where the mixed system shows periodicity only along a certain preferential direction [6].

1. *Physics of Organic Semiconductors*. Ed.: W. Brütting and C. Adachi, Wiley-VCH, Weinheim 2012, 2nd ed.
2. *Physical and Chemical Aspects of Organic Electronics*. (Ed.: C. Wöll), Wiley-VCH, Weinheim 2009.
3. U. Pietsch, V. Holý, T. Baumbach, *High Resolution X-ray Scattering: From Thin Films to Lateral Nanostructures*. New York: Springer 2009, 2nd ed.
4. A. Hinderhofer and F. Schreiber, *ChemPhysChem*, **13**, (2012) 628.
5. A. Opitz, J. Wagner, W. Brütting, A. Hinderhofer, F. Schreiber, *Phys. Status Solidi A*, **206**, (2009), 2683.
6. A. Aufderheide, K. Broch, J. Novák, A. Hinderhofer, R. Nervo, A. Gerlach, R. Banerjee, and F. Schreiber, *Phys. Rev. Lett.*, **109**, (2012), 156102.