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RESPONSIBLE EDITORS

Evgeny Antipov, Moscow State University, Department of Chemistry, Moscow 119991, Russia

Email: antipov@icr.chem.msu.ru; Fax: +7-495-9 39 47 88

Ulrich Bismayer, Universität Hamburg, Mineralogisch-Petrographisches Institut, Grindelallee 48, 20146 Hamburg, Germany

Email: ubis@uni-hamburg.de; Fax: +49-40-4 28 38-24 22

Hubert Huppertz, University of Innsbruck, Institute of General, Inorganic and Theoretical Chemistry, Innrain 52a, 6020 Innsbruck, Austria

Email: hubert.huppertz@uibk.ac.at; Fax: +43-512-507-29 34

Václav Petříček, Institute of Physics ASCR v.v.i., Cukrovarnicka 10, 162 00 Praha 6, Czech Republic

Email: petricek@fzu.cz; Fax: +42 0-2 33-34 3-1 84

Rainer Pöttgen, Universität Münster, Institut für Anorganische Chemie, Corrensstraße 30, 48149 Münster, Germany

Email: pottgen@uni-muenster.de; Fax: +49-2 51-83-3 60 02

Wolfgang W. Schmahl, Ludwig-Maximilians-Universität Munich, Applied Crystallography and Materials Science, Department of Earth- and Environmental Sciences, Theresienstraße 41, 80333 Munich, Germany

Email: wolfgang.schmahl@lrz.uni-muenchen.de; Fax: +49-89-21 80-43 34

Edward R. T. Tiekink, Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Email: Edward.Tiekink@gmail.com

Xiaodong Zou, Stockholm University, Department of Materials and Environmental Chemistry Berzelii center EXSELENT on Porous Materials, 106 91 Stockholm, Sweden

Email: xiaodong.zou@mmk.su.se; Fax: +46-8-15 21 87

JOURNAL MANAGER Birgit Zoglmeier, Oldenbourg Wissenschaftsverlag GmbH, a company of De Gruyter, Rosenheimer Str. 143, 81671 München, Germany, Tel.: +49 (0)89 76902-426, Fax: +49 (0)89 76902-491, Email: birgit.zoglmeier@oldenbourg-verlag.de

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Tel.: +49 (0)89 769 02-394, Fax: +49 (0)89 769 02-350, Email: Panagiota.Herbrand@degruyter.com

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COVER ILLUSTRATION *Front cover* with the friendly assistance of Rainer Pöttgen and Václav Petříček. Crystallographic Computing System JANA2006: General features (cf. Graphical Abstract Figure of Petříček, Dušek & Palatinus, pp. 345–352, this issue).



Graphical Synopsis

Review Article

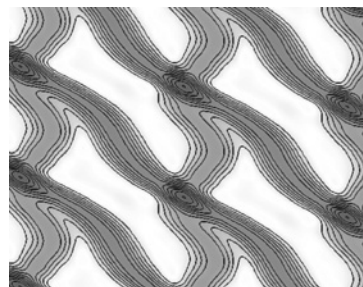
Václav Petříček, Michal Dušek and Lukáš Palatinus

Crystallographic Computing System JANA2006: General features

DOI 10.1515/zkri-2014-1737

Z. Kristallogr. 2014; 229(5): 345–352

Synopsis: JANA2006 is a crystallographic software for calculation of standard, modulated and magnetic structures from X-ray, neutron or electron diffraction data. The article summarizes features and possibilities of its latest version.



Inorganic Crystal Structures

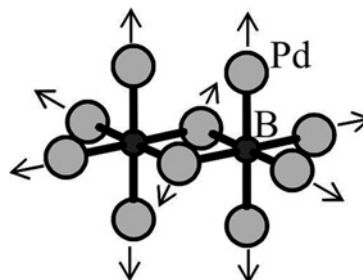
Andreas Leineweber, Tilmann Georg Berger, Alexander Udyansky, Volodymyr N. Bugaev and Viola Duppel

The incommensurate crystal structure of the $\text{Pd}_5\text{B}_{1-z}$ phase; B ordering driven by elastic interaction between B atoms

DOI 10.1515/zkri-2013-1710

Z. Kristallogr. 2014; 229(5): 353–367

Synopsis: The incommensurately modulated crystal structure of $\text{Pd}_5\text{B}_{1-z}$ is characterised by B ordering involving occurrence of B_2Pd_{10} double octahedra due to the predominance of elastic interaction between the B atoms.



Organic and Metalorganic Crystal Structures

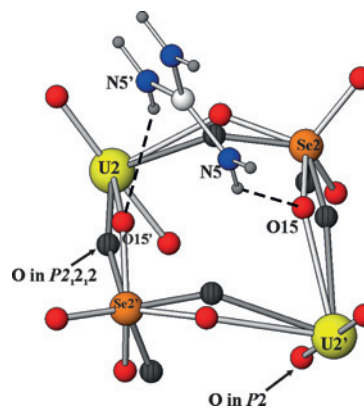
Vladislav V. Gurzhiy, Darya V. Tyshchenko, Sergey V. Krivovichev and Ivan G. Tananaev

Symmetry reduction in uranyl compounds with $[(\text{UO}_2)_2(\text{TO}_4)_3]^{2-}$ ($T = \text{Se}, \text{S}, \text{Mo}$) layers: crystal structures of the new guanidinium uranyl selenate and methylammonium uranyl sulfate

DOI 10.1515/zkri-2013-1651

Z. Kristallogr. 2014; 229(5): 368–377

Synopsis: The symmetry reduction of the new guanidinium uranyl selenate and methylammonium uranyl sulfate is induced by the hydrogen-bond interactions of amine groups emanated from organic substructure with the oxygen atoms from the inorganic layered complexes.



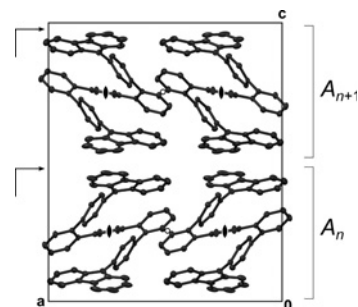
Berthold Stöger, Paul Kautny,
Daniel Lumpi, Erich Zobetz and
Johannes Fröhlich

**The pseudo-inversion symmetry of
9,9'-(1,3,4-oxadiazole-2,5-diyl)bis(1,1'-
biphenyl)-2',4-diyl)bis[9H-carbazole]
in the light of OD theory**

DOI 10.1515/zkri-2014-0001

Z. Kristallogr. 2014; 229(5): 378–384

Synopsis: The crystal structure of the title compound features pseudo-inversion strictly valid only for distinct layers. A parameter quantifying the deviation from perfect centrosymmetry is obtained by application of the order-disorder theory.



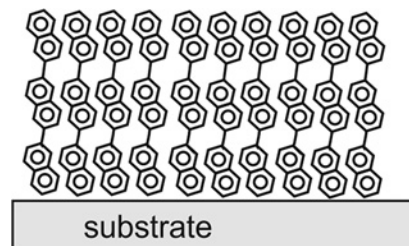
Alexander Pichler, Roland Resel,
Alfred Neuhold, Theo Dingemans,
Günther Schwabegger,
Massimo Moret, Clemens Simbrunner
and Ingo Salzmann

**Crystal structure determination
of organic thin-films: the example
of 2,2':6',2''-ternaphthalene**

DOI 10.1515/zkri-2013-1704

Z. Kristallogr. 2014; 229(5): 385–393

Synopsis: The solution of a crystal structure from a thin film is exemplarily shown for the molecule ternaphthalene using grazing incidence X-ray diffraction. The introduced method allows the study of specific polymorphs which are present only within thin films.



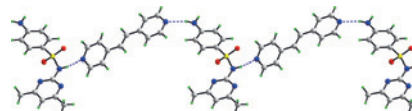
Hadi D. Arman, Trupta Kaulgud and
Edward R. T. Tiekink

**1:1 Co-crystals of sulfadimidine with
three bipyridine-type molecules:
Persistence of N–H...N hydrogen
bonded supramolecular chains**

DOI 10.1515/zkri-2013-1706

Z. Kristallogr. 2014; 229(5): 394–404

Synopsis: Non-linear supramolecular chains sustained by amino- and amide-H...N(pyridyl) hydrogen bonds feature in the co-crystals formed between sulfadimidine and pyridyl donors [4,4'-bipyridine, 4-[(E)-2-(pyridin-4-yl)ethenyl]pyridine and 4-[2-(pyridin-4-yl)ethyl]pyridine].



Crystallographic Computing

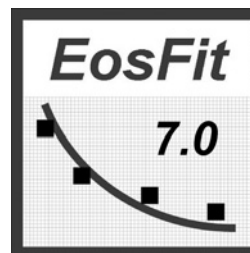
Ross J. Angel, Javier Gonzalez-Platas
and Matteo Alvaro

**EosFit7c and a Fortran module
(library) for equation of state
calculations**

DOI 10.1515/zkri-2013-1711

Z. Kristallogr. 2014; 229(5): 405–419

Synopsis: EosFit7c is a new program to perform EoS calculations and fitting for both volume and linear (unit-cell parameter) data in P, T and P-T. A new module for EoS calculations is provided in the CrysFML library.



Erratum

Author Index

Subject Index

Formulae Index