

List of Publications and Patents

Publications

- 141) Klaus Hunger, Martin U. Schmidt, Thomas Heber, Friedrich Reisinger, Stefan Wannemacher:
Industrial Organic Pigments: Production, Crystal Structures, Properties, Applications. 4th, completely revised edition,
Wiley-VCH, Weinheim, **2019**, ISBN: 978-3-527-32608-2.
- 140) Carina Schlesinger, Michael Bolte, Martin U. Schmidt*:
Challenging structure determination from powder diffraction data: two pharmaceutical salts and one cocrystal with $Z' = 2$,
Z. Kristallogr., **2018**, in press, doi: 10.1515/zkri-2018-2093.
- 139) Miriam Heine, Lothar Fink, Martin U. Schmidt*:
3-Cyanopyridine as a bridging and terminal ligand in coordination polymers,
CrystEngComm, **2018**, 20, 7556-7566.
- 138) B. Dittrich*, F. P. A. Fabbiani, J. Henn, M. U. Schmidt, P. Macchi, K. Meindl, M. A. Spackman:
Azulene revisited: solid-state structure, invariom modeling and lattice-energy minimization of a classical example of disorder,
Acta Cryst. Sect. B, Struct. Sci., **2018**, B74, 416-426.
- 137) Alexander Bodach, Lothar Fink, Martin U. Schmidt*:
Crystal structures of ordered and plastic-crystalline phases of iso-butyllithium by X-ray powder diffraction,
Chem. Commun., **2018**, 54, 10734-10737.
- 136) Carina Schlesinger, Lukas Tapmeyer, Silke D. Gumbert, Dragica Prill, Michael Bolte, Martin U. Schmidt, Christoph Saal*:
Bestimmung der absoluten Konfiguration pharmazeutischer Wirkstoffe durch Röntgenpulverdiffraktometrie,
Absolute Configuration of Pharmaceutical Research Compounds Determined by X-ray Powder Diffraction,
Angew. Chem., **2018**, 130, 9289-9293,
Angew. Chem. Int. Ed., **2018**, 57, 9150-9153.
- 135) Christian Czech, Jürgen Glinnemann, Kristoffer E. Johansson, Michael Bolte, Martin U. Schmidt*:
On the stacking disorder of DL-Norleucine,
Acta Cryst. Sect. B, Struct. Sci., **2017**, B73, 1075-1084.

- 134) Jérôme Roeser*, Dragica Prill, Michael J. Bojdys, Pierre Fayon, Abbie Trewin, Andrew N. Fitch, Martin U. Schmidt, Arne Thomas*:
Anionic silicate organic frameworks constructed from hexacoordinate silicon centres,
Nature Chemistry, **2017**, 9, 977–982.
- 133) Daniela Hempler, Martin U. Schmidt, Jacco van de Streek*:
Validation of missed space-group symmetry in X-ray powder diffraction structures with dispersion-corrected density functional theory,
Acta Cryst. Sect. B, Struct. Sci., **2017**, B73, 756-766.
- 132) Christian Czech, Lena Kalinowsky, Martin U. Schmidt*:
Local structure and stacking disorder of chloro(phthalocyaninato)aluminium,
Acta Cryst. Sect. B, Struct. Sci., **2017**, B73, 744-755.
- 131) Ira V. Rozhdestvenskaya, Enrico Mugnaioli*, Marco Schowalter, Martin U. Schmidt, Michael Czank, Wulf Depmeier*, Andreas Rosenauer:
The structure of denisovite, a fibrous nanocrystalline polytypic disordered ‘very complex’ silicate, studied by a synergistic multi-disciplinary approach employing methods of electron crystallography and X-ray powder diffraction,
IUCrJ, **2017**, 4, 223-242.
With cover picture.
- 130) Haishuang Zhao, Alexander Bodach, Miriam Heine, Yasar Krysiak, Jürgen Glinnemann, Edith Alig, Lothar Fink, Martin U. Schmidt*:
4-Cyanopyridine, a versatile mono- and bidentate ligand. Crystal structures of related coordination polymers determined by X-ray powder diffraction,
CrystEngComm, **2017**, 19, 2216-2228.
- 129) Franziska Fischer, Martin U. Schmidt, Sebastian Greisera, Franziska Emmerling*:
The challenging case of the theophylline–benzamide cocrystal,
Acta Cryst., Sect. C, Cryst. Struct. Commun., **2016**, 72, 217-224.
With cover picture.
- 128) Silke D. Gumbert, Meike Körbitzer, Edith Alig, Martin U. Schmidt*, Michelle R. Chierotti, Roberto Gobetto, Xiaozhou Li, Jacco van de Streek:
Crystal structure and tautomerism of Pigment Yellow 138 determined by X-ray powder diffraction and solid-state NMR,
Dyes and Pigments, **2016**, 131, 364-372.
- 127) Jaroslav L. Teteruk, Jürgen Glinnemann, Winfried Heyse, Kristoffer E. Johansson, Jacco van de Streek, Martin U. Schmidt*:
Local Structure in the Disordered Solid Solution of cis- and trans-Perinones,
Acta Cryst. Sect. B, Struct. Sci., **2016**, 72, 416-433.

- 126) Tatiana E. Gorelik*, Christian Czech, Sonja M. Hammer, Martin U. Schmidt:
Crystal structure of disordered nanocrystalline α^H -quinacridone determined by electron diffraction,
CrystEngComm, **2016**, *18*, 529-535.
With inside cover.
- 125) Dragica Prill, Pavol Juhás, Simon J. L. Billinge*, Martin U. Schmidt*:
Towards solution and refinement of organic crystal structures by fitting to the atomic pair distribution function,
Acta Cryst. Sect. A, Foundations and Advances, **2016**, *72*, 62-72.
- 124) Jürgen Brüning, Martin U. Schmidt*:
The determination of crystal structures of active pharmaceutical ingredients from X-ray powder diffraction data: a brief, practical introduction, with fexofenadine hydrochloride as example,
J. Pharm. Pharmacol., **2015**, *67*, 773-781.
- 123) C. Saal, M. Lange, C. Kuehn, H. Untenecker, A. Jonczyk, S. Peterson, G. Scholz, V. Buback, M. Dotzauer, H. Bauer, J. Foerster, J. Schumacher, A. Metz, M. Schmidt, K. Seemann:
Cilengitide – Exceptional pseudopolymorphism of a cyclic pentapeptide,
Eur. J. Pharm. Sci., **2015**, *71*, 1-11.
- 122) Sándor L. Bekö, Jan W. Bats, Martin U. Schmidt*:
One-dimensional zinc(II) fumarate coordination polymers,
J. Coord. Chem., **2015**, *21*, 118-129.
- 121) Sándor L. Bekö, Christian Czech, Marcus A. Neumann, Martin U. Schmidt*:
Determination of crystal structures and tautomeric states of 2-ammoniobenzenesulfonates by laboratory X-ray powder diffraction,
Z. Kristallogr., **2015**, *230*, 611-620.
- 120) Tatiana E. Gorelik*, Martin U. Schmidt, Ute Kolb, Simon J. L. Billinge:
Total-Scattering Pair-Distribution Function of Organic Material from Powder Electron Diffraction Data,
Microsc. Microanal., **2015**, *21*, 459-471.
- 119) Dragica Prill, Pavol Juhás, Martin U. Schmidt*, Simon J. L. Billinge*:
Modelling pair distribution functions (PDFs) of organic compounds: describing both intra- and intermolecular correlation functions in calculated PDFs,
J. Appl. Cryst., **2015**, *48*, 171-178.

- 118) Martin U. Schmidt*:
Nachruf: Prof. Dr. Erich F. Paulus,
GDCh Fachgruppe Analytische Chemie, Mitteilungsblatt, 2/2015, 33-34.
- 117) Philipp Mörschel, Martin U. Schmidt*:
Prediction of molecular crystal structures by a crystallographic QM/MM model with full space-group symmetry,
Acta Cryst. Sect. A, Foundations and Advances, 2015, 71, 26-35.
- 116) Yasar Krysiak, Lothar Fink*, Thomas Bernert, Jürgen Glinnemann, Martin Kapuscinski, Haishuang Zhao, Edith Alig, Martin U. Schmidt:
Crystal Structures and Polymorphism of Nickel and Copper Coordination Polymers with Pyridine Ligands,
Z. Anorg. Allg. Chem., 2014, 640, 3190-3196.
- 115) Susanne Wöhlert, Zbigniew Tomkowicz, Michal Rams, Stefan G. Ebbinghaus, Lothar Fink, Martin U. Schmidt, Christian Näther*:
Influence of the co-Ligand on the Magnetic and Relaxation Properties of Layered Cobalt(II) Thiocyanato Coordination Polymers,
Inorg. Chem., 2014, 53, 8298-8310.
- 114) H. C. Stephen Chan*, Grahame R. Woollam, Trixie Wagner, Martin U. Schmidt, Richard A. Lewis:
Can picolinamide be a promising cocrystal former?,
CrystEngComm, 2014, 16, 4365-4368.
- 113) Stefan Habermehl, Philipp Mörschel, Pierre Eisenbrandt, Sonja M. Hammer, Martin U. Schmidt*:
Structure determinations from powder data without prior indexing using similarity measure based on cross-correlation functions,
Acta Cryst. Sect. B, Struct. Sci., 2014, B70, 347-359.
- 112) Jaroslav L. Teteruk, Jürgen Glinnemann, Tatiana E. Gorelik, Anthony Linden, Martin U. Schmidt:
Explanation of the stacking disorder in the β -phase of Pigment Red 170,
Acta Cryst. Sect B, Struct. Sci., 2014, B70, 296-305.
- 111) Rangana Warshamanage, Anthony Linden, Martin U. Schmidt, Hans-Beat Bürgi:
Average structures of the disordered β -phase of Pigment Red 170: a single-crystal X-ray diffraction study,
Acta Cryst. Sect. B, Struct. Sci., 2014, B70, 283-295.
- 110) Sándor L. Bekő, Edith Alig, Martin U. Schmidt, Jacco van de Streek*:
On the correlation between hydrogen bonding and melting points in the inositols,
IUCrJ (Journal of the International Union of Crystallography), 2014, 1, 61-73.

- 109) Sándor L. Bekö, Silke D. Thoms, Martin U. Schmidt:
4,4'-{Diazenediylbis[(1,4-phenylene)bis(carbonyloxy)]}bis(2,2,6,6-tetramethylpiperidinyloxidanyl): the first crystal structure determination from powder data of a nitroxide radical,
Acta Cryst., Sect. C, Cryst. Struct. Commun., **2013**, C69, 1513-1515.
- 108) Sándor L. Bekö, Jan W. Bats, Edith Alig, Martin U. Schmidt:
The Influence of Different Solvents on 2-Ammonio-4-chloro-5-methylbenzenesulfonate, Including Its De- and Resulfonation,
J. Chem. Cryst., **2013**, 43, 655-663.
- 107) Susanne Wöhlert, Lothar Fink, Martin U. Schmidt, Christian Näther*:
Synthesis and Characterization of New 2D Coordination Polymers based on Mn(NCS)₂ and Ni(NCS)₂ with 1,2-Bis(4-pyridyl)-ethane as Co-Ligand,
Z. Anorg. Allg. Chem., **2013**, 639, 2186-2194.
- 106) Radha Bhola, Payam Payamyar, Daniel J. Murray, Bharat Kumar, Aaron J. Teator, Martin U. Schmidt, Sonja M. Hammer, Animesh Saha, Junji Sakamoto, A. Dieter Schlüter, Benjamin T. King*:
A Two-Dimensional Polymer from the Anthracene Dimer and Triptycene Motifs,
J. Am. Chem. Soc., **2013**, 135, 14134-14141.
- 105) Martin U. Schmidt*, Jürgen Glinnemann:
Explanation for the stacking disorder in tris(bicyclo[2.1.1]hexeno)benzene using lattice-energy minimisations,
Z. Kristallogr., **2013**, 227, 805-818.
- 104) Susanne Wöhlert, Lothar Fink, Martin Schmidt, Christian Näther*:
Exploration and synthesis of condensed coordination networks with modified magnetic properties,
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- 103) Bharat Kumar, Ruth L. Viboh, Margel C. Bonifacio, William B. Thompson, Jonathan C. Buttrick, Babe C. Westlake, Min-Soo Kim, Robert W. Zoellner, Sergey A. Varganov, Philipp Mörschel, Jaroslav Teteruk, Martin U. Schmidt, Benjamin T. King*:
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- 102) Sándor L. Bekö, David Urmann, Martin U. Schmidt*:
5'-Deoxy-5-Fluorouridine: Characterisation, Crystal Structure and Molecular Conformations Determined from X-Ray Powder Data,
J. Chem. Cryst., **2012**, 42, 933-940.

- 101) Sándor L. Bekö, Sonja M. Hammer, Martin U. Schmidt*:
Kristallstrukturen der Hydratstufen von Pigment Red 57:1,
Crystal Structures of the Hydration States of Pigment Red 57:1,
Angew. Chem., **2012**, *124*, 4814-4818,
Angew. Chem. Int. Ed., **2012**, *51*, 4735-4738.
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- 100) Jürgen Brüning, Tanja K. Trepte, Jan W. Bats, Martin U. Schmidt*:
Erythromycin A dimethyl sulfoxide disolvate 1.43-hydrate,
Acta Cryst., Sect. E, Struct. Rep. Online., **2012**, *E68*, o700-o701.
- 99) Sándor L. Bekö, Martin U. Schmidt*, Andrew D. Bond*:
An experimental screen for quinoline/fumaric acid salts and co-crystals,
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- 98) Sándor L. Bekö, David Urmann, Andrea Lakatos, Clemens Glaubitz, Martin U. Schmidt*:
Nimustine hydrochloride: the first crystal structure determination of a 2-chloroethyl-N-nitrosourea hydrochloride derivative by X-ray powder diffraction and solid-state NMR,
Acta Cryst., Sect. C, Cryst. Struct. Commun., **2012**, *C68*, o144-o148.
- 97) Jürgen Brüning, Dragica Podgorski, Edith Alig, Jan W. Bats, Martin U. Schmidt*:
Antidiarrhetic loperamide hydrochloride,
Acta Cryst., Sect. C, Cryst. Struct. Commun., **2012**, *C68*, o111-o113.
- 96) Alexandra K. Wolf, Stefan Brühne, Jürgen Glinnemann, Chunhua Hu, Michael T. Kirchner, Martin U. Schmidt*:
Local atomic order in sodium p-chlorobenzenesulfonate monohydrate studied by pair distribution function analyses and lattice-energy minimisations,
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- 95) Sándor L. Bekö, Jan W. Bats, Martin U. Schmidt*:
2-Ammonio-5-chloro-4-methylbenzenesulfonate, its 1-methyl-2-pyrrolidone and dimethyl sulfoxide monosolvates and a corrected structure of 2,2'-(1,4-phenylene)-di(4,5-dihydroimidazolium) bis(4-aminobenzene-sulfonate)dihydrate,
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- 94) Sándor L. Bekö, Silke D. Thoms, Michael Bolte, Martin U. Schmidt*:
Tizanidine and tizanidine hydrochloride: on the correct tautomeric form of tizanidine,
Acta Cryst., Sect. C, Cryst. Struct. Commun., **2012**, *C68*, o28-o32.
- 93) Christian Buchsbaum, Erich F. Paulus, Martin U. Schmidt*:
Crystal structures of thiazine-indigo pigments, determined from single-crystal and powder diffraction data,
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- 92) Jan Hüsche, Berce Dutağacı, Clemens Glaubitz, Tim Geppert, Gisbert Schneider, Meike Harms, C. C. Müller-Goymann, Lothar Fink, Martin U. Schmidt, Constanze Setzer, Jürgen Zirkel, Herbert Rebmann, Manfred Schubert-Zsilavecz, Mona Abdel-Tawab*: *Structural properties of so-called NSAID-phospholipid-complexes*, *Eur. J. Pharm. Sci.*, **2011**, *44*, 103-116.
- 91) Martin U. Schmidt*, Jürgen Brüning, Jürgen Glinnemann, Maximilian W. Hützlér, Philipp Mörschel, Svetlana N. Ivashevskaya, Jacco van de Streek, Dario Braga, Lucia Maini*, Michele R. Chierotti*, Roberto Gobetto: *Die thermodynamisch stabile Form von fester Barbitursäure: das Enol-Tautomer*, *The Thermodynamically Stable Form of Solid Barbituric Acid: The Enol Tautomer*, *Angew. Chem.*, **2011**, *123*, 8070-8072
Angew. Chem. Int. Ed., **2011**, *50*, 7924-7926.
- 90) Jan W. Bats*, Jürgen Brüning, Martin U. Schmidt: *1,5-Dianilinopentane-1,3,5-trione: a crystal structure containing two polymorphic domains*, *Acta Cryst., Sect. C, Cryst. Struct. Commun.*, **2011**, *C67*, o212-o218.
- 89) Jürgen Brüning, Edith Alig, Jacco van de Streek, Martin U. Schmidt*: *The use of dispersion-corrected DFT calculations to prevent an incorrect structure determination from powder data: the case of acetolone, C₁₁H₁₁N₃O₃*, *Z. Kristallogr.*, **2011**, *226*, 476-482.
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- 85) Yu Zhong Zhang, Kateryna Foyevtsova, Harald O. Jeschke, Martin U. Schmidt, Roser Valentí: *Can the Mott insulator TiOCl be metallized by doping? A first-principles study*, *Phys. Rev. Lett.*, **2010**, *104*, 146402/1-146402/4.

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- 79) Jürgen Brüning, Alexander Peters, Jan W. Bats, Martin U. Schmidt*:
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- 75) Karsten Sieg*, Elena Starokozhev, Martin U. Schmidt, Wilhelm Puettmann:
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- 73) Tatiana Gorelik, Martin U. Schmidt, Jürgen Brüning, Sándor Bekö, Ute Kolb*:
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