

## List of Publications and Patents of Prof. Dr. Martin U. Schmidt

July 2021

### Publications

- 153) Tatiana E. Gorelik\*, Stefan Habermehl, Aleksandr A. Shubin, Tim Gruene, Kaname Yoshida, Peter Oleynikov, Ute Kaiser, Martin U. Schmidt:  
*Crystal structure of copper perchlorophthalocyanine analysed by 3D electron diffraction*,  
*Acta Cryst.*, **2021**, B77, 662-675, doi.org/10.1107/S2052520621006806.
- 152) Lukas Tapmeyer, Daniel Eisenbeil, Michael Bolte, Martin U. Schmidt\*:  
*First crystal structure of a Pigment Red 52 compound: DMSO solvate hydrate of the monosodium salt*,  
*Acta Cryst.*, **2021**, E77, 402-405, doi.org/10.1107/S2056989021002577.
- 151) Maurice Beske, Stephanie Cronje, Martin U. Schmidt\*, Lukas Tapmeyer:  
*Disordered sodium alkoxides from powder data: crystal structures of sodium ethoxide, propoxide, butoxide and pentoxide, and some of their solvates*,  
*Acta Cryst.*, **2021**, B77, 68-82, doi.org/10.1107/S205252062001584X.
- 150) Fabian Jung, Manuela Thurn, Katharina Krollik, David Li, Jennifer Dressman, Edith Alig, Lothar Fink, Martin U. Schmidt, Matthias G. Wacker\*:  
*Sustained-release hot melt extrudates of the weak acid TMP-001: A case study using PBB modelling*,  
*Eur. J. Pharm. Biopharm.*, **2021**, 160, 23-34, doi.org/10.1016/j.ejpb.2021.01.007.
- 149) Lukas Tapmeyer, Michael Bolte, Michele R. Chierotti, Martin U. Schmidt\*:  
*Structure of the intermediates in the industrial separation of perinone isomers*,  
*Dyes and Pigments*, **2020**, 181, 108442, doi.org/10.1016/j.dyepig.2020.108442.
- 148) Carina Schlesinger, Sonja M. Hammer, Tatiana E. Gorelik, Martin U. Schmidt\*:  
*Orientalional disorder of monomethyl-quinacridone investigated by Rietveld refinement, structure refinement to the pair distribution function and lattice-energy minimizations*,  
*Acta Cryst.*, **2020**, B76, 353-365, doi: 10.1107/S2052520620003984.
- 147) Maurice Beske, Lukas Tapmeyer, Martin U. Schmidt\*:  
*Crystal structure of sodium ethoxide (C<sub>2</sub>H<sub>5</sub>ONa), unravelled after a 180 years*,  
*Chem. Commun.*, **2020**, 56, 3520-3523, doi: 10.1039/C9CC08907A.
- 146) Miriam Heine, Lothar Fink\*, Martin U. Schmidt:  
*4-Cyanopyridine complexes [MX<sub>2</sub>(4-CNpy)<sub>x</sub>]<sub>n</sub> (with X = Cl, Br and x = 1, 2): crystal structures, thermal properties and a comparison with [MX<sub>2</sub>(3-CNpy)<sub>x</sub>]<sub>n</sub> complexes*,  
*CrystEngComm*, **2020**, 22, 2067-2082, doi: 10.1039/C9CE02012H.
- 145) Martin U. Schmidt:

*Industrial organic pigments*, in: International Tables for Crystallography, Volume H, Powder Diffraction (Eds: C.J. Gilmore, J.A. Kaduk, H. Schenk), 1st edition, Wiley, **2019**, pp. 834-842. ISBN: 978-1-118-41628-0, doi: 10.1107/97809553602060000984.

- 144) 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.*, **2019**, 234, 257–268, doi: 10.1515/zkri-2018-2093.
- 143) Miriam Heine, Lothar Fink\*, Martin U. Schmidt:  
*Coordination compounds built up from  $M^{II}Cl_2$  and 3-cyanopyridine: double chains, single chains and isolated complexes,*  
*CrystEngComm*, **2019**, 21, 4305-4318, doi: 10.1039/C9CE00412B.
- 142) Inês C. B. Martins, Mariana Sardo, Edith Alig, Lothar Fink, Martin U. Schmidt, Luís Mafra\*, M. Teresa Duarte\*:  
*Enhancing adamantylamine solubility through salt formation: novel products studied by X-ray diffraction and solid-state NMR,*  
*Cryst. Growth Des.*, **2019**, 193, 1860-1873.
- 141) Klaus Hunger, Martin U. Schmidt:  
*Industrial organic pigments: production, crystal structures, properties, applications.*  
*4th, completely revised edition*, Wiley-VCH, Weinheim, **2018**, 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**, 234, 257-268, 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.  
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- 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.  
Mit Titelbild/With cover.
- 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  $\alpha^H$ -quinacridone determined by electron diffraction,*

*CrystEngComm*, **2016**, *18*, 529-535.

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- 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  $\beta$ -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  $\beta$ -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. Bekö, 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)<sub>2</sub> and Ni(NCS)<sub>2</sub> 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) Susanne Wöhlert, Lothar Fink, Martin Schmidt, Christian Näther\*:  
*Exploration and synthesis of condensed coordination networks with modified magnetic properties*,  
*CrystEngComm*, **2013**, *15*, 945-957.
- 104) Martin U. Schmidt\*, Jürgen Glinnemann:  
*Explanation for the stacking disorder in tris(bicyclo[2.1.1]hexeno)benzene using lattice-energy minimisations*,  
*Z. Kristallogr.*; **2012**, *227*, 805-818.
- 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\*:  
*Septulene: the heptagonal homologue of kekulene*,  
*Angew. Chem.*, **2012**, *124*, 12967-12972,  
*Angew. Chem. Int. Ed.*, **2012**, *51*, 12795-12800.  
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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*,  
*CrystEngComm*, **2012**, *14*, 1967-1971.
- 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*,  
*Z. Kristallogr.*, **2012**, 227, 113-121.
- 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*,  
*Acta Cryst., Sect. C, Cryst. Struct. Commun.*, **2012**, C68, o45-o50.
- 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*,  
*Z. Kristallogr.*, **2011**, 226, 822-831.
- 92) Jan Hüsich, Bercem Dutagaci, 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. Hützler, 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, C<sub>11</sub>H<sub>11</sub>N<sub>3</sub>O<sub>3</sub>*,  
*Z. Kristallogr.*, **2011**, 226, 476-482.
- 88) Sonja M. Hammer, Edith Alig, Lothar Fink, Martin U. Schmidt\*:  
*Predicted and experimental crystal structures of ethyl-tert-butyl ether*,  
*Acta Cryst., Sect. B, Struct. Sci.*, **2011**, B67, 155-162.

- 87) Jürgen Brüning, Anna Christine Petereit, Edith Alig, Michael Bolte, Jennifer B. Dressman, Martin U. Schmidt\*:  
*Characterization of a new solvate of risedronate,*  
*J. Pharm. Sci.,* **2011**, *100*, 863-873.
- 86) Christian Czech, Sonja M. Hammer, Boris Bonn, Martin U. Schmidt\*:  
*Adsorption sites, adsorption enthalpies and potential removal of terpenoids by atmospheric ice,*  
*Atmos. Environ.,* **2011**, *45*, 687-693.
- 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.
- 84) Alexandra K. Wolf, Jürgen Glinnemann, Lothar Fink, Edith Alig, Michael Bolte, Martin U. Schmidt\*:  
*Predicted crystal structures of tetramethylsilane and tetramethylgermane and an experimental low-temperature structure of tetramethylsilane,*  
*Acta Cryst., Sect. B, Struct. Sci.,* **2010**, *B66*, 229-236.
- 83) Sándor L. Bekö, Silke D. Thoms, Jürgen Brüning, Edith Alig, Jacco van de Streek, Andrea Lakatos, Clemens Glaubitz, Martin U. Schmidt\*:  
*X-ray powder diffraction, solid-state NMR and dispersion-corrected DFT calculations to investigate the solid-state structure of 2-ammonio-5-chloro-4-methylbenzenesulfonate,*  
*Z. Kristallogr.,* **2010**, *225*, 382-387.
- 82) Martin U. Schmidt\*, Erich F. Paulus, Nadine Rademacher, Graeme M. Day:  
*Experimental and predicted crystal structures of Pigment Red 168 and other dihalogenated anthanthrones,*  
*Acta Cryst., Sect. B, Struct. Sci.,* **2010**, *B66*, 515-526.
- 81) Jürgen Brüning, Desiree Heintz, Alke Meents, Michael Bolte, Martin U. Schmidt\*:  
*Monothioindigo, determined by microcrystal structure analysis,*  
*Acta Cryst., Sect. C, Cryst. Struct. Commun.,* **2010**, *C66*, o459-o462.
- 80) Jürgen Brüning, Edith Alig, Martin U. Schmidt\*:  
*Ezetimibe anhydrate, determined from laboratory powder diffraction data,*  
*Acta Cryst., Sect. C, Cryst. Struct. Commun.,* **2010**, *C66*, o341-o344.
- 79) Jürgen Brüning, Alexander Peters, Jan W. Bats, Martin U. Schmidt\*:  
*7-Methoxy-2,3-dioxo-1,4-dihydroquinoxalin-6-aminium chloride monohydrate,*  
*Acta Cryst., Sect. C, Cryst. Struct. Commun.,* **2010**, *C66*, o1-o4.
- 78) Jürgen Brüning, Edith Alig, Alke Meents, Jacco van de Streek, Martin U. Schmidt\*:  
*Structure determinations of three fluorescent organic pigments by powder diffraction and micro-crystal structure analysis,*  
*Z. Kristallogr.,* **2009**, *224*, 556-562.
- 77) Jürgen Brüning, Edith Alig, Jan W. Bats, Jacco van de Streek, Martin U. Schmidt\*:



*Crystal structure determination of N,N'-1,4-phenylenebis(3-oxobutanamide) from laboratory powder diffraction data,*  
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- 76) Jürgen Brüning, Jan W. Bats, Martin U. Schmidt\*:  
*2-Aminoterephthalic acid dimethyl ester,*  
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- 75) Karsten Sieg\*, Elena Starokozhev, Martin U. Schmidt, Wilhelm Puettmann:  
*Inverse temperature dependence of Henry's law coefficients for volatile organic compounds in supercooled water,*  
*Chemosphere*, **2009**, 77, 8-14.
- 74) Jürgen Brüning, Michael Bolte, Martin U. Schmidt\*:  
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*Acta Cryst., Sect. C, Cryst. Struct. Commun.*, **2009**, C65, o352-o356.
- 73) Tatiana Gorelik, Martin U. Schmidt, Jürgen Brüning, Sándor Bekö, Ute Kolb\*:  
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*Cryst. Growth Des.*, **2009**, 9, 3898-3903.
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*Two new cobalt(II) fumarates and a redetermination of tetraaquacobalt(II) fumarate monohydrate,*  
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- 71) Yurong Ma, Gerald Mehlretter, Carsten Plug, Nadine Rademacher, Martin U. Schmidt, Helmut Cölfen\*:  
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- 70) Yu-Zhong Zhang, Kateryna Foyevtsova, Harald O. Jeschke, Martin U. Schmidt, Roser Valentí:  
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- 69) Alexandra K. Wolf, Jürgen Glinnemann, Martin U. Schmidt\*, Jianwei Tong, Robert E. Dinnebier, Arndt Simon, Jürgen Köhler:  
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Vergleich von Atompaar-Verteilungsfunktionen mittels Kreuzkorrelationsfunktionen  
(Comparison of atomic pair distribution functions using cross-correlation functions)

*DE Application No. 10 2020 004 292.9, filed 17-07-2020.*

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Neue Kristallphasen von Flupirtin-Maleat  
(Novel crystal phases of flupirtine maleate)

*DE Application No. 10 2015 013 478 A1, filed 17-10-2015, published 20-04-2017;*

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Neue Kristallphasen von Pigment Orange 13  
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