

## List of Publications and Patents of Prof. Dr. Martin U. Piepenbring (formerly Schmidt)

June 2025

### Publications

This list also contains a few other major publications of the group of Martin U. Piepenbring, to which M.U. Piepenbring contributed, but is not listed as co-author. These publications are marked with "G".

- 168) Yaşar Krysiak\*, Sergi Plana-Ruiz, Lothar Fink, Edith Alig, Ulrich Bahnmüller, Ute Kolb, Martin U. Schmidt\*: *High temperature electron diffraction on organic crystals: in situ crystal structure determination of Pigment Orange 34*, *J. Am. Chem. Soc.*, **2024**, *146*, 9880-9887, <https://doi.org/10.1021/jacs.3c14800>.
- 167) Federica Bravetti, Robert Hühn, Simone Bordignon, Sylvia Reibeling, Martin U. Schmidt\*: *Crystal structure and tautomeric state of Pigment Red 48:2 from X-ray powder diffraction and solid-state NMR*, *Z. Kristallogr.*, **2024**, *239*, 283-297, <https://doi.org/10.1515/zkri-2023-0042>.
- 166) Federica Bravetti, Lukas Tapmeyer, Kathrin Skorodumov, Edith Alig, Stefan Habermehl, Robert Hühn, Simone Bordignon, Angelo Gallo, Carlo Nervi, Michele R. Chierotti, Martin U. Schmidt\*: *Leucopterin, the white pigment in butterfly wings: structural analysis by PDF fit, FIDEL fit, Rietveld refinement, solid-state NMR and DFT-D*, *IUCrJ*, **2023**, *10*, 448-463, [doi.org/10.1107/S2052252523004281](https://doi.org/10.1107/S2052252523004281).  
*With figure on the title cover.*
- 165) Jacco van de Streek\*, Svetlana N. Ivashevskaya, Martin U. Schmidt: *Crystal structures of two phases of Pigment Yellow 110 from X-ray powder diffraction data*, *Z. Kristallogr.*, **2023**, *238*, 217-223, [doi.org/10.1515/zkri-2023-0003](https://doi.org/10.1515/zkri-2023-0003).
- 164) Tatiana E. Gorelik\*, Sándor L. Bekö, Jaroslav Teteruk, Winfried Heyse, Martin U. Schmidt\*: *Analysis of diffuse scattering in electron diffraction data for the crystal structure determination of Pigment Orange 13, C<sub>32</sub>H<sub>24</sub>Cl<sub>2</sub>N<sub>8</sub>O<sub>2</sub>*, *Acta Cryst.* **2023**, *B79*, 122-137, [doi.org/10.1107/S2052520623000720](https://doi.org/10.1107/S2052520623000720).
- 163) Dominik Brey, Barbara Scherer, Martin U. Schmidt\*: *Lattice defects in quinacridone*, *Acta Cryst.* **2022**, *B78*, 763-780, [doi.org/10.1107/S205252062200779X](https://doi.org/10.1107/S205252062200779X).
- 162) Carina Schlesinger, Arnd Fitterer, Christian Buchsbaum, Stefan Habermehl, Michele R. Chierotti, Carlo Nervi, Martin U. Schmidt\*: *Ambiguous structure determination from powder data: four different structural models of 4,11-di-fluoro-quinacridone with similar X-ray powder patterns, fit to the PDF, SSNMR and DFT-D*, *IUCrJ*, **2022**, *9*, 406-424, [doi.org/10.1107/S2052252522004237](https://doi.org/10.1107/S2052252522004237).

Highlighted by a scientific commentary:

Angela Altomare:

*Solving molecular compounds from powder diffraction data: are results always reliable?*  
*IUCrJ*, **2022**, 9, 403–405, doi.org/10.1107/S2052252522006571.

- 161) A. I. Arns\*, D. Evans, R. Schiebel, L. Fink, M. Mezger, E. Alig, J. Linckens, K. P. Jochum, M. U. Schmidt, A. Jantschke, G. H. Haug:  
*Mesocrystalline architecture in hyaline foraminifer shells indicates a non-classical crystallisation pathway*,  
*Geochemistry, Geophysics, Geosystems*, **2022**, 23, e2022GC010445,  
doi.org/10.1029/2022GC010445.
- 160) Stefan Habermehl, Carina Schlesinger, Martin U. Schmidt\*:  
*Structure determination from unindexed powder data from scratch by a global optimization approach using pattern comparison based on cross-correlation functions*,  
*Acta Cryst.*, **2022**, B78, 195–213, doi.org/10.1107/S2052520622001500.  
Highlighted by a scientific commentary:  
Kenneth D. M. Harris:  
*Circumventing a challenging aspect of crystal structure determination from powder diffraction data*,  
*Acta Cryst.*, **2022**, B78, 96–99, doi.org/10.1107/S2052520622003717.
- 159) Federica Bravetti, Simone Bordignon, Edith Alig, Daniel Eisenbeil, Lothar Fink, Carlo Nervi\*, Roberto Gobetto, Martin U. Schmidt, Michele R. Chierotti\*:  
*Solid-state NMR-driven crystal structure prediction of molecular crystals: the case of mebendazole*,  
*Chem. Eur. J.*, **2022**, 28, e202103589/1–10, doi.org/10.1002/chem.202103589.
- 158) Jürgen Brüning, Svetlana N. Ivashevskaya, Jacco van de Streek, Edith Alig, Martin U. Schmidt\*:  
*Industrial azomethine nickel complex pigments. Four crystal structures from X-ray powder diffraction data*,  
*Z. Kristallogr.*, **2021**, 236, 105–115, doi.org/10.1515/zkri-2021-2005.
- 157) Jacco van de Streek, Tatiana E. Gorelik, Martin U. Schmidt\*:  
*Crystal structure and morphology of the bright orange  $\gamma$ -phase of Pigment Red 53:2 from XRPD, DFT+D and TEM*,  
*Dyes and Pigments*, **2021**, 196, 109456, doi.org/10.1016/j.dyepig.2021.109456.
- 156) 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.
- G155b) Carina Schlesinger, Stefan Habermehl, Dragica Prill\*:  
*Structure determination of organic compounds by a fit to the pair distribution function from scratch without prior indexing*,  
*J. Appl. Cryst.* **2021**, 54, 776–786, doi.org/10.1107/S1600576721002569.

- G155a) Stefan Habermehl, Carina Schlesinger, Dragica Prill\*:  
Comparison and evaluation of pair distribution functions, using a similarity measure based on cross-correlation functions,  
*J. Appl. Cryst.* **2021**, *54*, 612–623, doi.org/10.1107/S1600576721001722.
- 155) 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.
- 154) 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.
- 153) 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.
- 152) Carina Schlesinger, Edith Alig, Martin U. Schmidt\*:  
*Crystal structure of the anticancer drug carmustine determined by X-ray powder diffraction*,  
*Powder Diffraction*, **2021**, *36*, 148–150, doi.org/10.1017/S0885715621000294.
- 151) 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.
- 150) Carina Schlesinger, Sonja M. Hammer, Tatiana E. Gorelik, Martin U. Schmidt\*:  
*Oriental 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.org/10.1107/S2052520620003984.
- 149) 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*,  
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- G148a) Lukas Tapmeyer, Steven Hill, Michael Bolte, Wilhelm Maximilian Hützler:  
*Two monosodium salt hydrates of Colour Index Pigment Red 48*  
*Acta Cryst.* **2020**, *C76*, 716–722, doi.org/10.1107/S2053229620008530.
- 148) 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.org/10.1039/C9CE02012H.
- 147) Katharina Edkins\*, Garry J. McIntyre, Clive Wilkinson, Volker Kahlenberg, Daniel Többens, Ulrich J. Griesser, Jürgen Brüning, Martin U. Schmidt, and Jonathan W. Steed:

*Extensive sequential polymorphic interconversion in the solid state: two hydrates and ten anhydrous phases of hexamidine diisethionate*,  
*Cryst. Growth Des.*, **2019**, *19*, 7280–7289, doi.org/10.1021/acs.cgd.9b01170.

- 146) 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.org/10.1107/97809553602060000984.
- 145) 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.org/10.1039/C9CE00412B.
- 144) 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**, *19*, 1860–1873, doi.org/10.1021/acs.cgd.8b01830.
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*Two new polymorphs of cis-perinone: crystal structures, physical and electric properties*,  
*Acta Cryst.*, **2019**, *B75*, 384–392, doi.org/10.1107/S2052520619003287.
- 142) 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.
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*Challenging structure determination from powder diffraction data: two pharmaceutical salts and one cocrystal with  $Z' = 2$* ,  
*Z. Kristallogr.*, **2018**, *234*, 257–268, doi.org/10.1515/zkri-2018-2093.
- 140) Miriam Heine, Lothar Fink, Martin U. Schmidt\*:  
*3-Cyanopyridine as a bridging and terminal ligand in coordination polymers*,  
*CrystEngComm*, **2018**, *20*, 7556–7566, doi.org/10.1039/c8ce01568f.
- 139) 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, doi.org/10.1107/S2052520618010120.
- 138) 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, doi.org/10.1039/c8cc05918g.

- 137) 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, doi.org/10.1002/ange.201713168,  
*Angew. Chem. Int. Ed.*, **2018**, *57*, 9150-9153, doi.org/10.1002/anie.201713168.
- 136) Alexander G. Shtukenberg\*, Chunhua T. Hu, Qiang Zhu, Martin U. Schmidt, Wenqian Xu, Melissa Tan, Kahr, Bart:  
*The third ambient aspirin polymorph,*  
*Crystal Growth & Design*, **2017**, *17*, 3562-3566, doi.org/10.1021/acs.cgd.7b00673.
- 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,  
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- 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, doi.org/10.1038/NCHEM.2771.
- 133) Daniela Hempler, Martin U. Schmidt, Jacco van de Streek\*:  
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*Acta Cryst. Sect. B, Struct. Sci.*, **2017**, *B73*, 756-766, doi.org/10.1107/S2052520617005935.
- 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, doi.org/10.1107/S2052520617005017.
- 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, doi.org/10.1107/S2052252517002585.  
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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,*  
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- 129) Franziska Fischer, Martin U. Schmidt, Sebastian Greisera, Franziska Emmerling\*:  
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*Acta Cryst., Sect. C, Cryst. Struct. Commun.*, **2016**, 72, 217-224,  
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- 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, doi.org/10.1016/j.dyepig.2016.03.035.
- 127) Jaroslav L. Teteruk, Jürgen Glinnemann, Winfried Heyse, Kristoffer E. Johansson, Jacco van de Streek, Martin U. Schmidt\*:  
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- 126) Tatiana E. Gorelik\*, Christian Czech, Sonja M. Hammer, Martin U. Schmidt:  
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*CrystEngComm*, **2016**, 18, 529-535, doi.org/10.1039/c5ce01855b.  
Mit Titelbild (Innenseite) 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,  
doi.org/10.1107/S2053273315022457.
- 124) Jürgen Brüning, Martin U. Schmidt\*:  
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- 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:  
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*Eur. J. Pharm. Sci.*, **2015**, 71, 1-11, doi.org/10.1016/j.ejps.2015.01.017.
- 122) Sándor L. Bekö, Jan W. Bats, Martin U. Schmidt\*:  
*One-dimensional zinc(II) fumarate coordination polymers*,  
*J. Coord. Chem.*, **2015**, 68, 118-129, doi.org/10.1080/00958972.2014.978765.
- 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, doi.org/10.1515/zkri-2015-1845.
- 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 doi.org/10.1017/S1431927614014561.

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*J. Appl. Cryst.*, **2015**, *48*, 171-178, doi.org/10.1107/S1600576714026454.
- 118) Martin U. Schmidt:  
*Nachruf: Prof. Dr. Erich F. Paulus,*  
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- 117) Philipp Mörschel, Martin U. Schmidt\*:  
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*Acta Cryst. Sect. A, Foundations and Advances*, **2015**, *71*, 26-35,  
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- 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,*  
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*CrystEngComm*, **2014**, *16*, 4365-4368, doi.org/10.1039/c4ce00265b.
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*Acta Cryst. Sect. B, Struct. Sci.*, **2014**, *B70*, 347-359, doi.org/10.1107/S2052520613033994.
- 112) Jaroslav L. Teteruk, Jürgen Glinnemann, Tatiana E. Gorelik, Anthony Linden, Martin U. Schmidt:  
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*Acta Cryst. Sect B, Struct. Sci.*, **2014**, *B70*, 296-305, doi.org/10.1107/S2052520613031636.
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- 110) Sándor L. Bekö, Edith Alig, Martin U. Schmidt, Jacco van de Streek\*:  
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*IUCrJ (Journal of the International Union of Crystallography)*, **2014**, 1, 61-73,  
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*The influence of different solvents on 2-ammonio-4-chloro-5-methylbenzenesulfonate, including its de- and resulfonation*,  
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- 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*,  
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- 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, doi.org/10.1021/ja404351p.
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- 104) Martin U. Schmidt\*, Jürgen Glinnemann:  
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- 102) Sándor L. Bekö, David Urmann, Martin U. Schmidt\*:  
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*J. Chem. Cryst.*, **2012**, 42, 933-940, doi.org/10.1007/s10870-012-0339-0.
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*Angew. Chem.*, **2012**, *124*, 4814-4818, doi.org/ 10.1002/ange.201109082,  
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