

# **Crystal Engineering and Charge Density Studies on Pharmaceutically Active Derivatives of Sulfonamides**

Von der Fakultät für Mathematik, Informatik und Naturwissenschaften  
der RWTH Aachen University zur Erlangung des akademischen Grades  
eines Doktors der Naturwissenschaften vorgelegte Dissertation

vorgelegt von  
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	Univ. Prof.	Dr. Wolfgang Stahl

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Berichte aus der Chemie

**Fangfang Pan**

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The results reported in the present thesis have been achieved during my work in the Institute of Inorganic Chemistry, RWTH Aachen University under the supervision of Prof. Dr. Ulli Englert between October 2010 - June 2013.

Part of this work has been published:

1. F. Pan, R. Wang and U. Englert  
"Competing Protonation Sites in Sulfadiazine: Answers from Chemistry and Electron Density"  
*CrystEngComm.*, **2013**, 15, 1164-1172.
2. F. Pan, R. Wang and U. Englert  
"Switching from Bonding to Non-Bonding Temperature-dependent Metal Coordination in a Zn(II) sulfadiazine"  
*Inorg. Chem.*, **2012**, 51, 769-771.

or submitted:

1. C. Merckens, F. Pan and U. Englert  
"3-(4-Pyridyl)-2,4-Pentanedione-a Bridge between Coordinative, Halogen, and Hydrogen bonds"  
*CrystEngComm.*
2. F. Pan and U. Englert  
"A New Polymorph of N-(6-Methyl-2-Pyridyl)mesitylene-Sulfonamide"  
*Acta. Crystallogr., Sect. C.*
3. F. Pan, I. Kalf and U. Englert  
"Diamminebis[4-Amino-N-pyrimidin-2-yl-Benzenesulfonamido]copper(II): Aqua- or Ammine-Ligands?"  
*Acta. Crystallogr., Sect. C.*
4. V. L. Deringer, F. Pan, J. George, P. Müller, R. Dronskowski, and U. Englert  
"Intermolecular contacts in bromomalonic aldehyde – intuition, experiment, and theory"  
*Angew. Chem. Int. Ed.*

Other results have also been achieved and published in this period. But they are not directly related to the thesis. I contributed to these publications as a coauthor.

1. X. Liu, C. Wessel, F. Pan, R. Dronskowski  
"Synthesis and single-crystal structure determination of the zinc nitride halides  $Zn_2NX$  ( $X=Cl, Br, I$ )"  
*Journal of Solid State Chemistry* **2013**, 203, 31-36.
2. L. Wang, H. Huang, D. L. Priebsenow, F. Pan and C. Bolm  
"Copper-Catalyzed Oxidative Cross-Coupling of Sulfoximines and Alkynes"  
*Angew. Chem. Int. Ed.* **2013**, 52(12), 3478-3480.
3. C. Lichtenberg, F. Pan, T. P. Spaniol, U. Englert and J. Okuda  
"The Bis(allyl)bismuth Cation: A Reagent for Direct Allyl Transfer by Lewis Acid Activation and Controlled Radical Polymerization"  
*Angew. Chem. Int. Ed.* **2012**, 51(52), 13011-13015.
4. C. Gunanathan, M. Hölscher, F. Pan, and W. Leitner  
"Ruthenium Catalyzed Hydroboration of Terminal Alkynes to Z-Vinylboronates"  
*J. Am. Chem. Soc.*, **2012**, 134(35), 14349-14352.
5. J. Chen, W. Dong, M. Candy, F. Pan, M. Jorres, C. Bolm  
"Enantioselective Synthesis of Dihydropyrazoles by Formal [4+1] Cycloaddition of in Situ-Derived Azoalkenes and Sulfur Ylides"  
*J. Am. Chem. Soc.*, **2012**, 134(16), 6924-6927.
6. D. Chen, V. Leich, F. Pan and J. Klankermayer  
Enantioselective Hydrosilylation with Chiral Frustrated Lewis Pairs  
*Chem. Eur. J.*, **2012**, 18(17), 5184-5187.
7. J. Wan, C. C. J. Loh, F. Pan and D. Enders  
"Enantioselective Organocatalytic Domino Synthesis of Tetrahydropyridin-2-ols"  
*Chem. Commun.*, **2012**, 48, 10049-10051.
8. G. Ghattas, D. Chen, F. Pan and J. Klankermayer  
"Asymmetric Hydrogenation of Imines with a Recyclable Chiral Frustrated Lewis Pair Catalyst"  
*Dalton Trans.*, **2012**, 41, 9026-9028.
9. H. Zhang, P. Becker, H. Huang, R. Pirwerdjan, F. Pan, C. Bolm  
"Photochemically Induced Silylacetylations of Alkynes with Acylsilanes"  
*Adv. Synth. Catal.*, **2012**, 354(11-12), 2157-2161.

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