

Publikationen

- **Transferability of atomic volumes and charges in the peptide bond region in the solid state**
Birger Dittrich, Stephan Scheins, Carsten Paulmann, Peter Luger
J. Phys. Chem., **A107** (2003), *7471-7474*
- **Experimental charge density of octafluoro-1,2-dimethylenecyclobutane: atomic volumes and charges in a perfluorinated hydrocarbon**
Dieter Lentz, Mona Patzschke, Ansgar Bach, Stephan Scheins, Peter Luger
Org. Biomol. Chem. **1** (2003), *409-414*
- **High-resolution synchrotron data collection for charge-density work at 100 and 20 K**
Peter Luger, Marc Messerschmidt, Stephan Scheins, Armin Wagner
Acta Cryst., **A60** (2004), *390-396*
- **Atomic volumes and charges in a system with a strong hydrogen bond: L-tryptophan formic acid**
Stephan Scheins, Birger Dittrich, Marc Messerschmidt, Carsten Paulmann and Peter Luger
Acta Cryst., **B60(2)** (2004), *184-190*
- **Electron Density and Bonding at Inverted Carbon Atoms: An Experimental Study of a [1.1.1]Propellane Derivative**
Marc Messerschmidt, Stephan Scheins, Lutz Grubert, Michael Pätzelt, Günter Szeimies, Carsten Paulmann, Peter Luger
Angew. Chem., **117** (2005), *3993-3997*
Angew. Chem. int., **44** (2005), *3925-3928*
- **Charge density of (-)-strychnine from 100 to 15 K, a comparison of four data sets**
Marc Messerschmidt, Stephan Scheins, Peter Luger
Acta Cryst. **B61** (2005), *115-121*

- **Submolecular partitioning of morphine hydrate based on its experimental charge density at 25 K**

Stephan Scheins, Marc Messerschmidt, Peter Luger

Acta Cryst. **B61** (2005), 443-448

- **Bond Orders and Atomic Properties of the Highly Deformed Halogenated Fullerenes $C_{60}F_{18}$ and $C_{60}Cl_{30}$ Derives from their Charge Densities**

Christian Hübschle, Stephan Scheins, Manuela Weber, Peter Luger, Armin Wagner, Tibor Koritsánszky, Serghey I. Troyanov

Chem. Eur. J. (2007) in press

- **Charge Density Analysis of Opioids: A Comparative Study**

Stephan Scheins, Marc Messerschmidt, Wolfgang Morgenroth, Carsten Paulmann, Peter Luger

in progress

Vorträge auf Konferenzen:

- **Atomare Volumina und Ladungen in fluorierten Kohlenwasserstoffen**
Peter Luger, Mona Patschke, Ansgar Bach, Stephan Scheins, Marc Messerschmidt, und Manuela Weber
11. Jahrestagung der Deutschen Gesellschaft der Kristallographie(DGK), 2003, Berlin, Deutschland
- **High Resolution Synchrotron Data Collection for Charge Density Work at 100 K and 20 K**
Peter Luger, Marc Messerschmidt, Stephan Scheins
ECDM-III, 3rd European Charge Density Meeting. 24-29 Juni 2003, Sandbjerg, Dänemark
- **Topology and Submolecular Partitioning of Biologically Active molecules Based on Experimental Charge Density Determination at 100 K and at 20 K**
Peter Luger, Marc Messerschmidt, Stephan Scheins, Birger Dittrich
The Sixth Conference of the Asian Crystallographic Association (IUCr), AsCA'04, 27-30 June 2004, HongKong, China
- **Charge Density Investigations of the Highly Deformed Halogenated Fullerenes $C_{60}F_{18}$ and $C_{60}Cl_{30}$**
Stephan Scheins, Christian Hübschle, Serghey I. Troyanov, Manuela Weber, Armin Wagner, Tibor Koritsánszky, Peter Luger
AK14 (DGK) The Workshop "Electron Density - Theory and Applications, Computational Crystallography", Aachen, 19.-21.2.2006, Aachen, Deutschland

Posterpräsentationen auf internationalen Konferenzen:

- **Topological Analysis of 2,4,6,8-Tetraphenylbarbaralane based on a Synchrotron/CCD Area Detector Experiment at 110 K**
Stephan Scheins, Birger Dittrich, Peter Luger, Carsten Paulmann, Helmut Quast
IUCr XIX congress, **2002**, Geneva, Switzerland
- **Charge density of a [1.1.1]propellane**
Marc Messerschmidt, Stephan Scheins, Peter Luger
Gordon Research Conference on Electron Distribution and Chemical Bonding,
2004 South Hadley, USA
- **Charge density analysis of the opioids morphine hydrate and codeine from high resolution X-ray data measured at 25 K**
Stephan Scheins, Marc Messerschmidt, Peter Luger
Gordon Research Conference on Electron Distribution and Chemical Bonding,
2004 South Hadley, USA
- **Atomare Eigenschaften von Morphin-Hydrat**
Stephan Scheins, Marc Messerschmidt, Peter Luger
Atomare Eigenschaften von Morphin-Hydrat
12. Jahrestagung der Deutschen Gesellschaft der Kristallographie(DGK), **2004**,
Jena, Deutschland
- **Comparing charge densities of opioids: morphine, codeine and dextromethorphan.**
Stephan Scheins, Marc Messerschmidt, Peter Luger
IUCr XX congress, **2005**, Florence, Italy
- **Goldene Zeiten der Elektronendichtebestimmung: Hochaufgelste Röntgenbeugungsexperimente im Stundentakt**
Christian Hübschle, Armin Wagner, Stephan Scheins, Manuella Weber, Wolfgang Morgenroth, Peter Luger, Sergey I. Troyanov
Workshop zum Cluster „Moleküle“, **2005**, Berlin, Deutschland

- **Electron Density Analysis of unusual Bonds in Boronclusters**
 Diana Förster, Christian Hübschle, Stephan Scheins, Dieter Lentz, Peter Luger
 4th European Charge Density Meeting(ECDM IV), **2006**, Brandenburg/Havel,
 Deutschland
- **Charge Density Investigations of the Highly Deformed Halogenated Fullerenes $C_{60}F_{18}$ and $C_{60}Cl_{30}$**
 Stephan Scheins, Christian Hübschle, Serghey I. Troyanov, Manuela Weber, Armin
 Wagner, Tibor Koritsánszky, Peter Luger
 Tag der Chemie, **2006**, TU Berlin, Deutschland
- **Recent experimental and methodical advances in the charge density studies on tripeptides of the type Ala–Xxx–Ala**
 Lilianna Chechinska, Diana Förster, Eva Rödel, Stephan Scheins, Roman Kalinowski,
 Stefan Mebs, Christian Hübschle, Birger Dittrich, Wolfgang Morgenroth,
 Carsten Paulmann, Peter Luger
 AK14 (DGK) The Workshop "Electron Density - Theory and Applications, Computational
 Crystallography", **2006**, Aachen, Deutschland