

Publikationsliste

Veröffentlichungen in wissenschaftlichen Zeitschriften

1. A. Wagner, P. Luger.
"Charge Density and Topological Analysis of L-Glutamine"
J. Mol. Struct. **595** (2001), 39–46
2. A. Wagner, R. Flaig, D. Zobel, B. Dittrich, P. Bombicz, M. Strümpel, P. Luger, T. Koritsánszky, H.-G. Krane.
"Structure and Charge Density of a C₆₀-Fullerene Derivative Based on a High Resolution Synchrotron Diffraction Experiment at 100 K"
J. Phys. Chem. A **106** (2002), 6581–6590
3. M. Messerschmidt, A. Wagner, M. W. Wong, P. Luger
"Atomic Properties of N₂O₄ Based on Its Experimental Charge Density"
J. Am. Chem. Soc. **124** (2002), 732–733
4. R. Flaig, T. Koritsánszky, B. Dittrich, A. Wagner, P. Luger.
"Intra- and Intermolecular Topological Properties of Amino Acids: A Comparative Study of Experimental and Theoretical Results"
J. Am. Chem. Soc. **124** (2002), 3407–3417
5. B. Dittrich, T. Koritsánszky, M. Grosche, W. Scherer, R. Flaig, A. Wagner, H.-G. Krane, H. Kessler, C. Riemer, A. M. M. Schreurs, P. Luger.
"Reproducibility and Transferability of Topological Properties; Experimental Charge Density of the Hexapeptide cyclo-(D,L-Pro₂)-(L-Ala)₄ Monohydrate"
Acta Crystallogr. Sect. **B58** (2002), 721–727
6. R. Kingsford-Adaboh, B. Dittrich, A. Wagner, M. Messerschmidt, R. Flaig, P. Luger.
"Topological analysis of DL-Arginine monohydrate at 100 K"
Z. Kristallogr. **217** (2002), 168–173

7. I. M. Lyapkalo, H.-U. Reissig, A. Schaefer, A. Wagner.
"Study of Unusually High Rotation Barriers about S,N Bonds in Nonafluoro-1
butanesulfonamides: Electronic Nature of the Torsional Effect"
Helv. Chim. Acta **85** (2002), in press

Beträge bei nationalen und internationalen Konferenzen

- A. Wagner, B. Dittrich, H. Schmidt, H.-G. Krane, P. Luger
"Ladungsdichteuntersuchung an Vitamin B12"
9. Jahrestagung der Deutschen Gesellschaft der Kristallographie (DGK), Bayreuth
2001.
Vortrag
- A. Wagner, R. Flaig, T. Koritsánszky, P. Luger
"Ladungsdichteuntersuchungen an Penicillinderivaten"
8. Jahrestagung der Deutschen Gesellschaft für Kristallographie (DGK), Aachen
2000.
Vortrag
- A. Wagner, T. Koritsánszky, P. Luger
"Towards the Charge Density of Penicillins - An Experimental and Theoretical
Model Study"
Gordon Research Conference "Electron Density and Chemical Bonding", South
Hadley (USA) 2001.
Poster mit Kurzvortrag
- A. Wagner, P. Luger, T. Koritsánszky
"Charge Density Determination of non-centrosymmetric Thiazolidine-4-Carboxylic
Acid"
Indaba III "Workshop on Symmetry and Structure", Skukuza (Südafrika) 2000.
Auszeichnung für bestes Poster
- A. Wagner, R. Flaig, D. Zobel, B. Dittrich, P. Luger, T. Koritsánszky
"Charge Density of a Fullerene Derivative Based on a High Resolution Synchro-
tron Diffraction Experiment at 100 K"
IUCr, XIX Congress and General Assembly, Genf (Schweiz) 2002.
Poster
- A. Wagner, D. Zobel, T. Koritsánszky, P. Luger
"Experimental and theoretical Charge Density Study of non-centrosymmetric Thia-
zolidine-4-Carboxylic Acid"

9. Jahrestagung der Deutschen Gesellschaft der Kristallographie (DGK), Bayreuth 2001.

Poster

- A. Wagner, R. Flaig, P. Luger, T. Koritsánszky
"Is there a Relationship between the Charge Density and the Activity of Penicillins?"
2nd European Charge Density Meeting, Barcelona (Spanien) 1999.
Poster
- A. Wagner, P. Bombicz, R. Flaig, P. Luger, T. Koritsánszky
"Charge Density Study on Three Penicillin Derivatives"
IUCr, XVIII Congress and General Assembly, Glasgow (UK) 1999.
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