Universität Bielefeld

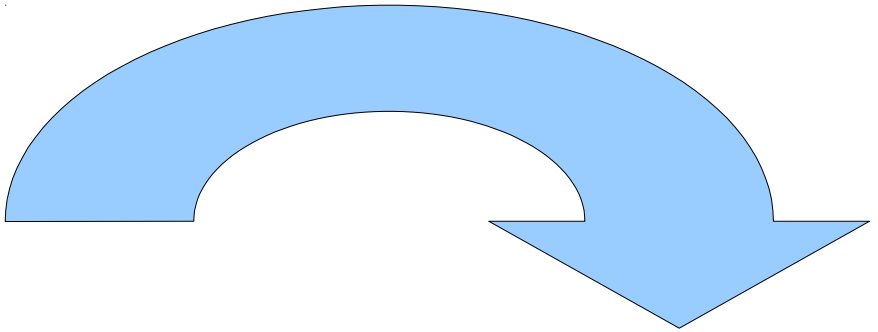
Rechenschaftsbericht 2012

Yury V. Vishnevskiy

Bielefeld, 22. Januar 2013

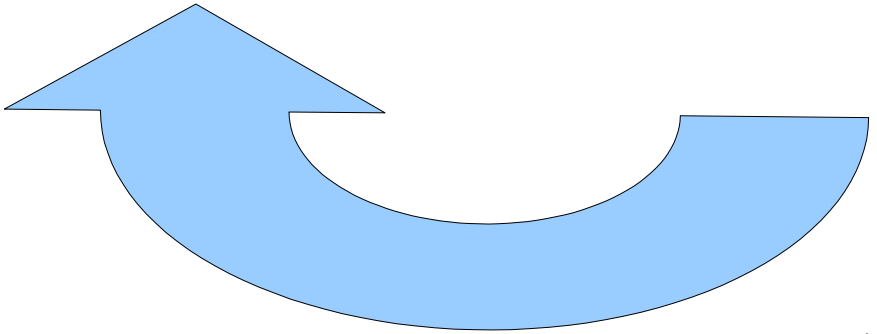
Unsere Arbeit

R-NCO, -NCS
R-SCN
R-SNO
R-NO2
CF3-CF2-C(O)-R
BAd



Strukturelle Untersuchungen

Entwiklung der Methode



UNEX 2
Experiment

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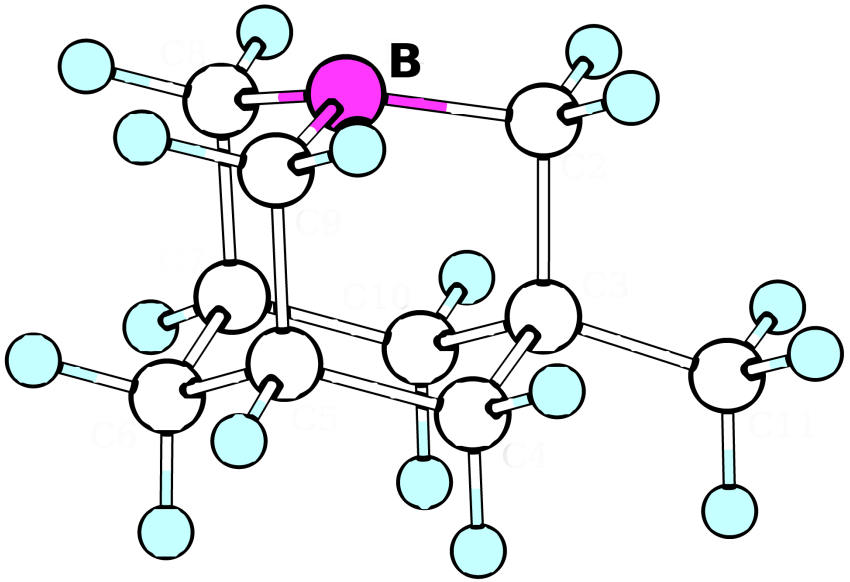
3-Methyl-1-boraadamantane



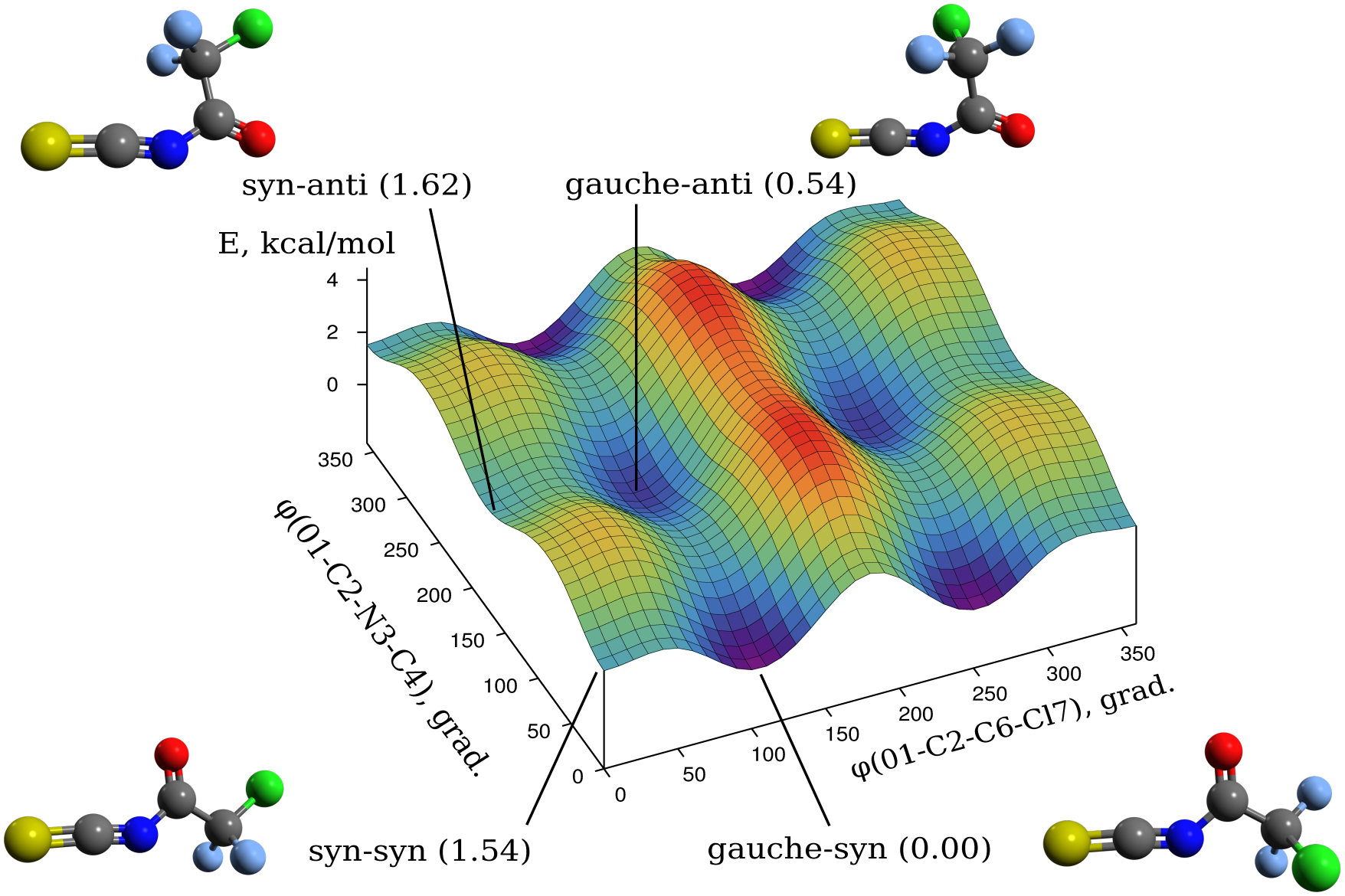
∠(C-X-C), grad.
116.5(2)
109.8(5), Adamantane

r_g(B-C), Å
1.565(5)
1.560(3), $B(CH=CH_2)_3$
1.578(3), BMe_3

Publiziert

[1] Yu. V. Vishnevskiy, M. A. Abaev, A. N. Rykov, M. E. Gurskii, P. A. Belyakov, S. Yu. Erdyakov, Yu. N. Bubnov, N. W. Mitzel, *Chem. Eur. J.*, 18 (2012) 10585.

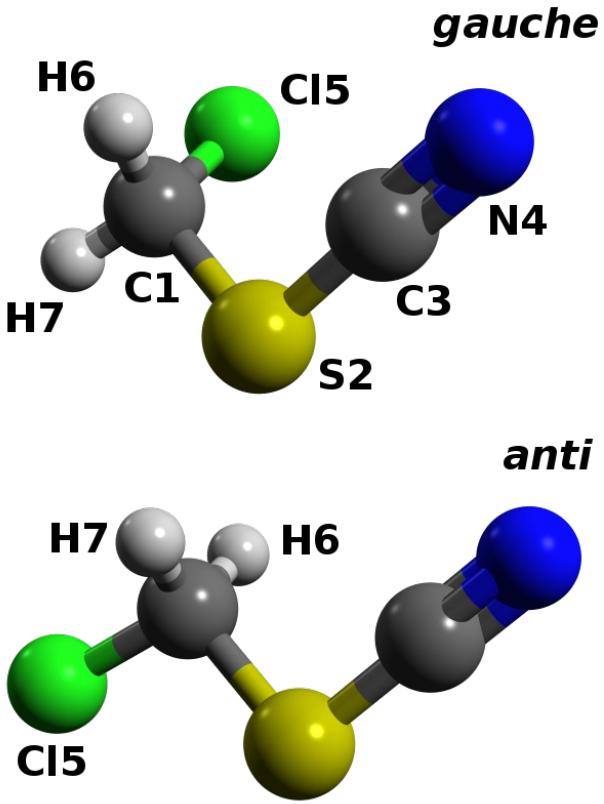
Cl_2FC-C(O)-NCO, -NCS

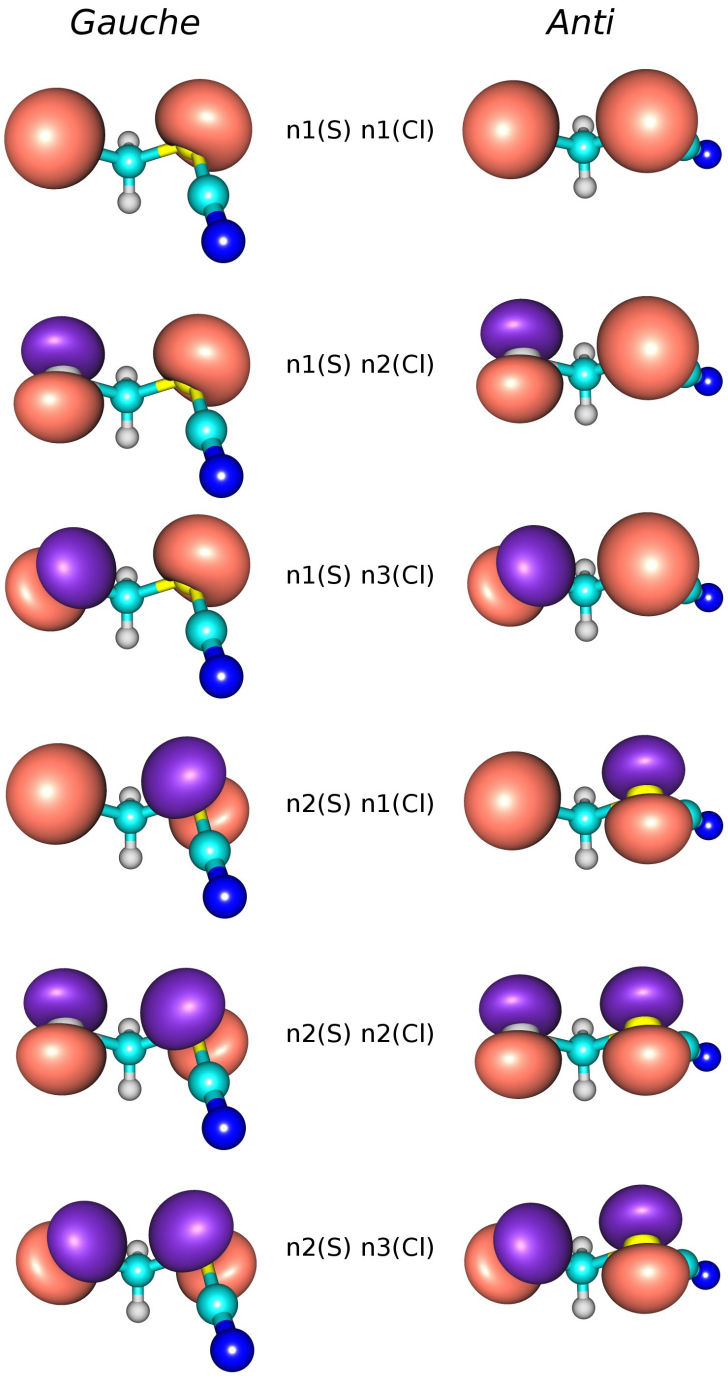


a) Publiziert; b) in Vorbereitung

[1] L. A. Ramos, S. E. Ulic, R. M. Romano, Yu. V. Vishnevskiy, R. J. F. Berger, N. W. Mitzel, H. Beckers, H. Willner, S. Tong, M. Ge, C. O. Della Védova, *J. Phys. Chem. A*, 116 (2012) 11586.

R-SCN (R=CCl_3, CCl_2F, $CClH_2$)

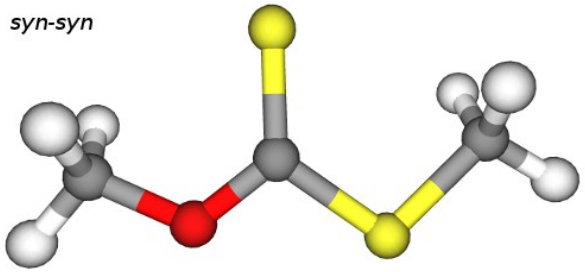


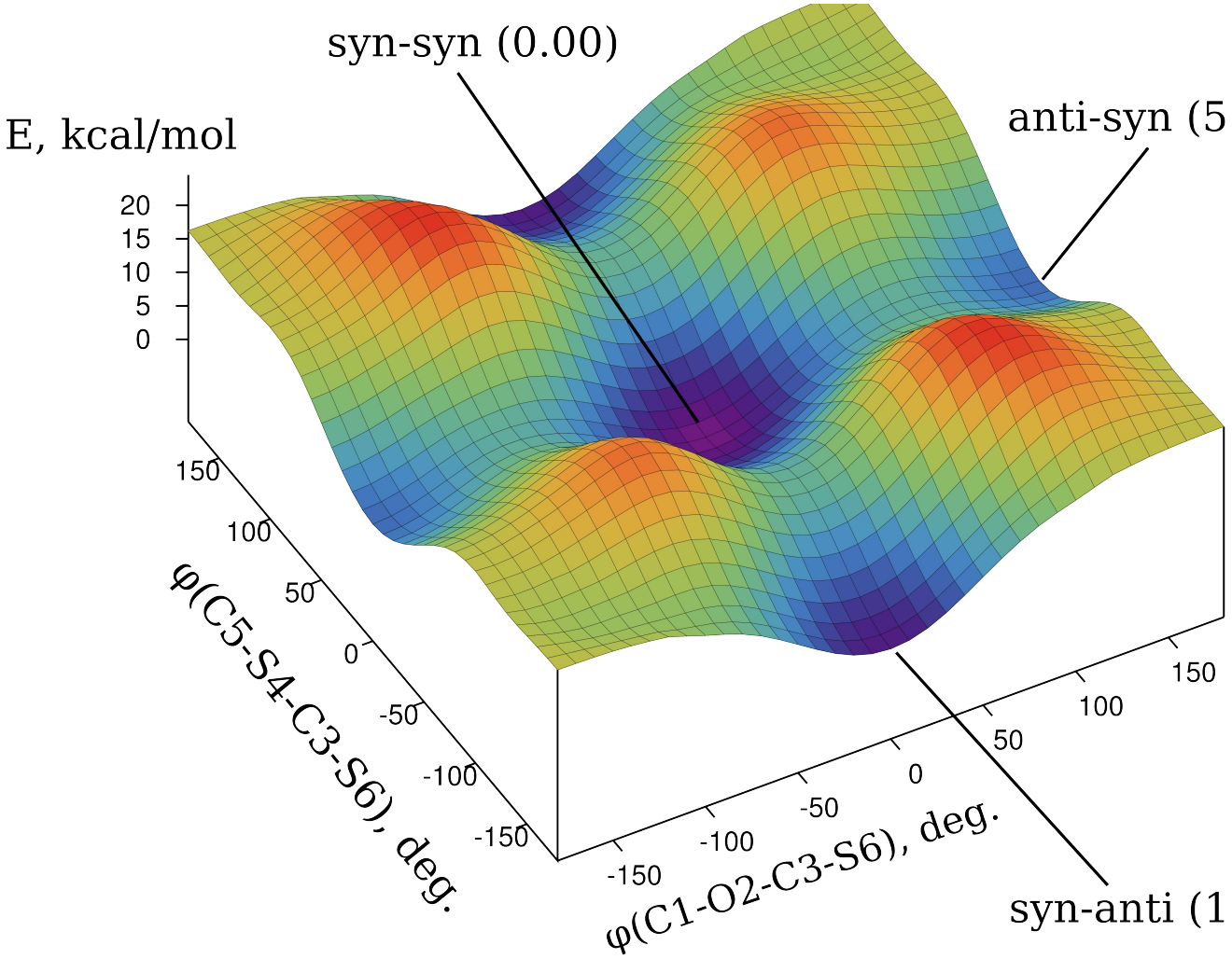


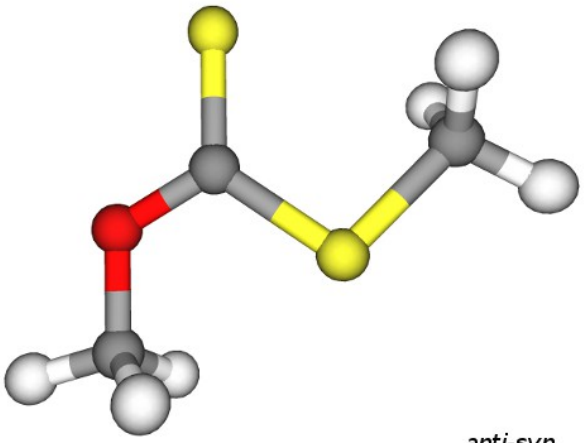
Gauche vs. Anti
XRD vs. GED
Elektronische vs. Sterische Effekte

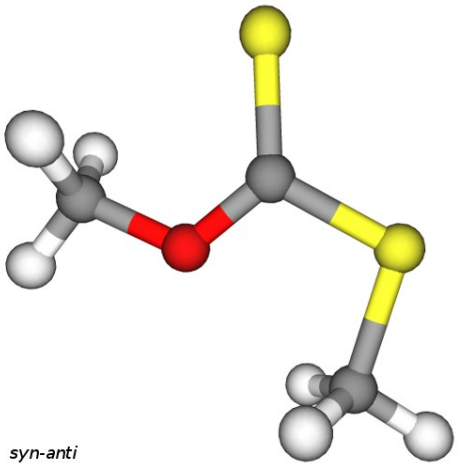
in Vorbereitung

$H_3CO\text{-}C(S)\text{-}SCH_3$

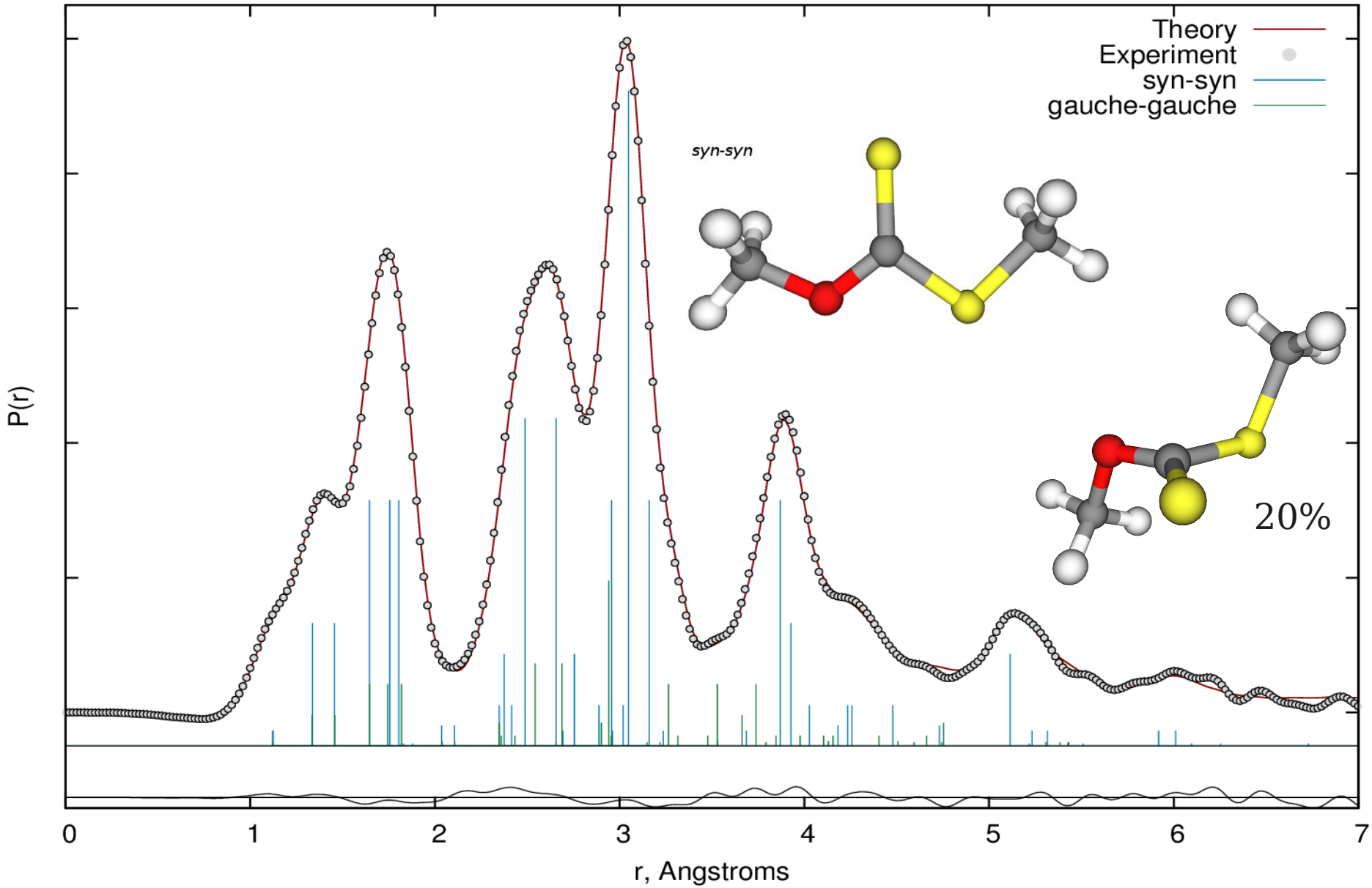






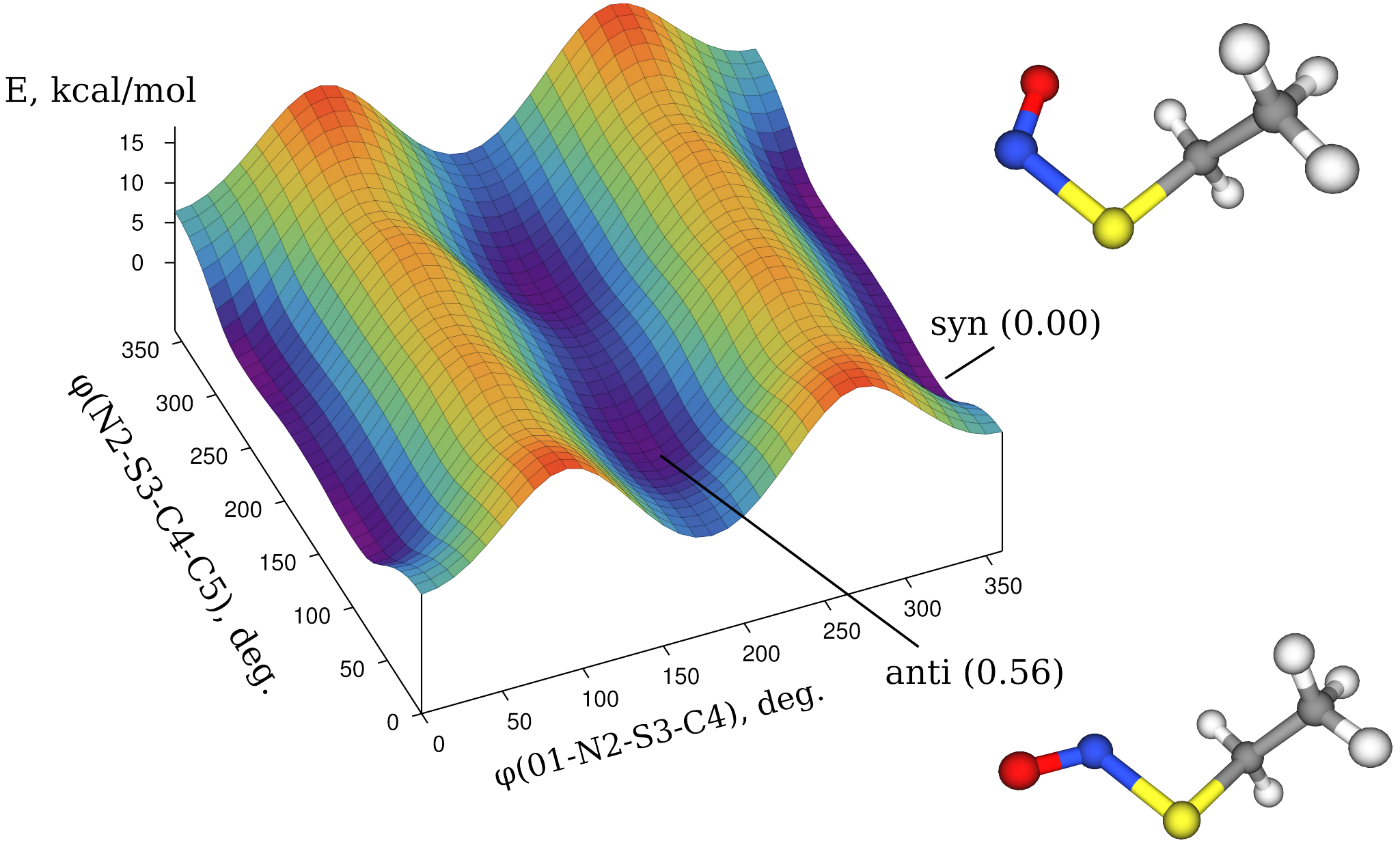


$H_3CO\text{-}C(S)\text{-}SCH_3$

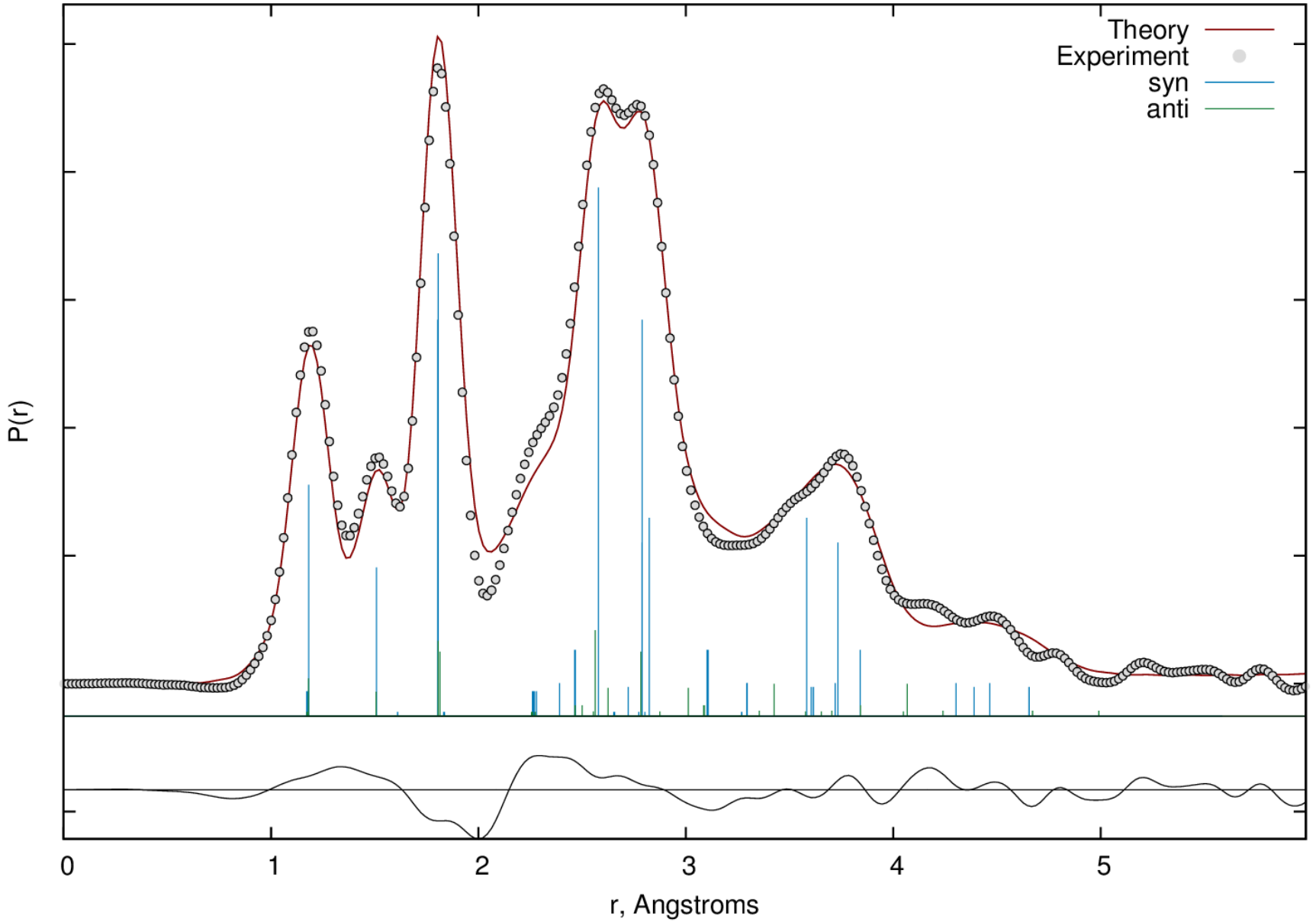


in Bearbeitung

R-SNO (R=CH_3CH_2, CF_3CH_2, $(CH_3)_3C$)



R-SNO (R=CH_3CH_2, CF_3CH_2, $(CH_3)_3C$)



in Bearbeitung

Universität Bielefeld

F-, Cl-, Br-$C(NO_2)_3$

nature chemistry

ARTICLES

PUBLISHED ONLINE: 3 MAY 2009 | DOI: 10.1038/NCHEM.179

Chlorotrinitromethane and its exceptionally short carbon–chlorine bond

Michael Göbel[1], Boris H. Tchitchanov[1], Jane S. Murray[2,3], Peter Politzer[2,3]* and Thomas M. Klapötke[1,4]*

$$r_\alpha(\text{Cl-C}) = 1.694(1)\ \text{Å}$$

Electron Diffraction Study of Gaseous $CH(NO_2)_3$ and $CCl(NO_2)_3$

By N. I. Sadova, N. I. Popik, L. V. Vilkov,* Ju. A. Pankrushev, and V. A. Shlyapochnikov

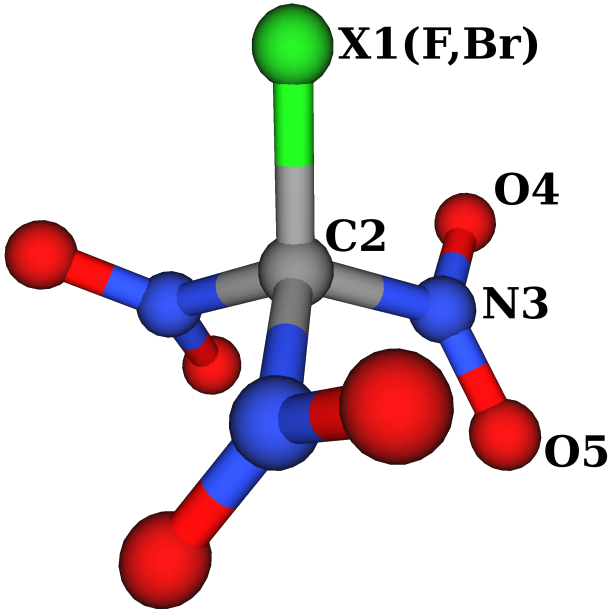
(*Department of Chemistry, Moscow State University, Moscow* 117234, *U.S.S.R.*)

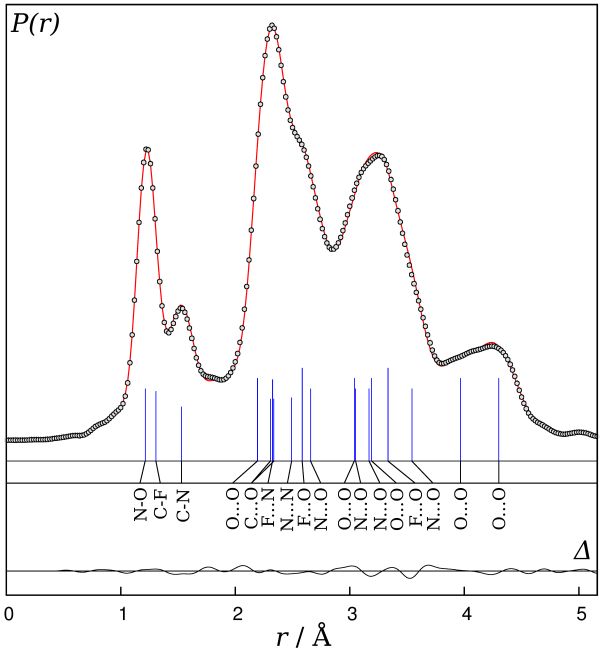
$$r_a(\text{Cl-C}) = 1.712(4)\ \text{Å}$$

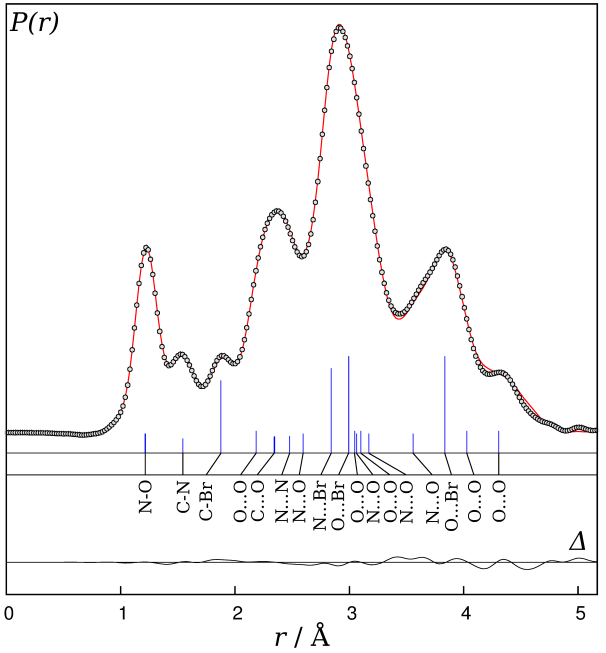
CCl_4: 1.767(2) Å

[1] M. Göbel, B. H. Tchitchanov, J. S. Murray, P. Politzer, T. M. Klapötke, *Nat. Chem.*, 1 (2009) 229.
[2] N. I. Sadova, N. I. Popik, L. V. Vilkov, A. Pankrushev, V. A. Shlyapochnikov, *J. Chem. Soc. Chem. Commun.*, 3 (1973) 708.
[3] S. Shibata, K. Iijima, R. Tani, I. Nakamura, *Reports of Faculty of Science, Shizuoka University*, 9 (1974) 33.

F-, Cl-, Br-$C(NO_2)_3$





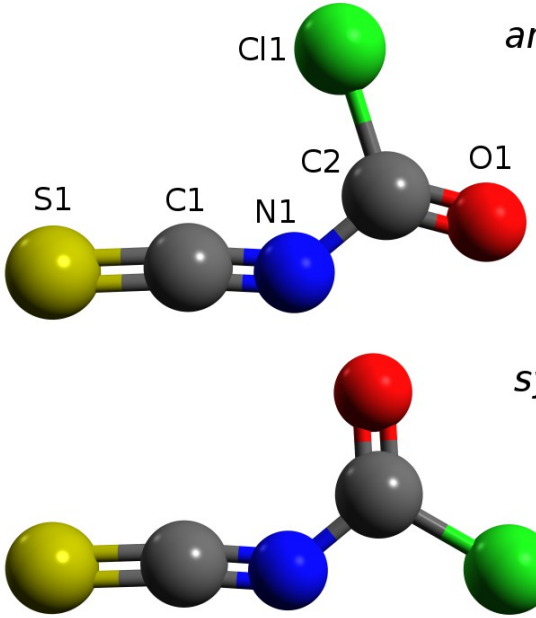


r_a(GED) und r_α(XRD) für C-X:

	X=F	X=Cl	X=Br
GED	1.307(4)	1.712(4)	1.876(2)
XRD	1.297(3)	1.694(1)	1.853(5)

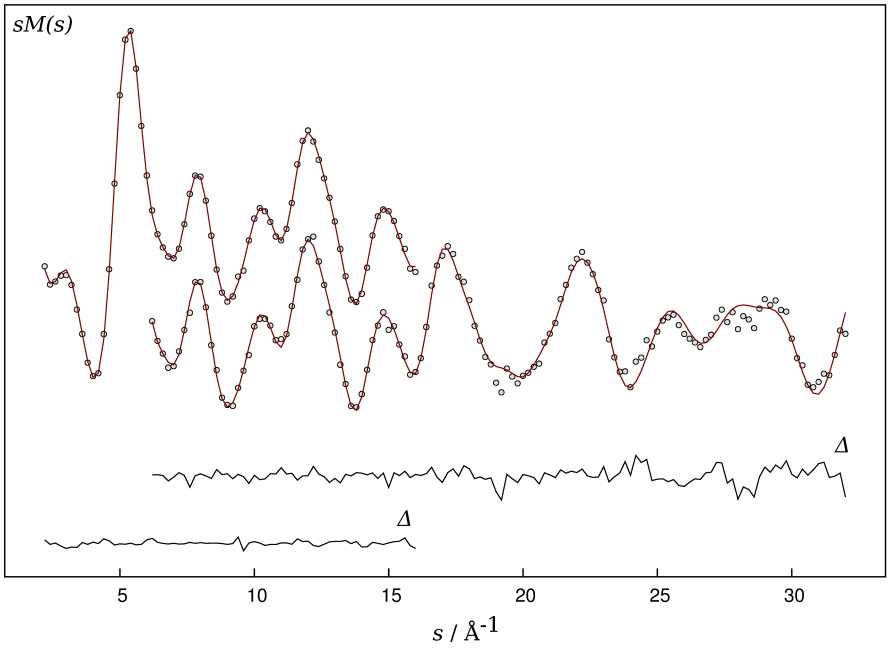
in Vorbereitung

F-, Cl-C(O)-R (R=SCN, NCS)



84(6) %

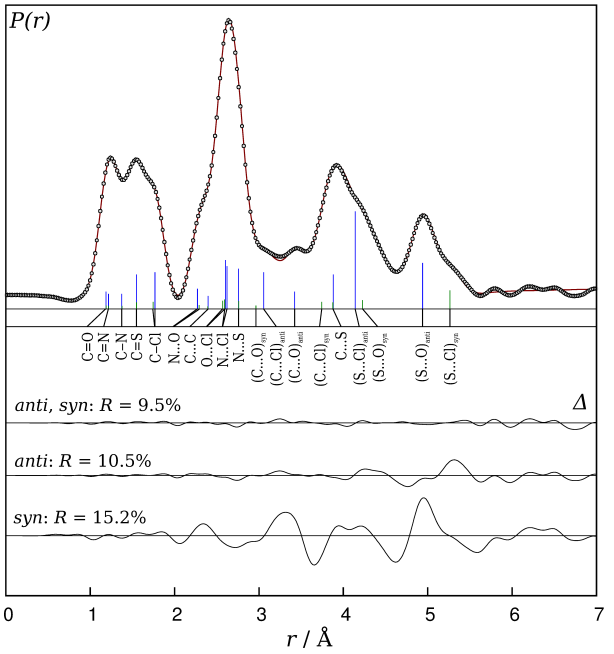
16(6) %



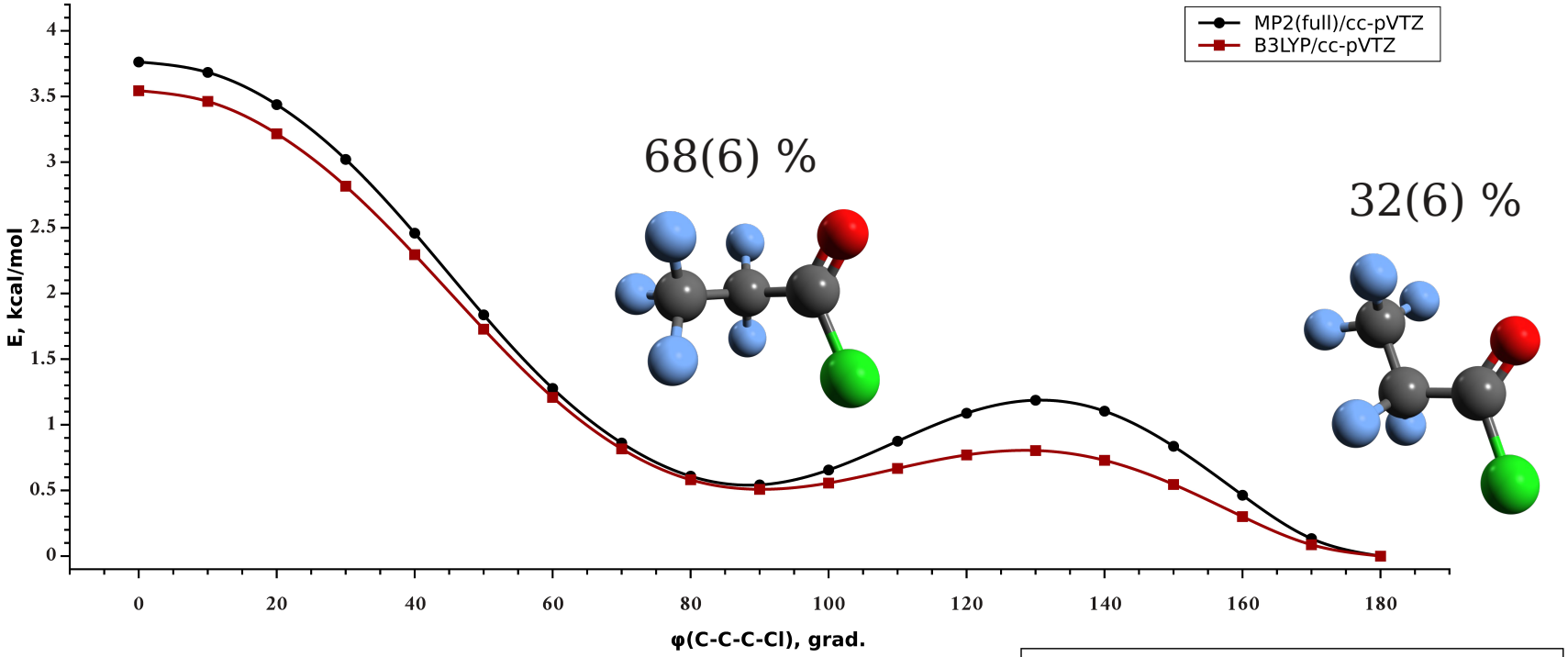
Cl-C(O)-NCS: **im Druck.**

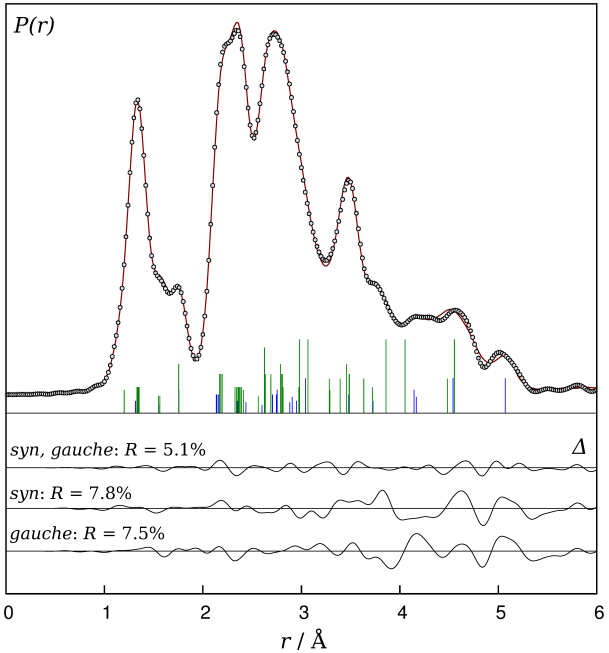
Cl-C(O)-SCN: **gescheitert.**

F-C(O)-SCN, -NCS: **noch zu messen.**



CF_3CF_2-C(O)-R (R=F, Cl, I, $OC(O)CF_2CF_3$)





CF_3CF_2-C(O)-Cl: **in Vorbereitung.**

CF_3CF_2-C(O)-F, -I, -O-C(O)-CF_2CF_3:
Daten sind vermessen.

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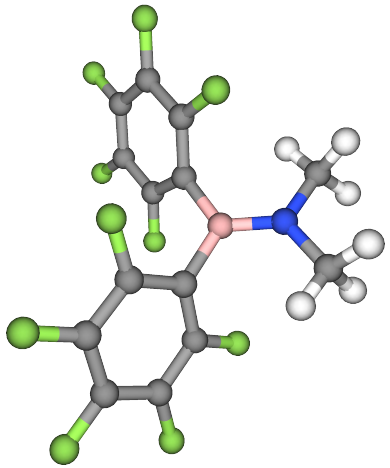
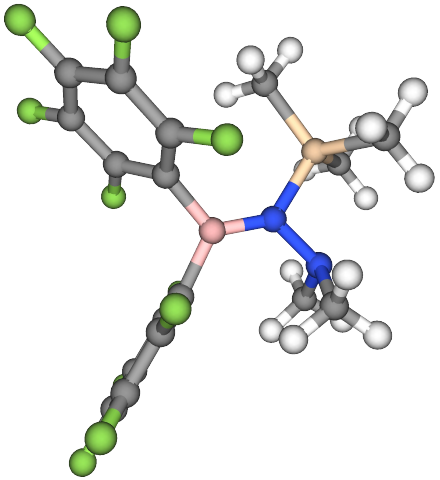
Theoretische Rechnungen

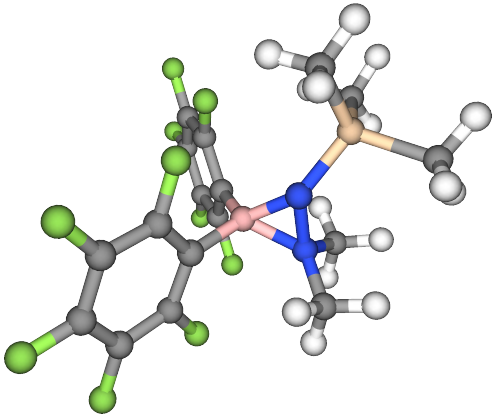
QTAIM für Daniel Winkelhaus:

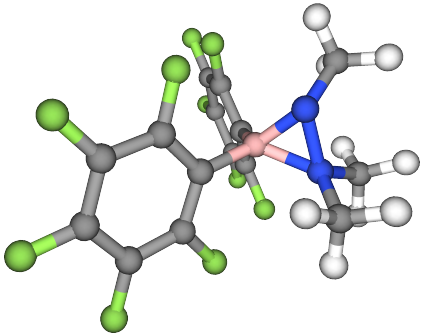


$(C_6F_5)_2B\text{-}N(CH_3)_2$

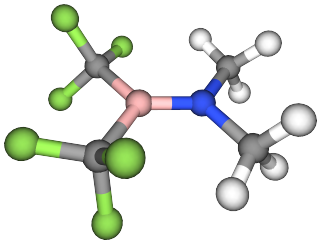


$(C_6F_5)_2B\text{-}N(Si(CH_3)_3)\text{-}N(CH_3)_2$

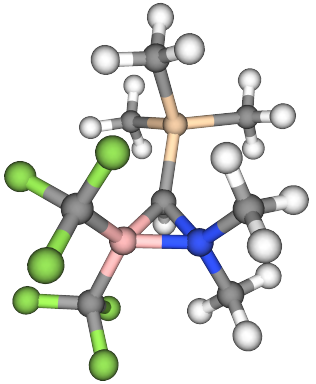




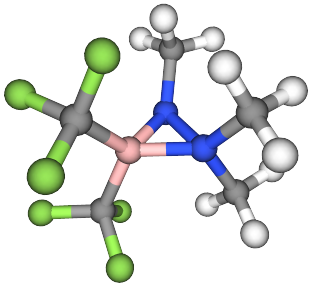
$(C_6F_5)_2B\text{-}N(CH_3)\text{-}N(CH_3)_2$



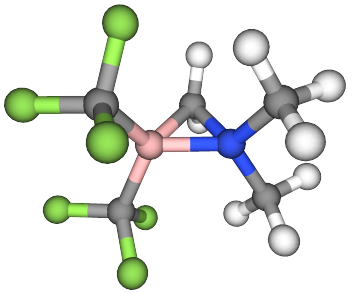
$(CF_3)_2B\text{-}N(CH_3)_2$



$(CF_3)_2B\text{-}CH(Si(CH_3)_3)\text{-}N(CH_3)_2$



$(CF_3)_2B\text{-}N(CH_3)\text{-}N(CH_3)_2$



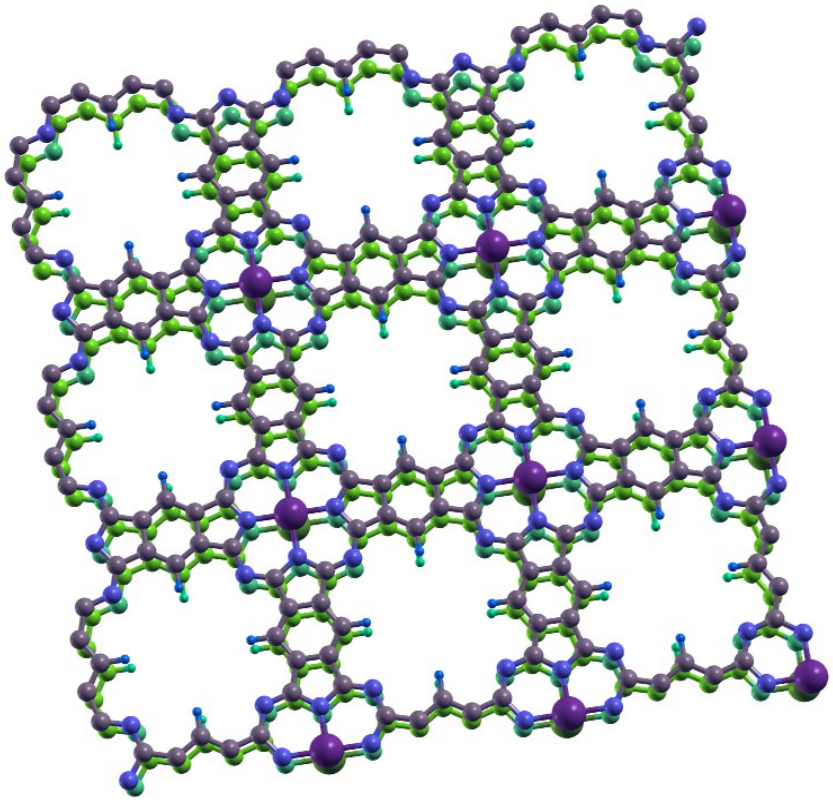
$(CF_3)_2B\text{-}CH_2\text{-}N(CH_3)_2$

a) Publiziert; b) im Druck

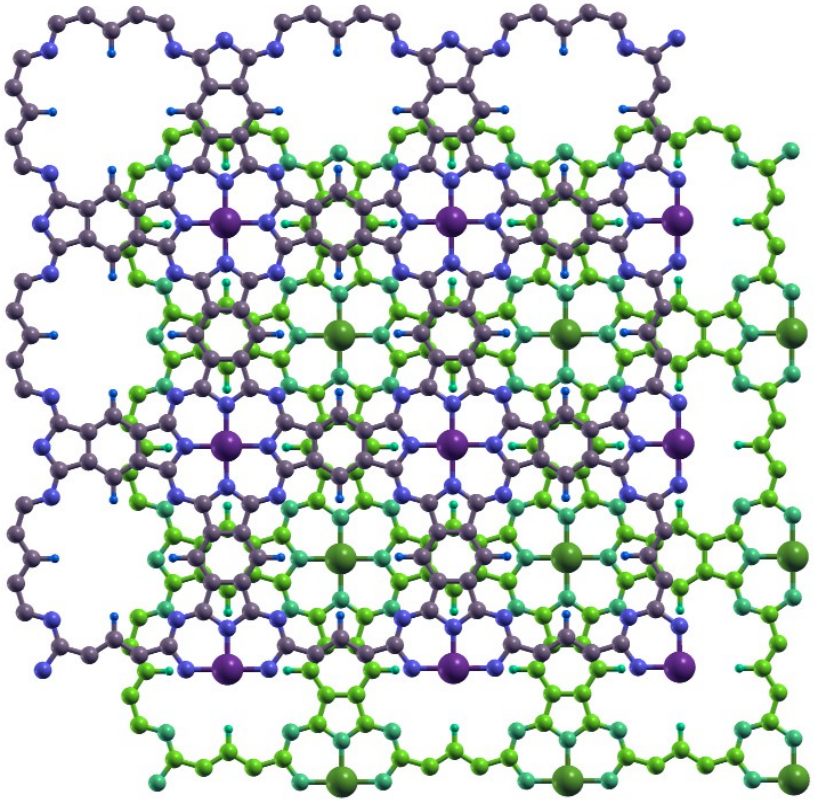
[1] D. Winkelhaus, B. Neumann, H.-G. Stammler, R. J. F. Berger, Yu. V. Vishnevskiy, N. W. Mitzel, *Chem. Eur. J.*, 18 (2012) 9312.
[2] D. Winkelhaus, Yu. V. Vishnevskiy, R. J. F. Berger, H.-G. Stammler, B. Neumann, N. W. Mitzel, *ZAAC*, in press.

Festkörperphysik: CuPPC

Kupfer(I) Phthalocyanin 2D Polymere : TEM, FTIR, UV-Vis, XRD, **QC**



AA

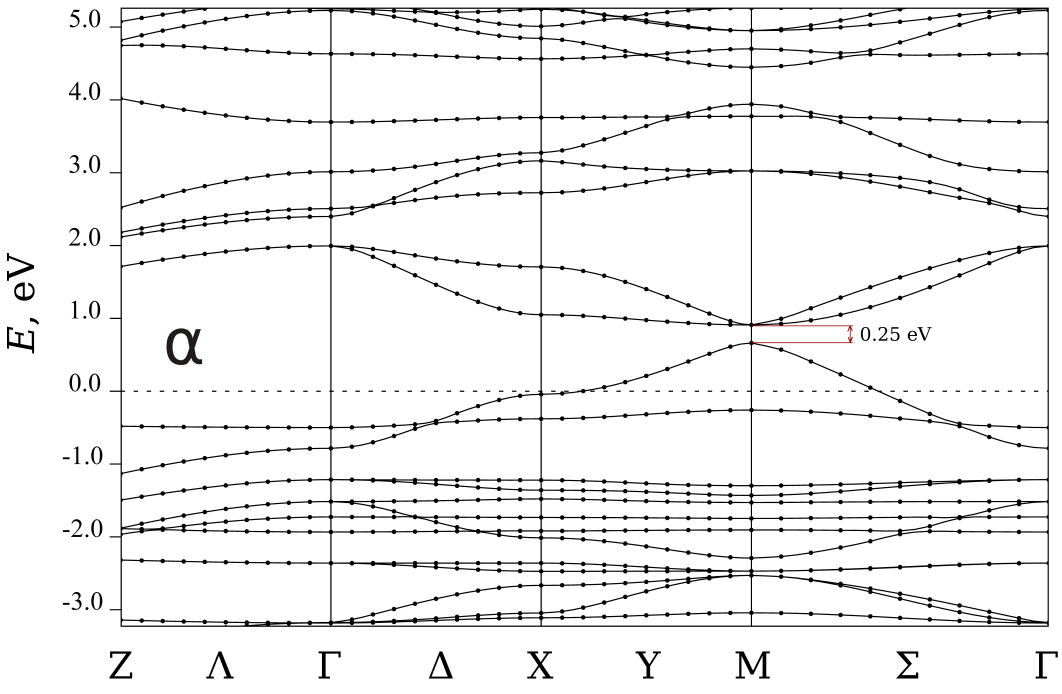


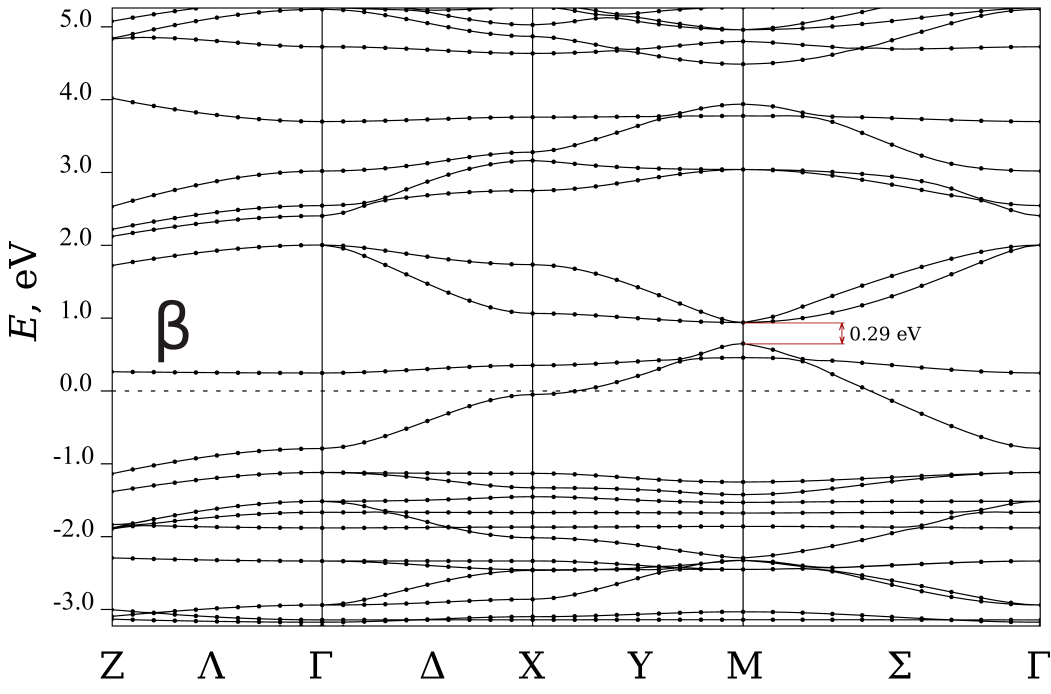
AB, ΔE= 0.96 kcal/mol
= 4.03 kJ/mol
= 0.04 eV pro Basis

Diamagnet? Antiferromagnet? Ferromagnet!

d, nm: 0.34 (TEM), 0.33 (XRD), 0.338 (QC).

Festkörperphysik: CuPPC Bandstruktur

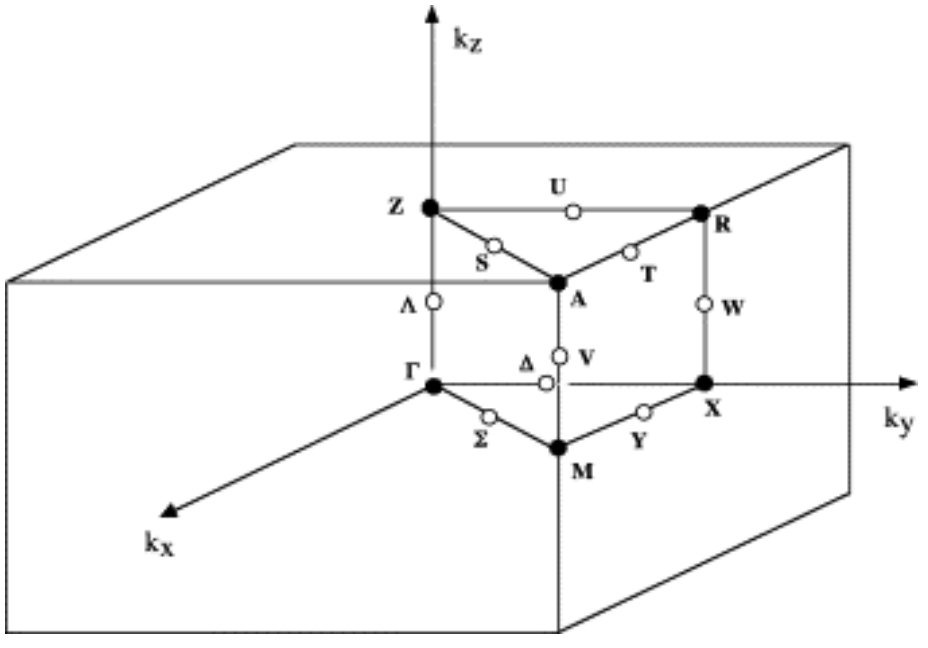




Brillouin-Zone P4/mmm

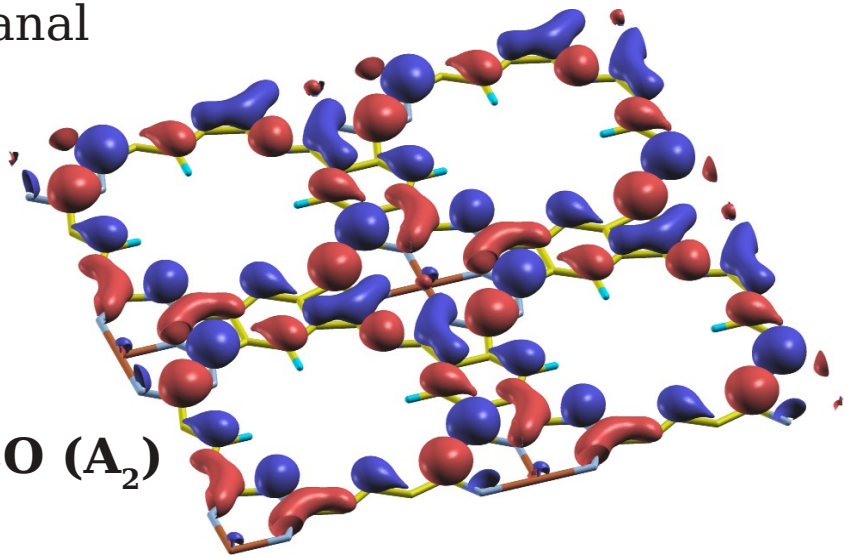
Bandlücke: 0.0 – 0.5 eV

<u>Widerstand</u>
CuPPC: 9-12 kOhm/sq
(Graphen: ~10 weniger)
(Cu: ~100 weniger)

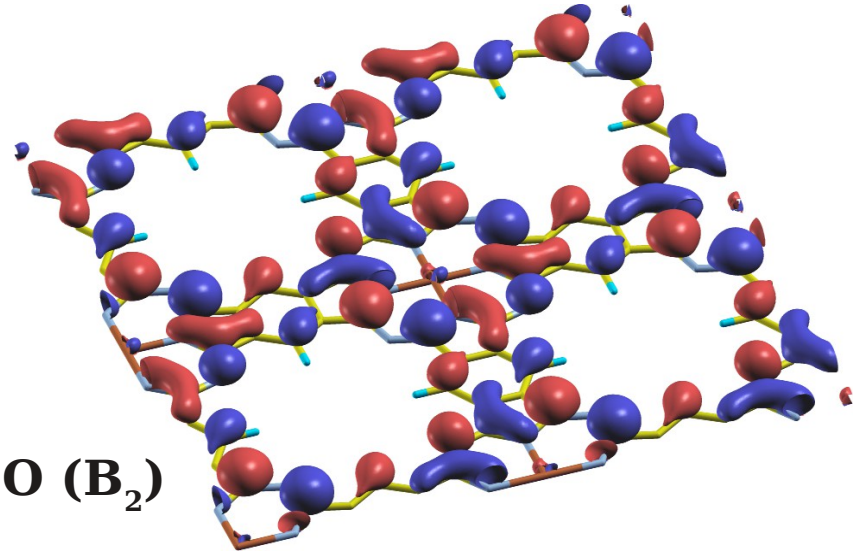


Festkörperphysik, CuPPC Orbitale

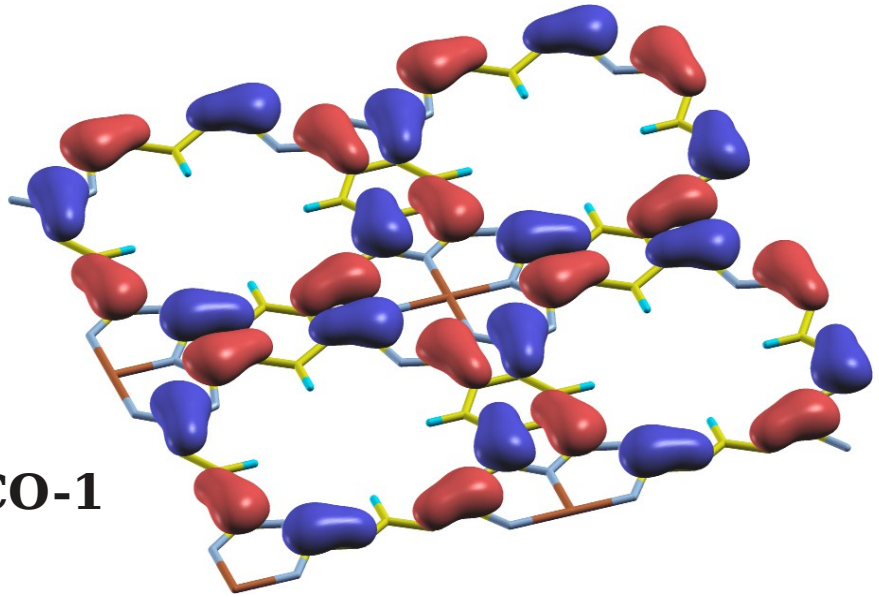
α-Kanal



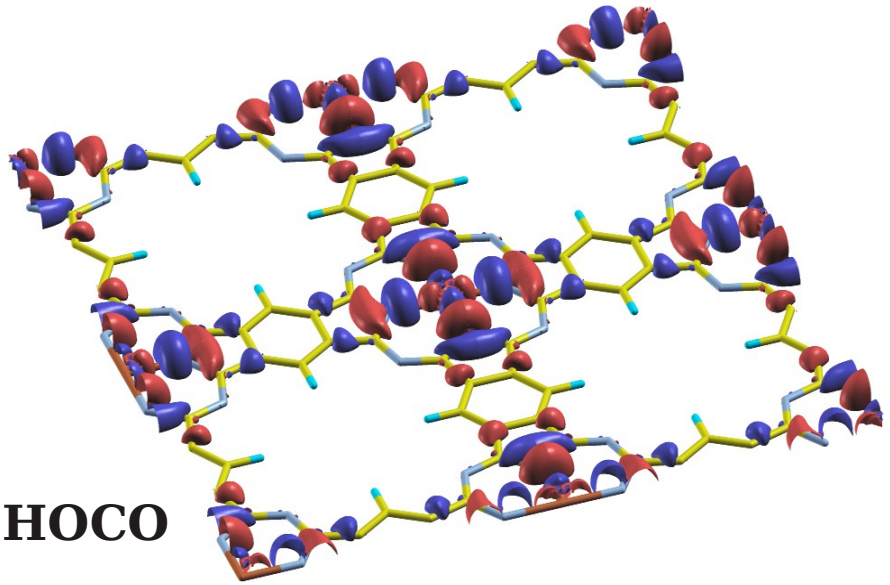
LUCO (A_2)



LUCO (B_2)



HOCO-1



HOCO

in Vorbereitung

Zusammenfassung

Artikel:

3 Publiziert

3 im Druck

5 in Vorbereitung

Danke für die Aufmerksamkeit!