

## Prof. Schmitt: Publikationen

Die Artikel können nur zum persönlichen Gebrauch heruntergeladen werden. Jede andere Verwendung bedarf der vorherigen Zustimmung des Autors und des Herausgebers.



<https://www.researcherid.com/rid/C-9708-2011>

ResearchGate

[https://www.researchgate.net/profile/Michael\\_Schmitt/](https://www.researchgate.net/profile/Michael_Schmitt/)



<https://orcid.org/0000-0002-7386-8092>



<https://orcid.org/0000-0002-7386-8092>

### Publications 2022

- 115 Marie-Luise Hebestreit, Hajo Böschen, Hilda Lartian, W. Leo Meerts und Michael Schmitt:  
**Rotationally resolved electronic spectroscopy of 6-methylindole: Structures, transition moments, and permanent dipole moments of ground and excited singlet states**  
J. Mol. Struct. **1252** (2022) 132053
- 114 Christian Brand und Michael Schmitt:  
**Vibronic coupling in serotonin studied by rotationally resolved electronic spectroscopy**  
J. Mol. Struct. **1250** (2022) 131819

### Publikationen 2021

- 113 Tony Ford, Sylvia Turrell, Michael Schmitt und Rui Fausto:  
**Austin Barnes**  
J. Mol. Struct. **1246** (2021) 131171
- 112 Mirko Matthias Lindic, Tim Axel Oberkirch, Jörg Tatchen und Michael Schmitt:  
**The excited state effective dipole moment of 2,3-benzofuran from thermochromic shifts in absorption and emission spectra**  
J. Photochem. Photobiol. A. **419** (2021) 113476

- 111 Vadim Ilyushin, Isabelle Kleiner, Masaaki Baba, Malgorzata Biczysko und Michael Schmitt:  
**Editorial**  
 Journal of Molecular Structure, Volume **1226** (2021), Part B, 129589
- 110 Marie-Luise Hebestreit, Hilda Lartian, Christian Henrichs, Ralf Kuehnemuth, W. Leo Meerts und Michael Schmitt:  
**Excited state dipole moments and lifetimes of 2-cyanoindole from rotationally resolved electronic Stark spectroscopy dagger**  
 Physical Chemistry Chemical Physics, Issue **17** (2021), 10196-10204
- 109 Christian Henrichs, Marie-Luise Hebestreit, Daniel Krügler und Michael Schmitt:  
**Structural changes upon electronic excitation in 1,3-dimethoxybenzene from Franck-Condon/rotational constants fits of the fluorescence emission spectra**  
 Journal of Molecular Structure, Volume **1233** (2021), 130106
- 108 Christian Henrichs, Stephan Zimmermann, Marie-Luise Hebestreit und Michael Schmitt:  
**Excited state structure of isolated 2-cyanoindole and the binary 2-cyanoindole-(H<sub>2</sub>O)<sub>1</sub> cluster from a combined Franck-Condon and rotational constants fit**  
 Journal of Molecular Structure, Volume **1233** (2021), 130055
- 107 Mirko Matthias Lindic und Michael Schmitt:  
**Ground and excited state dipole moments of 1-methylindole from thermochromic shifts in absorption and emission spectra**  
 Journal of Photochemistry and Photobiology A: Chemistry **406**, (2021) 112984
- 106 Christian Henrichs; Malte Reineke; Marie-Luise Hebestreit; Michael Schmitt:  
**Excited state structure of isolated 4-cyanoindole from a combined Franck-Condon and rotational constants analysis**  
 Journal of Molecular Structure, Volume **1223** (2021) 129241

### Publikationen 2020

- 105 Mirko Matthias Lindic, Matthias Zajonz, Marie-Luise Hebestreit, Michael Schneider, W Leo Meerts, Michael Schmitt:  
**Determination of excited state dipole moments in solution via thermochromic methods**  
 MethodsX **7** (2020) 101101-1 - 101101-12.
- 104 Christian Henrichs, Marie-Luise Hebestreit, Daniel Krügler, Michael Schmitt:  
**Structural changes upon electronic excitation in 1,2-dimethoxybenzene from Franck-Condon fits of the fluorescence emission spectra**  
 J. Mol. Struct. **1211** (2020) 127855  
 available online: 28.02.2020
- 103 Marie-Luise Hebestreit, Hilda Lartian, Michael Schneider, Ralf Kühnemuth, América Yareth Torres-Boy, Sergio Romero-Servin, José Arturo Ruiz-Santoyo, Leonardo Alvarez-Valtierra, W. Leo Meerts, Michael Schmitt:  
**Structure and excited state dipole moments of oxygen containing heteroaromatics: 2,3-benzofuran**  
 J. Mol. Struct. **1210** (2020) 127992

### Publikationen 2019

- 102 Mirko Matthias Lindic, Matthias Zajonz, Charlotte Gers-Panther, Thomas J.J. Müller, Michael Schmitt:

**The excited state dipole moment of 2-[(4-methoxyphenyl)ethynyl]-3-(1-methyl-1H-indol-3-yl)-quinoxaline from thermochromic shifts**

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (2020) 117574

- 101 Marie-Luise Hebestreit, Michael Schneider, Hilda Lartian, Vivienne Betz, Michael Heinrich, Mirko Lindic, Myong Yong Choi, Michael Schmitt:  
**Structures, dipole moments and excited state lifetime of isolated 4-cyanoindole in its ground and lowest electronically excited singlet states**  
Phys. Chem. Chem. Phys. **21** (2019) 14766-14774
- 100 Vasyl Yatsyna, Ranim Mallat, Tim Gorn, Michael Schmitt, Raimund Feifel, Anouk M. Rijs, Vitali Zhaunerchyk:  
**Competition between folded and extended structures of alanylalanine (Ala-Ala) in a molecular beam**  
Phys. Chem. Chem. Phys. **21** (2019) 14126-14132
- 99 Marie-Luise Hebestreit, Christian Henrichs, Michael Schneider, Martin Wilke, W. Leo Meerts, Daniel Krügler, Michael Schmitt:  
**Structural changes upon electronic excitation in 1,2-dimethoxybenzene from rotationally resolved electronic spectroscopy of various isotopologues**  
J. Mol. Struct. **1184** (2019) 139-145
- 98 Vasyl Yatsyna, Ranim Mallat, Tim Gorn, Michael Schmitt, Raimund Feifel, Anouk M. Rijs, Vitali Zhaunerchyk:  
**Conformational Preferences of Isolated Glycylglycine (Gly-Gly) Investigated with IRMPD-VUV Action Spectroscopy and Advanced Computational Approaches**  
J. Phys. Chem. A **123** (2019) 862-872

**Publikationen 2018**

- 97 Mirko Matthias Lindic, Matthias Zajonz, Marie-Luise Hebestreit, Michael Schneider, W. Leo Meerts, Michael Schmitt:  
**Additional data for evaluation of the excited state dipole moments of anisole**  
Data in Brief **21** (2018) 313-315
- 96 Michael Schneider, Marie-Luise Hebestreit, Mirko Matthias Lindic, Hilda Parsian, América Yareth Torres-Boy, Leonardo Álvarez-Valtierra, Leo Meerts, Ralf Kühnemuth, Michael Schmitt:  
**Rotationally resolved electronic spectroscopy of 3-cyanoindole and the 3-cyanoindole-water complex**  
PCCP **20** (2018) 23441-23452
- 95 Mirko Matthias Lindic, Matthias Zajonz, Marie-Luise Hebestreit, Michael Schneider, W. Leo Meerts, Michael Schmitt:  
**Excited state dipole moments of anisole in gas phase and solution**  
Journal of Photochemistry & Photobiology A: Chemistry **365** (2018) 213-219
- 94 Michael Schneider, Martin Wilke, Marie-Luise Hebestreit, Christian Henrichs, W. Leo Meerts, Michael Schmitt:  
**Excited-State Dipole Moments and Transition Dipole Orientations of Rotamers of 1,2-, 1,3, and 1,4-Dimethoxybenzene**  
ChemPhysChem **19** (2018) 307-318

## Publikationen 2017

- 93 Michael Schmitt, W. Leo Meerts:  
**Structures and Dipole Moments of Molecules in Their Electronically Excited States**  
Frontiers and Advances in Molecular Spectroscopy (2017) 143 - 194 Editor: Jaan Laane  
eBook ISBN: 9780128112212  
Paperback ISBN: 9780128112205
- 92 Michael Schneider, Martin Wilke, Marie-Luise Hebestreit, José Arturo Ruiz- Santoyo, Leonardo Álvarez-Valtierra, John T. Yi, W. Leo Meerts, David W. Pratt, Michael Schmitt:  
**Rotationally Resolved Electronic Spectroscopy of Rotamers of 1,3-Dimethoxybenzene Hot article**  
PCCP **19** (2017) 21364-21372
- 91 Martin Wilke, Christian Brand, Josefin Wilke, Michael Schmitt:  
**Influence of the position of the methoxy group on the stabilities of the *syn* and *anti* conformers of 4-, 5-, and 6-methoxyindole**  
J. Mol. Spectros. **337** (2017) 137-144
- 90 Felix Gmerek, Benjamin Stuhlmann, Elvedina Pehlivanovic, Michael Schmitt:  
**Franck Condon spectra of the 2-tolunitrile dimer and the binary 2-tolunitrile water cluster in the gas phase**  
J. Mol. Struct. **1143** (2017) 265-273
- 89 Martin Wilke, Michael Schneider, Josefin Wilke, José Arturo Ruiz-Santoyo, Jorge J. Campos-Amador, M. Elena González-Medina, Leonardo Álvarez- Valtierra, Michael Schmitt:  
**Rotationally resolved electronic spectroscopy study of the conformational space of 3-methoxyphenol**  
Journal of Molecular Structure **1140** (2017) 59-66
- 88 Josefin Wilke, Martin Wilke, Christian Brand, J. Dominik Spiegel, Christel M. Marian, Michael Schmitt:  
**Modulation of the  $L_a/L_b$  Mixing in an Indole Derivative: A Position-Dependent Study Using 4-, 5-, and 6-Fluoroindole**  
J. Phys. Chem. A **121** (2017) 1597

## Publikationen 2016

- 87 Michael Schmitt, Frans Spiering, Vitali Zhaunerchyk, Rienk T. Jongma, Sander Jaeqx, Anouk M. Rijs, Wim J. van der Zande:  
**Far-infrared spectra of the Tryptamine A conformer by IR-UV Ion Gain Spectroscopy**  
PCCP **18** (2016) 32116
- 86 Josefin Wilke, Martin Wilke, Christian Brand, W. Leo Meerts, Michael Schmitt: **On the Additivity of Molecular Fragment Dipole Moments of 5-Substituted Indole Derivatives**  
ChemPhysChem **17** (2016) 2736
- 85 Martin Wilke, Christian Brand, Josefin Wilke, Michael Schmitt:  
**The conformational space of the neurotransmitter serotonin: how the rotation of a hydroxyl group changes all**  
PCCP **18** (2016) 13538

- 84 Felix Gmerek, Benjamin Stuhlmann, Leonardo Álvarez-Valtierra, David W. Pratt, Michael Schmitt:  
**Electronic spectra of 2- and 3-tolunitrile in the gas phase. II. Geometry changes from Franck-Condon fits of fluorescence emission spectra**  
 J. Chem. Phys. **144** (2016) 084304
- 83 José Arturo Ruiz-Santoyo, Josefin Wilke, Martin Wilke, John T. Yi, David W. Pratt, Michael Schmitt, Leonardo Álvarez-Valtierra:  
**Electronic spectra of 2- and 3-tolunitrile in the gas phase. I. A study of methyl group internal rotation via rovibronically resolved spectroscopy** J. Chem. Phys. **144** (2016) 044303
- 82 Josefin Wilke, Martin Wilke, W. Leo Meerts, Michael Schmitt:  
**Determination of ground and excited state dipole moments via electronic Stark spectroscopy: 5-methoxyindole**  
 J. Chem. Phys. **144** (2016) 044201

### Publikation 2015

- 81 José Arturo Ruiz-Santoyo, Marcela Rodríguez-Matus, José Luis Cabellos, John T. Yi, David W. Pratt, Michael Schmitt, Gabriel Merino, Leonardo Álvarez-Valtierra:  
**Intramolecular structure and dynamics of mequinol and guaiacol in the gasphase: Rotationally resolved electronic spectra of their S<sub>1</sub> states**  
 J. Chem. Phys. **143** (2015) 94301143

### Publikationen 2014

- 80 Benjamin Stuhlmann, Felix Gmerek, Daniel Krügler, Michael Schmitt:  
**Determination of the geometry change of benzimidazole upon electronic excitation from a combined Franck-Condon/rotational constants fit**  
 J. Mol. Struct. **1072** (2014) 45-52
- 79 Benjamin Stuhlmann, Anna Gräßle, Michael Schmitt:  
**Determination of the geometry change of 5-cyanoindole upon electronic excitation from a combined Franck-Condon/rotational constants fit**  
 Phys. Chem. Chem. Phys. **16** (2014) 899-905

### Publikationen 2013

- 78 Christian Brand, Josefin Rolf, Martin Wilke, Michael Schmitt:  
**High Resolution Electronic Spectroscopy of Vibrationally Hot Bands of Benzimidazole**  
 J. Phys. Chem. A **117** (2013) 12812-12820
- 77 Christian Brand, Beatrice Happe, Olivia Oeltermann, Martin Wilke, Michael Schmitt:  
**High resolution spectroscopy of several rovibronically excited bands of 5-cyanoindole - The effect of vibrational averaging.**  
 J. Mol. Struct. **1044** (2013) 21-25
- 76 Christian Brand, Olivia Oeltermann, Martin Wilke, Michael Schmitt: Position matters: High resolution spectroscopy of 6-methoxyindole. J. Chem. Phys. **138** (2013) 024321
- 75 G. Engler, K. Seefeld, M. Schmitt, J. Tachen, O. Grotkopp, T. J. J. Müller, K. Kleineremanns:  
**Acetylation makes the difference: a joint experimental and theoretical study on low-lying electronically excited states of 9H-adenine and 9-acetyladenine.**  
 Phys. Chem. Chem. Phys. **15** (2013) 1025-1031

## Publikationen 2012

- 74 Olivia Oeltermann, Christian Brand, Martin Wilke, Michael Schmitt:  
Ground and Electronically Excited Singlet State Structures of the syn and anti Rotamers of 5-Hydroxyindole.  
J. Phys. Chem. A **116** (2012) 7873-7879
- 73 Christian Brand, Olivia Oeltermann, Martin Wilke, Jörg Tatchen, Michael Schmitt:  
**Ground and Electronically Excited Singlet-State Structures of 5-Fluoroindole Deduced from Rotationally Resolved Electronic Spectroscopy and *ab Initio* Theory.**  
Chem. Phys. Chem. **13** (2012) 3134
- 72 Olivia Oeltermann, Christian Brand, Bernd Engels, Jörg Tatchen, Michael Schmitt:  
**The structure of 5-cyanoindole in the ground and the lowest electronically excited singlet states, deduced from rotationally resolved electronic spectrascopy and *ab initio* theory.**  
Phys. Chem. Chem. Phys. **14** (2012) 10266-10270

## Publikationen 2011

- 71 Michael Schmitt, W. Leo Meerts:  
**Handbook of High Resolution Spectroscopy**  
Herausgeber: M. Quack and F. Merkt  
John Wiley and Sons, 2011, ISBN: 978-0-470-06653-9
- 70 John T Yi, Christian Brand, Miriam Wollenhaupt, David W Pratt, W. Leo Meerts, Michael Schmitt:  
**Rotationally resolved electronic spectroscopy of biomolecules in the gas phase. Melatonin.**  
J. Mol. Spectros. **268** (2011) 115
- 69 Christian Brand, W. Leo Meerts, Michael Schmitt:  
**How and why do transition dipole moment orientations depend on conformer structure?**  
J. Phys. Chem. A **115** (2011) 9612
- 68 Olivia Oeltermann, Christian Brand, W. Leo Meerts, Jörg Tatchen, Michael Schmitt:  
**Rotationally resolved electronic spectroscopy of 2,3-bridged indole derivatives: tetrahydrocarbazole.**  
J. Mol. Struct. **933** (2011) 2
- 67 Thi-Bao Chau Vu, Christian Brand, W. Leo Meerts, Michael Schmitt: **Rotationally resolved electronic spectroscopy of 1,4-benzodioxan: The anomeric effect in the ground and electronically excited state.**  
ChemPhysChem **12** (2011) 2035

## Publikationen 2010

- 66 Christian Brand, Olivia Oeltermann, David Pratt, Rainer Weinkauff, W. Leo Meerts, Wim van der Zande, Karl Kleinermanns, Michael Schmitt:  
Rotationally resolved electronic spectroscopy of 5-methoxyindole.  
J. Chem. Phys. **133** (2010) 024303
- 65 Jochen Küpper, David W. Pratt, W. Leo Meerts, Christian Brand Jörg Tatchen, Michael Schmitt:  
**Vibronic coupling in indole: II. Investigation of the  $^1L_a$ - $^1L_b$  interaction using rotationally resolved electronic spectroscopy. Hot article**

PCCP **12** (2010) 4980-4988

- 64 Christian Brand, Jochen Küpper, David W. Pratt, W. Leo Meerts, Daniel Krügler, Jörg Tatchen, Michael Schmitt:

Vibronic coupling in indole: I. Theoretical description of the 1La–1Lb interaction and the electronic spectrum. Hot article

PCCP **12** (2010) 4968-4979

### Publikationen 2009

- 63 Michael Schmitt, Lars Biemann, W. Leo Meerts, Karl Kleinermanns:  
Analysis of the FTIR spectrum of pyrazine using evolutionary algorithms.  
J. Mol. Spectros. **257** (2009) 74
- 62 Ivo Kalkman, Christian Brand, Thi-Bao Chau Vu, W. Leo Meerts, Yuriy N. Svartsov, Otto Dopfer, Xin Tong, Klaus Müller Dethlefs, Stefan Grimme, Michael

Schmitt:

The structure of phenol-Arn ( $n=1, 2$ ) clusters in their  $S_0$  and  $S_1$  states.

J. Chem. Phys. **130** (2009) 224303

- 61 Ivo Kalkman, Thi-Bao Chau Vu, Michael Schmitt, W. Leo Meerts:  
**Structure and internal rotation in the  $S_0$  and  $S_1$  states of o-toluidine studied by high resolution UV spectroscopy.**

Phys. Chem. Chem. Phys. **11** (2009) 4311

- 60 Thi Bao Chau Vu, Ivo Kalkman, W. Leo Meerts, Christian Brand, Yuriy N. Svartsov, Sascha Wiedemann, Rainer Weinkauff, Michael Schmitt:

**The conformational landscape of 5-methoxytryptamine studied by rotationally resolved fluorescence spectroscopy and resonant ionization spectroscopy.**

Phys. Chem. Chem. Phys. **11** (2009) 2433

- 59 Marcel Böhm, Jörg Tatchen, Daniel Krügler, Karl Kleinermanns, Michael G. D. Nix, Tracy A. LeGreve, Timothy S. Zwier, Michael Schmitt:

**High-resolution and Dispersed Fluorescence Examination of Vibronic bands of Tryptamine: Spectroscopic signatures for  $L_a/L_b$  mixing near a conical intersection.**

J. Phys. Chem. A **113** (2009) 2456

- 58 Marcel Böhm, Robert Brause, Christoph Jacoby, Michael Schmitt:

Conformational Relaxation Paths in Tryptamine.

J. Phys. Chem. A **113** (2009) 448

### Publikationen 2008

- 57 Michael Motsch, Markus Schenk, Martin Zeppenfeld, Michael Schmitt, W. Leo Meerts, Pepijn W.H. Pinkse, Gerhard Rempe:

**Spectroscopy of the  $\tilde{A}^1A_2 \leftarrow \tilde{X}^1A_1$  transition of formaldehyde in the 30140–30790  $\text{cm}^{-1}$  range: The  $2^1 4^3$  and  $2^2 4^1$  rovibrational bands.**

0 0 0 0

J. Mol. Spectrosc. **252** (2008) 25

- 56 Ivo Kalkman, Thi Bao Chau Vu, Michael Schmitt, W. Leo Meerts: **Tunneling splittings in the  $S_0$  and  $S_1$  states of the benzoic acid dimer determined by high-resolution UV spectroscopy.**

ChemPhysChem. **9** (2008) 1788

- 55 Thi Bao Chau Vu, Ivo Kalkman, W. Leo Meerts, Yuriy N. Svartsov, Christoph Jacoby, Michael Schmitt:

**Rotationally resolved electronic spectroscopy of water clusters of 7-azaindole.**

J. Chem. Phys. **128** (2008) 214311

54 Yuriy N. Svartsov, Michael Schmitt:

**Electronically excited states of water clusters of 7-azaindole: Structures, relative energies, and electronic nature of the excited states.**

J. Chem. Phys. **128** (2008) 214310

**Publikationen 2007**

53 Brause, R., Schmitt M., Kleinermanns, K.:

**Improved Determination of Structural Changes of 2-Pyridone-(H<sub>2</sub>O)<sub>1</sub> upon Electronic Excitation.**

J. Phys. Chem. A. **111** (2007) 3287

52 Robert Brause, Monika Santa, Michael Schmitt, Karl Kleinermanns: **Determination of the Geometry Change of the Phenol Dimer upon Electronic Excitation.**

ChemPhysChem **8** (2007) 1394

**Publikationen 2006**

51 Böhm, M., Ratzner, C., Schmitt, M.:

**The structure of p-chlorophenol and barrier to internal -OH rotation in the S<sub>1</sub>-state.**

J. Mol. Struct. **800** (2006) 55

50 Lee, Y., Kim, B., Schmitt, M., Kleinermanns, K.:

**Observation of Ultraviolet Rotational Band Contours of the DNA Base Adenine: Determination of the Transition Moment.**

J. Phys. Chem. A **110** (2006) 11819

49 Schmitt, M., Brause, R., Marian, C., Salzmann, S., Meerts, W. L.: Electronically excited states of tryptamine and its microhydrated complex. J. Chem. Phys. **125** (2006) 124309

48 Schmitt, M., Feng, K., Böhm, M., Kleinermanns, K.:

**Low frequency backbone vibrations of individual conformational isomers: tryptamine.**

J. Chem. Phys. **125** (2006) 144303

47 Meerts, W. L. und Schmitt, M.:

**Application of Genetic Algorithms in automated assignments of high resolution spectra.**

Int. Rev. Phys. Chem. **25** (2006) 353

46 Schmitt, M., Böhm, M., Ratzner, C., Krügler, D., Kleinermanns, K., Kalkman, I., Berden, G., Meerts, W. L.:

**Determining the intermolecular structure in the S<sub>0</sub> and S<sub>1</sub> states of the phenol dimer by rotationally resolved electronic spectroscopy.**

ChemPhysChem **7** (2006) 1241

45 Schmitt, M., Böhm, M., Ratzner, C., Siegert, S., van Beek, M., Meerts, W. L.:

Electronic excitation in the benzonitrile dimer: The intermolecular structure

in the S<sub>0</sub> and S<sub>1</sub> state determined by rotationally resolved electronic spectroscopy.

J. Mol. Struct. **795** (2006) 234



- 44 Jacoby, C., Böhm, M., Vu, C., Ratzer, C., Schmitt, M.:  
**Probing the acidity of p-substituted phenols in the excited state: electronic spectroscopy of the p-cyanophenol-water cluster.**  
 ChemPhysChem **7** (2006) 448
- 43 Schmitt, M., Krügler, D., Böhm, M., Ratzer, C., Bednarska, V., Kalkman, I., Meerts, W. L.:  
**A genetic algorithm based determination of the ground and excited <sup>1</sup>L<sub>b</sub> state structure and the orientation of the transition dipole moment of benzimidazole.**  
 Phys. Chem. Chem. Phys. **8** (2006) 228
- 42 Meerts, W. L. und Schmitt, M.:  
**A new automated assign and analysing method for high resolution rotational resolved spectra using Genetic Algorithms.**  
 Phys. Scripta **73** (2006) C47

### Publikationen 2005

- 41 Brause, R., Krügler, D., Schmitt, M., Kleinermanns, K., Nakajima, A., Miller, T. A.:  
**Determination of the excited state structure of 7-azaindole water cluster using a Franck-Condon analysis.**  
 J. Chem. Phys. **123** (2005) 224311
- 40 Myszkiewicz, G., Meerts, W. L., Ratzer, C., Schmitt, M.:  
**Structure Determination of Resorcinol Rotamers by High-Resolution UV Spectroscopy.**  
 ChemPhysChem **6** (2005) 2129
- 39 Schmitt, M., Böhm, M., Ratzer, C., Vu, C., Kalkman, I., Meerts, W. L.: **Structural selection by microsolvation: conformational locking of tryptamine.**  
 J. Am. Chem. Soc. **127** (2005), 10356
- 38 Myszkiewicz, G., Meerts, W. L., Ratzer, C., Schmitt, M.:  
**The structure of 4-methylphenol and its water cluster revealed by rotationally resolved UV-spectroscopy using a genetic algorithm approach.** J. Chem. Phys. **123** (2005) 044304
- 37 Myszkiewicz, G., Meerts, W. L., Ratzer, C., Schmitt, M.:  
**Rotational isomers of hydroxy deuterated o- and m-cresols studied by ultraviolet high resolution experiments.**  
 Phys. Chem. Chem. Phys. **7** (2005) 2142
- 36 Schmitt, M., Ratzer, C., Jacoby, C., Meerts, W. L.:

Structure and barrier to internal rotation of 4-methylstyrene in the S<sub>0</sub>- and S<sub>1</sub>-state.

J. Mol. Struct. **742** (2005) 123

### Publikationen 2004

- 35 Jacoby, C. und Schmitt, M.:  
**Torsional barriers in aromatic molecular clusters as probe of the electronic properties of the chromophore.**  
 Chem. Phys. Chem. **5** (2004) 1686
- 34 Schmitt, M., Ratzer, C., Kleinermanns, K. und Meerts, W. L.:

**Determination of the structure of 7-azaindole in the electronic ground and excited state using high resolution ultra-violet spectroscopy and an automated assignment based on a genetic algorithm.**

Mol. Phys. **102** (2004) 1605

- 33 Brause, R., Schmitt, M., Spangenberg, D. und Kleinermanns, K.:  
**Determination of the excited state structure of 7-azaindole using a Franck-Condon analysis.**  
Mol. Phys. **102** (2004) 1615
- 32 Meerts, W. L., Schmitt, M. und Groenenboom, G.:  
**New applications of the Genetic Algorithm for the interpretation of High Resolution Spectra.**  
Can. J. Chem. **82** (2004) 804
- 31 Schmitt, M., Ratzer, C. und Meerts, W. L.:  
**The structure of the phenol-nitrogen cluster. A joint experimental and *ab initio* study.**  
J. Chem. Phys. **120** (2004) 2752

### **Publikationen 2003**

- 30 Westphal, A., Jacoby, C., Ratzer, C., Reichelt, A. und Schmitt, M.: **Determination of the intermolecular geometry of the phenol-methanol cluster.**  
Phys. Chem. Chem. Phys. **5** (2003) 4114
- 29 Ratzer, C., Nispel, M. und Schmitt, M.:  
**Structure of p-fluorophenol and barrier to internal -OH torsion in the S<sub>1</sub>- state.**  
Phys. Chem. Chem. Phys. **5** (2003) 812

### **Publikationen 2002**

- 28 Küpper, J., Schmitt, M. und Kleinermanns, K.:  
The Rotationally Resolved Electronic Spectrum of p-Cyanophenol.  
Phys. Chem. Chem. Phys. **4** (2002) 4634
- 27 Ratzer, C., Küpper, J., Spangenberg, D. und Schmitt, M.:  
**The structure of phenol in the S<sub>1</sub>-state determined by high resolution UV-spectroscopy.**  
Chem. Phys. **283** (2002) 153
- 26 Plützer, C., Jacoby, C. und Schmitt, M.:  
**Internal rotation and intermolecular vibrations of the phenol-methanol cluster: A Comparison of Spectroscopic Results and *Ab Initio* Theory.** J. Phys. Chem.A **106** (2002) 399

### **Publikationen 2001**

- 25 Schmitt, M., Plützer, C. und Kleinermanns, K.:  
**Determination of the structures of benzotriazole(H<sub>2</sub>O)<sub>1,2</sub> clusters by IR-UV spectroscopy and *ab initio* theory.**  
Phys. Chem. Chem. Phys. **3** (2001) 4218
- 24 Küpper, J., Westphal, A. und Schmitt, M.:  
**The structure of the binary phenol-methanol cluster: A comparison of experiment and *ab initio* theory.**  
Chem. Phys. **263** (2001) 41

## Publikationen 2000

- 23 Schmitt, M., Küpper, J., Spangenberg, D. und Westphal, A.:  
**Determination of the structures and barriers to hindered internal rotation of the phenol-methanol cluster in the  $S_0$  and  $S_1$  state.**  
Chem. Phys. **254** (2000) 349
- 22 Schmitt, M., Jacoby, C., Gerhards, M., Unterberg, C., Roth, W. und Kleinermanns, K.:  
Structures and vibrations of phenol(NH<sub>3</sub>)<sub>2-4</sub> clusters.  
J. Chem. Phys. **113** (2000) 2995
- 21 Jacoby, C., Roth, W. und Schmitt, M.:  
**A comparison of intermolecular vibrations and tautomerism in benzimidazole, benzotriazole and their binary water clusters.** Appl. Phys. B **71** (2000) 643

## Publikationen 1991 - 1999

- 20 Roth, W., Spangenberg, D., Janzen, C., Westphal, A. und Schmitt, M.:  
**The relative stability of benzotriazole tautomers determined by a rotational band contour analysis of the N-H stretching vibration.**  
Chem. Phys. **248** (1999) 17
- 19 Jacoby, C., Hering, P., Schmitt, M., Roth, W. und Kleinermanns, K.: **Investigations of OH—N- and NH—O-type hydrogen-bonded clusters by UV laser spectroscopy.**  
Chem. Phys. **239** (1998) 23
- 18 Jacoby, C., Roth, W., Schmitt, M., Janzen, C., Spangenberg, D. und Kleinermanns, K.:  
**Intermolecular Vibrations of Phenol(H<sub>2</sub>O)<sub>2-5</sub> and Phenol(D<sub>2</sub>O)<sub>2-5-d<sub>1</sub></sub> Studied by UV Double-Resonance Spectroscopy and *ab Initio* Theory.**  
J. Phys. Chem. A **102** (1998) 4471
- 17 Schmitt, M., Jacoby, C. und Kleinermanns, K.:  
**Torsional splitting of the intermolecular vibrations of phenol (H<sub>2</sub>O)<sub>1</sub> and its deuterated isotopomers.**  
J. Chem. Phys. **108** (1998) 4486
- 16 Roth, W., Jacoby, C., Westphal, A. und Schmitt, M.:  
**A study of 2H- and 2D-benzotriazole in their lowest electronic states by UV-laser double-resonance spectroscopy.**  
J. Phys. Chem. A **102** (1998) 3048
- 15 Roth, W., Schmitt, M., Jacoby, C., Spangenberg, D., Janzen, C. und Kleinermanns, K.:  
**Double resonance spectroscopy of phenol(H<sub>2</sub>O)<sub>1-12</sub>: evidence for ice-like structures in aromate-water clusters?**  
Chem. Phys. **239** (1998) 1
- 14 Kleinermanns, K., Gerhards, M. und Schmitt, M.:  
**Electronic Spectroscopy of Aromatic Molecules in Jet-Cooled Hydrogen Bonded Clusters- Structure and Fluxionality.**  
Ber. Bunsenges. Phys. Chem. **101** (1997) 1785
- 13 Berden, G., Meerts, W. L., Schmitt, M. und Kleinermanns, K.:  
**High resolution UV spectroscopy of phenol and the hydrogen bonded phenol-water cluster.**

- J. Chem. Phys. **104** (1996) 972
- 12 Gerhards, M., Schmitt, M., Kleinermanns, K. und Stahl, W.:  
The structure of phenol(H<sub>2</sub>O) obtained by microwave spectroscopy.  
J. Chem. Phys. **104** (1996) 967
- 11 Schmitt, M., Müller, H., Henrichs, U., Gerhards, M., Perl, W., Deusen, C. und Kleinermanns, K.:  
**Structure and vibrations of phenol·CH<sub>3</sub>OH (CD<sub>3</sub>OD) in the electronic ground and excited state, revealed by spectral hole burning and dispersed fluorescence spectroscopy.**  
J. Chem. Phys. **103** (1995) 584
- 10 Schmitt, M., Henrichs, U., Müller, H. und Kleinermanns, K.:  
  
Intermolecular vibrations of the phenol dimer revealed by spectral hole burning and dispersed fluorescence spectroscopy.  
J. Chem. Phys. **103** (1995) 9918
- 9 Schiefke, A., Deusen, C., Jacoby, C., Gerhards, M., Schmitt, M., Kleinermanns, K. und Hering, P.:  
Structure and vibrations of the phenol-ammonia cluster.  
J. Chem. Phys. **102** (1995) 9197
- 8 Schmitt, M., Müller, H. und Kleinermanns, K.:  
**A study of intermolecular vibrational frequencies of phenol·(H<sub>2</sub>O)<sub>3</sub> by spectral hole burning spectroscopy.**  
Chem. Phys. Letters **218** (1994) 246
- 7 Kamps, R., Müller, H., Schmitt, M., Sommer, S., Wang, Z. und Kleinermanns, K.:  
**Photooxidation of exhaust pollutants. I. Degregation efficiencies, quantum yields and products of benzene photooxidation.**  
Chemosphere **27** (1993) 2127
- 6 Gerhards, M., Kimpfel, B., Pohl, M., Schmitt, M. und Kleinermanns, K.:  
Vibronic spectroscopy of jet-cooled hydrogen bonded clusters.  
J. Mol. Struct. **270** (1992) 301
- 5 Wolf, K., Kuge, H.-H., Schmitt, M. und Kleinermanns, K.:  
**Kinetics of Formation and Vibronic Spectroscopy of H-Bonded Clusters in Supersonic Jets.**  
Ber. Bunsenges. Phys. Chem. **96** (1992) 1309
- 4 Pohl, M., Schmitt, M. und Kleinermanns, K.:  
**Vibrational spectroscopy of size-assigned p-cresol/H<sub>2</sub>O-clusters in the S<sub>0</sub> and S<sub>1</sub> state.**  
Chem. Phys. Letters **177** (1991) 252
- 3 Schmitt, M., Pohl, M. und Kleinermanns, K.:  
**2-color ionization dip spectroscopy of size assigned hydrogen bonded clusters.**  
Internat. Phys. Conf. **114** (1991) 421
- 2 Pohl, M., Schmitt, M., Wolf, K. und Kleinermanns, K.:  
Microscopic shifts of size-assigned p-cresol(H<sub>2</sub>O)-cluster spectra.  
J. Chem. Phys. **94** (1991) 1717
- 1 Kleinermanns, K. und Schmitt, M.:  
Process for processing solid particles containing toxic chemicals.  
PCT Int. Appl. (2000). Patent WO 9118671 A1

