

## Prof. Schmitt: Publications

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### Publications 2022

- 115 Marie-Luise Hebestreit, Hajo Bösch, 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

### Publications 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

### **Publications 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

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**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

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- 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

## Publications 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

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**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

### Publications 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

### Publications 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

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**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
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**Acetylation makes the difference: a joint experimental and theoretical study on low-lying electronically excited states of 9H-adenine and 9-acetyladenine.**  
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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 spectroscopy and *ab initio* theory.**  
Phys. Chem. Chem. Phys. **14** (2012) 10266-10270

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- 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

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- 66 Christian Brand, Olivia Oeltermann, David Pratt, Rainer Weinkauf, 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:

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

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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

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**Structure and internal rotation in the  $S_0$  and  $S_1$  states of o-toluidine studied by high resolution UV spectroscopy.**

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

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- 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

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- 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.**

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

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

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

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

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

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

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

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**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.**  
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