

PUBLICATIONS

2021

- (125) B. E. Arenas, G. Batra, A. L. Steber, L. Bizzocchi, B. M. Giuliano, B. J. Harris, B. J. Pate, M. Schnell
“Rotational spectroscopy of imidazole: Three vibrationally excited states and a molecular structure based on an extended frequency range”
J. Mol. Spec., Festschrift Stefan Schlemmer, accepted (2021)
- (124) P. Stahl, B. E. Arenas, O. Zingsheim, M. Schnell, L. Margules, R. A. Motiyenko, G. W. Fuchs, T. F. Giesen
“Deciphering the rotational spectrum of the first excited torsional state of propylene oxide”
J. Mol. Spec., Festschrift Stefan Schlemmer, accepted (2021)
- (123) B. E. Arenas, M. Fatima, C. Perez, S. Fischer, A. L. Steber, M. Schnell
“Facilitating interstellar searches for simple amino alcohols with accurate rest frequencies up to the millimeter-wave regime: Alaninol, valinol, and leucinol”
Astrophys. J. accepted (2021).
- (122) M. Mar Quesada-Moreno, P. Pinacho, C. Perez, M. Sekutor, P. R. Schreiner, M. Schnell
“Do docking sites persist upon fluorination? The diadamantyl ether aromacts challenge for rotational spectroscopy and theory”
Chemistry – A European Journal (2021) doi.org/10.1002/chem.202100078
- (121) R. Tama Saragi, M. Juanes, C. Perez, P. Pinacho, D. S. Tikhonov, W. Caminati, M. Schnell, A. Lesarri
“Switching Hydrogen bonding to π -stacking: The thiophenol dimer and trimer”
J. Phys. Chem. Lett., **12** (2021) 1367-1373.
- (120) S. R. Domingos, C. Perez, N. M. Kreienborg, C. Merten, M. Schnell
“Dynamic chiral self-recognition in aromatic dimers of styrene oxide revealed by rotational spectroscopy”
Comm. Chemistry, **4** (2021) 32.
- (119) A. Lemmens, P. Chopra, D. Garg, A. L. Steber, M. Schnell, W. J. Buma, A. M. Rijs
“High resolution infrared spectroscopy of naphthalene and acenaphthene dimers”
Mol. Phys., Festschrift Dave Parker, **119** (2021) e1811908.
- (118) W. Li, M. Mar Quesada-Moreno, P. Pinacho, M. Schnell
“Unlocking the water trimer loop: Isotopic study of benzophenone-(H₂O)₁₋₃ clusters with rotational spectroscopy”
Angewandte Chemie Int. Ed. **60** (2021) 5323-5330.

2020

- (117) P. Pinacho, D. A. Obenchain, M. Schnell
“New findings from old data: A semi-experimental value for the eQq of the nitrogen atom”
J. Chem. Phys. **153** (2020) 234307. Editor’s choice.
- (116) M. Fatima, D. Maue, C. Perez, D. S. Tikhonov, D. Bernhard, A. Stamm, C. Medcraft, M. Gerhards, M. Schnell
“Structures and internal dynamics of diphenylether and its aggregates with water”
Physical Chemistry Chemical Physics **22** (2020) 27966-27978.
- (115) A. Lemmens, D. Rap, J. Thunnissen, S. Gruet, A.L. Steber, S. Panchagnula, A. Tielens, M. Schnell, W.J. Buma, A.M. Rijs
“Far-IR Absorption of Neutral PAHs: Light on the Mechanism of IR-UV Ion Dip Spectroscopy”
The Journal of Physical Chemistry Letters, **11** (2020) 8997-09002
- (114) S. R. Domingos, C. Perez, M. D. Marshall, H. O. Leung, M. Schnell
“Assessing the performance of rotational spectroscopy in chiral analysis”
(Minireview)
Chem. Science **11** (2020) 10863-10870.
- (113) P. Stahl, B. E. Arenas, S. R. Domingos, G. W. Fuchs, M. Schnell, T. F. Giesen
“Laboratory blueprints for interstellar searches of aromatic chiral molecules: rotational signatures of styrene oxide”
Physical Chemistry Chemical Physics **22** (2020) 21474-21487.
- (112) M. Mar Quesada-Moreno, P. Pinacho, C. Perez, M. Sekutor, P. R. Schreiner, M. Schnell
“London dispersion and hydrogen bonding interactions in bulky molecules: The diadamantyl ether case”
Chemistry- A European Journal, **26** (2020) 10817-10825.
- (111) V. L. Heywood, T. P. J. Alford, J. J. Roeleveld, S. J. Lekanne Deprez, A. Verhoofstad, J. I. van der Vlugt, S. R. Domingos, M. Schnell, A. P. Davis and T. J. Mooibroek
“Observations of tetrel bonding between sp^3 -carbon and THF”
Chem. Science, **11** (2020) 5289-5293.
- (110) S. Gruet, A. L. Steber, M. Schnell,
“Reconnaissance of the uncharted low energy vibrational motions of acenaphthene”
J. Mol. Spec., Special Issue for Astrochemistry, **371** (2020) 111296.

- (109) M. Fatima, , C. Perez, B. E. Arenas, M. Schnell, A. L. Steber
“Benchmarking a new segmented K-band chirped-pulse microwave spectrometer and its application to the conformationally rich amino alcohol isoleucinol”
Physical Chemistry Chemical Physics, **22** (2020) 17042-17051.
- (108) D. S. Tikhonov, A. Datta, P. Chopra, A. L. Steber, B. Manschwetus, M. Schnell
“Towards black-box calculations of pump-probe fragmentation dynamics of polyatomic molecules”
Zeitschrift für Physikalische Chemie, Special issue dedicated to the 65th birthday of Friedrich Temps **234** (2020) 1507-1531.
- (107) H. Gottschalk *et al.*,
“The first microsolvation step of furans: New experiments and benchmarking strategies”
Journal of Chemical Physics **152** (2020) 164303.
- (106) D. A. Obenchain, P. Pinacho Morante, S. Zinn, M. Schnell
“The low-barrier methyl internal rotation in the rotational spectrum of 3-methylphenylacetylene”
Journal of Molecular Structure **1213** (2020) 128109.
- (105) C. Perez, A. L. Steber, B. Temelso, Z. Kisiel, M. Schnell
“Water triggers hydrogen bond network reshaping in the glycoaldehyde dimer”
Angewandte Chemie Int. Edition **59** (2020) 8401-8405.
- 2019**
- (104) M. del Mar Quesada Moreno, A. Krin, M. Schnell
“Analysis of thyme essential oils using gas-phase broadband rotational spectroscopy”
Physical Chemistry Chemical Physics, **21** (2019) 26569-26579.
- (103) B. M. Giuliano, L. Bizzocchi, P. Caselli, B. E. Arenas, A. L. Steber, M. Schnell, B. J. Harris, B. H. Pate, A. Pietropolli Charmet, J.-C. Guillemin, A. Belloche
“Rotational spectroscopy of imidazole: improved rest frequencies for astrophysical searches”
Astronomy & Astrophysics **628** (2019) A53.
- (102) D. Bernhard, M. Fatima, A. Poblitzki, A. L. Steber, C. Perez, M. A. Suhm, M. Schnell, M. Gerhards
“Dispersion-controlled docking preference: multi-spectroscopic study on complexes of dibenzofuran with alcohols and water”
Phys. Chem. Chem. Phys. **21** (2019) 16032-16046.
- (101) S. R. Domingos, K. Martin, N. Avarvari, M. Schnell
“Water docking bias in [4]helicene ”

Angewandte Chemie Int. Edition **58** (2019) 11257-11261.

- (100) M. Fatima, A. L. Steber, A. Poblitzki, C. Perez, S. Zinn, M. Schnell
“Rotational signatures of dispersive stacking in the formation of aromatic dimers”
Angewandte Chemie Int. Edition **58** (2019) 3108-3113.
- (99) S. Gruet, O. Pirali, A. L. Steber, M. Schnell
“The structural determination and skeletal ring modes of tetrahydropyran”
Phys. Chem. Chem. Phys. **21** (2019) 3016-3023.
- (98) J. C. Lopez, C. Perez, S. Blanco, V. A. Shubert, B. Temelso, G. C. Shields, and M. Schnell
“Water induces the same crown shapes as Li⁺ or Na⁺ in 15-crown-5 ether: a broadband rotational spectroscopy study”
Phys. Chem. Chem. Phys. **21** (2019) 2875-2881.
- (97) A. K. Lemmens, S. Gruet, A. L. Steber, J. Antony, S. Grimme, M. Schnell, A. M. Rijs
“Far-IR and UV spectral signatures of controlled complexation and microhydration of the polycyclic aromatic hydrocarbon acenaphthene”
Phys. Chem. Chem. Phys. **21** (2019) 3414-3422.

2018

- (96) L. Surin, I. Tarabukin, C. Perez, M. Schnell
“Microwave spectra and nuclear quadrupole structure of the NH₃-N₂ van der Waals complex and its deuterated isotopologues”
J. Chem. Phys. **149** (2018) 224305.
- (95) S. R. Domingos, M. Schnell,
“Wet sunscreens in the gas phase: structures of isolated and micro-solvated oxybenzone”
Journal of Physical Chemistry Letters **9** (2018) 4963-4968.
- (94) S. Zinn and M. Schnell
“Flexibility at the fringes: Conformations of the steroid hormone β-estradiol”
ChemPhysChem **19** (2018) 2915-2920.
- (93) C. Perez, A. L. Steber, A. Krin, and M. Schnell
“State-specific enrichment of chiral conformers with microwave spectroscopy”
Journal of Physical Chemistry Letters **9** (2018) 4539-4543.
- (92) J. Graneek, W. C. Bailey, M. Schnell
“Electron-withdrawing effects on the molecular structure of 2- and 3-nitrobenzotrile revealed by broadband rotational spectroscopy and their comparison with 4-nitrobenzotrile”
Physical Chemistry Chemical Physics **20** (2018) 22210-22217.

- (91) D. Bernhard, F. Dietrich, M. Fatima, C. Perez, H. C. Gottschalk, A. Wuttke, R. A. Mata, M. Suhm, M. Schnell, and M. Gerhards
“The phenyl vinyl ether – methanol complex: a model system for quantum-chemistry benchmarking”
Beilstein Journal of Organic Chemistry **14** (2018) 1642-1654 (as a contribution to the themed series “Dispersion Interactions”)
- (90) F. Dietrich, D. Bernhard, M. Fatima, C. Perez, M. Schnell, and M. Gerhards
“The effect of dispersion on the structure of diphenyl ether aggregates”
Angewandte Chemie Int. Ed. **57** (2018) 9534-9537.
- (89) P. Pinacho, A. Krin, C. Perez, S. Zinn, J. C. Lopez, S. Blanco, and M. Schnell
“Microsolvated complexes of ibuprofen as revealed by high-resolution rotational spectroscopy”
Physical Chemistry Chemical Physics **20** (2018) 15635-15640.
- (88) S. R. Domingos, C. Perez, M. Schnell
“Sensing chirality with rotational spectroscopy”
Annual Reviews in Physical Chemistry **69** (2018) 499-519.
- (87) S. Gruet, C. Perez, A. L. Steber, M. Schnell
“Where’s water? The many binding sites of hydantoin”
Physical Chemistry Chemical Physics **20** (2018) 5545-5552 (part of the themed collection: Theory, experiment, and simulations in laboratory astrochemistry).
- 2017**
- (86) Amanda L. Steber, Cristóbal Pérez, Berhane Temelso, George C. Shields, Anouk M. Rijs, Brooks H. Pate, Zbigniew Kisiel, and Melanie Schnell
“Capturing the elusive water trimer from the stepwise growth of water on the surface of the polycyclic aromatic hydrocarbon acenaphthene”
J. Phys. Chem. Lett. **8** (2017) 5744-5750.
- (85) A. Krin, C. Perez, P. Pinacho, M. Mar Quesada-Moreno, J. J. Lopez-Gonzalez, J. R. Aviles-Moreno, S. Blanco, J. C. Lopez, M. Schnell
“Structure determination, conformational flexibility, internal dynamics, and chiral analysis of pulegone and its complex with water”
Chemistry- An European Journal **24** (2018) 721-729.
- (84) J. B. Graneek, C. Perez, M. Schnell
“Structural determination and population transfer of 4-nitroanisole by broadband microwave spectroscopy and tailored microwave pulses”
J. Chem. Phys. **147** (2017) 154306.
- (83) S. R. Domingos, C. Perez, M. Schnell
“On the structural intricacies of a metabolic precursor: Direct spectroscopic detection of water-induced conformational reshaping of mevalonolactone”

- J. Chem. Phys. Comm.* **147** (2017) 124310.
- (82) A. A. Fokin, T. S. Zhuk, S. Blomeyer, C. Perez, L. V. Chernish, A. E. Pashenko, J. Antony, Y. V. Vishnevsky, R. J. Berger, S. Grimme, C. Logemann, M. Schnell, N. W. Mitzel, P. R. Schreiner
“Intramolecular London dispersion interaction effects on gas-phase and solid-state structures of diamondoid dimers”
J. Am. Chem. Soc. **139** (2017) 16696-16707.
- (81) C. Perez, A. L. Steber, S. R. Domingos, A. Krin, D. Schmitz, M. Schnell
“Coherent enantiomer-selective population enrichment using tailored microwave pulses” (Very important paper)
Angew. Chem. Int. Ed. **56** (2017) 12512-12517.
- (80) D. Bernhard, F. Dietrich, M. Fatima, C. Perez, A. Poblitzki, G. Jansen, M. A. Suhm, M. Schnell, M. Gerhards
“Multi-spectroscopic and theoretical analyses on the diphenyl ether-tert-butyl alcohol complex in the electronic ground and electronically excited state”
Phys. Chem. Chem. Phys. **19** (2017) 18076-18088.
- (79) S. R. Domingos, A. Cnossen, W. J. Buma, W. R. Browne, B. L. Feringa and M. Schnell
“Cold Snapshot of a Molecular Rotary Motor Captured by High-Resolution Rotational Spectroscopy”
Angew. Chem. Int. Ed. **56** (2017) 11209-11212.
- (78) C. Perez, A. L. Steber, A. M. Rijs, B. Temelso, G. C. Shields, J. C. Lopez, Z. Kisiel, M. Schnell
“Corannulene and its complex with water: A tiny cup of water”
Phys. Chem. Chem. Phys. **19** (2017) 14214-14223.
- (77) B. E. Arenas, S. Gruet, A. L. Steber, M. Schnell
“A global study of 1,2-propanediol and new vibrationally excited states”
J. Mol. Spec. **337** (2017) 9-16.
- (76) B. E. Arenas, S. Gruet, A. L. Steber, B. M. Giuliano, M. Schnell
“Chirped-pulse Fourier transform millimeter-wave spectroscopy of ten vibrationally excited states of *i*-propyl cyanide: exploring the far-infrared region”
Phys. Chem. Chem. Phys. **19** (2017) 1751-1756.
- 2016**
- (75) C. Perez, J. C. Lopez, S. Blanco, M. Schnell
“Water-induced structural changes in crown ethers from broadband rotational spectroscopy”
J. Phys. Chem. Lett., **7** (2016) 4053-4058.

- (74) S. R. Domingos, C. Perez, M. Schnell
“Structural locking mediated by a water wire: A high-resolution rotational spectroscopy study on hydrated forms of a chiral biphenyl derivative”
J. Chem. Phys. Communications **145** (2016) 16113.
- (73) C. Medcraft, S. Zinn, M. Schnell*, A. Poblitzki, J. Altnöder, M. Heger, M. A. Suhm*, D. Bernhard, A. Stamm, F. Dietrich, M. Gerhards*
“Aromatic embedding wins over classical hydrogen bonding – a multi-spectroscopic approach for the diphenyl ether–methanol complex”
Phys. Chem. Chem. Phys. **18** (2016) 25975-25983.
- (72) J. B. Graneek, S. Merz, T. Betz, D. Patterson, M. Schnell
“Simulating spatial microwave manipulation of polyatomic asymmetric-top molecules using a multi-level approach”
ChemPhysChem **17** (2016) 3624-3630.
- (71) S. R. Domingos, C. Perez, C. Medcraft, P. Pinacho, M. Schnell
“Flexibility unleashed in acyclic monoterpenes: conformational space of citronellal revealed by broadband rotational spectroscopy”
Physical Chemistry Chemical Physics **18** (2016) 16682-16689,
- (70) S. Zinn, C. Medcraft, T. Betz, M. Schnell
“High-resolution rotational spectroscopy study of the smallest sugar dimer: Interplay of hydrogen bonds in the glycolaldehyde dimer”
Angewandte Chemie International Edition **128** (2016) 6079-6084.
- (69) C. Perez, A. Krin, A. L. Steber, J. C. Lopez, Z. Kisiel, M. Schnell
“Wetting camphor: Multi-isotopic substitution identifies the complementary roles of hydrogen bonding and dispersive forces”
The Journal of Physical Chemistry Letters **7** (2016) 154-160.
- (68) V.A. Shubert, D. Schmitz, C. Perez, C. Medcraft, A. Krin, S. R. Domingos, D. Patterson, M. Schnell
“Chiral analysis using broadband rotational spectroscopy”
The Journal of Physical Chemistry Letters **7** (2016) 341-350. **INVITED PERSPECTIVE ARTICLE.**
- (67) C. Medcraft, M. Schnell
“A comparative study of two bicyclic ethers, eucalyptol and 1,4-cineole, by broadband rotational spectroscopy”
Zeitschrift für Physikalische **230** (2016) 1.
- 2015**
- (66) V.A. Shubert, D. Schmitz, C. Medcraft, A. Krin, D. Patterson, John M. Doyle, M. Schnell
“Rotational Spectroscopy and Three-Wave Mixing of 4-carvomenthenol: A Technical Guide to Measuring Chirality in the Microwave Regime”
The Journal of Chemical Physics **142** (2015) 214201. **JCP EDITOR’S CHOICE 2015**
- (65) S. Zinn, C. Medcraft, T. Betz, M. Schnell

- “Structure determination of *trans*-cinnamaldehyde by broadband microwave spectroscopy”
Physical Chemistry Chemical Physics **17** (2015) 16080-16085. (*open access*)
- (64) D. Schmitz, V. A. Shubert, D. Patterson, A. Krin, M. Schnell
“On the phase dependence of double-resonance experiments in rotational spectroscopy”
Journal of Physical Chemistry Letters **6** (2015) 1493-1498.
- (63) D. Schmitz, V. A. Shubert, T. Betz, M. Schnell
“The conformational landscape of menthone and menthol”
Frontiers in Physical Chemistry and Chemical Physics **3** (2015) 15. (*open access*)
- (62) T. Betz, S. Zinn, M. Schnell
“The Shape of Ibuprofen in the Gas Phase”
Physical Chemistry Chemical Physics, **17** (2015) 4538-4541. (*open access*)
- 2014**
- (61) C. Medcraft, R. Wolf, M. Schnell
“High-Resolution Spectroscopy of the Chiral Metal Complex [CpRe(CH₃)(CO)(NO)]: A Potential Candidate for Probing Parity Violation”
Angewandte Chemie International Edition **53** (2014) 11656-11659.
- (60) D. Schmitz, V.A. Shubert, B.M. Giuliano, M. Schnell
“The broadband microwave spectra of the monoterpenoids thymol and carvacrol: Conformational landscape and internal dynamics”
The Journal of Chemical Physics **141** (2014) 034304.
- (59) T. Betz, S. Zinn, J.B. Graneek, M. Schnell
“Nuclear Quadrupole Coupling Constants of Two Chemically Distinct Nitrogen Atoms in 4-Aminobenzonitrile”
The Journal of Physical Chemistry A **118** (2014) 5164-5169.
- (58) V.A. Shubert, D. Schmitz, M. Schnell
“Enantiomer-sensitive investigations of a chiral molecule containing two stereogenic centers – microwave three-wave mixing of menthone”
Journal of Molecular Spectroscopy, special issue: “Molecular Spectroscopy Tests of Fundamental Physics” **300** (2014) 31-36.
- (57) D. Patterson, M. Schnell
“New Studies on Molecular Chirality: Enantiomer Differentiation and Determination of Enantiomeric Excess and Molecular Handedness”
Physical Chemistry Chemical Physics **16** (2014) 11114-11123. **INVITED PERSPECTIVE ARTICLE.**
- (56) V.A. Shubert, D. Schmitz, D. Patterson, J.M. Doyle, M. Schnell*
“Identifying Enantiomers in Mixtures of Chiral Molecules with Broadband Microwave Spectroscopy”
Angewandte Chemie International Edition **53** (2014) 1152-1155.

2013

- (55) M. Schnell*, P.R. Bunker, G. v. Helden, J.-U. Grabow, G. Meijer, A. van der Avoird
“Stark Effect in the Benzene Dimer”

- The Journal of Physical Chemistry A* **117** (2013) 13775-13778.
- (54) D. Patterson, M. Schnell, J.M. Doyle
“Enantiomer-Specific Detection of Chiral Molecules via Microwave Spectroscopy”
Nature **497** (2013) 475. **(Cover Article and Featured as Nature News&Views)**
- (53) M. Schnell*, U. Erlekam, P.R. Bunker, G. v. Helden, J.-U. Grabow, G. Meijer, A. van der Avoird
“Unraveling the internal dynamics of the benzene dimer: a combined theoretical and microwave spectroscopy study”
Physical Chemistry Chemical Physics **15** (2013) 10207-10223.
- (52) V.A. Shubert, D. Schmitz, M. Schnell*
“Communication through the Phenyl Ring: Internal Rotation and Nuclear Quadrupole Splitting in p-halotoluenes”
Molecular Physics **111** (2013) 2189-2197.
- (51) S. Merz, C. Brieger, N. Vanhaecke, G. Meijer, M. Schnell*
“Microwave Manipulation of Polar Molecules”
Molecular Physics **111** (2013) 1855-1864.
- (50) M. Schnell*, U. Erlekam, P.R. Bunker, G. v. Helden, J.-U. Grabow, G. Meijer, A. van der Avoird
“Structure of the benzene dimer – governed by dynamics”
Angewandte Chemie International Edition **52** (2013) 5180-5183, **(VERY IMPORTANT PAPER)**.
- (49) M. Schnell
“Chirped-pulse rotational spectroscopy for molecular structure and dynamics studies”
INVITED REVIEW ARTICLE, *Zeitschrift für Physikalische Chemie*, **227** (2013) 1-21

2012

- (48) D. Schmitz, V.A. Shubert, T. Betz, M. Schnell*
“Multi-Resonance Effects within a Single Chirp in Broadband Rotational Spectroscopy: The Rapid Adiabatic Passage Regime for Benzonitrile”
Journal of Molecular Spectroscopy **280** (2012) 77-84.
- (47) S. Merz, N. Vanhaecke, W. Jäger, M. Schnell*, G. Meijer*
“Decelerating molecules with microwave fields”
Physical Review A, **85** (2012) 063411.

2011

- (46) M. Schnell
“Group theory for high-resolution spectroscopy of non-rigid molecules”
Refereed bookchapter in *Handbook of High-Resolution Spectroscopy*, edited by M. Quack and F. Merkt, Wiley VCH, Sept. 2011
- (45) M. Schnell*, J. Küpper
“Tailored molecular samples for precision spectroscopy experiments”
Faraday Discussions **150** (2011) 33-49.

2010

- (44) S. Merz, H. Odashima, K. Enomoto, M. Schnell*, G. Meijer
"A microwave lens for polar molecules"
Physical Review Letters **104** (2010) 253001
- (43) A. van der Avoird, R. Podeszwa, K. Szalewicz, C. Leforestier, R. van Harreveld, P.R. Bunker, M. Schnell, G. von Helden, G. Meijer
"Vibration-rotation-tunneling states of the benzene dimer: an ab initio study"
Physical Chemistry Chemical Physics **12** (2010) 8219-8240.
- (42) M. Schnell
"Understanding high-resolution spectra of non-rigid molecules using group theory" (review article)
ChemPhysChem. **11** (2010) 758-780.

2009

- (41) M. Schnell*, G. Meijer
„Kalte Moleküle: Darstellung, Anwendungen und Herausforderungen“
(EINGELADENER ÜBERSICHTSARTIKEL)
Angewandte Chemie **121** (2009) 6124-6147.
"Cold Molecules: Preparation, Applications and Challenges"
(INVITED REVIEW ARTICLE)
Angewandte Chemie International Edition **48** (2009) 6010-6031.
- (40) M. Kirste, B. Sartakov, M. Schnell*, G. Meijer
"Non-adiabatic transitions in electrostatically trapped ammonia molecules"
Physical Review A **79** (2009) 051401(R).

2008

- (39) P. Lützow, M. Schnell*, G. Meijer
"Instabilities of molecule motion in a linear AC trap"
Physical Review A **77** (2008) 063402.
- (38) M. Schnell*, J.-U. Grabow, J. T. Hougen
"Towards the complete analysis of the rotational spectrum of (CH₃)₃SnCl"
Journal of Molecular Spectroscopy **251** (2008) 38-55.
- (37) F. Filsinger, K. Wohlfart, M. Schnell, J.-U. Grabow, J. Küpper
"Precise dipole moments and quadrupole coupling constants of the cis and trans conformers of 3-aminophenol: Determination of the absolute conformation"
Physical Chemistry Chemical Physics **10** (2008) 666-673.
- (36) K. Wohlfart, M. Schnell, J.-U. Grabow, J. Küpper
"Precise dipole moment and quadrupole coupling constants of benzonitrile"
Journal of Molecular Spectroscopy **247** (2008) 119-121.
- (35) M. Schnell*, J.-U. Grabow
"Three-dimensional intramolecular dynamics: Internal rotation of (CH₃)₃GeBr"

Special issue dedicated to Sigrid D. Peyerimhoff,
Chemical Physics **343** (2008) 121-128.

2007

- (34) M. Schnell*, P. Lützow, J. van Veldhoven, H. L. Bethlem, J. Küpper, B. Friedrich, M. Schleier-Smith, H. Haak, G. Meijer
“A linear AC trap for polar molecules in their ground state”
Roger E. Miller memorial issue,
Journal of Physical Chemistry A **111** (2007) 7411-7419.
- (33) L. H. Coudert, W. Caminati, M. Schnell, J.-U. Grabow
“Hyperfine coupling and large-amplitude motions interaction in the water dimer”
Journal of Molecular Spectroscopy **242** (2007) 118-128.
- (32) P. Ottaviani, W. Caminati, M. Schnell, J.-U. Grabow
“The mm-Wave Rotational Spectrum of Dichlorodimethylgermane”
Inorganica Chimica Acta **360** (2007) 1240-1243.

2006

- (31) H. L. Bethlem, J. van Veldhoven, M. Schnell, G. Meijer
“Trapping polar molecules in an ac trap”
Physical Review A **74** (2006) 063403.
- (30) J. van Veldhoven, H. L. Bethlem, M. Schnell, G. Meijer
“A versatile electrostatic trap”
Physical Review A **73** (2006) 063408.
- (29) M. Schnell, J.-U. Grabow
“Multi-dimensional large-amplitude motions: Revealing concurrent tunneling pathways”
Angewandte Chemie International Edition **45** (2006) 3465-3470.
- (28) M. Schnell*, J.-U. Grabow
“Internal dynamics in organometallic molecules: Rotational spectrum of (CH₃)₃GeCl”
Physical Chemistry Chemical Physics **8** (2006) 2225-2231.

2005

- (27) D. Banser, M. Schnell, J.-U. Grabow, E. J. Cocinero, A. Lessari, J. L. Alonso
“The Internuclear Potential, Electronic Structure, and Chemical Bond of Tellurium Selenide”
Angewandte Chemie International Edition **44** (2005) 6311-6315 („Very Important Paper“).
- (26) S. Zink, T. Eichner, M. Schnell, J. Woenckhaus
“Electrospray mass spectra of oligo germanium acids and oligo chloro germanium acids appearing during germanium tetra-ethoxide hydrolysis”
Zeitschrift für Physikalische Chemie **219** (2005) 1355-1371.
- (25) M. Schnell, J. S. Francisco, S. D. Peyerimhoff

- “MRD-CI study of the photodissociative behavior of HOOC₂Cl, a molecule relevant to atmospheric chemistry”
Physical Chemistry Chemical Physics **7** (2005) 1912-1917.
- (24) F. J. Lovas, R. J. McMahon, J.-U. Grabow, M. Schnell, J. Mack, L. T. Scott, R. L. Kuczkowski
“Interstellar chemistry: A strategy for detecting polycyclic aromatic hydrocarbons by radio astronomy”
Journal of the American Chemical Society **127** (2005) 4345-4349.
- (23) W. Caminati, S. Melandri, M. Schnell, D. Banser, J.-U. Grabow, J. L. Alonso
“The Fourier transform rotational spectrum of difluoromethane-water: internal motion of water”
special issue dedicated to Walter Lafferty,
Journal of Molecular Structure **742** (2005) 87-90.
- (22) B. M. Giuliano, P. Ottaviani, W. Caminati, M. Schnell, D. Banser, J.-U. Grabow
“Molecular complexes of organo-metallic molecules with rare gases: the rotational spectrum of difluorodimethylsilane-argon”
Chemical Physics **312** (1-3) (2005) 111-117.
- (21) M. Schnell, J.-U. Grabow, H. Hartwig, N. Heineking, M. Meyer, W. Stahl, W. Caminati
“Structure and methyl group internal rotation of difluorodimethylsilane”
Journal of Molecular Spectroscopy **229** (2005) 1-8.
- 2004**
- (20) M. Schnell, C. Herwig, J. A. Becker
“Polyanionic selenium fragments and vibrations in Na_mSe_n clusters”
Zeitschrift für Physikalische Chemie, **218** (2004) 1-10.
- (19) P. Ottaviani, S. Melandri, W. Caminati, D. Banser, M. Schnell, J.-U. Grabow
“Molecular complexes of organo metallic molecules with rare gases: the rotational spectrum of dimethylsilane-argon”
ChemPhysChem **5** (2004) 1772-1778.
- (18) C. Herwig, D. Banser, M. Schnell, J. A. Becker
“Stability, structure, and vibrations of metal doped selenium clusters”
Journal of Physical Chemistry A, **108** (2004) 3151-3155.
- (17) C. Herwig, M. Schnell, J. A. Becker
“Raman band of matrix isolated Na_mSe_n clusters”
Chemical Physics Letters **385** (2004) 462-466.
- (16) M. Schnell, D. Banser, J.-U. Grabow
“Coaxially aligned electrodes for Stark-effect applied in resonators using a supersonic jet Fourier transform microwave spectrometer”
Review of Scientific Instruments **75** (2004) 2111-2115.
- (15) M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff
“Can the methoxyradical CH₃O act as a sink for Cl and ClO in the atmosphere?”
Journal of Physical Chemistry A **108** (2004) 1298-1304.

2003

- (14) M. Mühlhäuser, M. Schnell, S. D. Peyerimhoff
"The importance of photodissociative trichloromethanol for atmospheric chemistry"
Collection of Czechoslovak Chemical Communications **68** (2003), 2297-2308.
- (13) A. Mavrandonakis, G. E. Froudakis, M. Schnell, M. Mühlhäuser
"From Pure Carbon to Silicon-Carbon Nanotubes: An *ab initio* Study"
Nano Letters **11** (2003), 1481-1484.
- (12) G. E. Froudakis, M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff, A. N. Andriotis, M. Menon, R. M. Sheets
"Pathways for oxygen adsorption on single-wall carbon nanotubes"
Physical Reviews B **68** (2003), 115435.
- (11) M. Schnell, M. Mühlhäuser, A. Lesar, S. D. Peyerimhoff
"The Electronic Spectra of CH_2XOH (X = F, Cl, Br): A Comparative Study"
Journal of Physical Chemistry A **107** (2003), 6489-6494.
- (10) M. Schnell, C. Herwig, J. A. Becker
"Analysis of Semiconductor Cluster Beam Polarization Taking Small Permanent Dipole Moments Into Account"
Zeitschrift für Physikalische Chemie **217** (2003), 1-28.

2002

- (9) A. Lesar, M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff
"*Ab initio* investigation of the photofragmentation of bromomethanol"
Chemical Physics Letters **366** (2002), 350-356.
- (8) M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff
"The electronic spectrum of trichloromethanol Cl_3COH : An *ab initio* study"
Chemical Physics Letters **361** (2002), 1-7.
- (7) M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff
"*Ab initio* MRD-CI investigation of the electronic spectrum of dichloromethanol Cl_2CHOH "
Journal of Molecular Spectroscopy **214** (2002) 124-128.
- (6) M. Mühlhäuser, M. Schnell, S. D. Peyerimhoff
"*Ab initio* MRD-CI investigation of the electronic spectrum of 1-chloromethyl hypochlorite ClCH_2OCl in comparison with isomeric dichloromethanol Cl_2CHOH "
Molecular Physics **100** (2002) 2719-2725.
- (5) M. Mühlhäuser, M. Schnell, S. D. Peyerimhoff
"Photofragmentation of dichloromethanol Cl_2CHOH along C-O and C-Cl cleavage: A theoretical study."
Photochemistry and Photobiology **76** (2002) 176-180.
- (4) E. Drougas, A. M. Kosmas, M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff
"*Ab initio* and RRKM studies of decomposition and interconversion pathways of ClCH_2OH and CH_3OCl isomeric species"
Molecular Physics **100** (2002) 2653-2658.

- (3) M. Mühlhäuser, M. Schnell, S. D. Peyerimhoff
“The electronic spectrum of chloromethanol ClCH_2OH in comparison with isomeric methylhypochlorite CH_3OCl ”
Molecular Physics **100** (2002) 509-515.

2001

- (2) M. Schnell, M. Mühlhäuser, S. D. Peyerimhoff
“*Ab initio* MRD-CI study of excited states of chloromethanol ClCH_2OH and photofragmentation along C-O and C-Cl cleavage”
Chemical Physics Letters **344** (2001) 519-526.
- (1) M. Schnell, M. Mühlhäuser, G. E. Froudakis, S. D. Peyerimhoff
“*Ab initio* CCSD(T) and MRD-CI study of excited states and the electronic spectrum of linear C_5^+ ”
Chemical Physics Letters **340** (2001) 559-564.