# Martin A Suhm

List of Publications by Year
in descending order

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| 207 | 7,934 | 41344 | 76900 |
|---|---|---|---|
| papers | citations | 49 h-index | 74 g-index |

| 222 | 222 | 222 | 3676 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Potential energy surfaces, quasiadiabatic channels, rovibrational spectra, and intramolecular dynamics of (HF)2 and its isotopomers from quantum Monte Carlo calculations. Journal of Chemical Physics, 1991, 95, 28-59. | 3.0 | 278 |
| 2 | Quantum Monte Carlo studies of vibrational states in molecules and clusters. Physics Reports, 1991, 204, 293-329. | 25.6 | 247 |
| 3 | Chirality Recognition between Neutral Molecules in the Gas Phase. Angewandte Chemie - International Edition, 2008, 47, 6970-6992. | 13.8 | 221 |
| 4 | A new six-dimensional analytical potential up to chemically significant energies for the electronic ground state of hydrogen peroxide. Journal of Chemical Physics, 1999, 111, 2565-2587. | 3.0 | 175 |
| 5 | FTIR-spectroscopy of molecular clusters in pulsed supersonic slit-jet expansions. Physical Chemistry Chemical Physics, 1999, 1, 5573-5582. | 2.8 | 168 |
| 6 | HF dimer: Empirically refined analytical potential energy and dipole hypersurfaces from ab initio calculations. Journal of Chemical Physics, 1998, 108, 10096-10115. | 3.0 | 157 |
| 7 | Hydrogen-bonded OH stretching modes of methanol clusters: A combined IR and Raman isotopomer study. Journal of Chemical Physics, 2007, 126, 194307. | 3.0 | 153 |
| 8 | A monomers-in-dimers model for carboxylic acid dimers. Journal of Chemical Physics, 2003, 118, 2242-2255. | 3.0 | 121 |
| 9 | Benchmarking Quantum Chemical Methods: Are We Heading in the Right Direction?. Angewandte Chemie - International Edition, 2017, 56, 11011-11018. | 13.8 | 119 |
| 10 | Dipole moment function and equilibrium structure of methane in an analytical, anharmonic nineâ€dimensional potential surface related to experimental rotational constants and transition moments by quantum Monte Carlo calculations. Journal of Chemical Physics, 1994, 101, 3588-3602. | 3.0 | 105 |
| 11 | The Last Globally Stable Extended Alkane. Angewandte Chemie - International Edition, 2013, 52, 463-466. | 13.8 | 105 |
| 12 | Ragout-jet FTIR spectroscopy of cluster isomerism and cluster dynamics: from carboxylic acid dimers to N2O nanoparticles. Faraday Discussions, 2001, 118, 331-359. | 3.2 | 99 |
| 13 | A new ab initio based six-dimensional semi-empirical pair interaction potential for HF. Chemical Physics Letters, 1996, 261, 35-44. | 2.6 | 86 |
| 14 | A critical analysis of electronic density functionals for structural, energetic, dynamic, and magnetic properties of hydrogen fluoride clusters. Journal of Computational Chemistry, 1997, 18, 1695-1719. | 3.3 | 85 |
| 15 | Hydrogen Bonding in 2-Propanol. The Effect of Fluorinationâ€. Journal of Physical Chemistry A, 2000, 104, 265-274. | 2.5 | 84 |
| 16 | High resolution 1.3 Î¼m overtone spectroscopy of HF dimer in a slit jet: Ka=0â†0 and Ka=1â†0 subbands of vacc=2â†0. Journal of Chemical Physics, 1992, 97, 5341-5354. | 3.0 | 81 |
| 17 | Acidic protons before take-off: A comparative jet Fourier transform infrared study of small HClâ€“ and HBrâ€“solvent complexes. Journal of Chemical Physics, 2003, 118, 10120-10136. | 3.0 | 80 |
| 18 | Raman jet spectroscopy of formic acid dimers: low frequency vibrational dynamics and beyond. Physical Chemistry Chemical Physics, 2007, 9, 4528. | 2.8 | 80 |

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|---|---|---|---|
| 19 | Elementary Peptide Motifs in the Gas Phase: FTIR Aggregation Study of Formamide, Acetamide, N-Methylformamide, and N-Methylacetamide. Journal of Physical Chemistry A, 2008, 112, 7530-7542. | 2.5 | 79 |
| 20 | A combined Raman- and infrared jet study of mixed methanolâ€“water and ethanolâ€“water clusters. Physical Chemistry Chemical Physics, 2011, 13, 14050. | 2.8 | 77 |
| 21 | The Raman spectrum of isolated water clusters. Physical Chemistry Chemical Physics, 2014, 16, 9849. | 2.8 | 77 |
| 22 | Glycidol dimer: anatomy of a molecular handshakePresented at the LANMAT 2001 Conference on the Interaction of Laser Radiation with Matter at Nanoscopic Scales: From Single Molecule Spectroscopy to Materials Processing, Venice, 3â€“6 October, 2001.. Physical Chemistry Chemical Physics, 2002, 4, 2721-2732. | 2.8 | 76 |
| 23 | Communication: The highest frequency hydrogen bond vibration and an experimental value for the dissociation energy of formic acid dimer. Journal of Chemical Physics, 2012, 136, 151101. | 3.0 | 76 |
| 24 | Observation and assignment of the hydrogen bond exchange disrotatory in-plane bending vibration v5 in (HF)2. Chemical Physics Letters, 1990, 171, 517-524. | 2.6 | 75 |
| 25 | Femtisecond single-mole infrared spectroscopy of molecular clusters. Physical Chemistry Chemical Physics, 2013, 15, 10702. | 2.8 | 75 |
| 26 | Intra- vs. intermolecular hydrogen bonding: dimers of alpha-hydroxyesters with methanol. Physical Chemistry Chemical Physics, 2006, 8, 4449. | 2.8 | 71 |
| 27 | Chirality-Induced Switch in Hydrogen-Bond Topology: Tetrameric Methyl Lactate Clusters in the Gas Phase. Angewandte Chemie - International Edition, 2006, 45, 3440-3445. | 13.8 | 71 |
| 28 | Nâ€“Hâ‹¯Ï€ interactions in pyrroles: systematic trends from the vibrational spectroscopy of clusters. Physical Chemistry Chemical Physics, 2008, 10, 2827. | 2.8 | 70 |
| 29 | Accurate quantum Monte Carlo calculations of the tunneling splitting in (HF)2 on a six-dimensional potential hypersurface. Chemical Physics Letters, 1995, 234, 71-76. | 2.6 | 68 |
| 30 | A first glimpse at the acidic proton vibrations in HClâ€“water clusters via supersonic jet FTIR spectroscopy. Physical Chemistry Chemical Physics, 2002, 4, 3933-3937. | 2.8 | 68 |
| 31 | Highâ€resolution infrared spectroscopy of DF trimer: A cyclic ground state structure and DF stretch induced intramolecular vibrational coupling. Journal of Chemical Physics, 1993, 98, 5985-5989. | 3.0 | 67 |
| 32 | Probing the stiffness of the simplest double hydrogen bond: The symmetric hydrogen bond modes of jet-cooled formic acid dimer. Journal of Chemical Physics, 2009, 131, 054301. | 3.0 | 65 |
| 33 | Observation and assignment of tunnelling-rotational transitions in the far infrared spectrum of (HF)2. Molecular Physics, 1988, 65, 1025-1045. | 1.7 | 64 |
| 34 | Self-organization of lactates in the gas phase. Organic and Biomolecular Chemistry, 2003, 1, 4351. | 2.8 | 64 |
| 35 | Combined jet relaxation and quantum chemical study of the pairing preferences of ethanol. Physical Chemistry Chemical Physics, 2005, 7, 991-997. | 2.8 | 64 |
| 36 | Potential energy surface and energy levels of (HF)2 and its D isotopomers. Molecular Physics, 1990, 69, 791-801. | 1.7 | 63 |

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| 37 | Hydrogen bonded rings, chains and lassos: the case of t-butyl alcohol clusters. Molecular Physics, 2001, 99, 413-425. | 1.7 | 62 |
| 38 | Concerted proton motion in hydrogen-bonded trimers: A spontaneous Raman scattering perspective. Physical Chemistry Chemical Physics, 2006, 8, 2826. | 2.8 | 61 |
| 39 | A peptide co-solvent under scrutiny: self-aggregation of 2,2,2-trifluoroethanol. Physical Chemistry Chemical Physics, 2007, 9, 4472. | 2.8 | 61 |
| 40 | Evidence for the (HF) 5 complex in the HF stretching FTIR absorption spectra of pulsed and continuous supersonic jet expansions of hydrogen fluoride. Chemical Physics Letters, 1993, 208, 446-452. | 2.6 | 60 |
| 41 | Vibrational dynamics of (HF)n aggregates from an ab initio based analytical (1+2+3)-body potential. Journal of Molecular Structure, 1993, 294, 33-36. | 3.6 | 59 |
| 42 | The complexes of halothane with benzene: the temperature dependent direction of the complexation shift of the aliphatic Câ€“H stretching. Physical Chemistry Chemical Physics, 2010, 12, 14034. | 2.8 | 59 |
| 43 | Potential surfaces and dynamic of weakly bound trimers: perspectives from high resolution IR spectroscopy. Chemical Society Reviews, 1995, 24, 45. | 38.1 | 58 |
| 44 | OH-Stretching Red Shifts in Bulky Hydrogen-Bonded Alcohols:Â Jet Spectroscopy and Modeling. Journal of Physical Chemistry A, 2006, 110, 9839-9848. | 2.5 | 58 |
| 45 | Proton tunneling estimates for malonaldehyde vibrations from supersonic jet and matrix quenching experiments. Physical Chemistry Chemical Physics, 2006, 8, 2344. | 2.8 | 56 |
| 46 | Structural Preferences, Argon Nanocoating, and Dimerization ofn-Alkanols As Revealed by OH Stretching Spectroscopy in Supersonic Jetsâ€. Journal of Physical Chemistry A, 2007, 111, 7437-7448. | 2.5 | 55 |
| 47 | Ethanol Monomers and Dimers Revisited: A Raman Study of Conformational Preferences and Argon Nanocoating Effects. Journal of Physical Chemistry A, 2010, 114, 8223-8233. | 2.5 | 55 |
| 48 | On FTIR Spectroscopy in Asynchronously Pulsed Supersonic Free Jet Expansions and on the Interpretation of Stretching Spectra of HF Clusters. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 457-468. | 0.9 | 53 |
| 49 | A chemical approach towards the spectroscopy of carboxylic acid dimer isomerism. Physical Chemistry Chemical Physics, 2003, 5, 3094. | 2.8 | 51 |
| 50 | Analytical three-body interaction potentials and hydrogen bond dynamics of hydrogen fluoride aggregates, (HF) n , n â‰¥3. Journal of Molecular Structure, 2001, 599, 381-425. | 3.6 | 50 |
| 51 | FTIR spectroscopy of hydrogen fluoride clusters in synchronously pulsed supersonic jets. Isotopic isolation, substitution and 3-d condensation. Chemical Physics Letters, 1997, 269, 29-38. | 2.6 | 48 |
| 52 | Dimerization of Pyrazole in Slit Jet Expansions. Zeitschrift Fur Physikalische Chemie, 2005, 219, 379-388. | 2.8 | 48 |
| 53 | From hydrogen bond donor to acceptor: the effect of ethanol fluorination on the first solvating water molecule. Physical Chemistry Chemical Physics, 2013, 15, 16065. | 2.8 | 48 |
| 54 | Observation and quantification of the hydrogen bond effect on Oâ€“H overtone intensities in an alcohol dimer. Chemical Physics, 2008, 346, 167-175. | 1.9 | 46 |

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| 55 | Dimer formation in nicotinamide and picolinamide in the gas and condensed phases probed by infrared spectroscopy. Physical Chemistry Chemical Physics, 2008, 10, 7010. | 2.8 | 46 |
| 56 | The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie - International Edition, 2019, 58, 5080-5084. | 13.8 | 46 |
| 57 | Quasiadiabatic channels and effective transition-state barriers for the disrotatory in-plane hydrogen-bond exchange motion in (HF)2. Chemical Physics Letters, 1991, 183, 187-194. | 2.6 | 45 |
| 58 | Chiral self-recognition in the gas phase: the case of glycidol dimers. Physical Chemistry Chemical Physics, 2001, 3, 1945-1948. | 2.8 | 45 |
| 59 | Chirality-dependent sublimation of -(trifluoromethyl)-lactic acid: Relative vapor pressures of racemic, eutectic, and enantiomerically pure forms, and vibrational spectroscopy of isolated (S,S) and (S,R) dimers. Journal of Fluorine Chemistry, 2010, 131, 495-504. | 1.7 | 44 |
| 60 | Quantum-chemical study and FTIR jet spectroscopy of CHCl3â€“NH3 association in the gas phase. Physical Chemistry Chemical Physics, 2010, 12, 13555. | 2.8 | 44 |
| 61 | The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301. | 3.0 | 44 |
| 62 | Explicitly correlated coupled cluster calculations of the dissociation energies and barriers to concerted hydrogen exchange of (HF)n oligomers (n = 2,3,4,5). Molecular Physics, 1998, 94, 105-119. | 1.7 | 44 |
| 63 | Alcohol dimers â€“ how much diagonal OH anharmonicity?. Physical Chemistry Chemical Physics, 2014, 16, 15948-15956. | 2.8 | 43 |
| 64 | HF Vapor. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 1159-1167. | 0.9 | 42 |
| 65 | Chiral recognition between lactic acid derivatives and an aromatic alcohol in a supersonic expansion: electronic and vibrational spectroscopy. Physical Chemistry Chemical Physics, 2006, 8, 1007-1016. | 2.8 | 42 |
| 66 | Cooperative organic hydrogen bonds: The librational modes of cyclic methanol clusters. Journal of Chemical Physics, 2006, 125, 154314. | 3.0 | 41 |
| 67 | Control over the Hydrogenâ€Bond Docking Site in Anisole by Ring Methylation. Angewandte Chemie - International Edition, 2016, 55, 1921-1924. | 13.8 | 41 |
| 68 | Infrared spectrum and dynamics of the hydrogen bonded dimer (HF)2. Infrared Physics, 1989, 29, 535-539. | 0.5 | 40 |
| 69 | The permanentectric dipole moment of CH2D2: FIR el spectroscopy. Molecular Physics, 1996, 89, 297-313. | 1.7 | 40 |
| 70 | Tipping the Scales: Spectroscopic Tools for Intermolecular Energy Balances. Journal of Physical Chemistry Letters, 2017, 8, 5656-5665. | 4.6 | 40 |
| 71 | Breaking symmetry with hydrogen bonds: Vibrational predissociation and isomerization dynamics in HFâ€“DF and DFâ€“HF isotopomers. Journal of Chemical Physics, 1996, 104, 9313-9331. | 3.0 | 39 |
| 72 | Tailor-made aggregates of Î±-hydroxy esters in supersonic jets. Physical Chemistry Chemical Physics, 2004, 6, 2885-2890. | 2.8 | 39 |

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| 73 | Correcting the record: the dimers and trimers of trans-N-methylacetamide. Physical Chemistry Chemical Physics, 2017, 19, 10727-10737. | 2.8 | 39 |
| 74 | Raman spectroscopic evidence for the most stable water/ethanol dimer and for the negative mixing energy in cold water/ethanol trimers. Physical Chemistry Chemical Physics, 2008, 10, 5953. | 2.8 | 38 |
| 75 | Communication: Where does the first water molecule go in imidazole?. Journal of Chemical Physics, 2011, 135, 061102. | 3.0 | 38 |
| 76 | Chirality-dependent balance between hydrogen bonding and London dispersion in isolated (Â±)-1-indanol clusters. Physical Chemistry Chemical Physics, 2013, 15, 10167. | 2.8 | 38 |
| 77 | On hydrogen-bonded complexes: the case of (HF). Theoretica Chimica Acta, 1996, 93, 61. | 0.8 | 37 |
| 78 | Cooperative and anticooperative mixed trimers of HCl and methanol. Journal of Molecular Structure, 2006, 790, 18-26. | 3.6 | 35 |
| 79 | Hydrogen bonding lights up overtones in pyrazoles. Journal of Chemical Physics, 2007, 127, 234309. | 3.0 | 35 |
| 80 | Periodic bond breaking and making in the electronic ground state on a sub-picosecond timescale: OH bending spectroscopy of malonaldehyde in the frequency domain at low temperature. Physical Chemistry Chemical Physics, 2010, 12, 8201. | 2.8 | 35 |
| 81 | Chirality influence on the aggregation of methyl mandelate. New Journal of Chemistry, 2010, 34, 1266. | 2.8 | 35 |
| 82 | Vibrational tuning of the Hydrogen transfer in malonaldehyde â€“ a combined FTIR and Raman jet study<sup>â€</sup>. Molecular Physics, 2013, 111, 2211-2227. | 1.7 | 35 |
| 83 | Low Temperature Infrared Spectroscopy Study of Pyrazinamide: From the Isolated Monomer to the Stable Low Temperature Crystalline Phase. Journal of Physical Chemistry A, 2010, 114, 151-161. | 2.5 | 34 |
| 84 | Weak hydrogen bonds â€“ strong effects?. Physical Chemistry Chemical Physics, 2011, 13, 13858. | 2.8 | 34 |
| 85 | Quantitative chirality synchronization in trifluoroethanol dimers. Physical Chemistry Chemical Physics, 2006, 8, 4664-4667. | 2.8 | 33 |
| 86 | Tuning the Hydrogen Bond Donor/Acceptor Isomerism in Jet-Cooled Mixed Dimers of Aliphatic Alcohols. Journal of Physical Chemistry A, 2006, 110, 2906-2915. | 2.5 | 33 |
| 87 | Isomerization around Câ€“C and Câ€“O bonds in 1-propanol: Collisional relaxation in supersonic jets and selective IR photo-isomerization in cryogenic matrices. Journal of Molecular Structure, 2012, 1025, 20-32. | 3.6 | 33 |
| 88 | The effect of hydrogen bonding on torsional dynamics: A combined far-infrared jet and matrix isolation study of methanol dimer. Journal of Chemical Physics, 2014, 141, 174314. | 3.0 | 33 |
| 89 | To Ï€ or not to Ï€ â€“ how does methanol dock onto anisole?. Physical Chemistry Chemical Physics, 2015, 17, 13045-13052. | 2.8 | 33 |
| 90 | Anisotropic molecular reorientation of liquid benzene revisited. A study using13C magnetic relaxation through chemical shift anisotropy and spin rotation. Journal of Chemical Physics, 1991, 94, 3361-3365. | 3.0 | 32 |

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| 91 | Extension of panoramic cluster jet spectroscopy into the far infrared: Low frequency modes of methanol and water clusters. Physical Chemistry Chemical Physics, 2004, 6, 3315. | 2.8 | 32 |
| 92 | Explicitly correlated coupled cluster calculations of the dissociation energies and barriers to concerted hydrogen exchange of (HF)n oligomers (n=2,3,4,5). Molecular Physics, 1998, 94, 105-119. | 1.7 | 31 |
| 93 | Experimental and theoretical study of the microsolvation of sodium atoms in methanol clusters: differences and similarities to sodiumâ€“water and sodiumâ€“ammonia. Physical Chemistry Chemical Physics, 2008, 10, 83-95. | 2.8 | 31 |
| 94 | Size-selected methyl lactate clusters: fragmentation and spectroscopic fingerprints of chiral recognition. Physical Chemistry Chemical Physics, 2006, 8, 1148. | 2.8 | 29 |
| 95 | On the weakly Câ€“Hâ‹¯Ï€ hydrogen bonded complexes of sevoflurane and benzene. Physical Chemistry Chemical Physics, 2011, 13, 14142. | 2.8 | 29 |
| 96 | Vibrational exciton coupling in homo and hetero dimers of carboxylic acids studied by linear infrared and Raman jet spectroscopy. Journal of Chemical Physics, 2018, 149, 104307. | 3.0 | 29 |
| 97 | Hybrid diatomics-in-molecules-based quantum mechanical/molecular mechanical approach applied to the modeling of structures and spectra of mixed molecular clusters Arn(HCl)m and Arn(HF)m. Journal of Chemical Physics, 2004, 120, 3732-3743. | 3.0 | 28 |
| 98 | Communication: Towards the binding energy and vibrational red shift of the simplest organic hydrogen bond: Harmonic constraints for methanol dimer. Journal of Chemical Physics, 2014, 141, 101105. | 3.0 | 28 |
| 99 | Stretching and folding of 2-nanometer hydrocarbon rods. Soft Matter, 2014, 10, 4885-4901. | 2.7 | 28 |
| 100 | The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303. | 3.0 | 28 |
| 101 | Competing hydrogen bond topologies in 2-fluoroethanol dimer. Journal of Molecular Structure, 2006, 786, 86-95. | 3.6 | 27 |
| 102 | Aromatic embedding wins over classical hydrogen bonding â€“ a multi-spectroscopic approach for the diphenyl etherâ€“methanol complex. Physical Chemistry Chemical Physics, 2016, 18, 25975-25983. | 2.8 | 27 |
| 103 | Comparative FTIR Spectroscopy of HX Adsorbed on Solid Water:â€‰ Ragout-Jet Water Clusters vs Ice Nanocrystal Arrays. Journal of Physical Chemistry A, 2005, 109, 955-958. | 2.5 | 26 |
| 104 | On the low volatility of cyclic esters: an infrared spectroscopy comparison between dimers of Î³-butyrolactone and methyl propionate. Physical Chemistry Chemical Physics, 2009, 11, 11157. | 2.8 | 26 |
| 105 | Chirality Recognition in Menthol and Neomenthol: Preference for Homoconfigurational Aggregation. Angewandte Chemie - International Edition, 2010, 49, 6203-6206. | 13.8 | 26 |
| 106 | Soft hydrogen bonds to alkenes: the methanolâ€“ethene prototype under experimental and theoretical scrutiny. Chemical Science, 2015, 6, 3738-3745. | 7.4 | 26 |
| 107 | FTIR investigation of non-volatile molecular nanoparticles. Chemical Physics Letters, 2000, 329, 52-60. | 2.6 | 25 |
| 108 | Identifying the first folded alkylbenzene via ultraviolet, infrared, and Raman spectroscopy of pentylbenzene through decylbenzene. Chemical Science, 2017, 8, 5305-5318. | 7.4 | 25 |

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| 109 | Spectroscopy and quantum dynamics of hydrogen fluoride clusters. Advances in Molecular Vibrations and Collision Dynamics, 1998, , 205-248. | 0.8 | 25 |
| 110 | Spectroscopic characterization of N2O aggregates: from clusters to the particulate state. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2855-2865. | 3.9 | 24 |
| 111 | Adding more weight to a molecular recognition unit: the low-frequency modes of carboxylic acid dimers. Molecular Physics, 2010, 108, 2279-2288. | 1.7 | 24 |
| 112 | Temperature-dependent intensity anomalies in amino acid esters: weak hydrogen bonds in protected glycine, alanine and valine. Physical Chemistry Chemical Physics, 2011, 13, 14119. | 2.8 | 24 |
| 113 | Supersonic jet FTIR and quantum chemical investigations of ammonia/acetylene clusters. Physical Chemistry Chemical Physics, 2004, 6, 4642-4651. | 2.8 | 23 |
| 114 | Infrared spectroscopy of pyrrole-2-carboxaldehyde and its dimer: A planar Î²-sheet peptide model?. Journal of Chemical Physics, 2007, 126, 134313. | 3.0 | 23 |
| 115 | Weak Hydrogen Bonds Make a Difference: Dimers of Jet-Cooled Halogenated Ethanols. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1407-1452. | 2.8 | 23 |
| 116 | The stiffness of a fully stretched polyethylene chain: A Raman jet spectroscopy extrapolation. Journal of Chemical Physics, 2009, 131, 161108. | 3.0 | 23 |
| 117 | Origin of the Argon Nanocoating Shift in the OH Stretching Fundamental of n-Propanol: A Combined Experimental and Quantum Chemical Study. Journal of Physical Chemistry C, 2009, 113, 10929-10938. | 3.1 | 23 |
| 118 | Phenyl- vs Cyclohexyl-Substitution in Methanol: Implications for the OH Conformation and for Dispersion-Affected Aggregation from Vibrational Spectra in Supersonic Jets. Journal of Physical Chemistry A, 2014, 118, 3266-3279. | 2.5 | 22 |
| 119 | Molecular Docking via Olefinic OHÂ·Â·Â·Ï€ Interactions: A Bulky Alkene Model System and Its Cooperativity. Journal of Physical Chemistry A, 2015, 119, 1723-1730. | 2.5 | 22 |
| 120 | Multidimensional vibrational quantum Monte Carlo technique using robust interpolation from static or growing sets of discrete potential energy points. Chemical Physics Letters, 1993, 214, 373-380. | 2.6 | 21 |
| 121 | How Broad Are Water Dimer Bands?. Science, 2004, 304, 823-824. | 12.6 | 21 |
| 122 | Size-selective vibrational spectroscopy of methyl glycolate clusters: comparison with ragout-jet FTIR spectroscopy. Physical Chemistry Chemical Physics, 2004, 6, 4614-4620. | 2.8 | 21 |
| 123 | Conformation-Changing Aggregation in Hydroxyacetone: A Combined Low-Temperature FTIR, Jet, and Crystallographic Study. Journal of the American Chemical Society, 2011, 133, 20194-20207. | 13.7 | 21 |
| 124 | Dispersion-controlled docking preference: multi-spectroscopic study on complexes of dibenzofuran with alcohols and water. Physical Chemistry Chemical Physics, 2019, 21, 16032-16046. | 2.8 | 21 |
| 125 | The benefits of alternation and alkylation: large amplitude hydrogen bond librational modes of alcohol trimers and tetramers. Physical Chemistry Chemical Physics, 2010, 12, 8152. | 2.8 | 20 |
| 126 | Subtle solvation behaviour of a biofuel additive: the methanol complex with 2,5-dimethylfuran. Physical Chemistry Chemical Physics, 2016, 18, 27265-27271. | 2.8 | 20 |

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| 127 | Soft experimental constraints for soft interactions: a spectroscopic benchmark data set for weak and strong hydrogen bonds. Physical Chemistry Chemical Physics, 2019, 21, 18799-18810. | 2.8 | 20 |
| 128 | Stretching ofcis-formic acid: warm-up and cool-down as molecular work-out. Chemical Science, 2019, 10, 6285-6294. | 7.4 | 20 |
| 129 | The Chiral Trimer and a Metastable Chiral Dimer of Achiral Hexafluoroisopropanol: A Multiâ€Messenger Study. Angewandte Chemie, 2019, 131, 5134-5138. | 2.0 | 20 |
| 130 | Dipole Moment Function of Methane and Analytical Anharmonic, 9â€dimensional Potential Surface: Theory and Experiment for the Permanent Electric Dipole Moment of CH<sub>2</sub>D<sub>2</sub> Using Quantum Monte Carlo Calculations and FIR Spectroscopy. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1995, 99, 275-281. | 0.9 | 19 |
| 131 | A Symmetric Recognition Motif between Vicinal Diols: The Fourfold Grip in Ethylene Glycol Dimer. Angewandte Chemie - International Edition, 2016, 55, 4591-4595. | 13.8 | 19 |
| 132 | Molecular Recognition in Glycolaldehyde, the Simplest Sugar: Two Isolated Hydrogen Bonds Win Over One Cooperative Pair. ChemistryOpen, 2012, 1, 269-275. | 1.9 | 18 |
| 133 | Microscopic Roots of Alcoholâ€“Ketone Demixing: Infrared Spectroscopy of Methanolâ€“Acetone Clusters. Journal of Physical Chemistry A, 2015, 119, 2225-2232. | 2.5 | 18 |
| 134 | On hydrogen-bonded complexes: the case of (HF)2. Theoretica Chimica Acta, 1996, 93, 61-65. | 0.8 | 17 |
| 135 | Variations of bite angle and coupling patterns in double hydrogen bonds: The case of oxime dimers. Journal of Molecular Structure, 2008, 880, 2-13. | 3.6 | 17 |
| 136 | Potential Energy Hypersurfaces for Hydrogen Bonded Clusters (HF) n. , 1997, , 415-463. | | 17 |
| 137 | Increasing the weights in the molecular work-out of cis- and trans-formic acid: extension of the vibrational database via deuteration. Physical Chemistry Chemical Physics, 2020, 22, 25492-25501. | 2.8 | 17 |
| 138 | Exploring a hydrogen-bond terminus: spectroscopy of eucalyptolâ€“alcohol clusters. Physical Chemistry Chemical Physics, 2000, 2, 3555-3563. | 2.8 | 16 |
| 139 | Infrared spectra of phenanthrene particles generated by pulsed rapid expansion of CO2solutions. Physical Chemistry Chemical Physics, 2004, 6, 4652-4657. | 2.8 | 16 |
| 140 | Dimers of cyclic carbonates: chirality recognition in battery solvents and energy storage. Physical Chemistry Chemical Physics, 2011, 13, 14176. | 2.8 | 16 |
| 141 | Soluteâ€“solvent interactions in cryosolutions: a study of halothaneâ€“ammonia complexes. Physical Chemistry Chemical Physics, 2012, 14, 6469. | 2.8 | 16 |
| 142 | Adaptive Aggregation of Peptide Model Systems. Journal of Physical Chemistry A, 2013, 117, 7050-7063. | 2.5 | 16 |
| 143 | Multi-spectroscopic and theoretical analyses on the diphenyl etherâ€“tert-butyl alcohol complex in the electronic ground and electronically excited state. Physical Chemistry Chemical Physics, 2017, 19, 18076-18088. | 2.8 | 16 |
| 144 | Dinitrogen as a Sensor for Metastable Carboxylic Acid Dimers and a Weak Hydrogen Bond Benchmarking Tool. Journal of Physical Chemistry A, 2018, 122, 2933-2946. | 2.5 | 16 |

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| 145 | The reduced cohesion of homoconfigurational 1,2-diols. Physical Chemistry Chemical Physics, 2020, 22, 1122-1136. | 2.8 | 16 |
| 146 | Torsional isomers in methylated aminoethanols - A jet-FT-IR study. Canadian Journal of Chemistry, 2004, 82, 1006-1012. | 1.1 | 15 |
| 147 | Infrared absorption imaging of 2D supersonic jet expansions: Free expansion, cluster formation, and shock wave patterns. Journal of Chemical Physics, 2013, 139, 024201. | 3.0 | 15 |
| 148 | The OH stretching spectrum of warm water clusters. Journal of Chemical Physics, 2014, 140, 064312. | 3.0 | 15 |
| 149 | Concerted Pair Motion Due to Double Hydrogen Bonding: The Formic Acid Dimer Case. Journal of the Indian Institute of Science, 2020, 100, 5-19. | 1.9 | 15 |
| 150 | A Rather Universal Vibrational Resonance in 1:1 Hydrates of Carbonyl Compounds. Journal of Physical Chemistry Letters, 2021, 12, 138-144. | 4.6 | 15 |
| 151 | The Hydrates of TEMPO: Water Vibrations Reveal Radical Microsolvation. Angewandte Chemie - International Edition, 2021, 60, 19013-19017. | 13.8 | 15 |
| 152 | Understanding benzyl alcohol aggregation by chiral modification: the pairing step. Physical Chemistry Chemical Physics, 2020, 22, 25538-25551. | 2.8 | 15 |
| 153 | Reliable determination of multidimensional analytical fitting bias. Chemical Physics Letters, 1994, 223, 474-480. | 2.6 | 14 |
| 154 | Brightening and Locking a Weak and Floppy Nâ”H Chromophore: The Case of Pyrrolidine. Journal of Physical Chemistry A, 2010, 114, 10492-10499. | 2.5 | 14 |
| 155 | Quantenchemische Methoden im Leistungsvergleich: Stimmt die Richtung noch?. Angewandte Chemie, 2017, 129, 11155-11163. | 2.0 | 14 |
| 156 | Experimental Reference Data for Hexafluorinated Propanol by Exploring an Unusual Intermolecular Torsional Balance. Angewandte Chemie - International Edition, 2017, 56, 12672-12676. | 13.8 | 13 |
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