

**2024**

295. A. Chakraborty, S. Henkel, G. Schwaab, M. Havenith  
*Structural characterization of pyruvic acid dimer formed inside helium nanodroplets by infrared spectroscopy and ab initio study*  
J. Phys. Chem. A, accepted (2024).
294. B. König, S. Pezzotti, S. Ramos, G. Schwaab, M. Havenith  
*Real time measure of solvation free energy changes upon liquid-liquid phase separation of  $\alpha$ -Elastin*  
Biophys. J. **123**, 1367–1375, (2024). DOI: 10.1016/j.bpj.2023.07.023
293. M. Koga, D.H. Kang, Z.N. Heim, P. Meyer, B.A. Erickson, N. Haldar, N. Baradaran, M. Havenith, D.M. Neumark  
*Extreme ultraviolet time-resolved photoelectron spectroscopy of adenine, adenosine and adenosine monophosphate in a liquid flat jet*  
Phys. Chem. Chem. Phys. **26**, 13106–13117 (2024). DOI: 10.1039/D4CP00856A
292. Y.H. Tao, S. Schulke, G. Schwaab, G.L. Nealon, S. Pezzotti, S.I. Hodgetts, A.R. Harvey, V.P. Wallace, M. Havenith  
*Hydration water drives the self-assembly of guanosine monophosphate*  
Biophys. J. **123**, 931–939 (2024). DOI: 10.1016/j.bpj.2024.03.005
291. D. Das Mahanta, D. Robinson Brown, T. Webber, S. Pezzotti, G. Schwaab, S. Han, M.S. Shell, M. Havenith  
*Bridging the gap in cryopreservation mechanism: Unraveling the interplay between structure, dynamics, and thermodynamics in cryoprotectant aqueous solutions*  
J. Phys. Chem. B **128**, 3720–3731 (2024). DOI: 10.1021/acs.jpcc.4c00264
290. S. Murke, W. Chen, S. Pezzotti, M. Havenith  
*Tuning acid-base chemistry at an electrified gold/water interface*  
J. Am. Chem. Soc. **146**, 12423–12430 (2024). DOI: 10.1021/jacs.3c13633  
(Cover article – <https://pubs.acs.org/toc/jacsat/146/18>)
289. S. Mukherjee, S. Ramos, S. Pezzotti, A. Kalarikkal, T.M. Prass, L. Galazzo, D. Gendreizig, N. Barbosa, E. Bordignon, M. Havenith, L. Schäfer  
*Entropy tug-of-war determines solvent effects in the liquid-liquid phase separation of a globular protein*  
J. Phys. Chem. Lett. **15**, 4047–4055 (2024). DOI: 10.1021/acs.jpcclett.3c03421
288. S. Schulke, M. Nolten, G. Schwaab, M. Havenith  
*Studying local electrostatics by terahertz spectroscopy using amines as a probe*  
ChemPhysChem **25**, e202300389 (2024). DOI: 10.1002/cphc.202300389

**2023**

287. T. Ockelmann, C. Hoberg, A. Buchmann, F. Novelli, M. Havenith  
*Energy dissipation into the solvent during proton transfer occurs via acoustic phonons*  
J. Phys. Chem. B **127**, 9560–9565 (2023). DOI: 10.1021/acs.jpcc.3c04874
286. S. Bag, S. Pezzotti, D. Das Mahanta, S. Schulke, G. Schwaab, M. Havenith

- From local hydration motifs in aqueous acetic acid solutions to macroscopic mixing thermodynamics: A quantitative connection from THz-calorimetry*  
J. Phys. Chem. B **127**, 9204–9210 (2023). DOI: 10.1021/acs.jpcc.3c06328
285. S. Ramos, J. Kamps, S. Pezzotti, K.F. Winklhofer, J. Tatzelt, M. Havenith  
*Hydration makes a difference! How to tune protein complexes between liquid–liquid and liquid–solid phase separation*  
Phys. Chem. Chem. Phys. **25**, 28063–28069 (2023). DOI: 10.1039/d3cp03299j
284. D. Das Mahanta, D.R. Brown, S. Pezzotti, S. Han, G. Schwaab, M.S. Shell, M. Havenith  
*Local solvation structures govern the mixing thermodynamics of glycerol–water solutions*  
Chem. Sci. **14**, 7381–7392 (2023). DOI: 10.1039/d3sc00517h
283. S. Pezzotti, A. Serva, C.J. Stein, M. Havenith  
*Adsorption of ions and solutes at electrified metal–aqueous interfaces: insights from THz spectroscopy and simulations*  
Reference Module in Chemistry, Molecular Sciences and Chemical Engineering  
Elsevier, ISBN 9780124095472 (2023). DOI: 10.1016/B978-0-323-85669-0.00092-1
282. A.W. Hauser, M. Havenith, M. Koch, M. Sterrer  
*Festschrift for Wolfgang E. Ernst – electronic and nuclear dynamics and their interplay in molecules, clusters and on surfaces*  
Phys. Chem. Chem. Phys. **25**, 11880–11882 (2023). DOI: 10.1039/d3cp90052e
281. A. Leitenstorfer, ..., M. Havenith, ..., J. Cunningham  
*The 2023 terahertz science and technology roadmap*  
J. Phys. D: Appl. Phys. **56**, 223001 (2023). DOI: 10.1088/1361-6463/acbe4c
280. C. Hoberg, J.J. Talbot, J. Shee, T. Ockelmann, D. Das Mahanta, F. Novelli, M. Head-Gordon, M. Havenith  
*Caught in the act: real-time observation of the solvent response that promotes excited-state proton transfer in pyranine*  
Chem. Sci. **14**, 4048–4058 (2023). DOI: 10.1039/d2sc07126f
279. S. Pezzotti, B. König, S. Ramos, G. Schwaab, M. Havenith  
*Liquid–liquid phase separation? Ask the water!*  
J. Phys. Chem. Lett. **14**, 1556–1563 (2023). DOI: 10.1021/acs.jpcclett.2c02697
278. F. Novelli, K. Chen, A. Buchmann, T. Ockelmann, C. Hoberg, T. Head-Gordon, M. Havenith  
*The birth and evolution of solvated electrons in the water*  
PNAS **120**, e2216480120 (2023). DOI: 10.1073/pnas.2216480120
277. H. Hao, E.M. Adams, S. Funke, G. Schwaab, M. Havenith, T. Head-Gordon  
*Highly altered state of proton transport in acid pools in charged reverse micelles*  
J. Am. Chem. Soc. **145**, 1826–1834 (2023). DOI: 10.1021/jacs.2c11331
276. S. Murke, K. Wonner, S. Alfarano, C. Rurainsky, P. Cignoni, K. Tschulik, M. Havenith  
*SERS reveals presence of Au–O–O–H and enhanced catalytic activity of electrochemically dealloyed AgAu nanoparticles*  
J. Phys. Chem. C **127**, 1071–1076 (2023). DOI: 10.1021/acs.jpcc.2c06515

275. E.P. van Dam, B. König, S. Ramos, E.M. Adams, G. Schwaab, M. Havenith  
*Observation of dissipating solvated protons upon hydrogel formation*  
Phys. Chem. Chem. Phys. **24**, 27893–27899 (2022). DOI: 10.1039/d2cp01949c
274. S. Ruiz-Barragan, F. Sebastiani, P. Schienbein, J. Abraham, G. Schwaab, R. Raveendran, M. Havenith, D. Marx  
*Nanoconfinement effects on water in narrow graphene-based slit pores as revealed by THz spectroscopy*  
Phys. Chem. Chem. Phys. **24**, 24734–24747 (2022). DOI: 10.1039/d2cp02564g
273. S. Jäger, P. Meyer, K.-S. Feichtner, S. Henkel, G. Schwaab, V.H. Gessner, M. Havenith  
*Reaction of lithium hexamethyldisilazide (LiHMDS) with water at ultracold conditions*  
Phys. Chem. Chem. Phys. **24**, 24089–24094 (2022). DOI: 10.1039/d2cp03372k
272. D. Mani, T.K. Roy, J. Khatri, G. Schwaab, S. Blach, C. Hölzl, H. Forbert, D. Marx, M. Havenith  
*Internal electric field-induced formation of exotic linear-acetonitrile chains*  
J. Phys. Chem. Lett. **13**, 6852–6858 (2022). DOI: 10.1021/acs.jpcclett.2c01482
271. F.N. Brünig, M. Rammler, E.M. Adams, M. Havenith, R.R. Netz  
*Spectral signatures of excess-proton waiting and transfer-path dynamics in aqueous hydrochloric acid solutions*  
Nat. Commun. **13**, 4210 (2022). DOI: 10.1038/s41467-022-31700-x
270. S. Pezzotti, F. Sebastiani, E.P. van Dam, S. Ramos, V. Conti Nibali, G. Schwaab, M. Havenith  
*Spectroscopic fingerprints of cavity formation and solute insertion as a measure of hydration entropic loss and enthalpic gain*  
Angew. Chem. Int. Ed. **61**, e202203893 (2022). DOI: 10.1002/anie.202203893  
Angew. Chem. **134**, e202203893 (2022). DOI: 10.1002/ange.202203893
269. G. Schwaab, R. Pérez de Tudela, D. Mani, N. Pal, T.K. Roy, F. Gabas, R. Conte, L. Durán Caballero, M. Ceotto, D. Marx, M. Havenith  
*Zwitter ionization of glycine at outer space conditions due to microhydration by six water molecules*  
Phys. Rev. Lett. **128**, 033001 (2022). DOI: 10.1103/PhysRevLett.128.033001
268. K. Wonner, S. Murke, S.R. Alfarano, P. Hosseini, M. Havenith, K. Tschulik  
*Operando electrochemical SERS monitors nanoparticle reactions by capping agent fingerprints*  
Nano Res. **15**, 4517–4524 (2022). DOI: 10.1007/s12274-021-3999-2
267. F. Novelli, C. Hoberg, E.M. Adams, J.M. Klopff, M. Havenith  
*Reply to the ‘Comment on “Terahertz pump–probe of liquid water at 12.3 THz”’ by A. F. G. van der Meer, PCCP, 2022, 24, D1CP05216K*  
Phys. Chem. Chem. Phys. **24**, 13413–13415 (2022). DOI: 10.1039/d2cp00565d
266. F. Novelli, C. Hoberg, E.M. Adams, J.M. Klopff, M. Havenith  
*Terahertz pump–probe of liquid water at 12.3 THz*  
Phys. Chem. Chem. Phys. **24**, 653–665 (2022). DOI: 10.1039/d1cp03207k  
(Inside front cover: Phys. Chem. Chem. Phys. **24**, 598–598 (2022). DOI: 10.1039/d2cp90007f)

**2021**

265. A. Serva, M. Havenith, S. Pezzotti

- The role of hydrophobic hydration in the free energy of chemical reactions at the gold/water interface: Size and position effects*  
J. Chem. Phys. **155**, 204706 (2021). DOI: 10.1063/5.0069498
264. T.K. Roy, K. Chatterjee, J. Khatri, G. Schwaab, M. Havenith  
*Helium nanodroplet infrared spectroscopy of oxazole-(water)<sub>n</sub> (n = 1,2) clusters*  
AIP Adv. **11**, 115112 (2021). DOI: 10.1063/5.0066419
263. S.R. Alfarano, S. Pezzotti, C.J. Stein, Z. Lin, F. Sebastiani, S. Funke, C. Hoberg, I. Kolling, C.Y. Ma, K. Mauelshagen, T. Ockelmann, G. Schwaab, L. Fu, J.-B. Brubach, P. Roy, M. Head-Gordon, K. Tschulik, M.-P. Gaigeot, M. Havenith  
*Stripping away ion hydration shells in electrical double layer formation: Water networks matter*  
PNAS **118**, e2108568118 (2021). DOI: 10.1073/pnas.2108568118
262. T.K. Roy, D. Mani, G. Schwaab, M. Havenith  
*An infrared spectroscopic study of trifluoromethoxybenzene···methanol complexes formed in superfluid helium nanodroplets*  
Phys. Chem. Chem. Phys. **23**, 25180–25187 (2021). DOI: 10.1039/d1cp03136h
261. C.Y. Ma, S. Pezzotti, G. Schwaab, M. Gebala, D. Herschlag, M. Havenith  
*Cation enrichment in the ion atmosphere is promoted by local hydration of DNA*  
Phys. Chem. Chem. Phys. **23**, 23203–23213 (2021). DOI: 10.1039/d1cp01963e
260. E.M. Adams, H. Hao, I. Leven, M. Rüttermann, H. Wirtz, M. Havenith, T. Head-Gordon  
*Proton traffic jam: Effect of nanoconfinement and acid concentration on proton hopping mechanism*  
Angew. Chem. Int. Ed. **60**, 25419–25427 (2021). DOI: 10.1002/anie.202108766  
Angew. Chem. **133**, 25623–25631 (2021). DOI: 10.1002/ange.202108766
259. J. Khatri, T.K. Roy, K. Chatterjee, G. Schwaab, M. Havenith  
*Vibrational spectroscopy of benzonitrile-(water)<sub>1-2</sub> clusters in helium droplets*  
J. Phys. Chem. A **125**, 6954–6963 (2021). DOI: 10.1021/acs.jpca.1c04553
258. K. Chatterjee, T.K. Roy, J. Khatri, G. Schwaab, M. Havenith  
*Unravelling the microhydration frameworks of prototype PAH by infrared spectroscopy: Naphthalene-(water)<sub>1-3</sub>*  
Phys. Chem. Chem. Phys. **23**, 14016–14026 (2021). DOI: 10.1039/d1cp01789f
257. K. Orend, C. Baer, F. Novelli, D. Welzel, T. Musch, M. Havenith  
*Designing a dielectric RF applicator cell for terahertz transmission*  
2021 ICEAA, IEEE, 177–182 (2021). DOI: 10.1109/ICEAA52647.2021.9539564
256. T.K. Roy, K. Chatterjee, J. Khatri, G. Schwaab, M. Havenith  
*Stepwise microhydration of isoxazole: Infrared spectroscopy of isoxazole-(water)<sub>n≤2</sub> clusters in helium nanodroplets*  
J. Phys. Chem. A **125**, 4766–4774 (2021). DOI: 10.1021/acs.jpca.1c01974
255. E. Adams, S. Pezzotti, J. Ahlers, M. Rüttermann, M. Levin, A. Goldenzweig, Y. Peleg, S. Fleischmann, I. Sagi, M. Havenith  
*Local mutations can serve as a game changer for global protein solvent interaction*  
JACS Au **1**, 1076–1085 (2021). DOI: 10.1021/jacsau.1c00155
254. I. Kolling, C. Hölzl, S. Imoto, S.R. Alfarano, H. Vondracek, L. Knake, F. Sebastiani, F. Novelli, C. Hoberg, J.-B. Brubach, P. Roy, H. Forbert, G. Schwaab, D. Marx, M. Havenith

- Aqueous TMAO solution under high hydrostatic pressure*  
Phys. Chem. Chem. Phys. **23**, 11355–11365 (2021). DOI: 10.1039/d1cp00703c
253. S. Pezzotti, A. Serva, F. Sebastiani, F. Siro Brigiano, D.R Galimberti, L. Potier, S. Alfarano, G. Schwaab, M. Havenith, M.-P. Gaigeot  
*Molecular fingerprints of hydrophobicity at aqueous interfaces from theory and vibrational spectroscopies*  
J. Phys. Chem. Lett. **12**, 3827–3836 (2021). DOI: 10.1021/acs.jpcclett.1c00257
252. A. Serva, M. Salanne, M. Havenith, S. Pezzotti  
*Size-dependence of hydrophobic hydration at electrified gold/water interfaces*  
PNAS **118**, e2023867118 (2021). DOI: 10.1073/pnas.2023867118
251. J. Ahlers, E.M. Adams, V. Bader, S. Pezzotti, K.F. Winklhofer, J. Tatzelt, M. Havenith  
*The key role of solvent in condensation: mapping water in liquid-liquid phase-separated FUS*  
Biophys. J. **120**, 1266–1275 (2021). DOI: 10.1016/j.bpj.2021.01.019
250. F. Sebastiani; C.Y. Ma, S. Funke, A. Bäumer, D. Decka, C. Hoberg, A. Esser, H. Forbert, G. Schwaab, D. Marx, M. Havenith  
*Probing local electrostatics of glycine in aqueous solution by THz spectroscopy*  
Angew. Chem. Int. Ed. **60**, 3768–3772 (2021). DOI: 10.1002/anie.202014133
- 2016-2020**
249. F. Sebastiani, T.A. Bender, S. Pezzotti, W.-L. Li, G. Schwaab, R.G. Bergman, K.N. Raymond, F.D. Toste, T. Head-Gordon, M. Havenith  
*An isolated water droplet in the aqueous solution of a supramolecular tetrahedral cage*  
PNAS **117**, 32954–32961 (2020). DOI: 10.1073/pnas.2012545117
248. T.K. Roy, D. Mani, G. Schwaab, M. Havenith  
*A close competition between O-H···O and O-H··· $\pi$  hydrogen bonding: IR spectroscopy of anisole-methanol complex in helium nanodroplets*  
Phys. Chem. Chem. Phys. **22**, 22408–22416 (2020). DOI: 10.1039/d0cp02589e
247. F. Novelli, C.Y. Ma, N. Adhlakha, E.M. Adams, T. Ockelmann, D. Das Mahanta, P. Di Pietro, A. Perucchi, M. Havenith  
*Nonlinear terahertz transmission by liquid water at 1 THz*  
Appl. Sci. **10**, 5290 (2020). DOI: 10.3390/app10155290
246. V. Conti Nibali, S. Pezzotti, F. Sebastiani, D. Galimberti, G. Schwaab, M. Heyden, M.-P. Gaigeot, M. Havenith  
*Wrapping up hydrophobic hydration: Locality matters*  
J. Phys. Chem. Lett. **11**, 4809–4816 (2020). DOI: 10.1021/acs.jpcclett.0c00846
245. F. Novelli, L. R. Pestana, K. C Bennett, F. Sebastiani, E.M. Adams, N. Stavrias, T. Ockelmann, A. Colchero, C. Hoberg, G. Schwaab, T. Head-Gordon, M. Havenith  
*Strong anisotropy in liquid water upon librational excitation using terahertz laser fields*  
J. Phys. Chem. B **124**, 4989–5001 (2020). DOI: 10.1021/acs.jpccb.0c02448
244. F. Sebastiani, A.V. Verde, M. Heyden, G. Schwaab, M. Havenith  
*Cooperativity and ion pairing in magnesium sulfate aqueous solutions from the dilute regime to the solubility limit*  
Phys. Chem. Chem. Phys. **22**, 12140–12153 (2020). DOI: 10.1039/c9cp06845g

243. R. Schwan, C. Qu, D. Mani, N. Pal, G. Schwaab, J.M. Bowman, G.S. Tschumper, M. Havenith  
*Observation of the low frequency spectrum of water trimer as a sensitive test of the water trimer potential and the dipole moment surface*  
Angew. Chem. Int. Ed. **59**, 11399–11407(2020). DOI: 10.1002/anie.202003851  
(Frontispiece / Hot Paper: <https://onlinelibrary.wiley.com/doi/epdf/10.1002/anie.202082862>)
242. F. Novelli, B. Guchhait, M. Havenith  
*Towards intense THz spectroscopy on water: Characterization of optical rectification by GaP, OH1, and DSTMS at OPA wavelengths*  
MDPI Materials **13**, 1311 (2020). DOI: 10.3390/ma13061311
241. E. Adams, O. Lampret, B. König, T. Happe, M. Havenith  
*Solvent dynamics play a decisive role in the complex formation of biologically relevant redox proteins*  
Phys. Chem. Chem. Phys. **22**, 7451–7459 (2020). DOI: 10.1039/d0cp00267d
240. J. Deichmüller, F. Kogelheide, S. Murke, D. Hüther, G. Schwaab, P. Awakowicz, M. Havenith  
*Does plasma-induced methionine degradation provide alternative reaction paths for cell death?*  
J. Phys. D. **53**, 355401 (2020). DOI: 10.1088/1361-6463/ab8cea
239. S. Alfarano, H. Vondracek, F. Sebastiani, F. Novelli, C. Hoberg, I. Kolling, J.-B. Brubach, P. Roy, G. Schwaab, M. Havenith  
*Does hydrated glycine act as solidification nucleus at multi-kilobar conditions?*  
Biophys. Chem. **253**, 106215 (2019). DOI: 10.1016/j.bpc.2019.106215
238. D. Mani, R. Pèrez de Tudela, R. Schwan, N. Pal, S. Körning, H. Forbert, B. Redlich, A.F.G. van der Meer, G. Schwaab, D. Marx, M. Havenith  
*Acid solvation versus dissociation at "stardust conditions": Reaction sequence matters*  
Sci. Adv. **5**, eaav8179 (2019). DOI: 10.1126/sciadv.aav8179
237. S. Funke, F. Sebastiani, G. Schwaab, M. Havenith  
*Spectroscopic fingerprints in the low frequency spectrum of ice (Ih), clathrate hydrates, supercooled water and hydrophobic hydration reveal similarities in the hydrogen bond network motifs*  
J. Chem. Phys. **150**, 224505 (2019). DOI: 10.1063/1.5097218
236. C. Hoberg, P. Balzerowski, M. Havenith  
*Integration of a rapid scanning technique into THz time-domain spectrometers for nonlinear THz spectroscopy measurements*  
AIP Adv. **9**, 035348 (2019). DOI: 10.1063/1.5080653
235. K. Lotz, A. Wütscher, H. Düdler, C. Berger, C. Russo, K. Mukherjee, G. Schwaab, M. Havenith, M. Muhler  
*Tuning the properties of iron-doped porous graphitic carbon synthesized by hydrothermal carbonization of cellulose and subsequent pyrolysis*  
ACS Omega **4**, 4448–4460 (2019). DOI: 10.1021/acsomega.8b03369
234. D. Mani, N. Pal, M. Smialkowski, C. Beakovic, G. Schwaab, M. Havenith  
*Accessing different binding sites of a multifunctional molecule: IR spectroscopy of propargyl alcohol...Water complexes in helium droplets*  
Phys. Chem. Chem. Phys. **21**, 20582–20587 (2019). DOI: 10.1039/c9cp02055a

- (Inside front cover: *Phys. Chem. Chem. Phys.* **21**, 20504–20504 (2019). DOI: 10.1039/c9cp90233c)
233. R. Schwan, C. Qu, D. Mani, N. Pal, L. van der Meer, B. Redlich, C. Leforestier, J.M. Bowman, G. Schwaab, M. Havenith  
*Observation of the low frequency spectrum of water dimer as a sensitive test of the water dimer potential and dipole moment surfaces*  
*Angew. Chem. Int. Ed.* **58**, 13119–13126 (2019). DOI: 10.1002/anie.201906048
232. H. Vondracek, S. Alfarano, C.M. Hoberg, I. Kolling, F. Novelli, S. Sebastiani, J.-B. Brubach, P. Roy, G. Schwaab, M. Havenith  
*Urea's match in the hydrogen-bond network? A high pressure THz study*  
*Biophys. Chem.* **254**, 106240 (2019). DOI: 10.1016/j.bpc.2019.106240
231. G. Schwaab, F. Sebastiani, M. Havenith  
*Ion hydration and ion pairing as probed by THz spectroscopy*  
*Angew. Chem. Int. Ed.* **58**, 3000–3013 (2019). DOI: 10.1002/anie.201805261
230. G. Schwaab, F. Sebastiani, M. Havenith  
*Untersuchung von Ionenhydratation und Ionenpaarbildung mittels THz-Spektroskopie*  
*Angew. Chem.* **131**, 3030–3044 (2019). DOI: 10.1002/ange.201805261
229. H. Vondracek, S. Imoto, L. Knake, G. Schwaab, D. Marx, M. Havenith  
*Hydrogen-bonding in liquid water at multikilobar pressures*  
*J. Phys. Chem. B* **123**, 7748–7753 (2019). DOI: 10.1021/acs.jpcc.9b06821
228. F. Novelli, M. Bernal Lopez, G. Schwaab, B. Roldan Cuenya, M. Havenith  
*Water solvation of charged and neutral gold nanoparticles*  
*J. Phys. Chem. B* **123**, 6521–6528 (2019). DOI: 10.1021/acs.jpcc.9b02358
227. K. Mukherjee, G. Schwaab, M. Havenith  
*Cation-specific interactions of protein surface charges in dilute aqueous salt solutions: A combined study using dielectric relaxation spectroscopy and Raman spectroscopy*  
*Phys. Chem. Chem. Phys.* **20**, 29306–29313(2018). DOI: 10.1039/c8cp05011b
226. H. Wirtz, S. Schäfer, C. Hoberg, K. Reid, D. Leitner, M. Havenith  
*Hydrophobic collapse of ubiquitin generates rapid protein-water motions*  
*Biochemistry* **57**, 3650–3657 (2018). DOI: 10.1021/acs.biochem.8b00235
225. A. Esser, H. Forbert, F. Sebastiani, G. Schwaab, M. Havenith, D. Marx  
*Hydrophilic solvation dominates the terahertz fingerprint of amino acids in water*  
*J. Phys. Chem. B* **122**, 1453–1459 (2018). DOI: 10.1021/acs.jpcc.7b08563
224. H. Wirtz, S. Schäfer, C. Hoberg, M. Havenith  
*Differences in hydration structure around hydrophobic and hydrophilic model peptides probed by THz spectroscopy*  
*J. Infrared Millim. Terahertz Waves* **39**, 816–827 (2018). DOI: 10.1007/s10762-018-0478-2
223. V. Conti Nibali, G. Morra, M. Havenith, G. D'Angelo, G. Colombo  
*Concerted motions on allosteric model proteins at terahertz frequencies*  
*AAPP* **96**, A6 (2018). DOI: 10.1478/AAPP.961A6
222. C. Klinkhammer, F. Böhm, V. Sharma, M. Seitz, G. Schwaab, M. Havenith  
*Anion dependent ion pairing in concentrated ytterbium halide solutions*

- J. Chem. Phys. **148**, 222802 (2018). DOI: 10.1063/1.5016549
221. M. Senske, Y. Xu, A. Bäumer, S. Schäfer, H. Wirtz, J. Savolainen, H. Weingärtner, M. Havenith  
*Local chemistry of the surfactant's head groups determines protein stability in reverse micelles*  
Phys. Chem. Chem. Phys. **20**, 8515–8522 (2018). DOI: 10.1039/c8cp00407b
220. D. Mani, T. Fischer, R. Schwan, A. Dey, B. Redlich, A.F.G. Van der Meer, G. Schwaab, M. Havenith  
*A helium nanodroplet setup for mid and far-infrared spectroscopy using pulsed-free-electron lasers: Vibrational spectra of propargyl alcohol*  
RSC Adv. **7**, 54318–54325 (2017). DOI: 10.1039/c7ra08102b
219. F. Sebastiani, S. Wolf, B. Born, T.Q. Luong, H. Cölfen, D. Gebauer, M. Havenith,  
*Water dynamics from THz spectroscopy reveals the locus of a liquid-liquid binodal limit in aqueous CaCO<sub>3</sub> solutions*  
Angew. Chem. Int. Ed. **56**, 490–495 (2017). DOI: 10.1002/anie.201610554
218. F. Sebastiani, S. Wolf, B. Born, T.Q. Luong, H. Cölfen, D. Gebauer, M. Havenith  
*THz-Spektroskopie erlaubt Rückschlüsse auf die Wasserdynamik und die Lage einer flüssig-flüssig-binodalen Grenze in wässrigen CaCO<sub>3</sub>-Lösungen*  
Angew. Chem. **129**, 504–509 (2017). DOI: 10.1002/ange.201610554
217. V. Conti Nibali, G. Morra, M. Havenith, G. Colombo  
*Role of terahertz (THz) fluctuations in the allosteric properties of the PDZ domains*  
J. Phys. Chem. B **121**, 10200–10208 (2017). DOI: 10.1021/acs.jpcc.7b06590
216. K. Aoki, J. Savolainen, M. Havenith  
*Broadband terahertz pulse generation by optical rectification in GaP crystals*  
Appl. Phys. Lett. **110**, 201103 (2017). DOI: 10.1063/1.4983371
215. K. Sommer, M. Havenith  
*Lösungsmittel im Fokus der Forschung*  
Chem. Unserer Zeit **51**, 3 (2017). DOI: 10.1002/ciuz.201790003
214. M. Di Tucci, F. Böhm, G. Schwaab, E.R. Williams, M. Havenith  
*Effects of multivalent hexacyanoferrates and their ion pairs on water molecule dynamics measured with terahertz spectroscopy*  
Phys. Chem. Chem. Phys. **19**, 7297–7306 (2017). DOI: 10.1039/c6cp08423k
213. P. Schienbein, G. Schwaab, H. Forbert, M. Havenith, D. Marx  
*Correlations in the solute-solvent dynamics reach beyond the first hydration shell of ions*  
J. Phys. Chem. Lett. **8**, 2373–2380, (2017). DOI: 10.1021/acs.jpcllett.7b00713
212. E. Feresin, M. Havenith  
*Solvatationsforschung ermittelt Rolle des Solvens: Das Lösungsmittel im Fokus*  
Chem. Unserer Zeit **51**, 18–24 (2017). DOI: 10.1002/ciuz.201700781
211. D. Leicht, M. Kaufmann, N. Pal, G. Schwaab, M. Havenith  
*From the tunneling dimer to the onset of microsolvation: Infrared spectroscopy of allyl radical water aggregates in helium nanodroplets*  
J. Chem. Phys. **146**, 114306 (2017). DOI: 10.1063/1.4978482
210. F. Böhm, G. Schwaab, M. Havenith  
*Mapping hydration water around alcohol chains by THz calorimetry*



- Angew. Chem. Int. Ed. **56**, 9981–9985 (2017). DOI: 10.1002/anie.201612162
209. F. Böhm, G. Schwaab, M. Havenith  
*Kartierung des Hydratwassers um Alkoholketten mittels THz-Kalorimetrie*  
Angew. Chem. **129**, 10113–10117 (2017). DOI: 10.1002/ange.201612162
208. P.E. Decaneto, T. Vasilevskaya, Y. Kutin, H. Ogata, M. Grossman, I. Sagi, M. Havenith, W. Lubitz, W. Thiel, N. Cox  
*Solvent water interactions within the active site of the membrane type I matrix metalloproteinase*  
Phys. Chem. Chem. Phys. **19**, 30316–30331 (2017). DOI: 10.1039/c7cp05572b
207. C. Klinkhammer, C. Verlackt, D. Smilowicz, F. Kogelheide, A. Bogaerts, N. Metzler-Nolte, K. Stapelmann, M. Havenith, J. Lackmann  
*Elucidation of plasma-induced chemical modifications on glutathione and glutathione disulphide*  
Sci. Rep. **7**, 13828- (2017). DOI: 10.1038/s41598-017-13041-8
206. D. Gnutt, O. Brylski, E. Edengeiser, M. Havenith, S. Ebbinghaus  
*Imperfect crowding adaptation of mammalian cells towards osmotic stress and its modulation by osmolytes*  
Mol. BioSyst. **13**, 2218–2221 (2017). DOI: 10.1039/C7MB00432J
205. M. Engelhardt, K. Kartaschew, N. Bibino, M. Havenith, P. Awakowicz  
*Silicon surface modifications produced by non-equilibrium He, Ne, and Kr plasma jets*  
J. Phys. D **50**, 015206 (2017). DOI: 10.1088/1361-6463/50/1/015206
204. J.-W. Lackmann, M. Fiebrandt, M. Raguse, K. Kartaschew, M. Havenith, J. Bandow, R. Moeller, P. Awacowicz, K. Stapelmann  
*A combined low-pressure hydrogen peroxide evaporation plus hydrogen plasma treatment method for sterilization - Part 2: An intercomparison study of different biological systems*  
Plasma Process Polym. **14**, 1600199 (2017). DOI: 10.1002/ppap.201600199
203. A. Pougin, A. Lüken, C. Klinkhammer, D. Hiltrop, M. Kauer, K. Tölle, M. Havenith, K. Morgenstern, W. Grünert, M. Muhler, J. Strunk  
*Probing oxide reduction and phase transformations at the Au-TiO<sub>2</sub> interface by vibrational spectroscopy*  
Top. Catal. **60**, 1744–1753 (2017). DOI: 10.1007/s11244-017-0851-8
202. H. Jähme, G. Di Florio, V. Conti Nibali, C. Esen, A. Ostendorf, M. Grafen, E. Henke, J. Soetebier, C. Brenner, M. Havenith, M.R. Hofmann  
*Recognition of pharmaceuticals with compact mini-Raman-spectrometer and automatized pattern recognition algorithms*  
Proceedings of SPIE **9899**, 98992M (2016). DOI: 10.1117/12.2228070
201. K. Kartaschew, S. Baldus, M. Mischo, E. Bründermann, P. Awakowicz, M. Havenith  
*Cold atmospheric-pressure plasma and bacteria: Understanding the mode of action using vibrational microspectroscopy*  
J. Phys. D. **49**, 374003 (2016). DOI: 10.1088/0022-3727/49/37/374003
200. M. Senske, D. Constantinescu-Aruxandei, M. Havenith, C. Herrmann, H. Weingärtner, S. Ebbinghaus

- The temperature dependence of the Hofmeister series: Thermodynamic fingerprints of cosolute-protein interactions*  
Phys. Chem. Chem. Phys. **18**, 29698–29708 (2016). DOI: 10.1039/c6cp05080h
199. M. Engelhardt, R. Pothiraja, K. Kartaschew, N. Bibinov, M. Havenith, P. Awakowicz  
*Interaction of an argon plasma jet with a silicon wafer*  
J. Phys. D **49**, 145201 (2016). DOI: 10.1088/0022-3727/49/14/145201
198. D. Leicht, M. Kaufmann, R. Schwan, J. Schäfer, G. Schwaab, M. Havenith  
*Understanding the microsolvation of radicals: Infrared spectroscopy of benzyl radical water clusters*  
J. Chem. Phys. **145**, 204305 (2016). DOI: 10.1063/1.4968214
197. A. Bäumer, J. Duman, M. Havenith  
*Ice nucleation of an insect lipoprotein ice nucleator (LPIN) correlates with retardation of the hydrogen bond dynamics at the myo-inositol ring*  
Phys. Chem. Chem. Phys. **18**, 19318–19323 (2016). DOI: 10.1039/c6cp02399a
196. R. Schwan, M. Kaufmann, D. Leicht, G. Schwaab, M. Havenith  
*Infrared spectroscopy of the  $\nu_2$  band of the water monomer and small water clusters  $(\text{H}_2\text{O})_{n=2,3,4}$  in helium droplets*  
Phys. Chem. Chem. Phys. **18**, 24063–24069 (2016). DOI: 10.1039/c6cp04333j
195. D. Leicht, M. Kaufmann, G. Schwaab, M. Havenith  
*Infrared spectroscopy of the helium solvated cyclopentadienyl radical in the CH stretch region*  
J. Chem. Phys. **145**, 074304 (2016). DOI: 10.1063/1.4960781
194. M.-C. Bellissent-Funel, A. Hassanali, M. Havenith, R. Henchman, P. Pohl, F. Sterpone, D. van der Spoel, Y. Xu, A.E. Garcia  
*Water determines the structure and dynamics of proteins*  
Chem. Rev. **116**, 7673–7697 (2016). DOI: 10.1021/acs.chemrev.5b00664
193. N. Samanta, T. Luong, D. Das Mahanta, R. Mitra, M. Havenith  
*Effect of short chain poly(ethylene glycol)s on the hydration structure and dynamics around human serum albumin*  
Langmuir **32**, 831–837 (2016). DOI: 10.1021/acs.langmuir.5b03884
192. P. Balzerowski, E. Bründermann, M. Havenith  
*Fabry-Pérot cavities for the terahertz spectral range based on high reflectivity multilayer mirrors*  
IEEE Trans. THz Sci. Technol. **6**, 563–567 (2016). DOI: 10.1109/TTHZ.2016.2572361
191. Y. Xu, A. Bäumer, K. Meister, C. Bischak, A. DeVries, D.M. Leitner, M. Havenith  
*Protein-water dynamics in antifreeze protein III activity*  
Chem. Phys. Lett. **647**, 1–6 (2016). DOI: 10.1016/j.cplett.2015.11.030  
(Cover article / Frontiers article)
190. L. Knake, H. Vondracek, M. Havenith  
*A novel set-up to investigate the low-frequency spectra of aqueous solutions at high hydrostatic pressure*  
Rev. Sci. Instrum. **87**, 104101 (2016). DOI: 10.1063/1.4964099
189. T.Q. Luong, Y. Xu, E. Bründermann, D.M. Leitner, M. Havenith

- Hydrophobic collapse induces changes in the collective protein and hydration low frequency modes*  
Chem. Phys. Lett. **651**, 1–7 (2016). DOI: 10.1016/j.cplett.2016.02.036  
(Cover article / Frontiers article)
188. M. Kaufmann, D. Leicht, R. Schwan, D. Mani, G. Schwaab, M. Havenith  
*Helium droplet infrared spectroscopy of glycine and glycine-water aggregates*  
Phys. Chem. Chem. Phys. **18**, 28082–28090 (2016). DOI: 10.1039/c6cp05042e
187. M. Kaufmann, D. Leicht, M. Havenith, B.M Broderick, G.E. Douberly  
*Infrared spectroscopy of the tropyli radical in helium droplets*  
J. Phys. Chem. A **120**, 6768–6773 (2016). DOI: 10.1021/acs.jpca.6b06522
186. T. Fobbe, S. Markmann, F. Fobbe, N. Hekmat; H. Nong, S. Pal, P. Balzerowski, J. Savolainen, M. Havenith, A.D. Wieck, N. Jukam  
*Broadband terahertz dispersion control in hybrid waveguides*  
Opt. Express **24**, 22319–22333 (2016). DOI: 10.1364/oe.24.022319
185. F. Kogelheide, K. Kartaschew, M. Strack, S. Baldus, N. Metzler-Nolte, M. Havenith, P. Awakowicz, K. Stapelmann, J.-W. Lackmann  
*FTIR spectroscopy of cysteine as a ready-to-use method for the investigation of plasma-induced chemical modifications of macromolecules*  
J. Phys. D **49**, 084004 (2016). DOI: 10.1088/0022-3727/49/8/084004

**2011-2015**

184. E. Edengeiser, K. Meister, E. Bründermann, S. Büning, S. Ebbinghaus, M. Havenith  
*Non-invasive chemical assessment of living human spermatozoa*  
RSC Adv. **5**, 10424–10429 (2015). DOI: 10.1039/C4RA12158A
183. K. Kartaschew, M. Mischo, S. Baldus, E. Bründermann, P. Awakowicz, M. Havenith  
*Unraveling the interactions between cold atmospheric plasma and skin-components with vibrational microspectroscopy*  
Biointerphases **10**, 029516 (2015). DOI: 10.1116/1.4919610
182. R. Pothiraja, K. Kartaschew, N. Bibinov, M. Havenith, P. Awakowicz  
*Diamond single micro-crystals and graphitic micro-balls formation in plasmoids under atmospheric pressure*  
J. Phys. D **48**, 115201 (2015). DOI: 10.1088/0022-3727/48/11/115201
181. M. Havenith  
*Solvation Science: A new interdisciplinary field*  
Angew. Chem. Intl. Ed. **55**, 1218–1219 (2015). DOI: 10.1002/anie.201510614
180. D. Decka, G. Schwaab, M. Havenith  
*A THz/FTIR fingerprint of the solvated proton: Evidence for Eigen structure and Zundel dynamics*  
Phys. Chem. Chem. Phys. **17**, 11898–11907 (2015). DOI: 10.1039/C5CP01035G
179. F. Böhm, V. Sharma, G. Schwaab, M. Havenith  
*The low frequency modes of solvated ions and ion pairs in aqueous electrolyte solutions: iron(II) and iron(III) chloride*  
Phys. Chem. Chem. Phys. **17**, 19582–19591 (2015). DOI: 10.1039/C5CP03157E

- 
178. L. Knake, G. Schwaab, K. Kartaschew, M. Havenith  
*Solvation dynamics of trimethylamine N-Oxide in aqueous solution probed by terahertz spectroscopy*  
J. Phys. Chem. B **119**, 13842–13851 (2015). DOI: 10.1021/acs.jpcc.5b04152
177. E. Decaneto, S. Suladze, Chr. Rosin, M. Havenith, W. Lubitz, R. Winter  
*Pressure and temperature effects on the activity and structure of the catalytic domain of human MT1-MMP*  
Biophys. J. **109**, 2371–2381 (2015). DOI: 10.1016/j.bpj.2015.10.023
176. S. Bauer, J. Stern, F. Böhm, C. Gainaru, M. Havenith, T. Loerting, R. Böhmer  
*Vibrational study of anharmonicity, supramolecular structure, and hydrogen bonding in two octanol isomers*  
Vib. Spectrosc. **79**, 59–65 (2015). DOI: 10.1016/j.vibspec.2015.05.001
175. D. Leicht, D. Habig, G. Schwaab, M. Havenith  
*Complexation of allyl radicals and hydrochlorid acid in helium nanodroplets*  
J. Phys. Chem. A **119**, 1007–1012 (2015). DOI: 10.1021/jp511708s
174. Y. Xu, M. Havenith  
*Perspective: Watching low-frequency vibrations of water in biomolecular recognition by THz spectroscopy*  
J. Chem. Phys. **143**, 170901 (2015). DOI: 10.1063/1.4934504
173. D. Habig, D. Leicht, G. Schwaab, M. Havenith  
*Reassignment of  $\nu_{2,3}$  IR band of the allyl radical in liquid helium nanodroplets*  
J. Chem. Phys. **143**, 024308 (2015). DOI: 10.1063/1.4923214
172. K. Hanke, M. Kaufmann, G. Schwaab, M. Havenith, C.T. Wolke, O. Gotlova, M.A. Johnson, B. Kar, W. Sander, E. Sánchez-García  
*Understanding the ionic liquid [NC<sub>4111</sub>][NTf<sub>2</sub>] from individual building blocks: An IR-spectroscopic study*  
Phys. Chem. Chem. Phys. **17**, 8518–8529 (2015). DOI: 10.1039/c5cp00116a
171. D. Marx, K. Morgenstern, M. Havenith, M. Muhler  
*At the heart of the Ruhr metropolis: Bochum explores solvation science*  
Bunsen-Magazin **17**, 33–35 (2015).
170. K. Morgenstern, M. Havenith, D. Marx, M. Muhler  
*Solvation science – main topic of the Bunsentagung 2015*  
Bunsen-Magazin **17**, 36–37 (2015).
169. K. Morgenstern, D. Marx, M. Havenith, M. Muhler  
*Editorial of the PCCP themed issue on "Solvation Science"*  
Phys. Chem. Chem. Phys. **17**, 8295–8296 (2015). DOI: 10.1039/C5CP90022K
168. E. Edengeiser, J.-W. Lackmann, E. Bründermann, S. Schneider, J. Benedikt, J. E. Bandow, M. Havenith  
*Synergetic effects of atmospheric pressure plasma-emitted components on DNA oligomers: A Raman spectroscopic study*  
J. Biophotonics **8**, 918–924 (2015). DOI: 10.1002/jbio.201400123
167. H. Vondracek, J. Dielmann-Gessner, W. Lubitz, M. Knipp, M. Havenith  
*THz absorption spectroscopy of solvated  $\beta$ -lactoglobulin*

- J. Chem. Phys. **141**, 22D534 (2014). DOI: 10.1063/1.4903237
166. B. Born, M. Heyden, S. Ebbinghaus, M. Havenith  
*Probing solvation dynamics by terahertz absorption spectroscopy*  
In Terahertz biomedical science & technology, Editor J.-H. Son., CRC Press, 135–152 (2014).
165. J. Dielmann-Gessner, M. Grossman, V. Conti Nibali, B. Born, I. Solomonov, G.B. Fields, M. Havenith, I. Sagi  
*Enzymatic turnover of macromolecules generates long-lasting protein-water-coupled motions beyond reaction steady state*  
PNAS **111**, 17857–17862 (2014). DOI: 10.1073/pnas.1410144111
164. V. Sharma, F. Böhm, G. Schwaab, M. Havenith  
*The low frequency motions of solvated Mn(II) and Ni(II) ions and their halide complexes*  
Phys. Chem. Chem. Phys. **16**, 25101–25110 (2014). DOI: 10.1039/c4cp03989k
163. G. Di Florio, E. Bründermann, N.S. Yadavalli, S. Santer, M. Havenith  
*Graphene multilayer as nano-sized optical strain gauge for polymer surface relief gratings*  
Nano Lett. **14**, 5754–5760 (2014). DOI: 10.1021/nl502631s
162. M. Heyden, G. Schwaab, M. Havenith,  
*Comment on "Hydration and mobility of trehalose in aqueous solution"*  
J. Phys. Chem. B. **118**, 10802–10805 (2014). DOI: 10.1021/jp508089t
161. M. Banerjee, V.-S. Dang; M. Bledowski, R. Radim; H.-W. Becker, D. Rogalla, E. Edengeiser, M. Havenith, A. Wieck, A. Devi,  
*MOCVD of TiO<sub>2</sub> thin films using a heteroleptic titanium complex: Precursor evaluation and investigation of optical, photoelectrochemical and electrical properties*  
Chem. Vap. Deposition **20**, 224–233 (2014). DOI: 10.1002/cvde.201407125
160. V. Conti Nibali, M. Havenith  
*New insights into the role of water in biological function: Studying solvated biomolecules using terahertz absorption spectroscopy in conjunction with molecular dynamics simulations*  
J. Am. Chem. Soc. **136**, 12800–12807 (2014). DOI: 10.1021/ja504441h
159. D. Habig, D. Leicht, M. Kaufmann, G. Schwaab, M. Havenith  
*IR-spectroscopic study of the allyl + NO reaction in helium nanodroplets*  
J. Chem. Phys. **141**, 044312 (2014). DOI: 10.1063/1.4890366
158. G. Di Florio, E. Bründermann, N.S. Yadavalli, S. Santer, M. Havenith  
*Confocal Raman microscopy and AFM study of the interface between the photosensitive polymer layer and multilayer graphene*  
Soft Mater. **12**, 98–105 (2014). DOI: 10.1080/1539445X.2014.945040
157. A. Patra, T.Q. Luong, R.K. Mitra, M. Havenith  
*The influence of charge on the structure and dynamics of water encapsulated in reverse micelles*  
Phys. Chem. Chem. Phys. **16**, 12875–12883 (2014). DOI: 10.1039/c4cp00386a
156. M. Senske, L. Törk, B. Born, M. Havenith, C. Herrmann, S. Ebbinghaus  
*Protein stabilization by macromolecular crowding through enthalpy rather than entropy*  
J. Am. Chem. Soc. **136**, 9036–9041 (2014). DOI: 10.1021/ja503205y
155. K. Meister, J. Duman, Y. Xu, A. DeVries, D. Leitner, M. Havenith

- The role of sulfates on antifreeze protein activity*  
J. Phys. Chem. B **118**, 7920–7924 (2014). DOI: 10.1021/jp5006742
154. M. Mischo, L. von Kobyletzki, E. Bründermann, D. Schmidt, A. Pothhoff, N.H. Brockmeyer, M. Havenith  
*Similar appearance, different mechanisms: Xerosis in HIV, atopic dermatitis and aging*  
Exp. Dermatol. **23**, 446–448 (2014). DOI: 10.1111/exd.12425
153. E.T. Spielberg, E. Edengeiser, B. Mallick, M. Havenith, A.-V. Mudring  
*(1-Butyl-4-methyl-pyridinium)[Cu(SCN)<sub>2</sub>]: A coordination polymer and ionic liquid*  
Chem. Eur. J. **20**, 5338–5345 (2014). DOI: 10.1002/chem.201302777
152. J. Sun, G. Niehues, H. Forbert, D. Decka, G. Schwaab, D. Marx, M. Havenith  
*Understanding THz spectra of aqueous solutions: Glycine in light and heavy water*  
J. Am. Chem. Soc. **136**, 5031–5038 (2014). DOI: 10.1021/ja4129857
151. P. Nieto, M. Letzner, T. Endres, G. Schwaab, M. Havenith  
*IR spectroscopy of pyridine-water conformers in helium nanodroplets*  
Phys. Chem. Chem. Phys. **16**, 8384–8391 (2014). DOI: 10.1039/c3cp55284e
150. H. Ogata, E. Decaneto, M. Grossman, M. Havenith, I. Sagi, W. Lubitz, M. Knipp  
*Crystallization and preliminary X-ray crystallographic analysis of the catalytic domain of membrane type 1 matrix metalloproteinase*  
Acta Cryst. **F70**, 232–235 (2014). DOI: 10.1107/S2053230X13034857
149. G. Di Florio, E. Bründermann, N.S. Yadavalli, S. Santer, M. Havenith  
*Polarized 3D Raman and nanoscale near-field optical microscopy of optically inscribed surface relief gratings: chromophore orientation in azo-doped polymer films*  
Soft Matter **10**, 1544–1554 (2014). DOI: 10.1039/c3sm51787j
148. V.-S. Dang, H. Parala, J.H. Kim, K. Xu, N.B. Srinivasan, E. Edengeiser, M. Havenith, A.D. Wieck, T. de los Arcos, R.A. Fischer, A. Devi  
*Electrical and optical properties of TiO<sub>2</sub> thin films prepared by plasma-enhanced atomic layer deposition*  
Physica Status Solidi A **211**, 416–424 (2014). DOI: 10.1002/pssa.201330115
147. D. Peeters, G. Carraro, C. Maccato, H. Parala, A. Gasparatto, D. Barreca, C. Sada, K. Kartaschew, M. Havenith, D. Rogalla, H.-W. Becker, A. Devi  
*Tailoring iron (III) oxide nanomorphology by chemical vapor deposition: Growth and characterization*  
Physica Status Solidi A **211**, 316–322 (2014). DOI: 10.1002/pssa.201330079
146. J.-W. Lackmann, E. Edengeiser, S. Schneider, J. Benedikt, M. Havenith, J.E. Bandow  
*Effects of the effluent of a microscale atmospheric pressure plasma jet operated with He/O<sub>2</sub> gas on bovine serum albumin*  
Plasma Medicine **3**, 115–124 (2013). DOI: 10.1615/PlasmaMed.2014008858
145. M. Letzner, S. Grün, D. Habig, K. Hanke, T. Endres, P. Nieto, G. Schwaab, Ł. Walewski, M. Wollenhaupt, H. Forbert, D. Marx, M. Havenith  
*High resolution spectroscopy of HCl–water clusters: IR bands of undissociated and dissociated clusters revisited*  
J. Chem. Phys. **139**, 154304 (2013). DOI: 10.1063/1.4824858

144. J.-W. Lackmann, S. Schneider, E. Edengeiser, F. Jarzina, S. Brinkmann, E. Steinborn, M. Havenith, J. Benedikt, J. Bandow  
*Photons and particles emitted from cold atmospheric-pressure plasma inactivate bacteria and biomolecules independently and synergistically*  
J. R. Soc. Interface **10**, 20130591 (2013). DOI: 10.1098/rsif.2013.0591
143. V. Sharma, F. Böhm, M. Seitz, G. Schwaab, M. Havenith  
*From solvated ions to ion-pairing: A THz study of lanthanum (III) hydration*  
Phys. Chem. Chem. Phys. **15**, 8383–8391 (2013). DOI: 10.1039/c3cp50865j
142. B. Born, M. Heyden, M. Grossman, I. Sagi, M. Havenith  
*Protein-water network dynamics during metalloenzyme hydrolysis observed by kinetic THz absorption (KITA)*  
Proceedings of SPIE **8585**, 85850E (2013). DOI: 10.1117/12.2000715
141. K. Meister, S. Ebbinghaus, Y. Xu, J.G. Duman, A. DeVries, M. Gruebele, D.M. Leitner, M. Havenith  
*Long-range protein-water dynamics in hyperactive insect antifreeze proteins*  
PNAS **110**, 1617–1622 (2013). DOI: 10.1073/pnas.1214911110
140. A. Patra, T.Q. Luong, R.K. Mitra, M. Havenith  
*Solvent dynamics in reverse micellar water-pool: A spectroscopic investigation of DDAB-cyclohexane-water systems*  
Phys. Chem. Chem. Phys. **15**, 930–939 (2013). DOI: 10.1039/c2cp42560b
139. D.M. Leitner, M. Gruebele, M. Havenith  
*THz technology and THz spectroscopy: Modeling and experiments to study solvation dynamics of biomolecules*  
In Methods in Physical Chemistry, Vol. 1, Wiley-VCH, 687–710 (2012).  
DOI: 10.1002/9783527636839.ch22
138. L. von Kobyletzki, M. Mischo, D.A. Schmidt, E. Bründermann, N.H. Brockmeyer, A. Potthoff, M. Havenith  
*Probing epidermis and dermis by Raman spectroscopy: changes in antioxidant and lipid network with age and disease*  
Int. J. Cosmet. Sci. **34**, 372–373 (2012).
137. L. von Kobyletzki, M. Mischo, D.A. Schmidt, E. Bründermann, N.H. Brockmeyer, A. Potthoff, M. Havenith  
*Changes in antioxidant and lipid network in HIV patients compared to young and old patients: Probing epidermis and dermis by Raman spectroscopy*  
J. Dtsch. Dermatol. Ges. **10**, 15 (2012).
136. S. Funkner, M. Havenith, G. Schwaab  
*Urea, a structure breaker? Answers from THz absorption spectroscopy*  
J. Phys. Chem. **116**, 13374–13380 (2012). DOI: 10.1021/jp308699w
135. M.A. Sliem, D.A. Schmidt, A. Betard, S.B. Kalidindi, S. Gross, M. Havenith, A. Devi, R.A. Fischer  
*Surfactant induced nonhydrolytic synthesis of phase-pure ZrO<sub>2</sub> nanoparticles from metal-organic and oxocluster precursors*  
Chem. Mat. **24**, 4274–4282 (2012). DOI: 10.1021/cm301128a
134. I. Kopf, H.W. Peindy N'Dongo, F. Ballout, U. Schatzschneider, E. Bründermann, M. Havenith

- Introducing cymantrene labels into scattering scanning near-field infrared microscopy*  
*Analyst* **137**, 4995–5001 (2012). DOI: 10.1039/c2an16201f
133. J. Soetebier, M. Havenith  
*Der THz-Tanz des Wassers: Experimentelle Möglichkeiten der THz-Spektroskopie*  
*GIT Labor-Fachzeitschrift* **56**, 342–344 (2012)
132. B. Born, I. Sagi, M. Havenith  
*Water's contribution and enzyme's work – A KITA study*  
*Proceedings of SPIE* **8225**, 822518 (2012). DOI: 10.1117/12.907770
131. G. Niehues, A.L. Kaledin, J.M. Bowman, M. Havenith  
*Driving a small solvated peptide in the IR and THz range – A comparative study of energy flow*  
*J. Phys. Chem. B* **116**, 10020–10025 (2012). DOI: 10.1021/jp3021358
130. M. Heyden, J. Sun, H. Forbert, G. Mathias, M. Havenith, D. Marx  
*Understanding the origins of dipolar couplings and correlated motion in the vibrational spectrum of water*  
*J. Phys. Chem. Lett.* **3**, 2135–2140 (2012). DOI: 10.1021/jz300748s
129. S. Ebbinghaus, K. Meister, M.B. Proghozin, A.L. DeVries, M. Havenith, J. Dzubiella, M. Gruebele  
*Functional importance of short-range binding and long-range solvent interactions in helical antifreeze peptides*  
*Biophys. J.* **103**, L20–L22 (2012). DOI: 10.1016/j.bpj.2012.06.013
128. N. Pérez-Hernández, T.Q. Luong, M. Febles, C. Marco, H.-H. Limbach, M. Havenith, C. Pérez, M.V. Roux, R. Pérez, J. Martín  
*The mobility of water molecules through hydrated pores*  
*J. Phys. Chem. C* **116**, 9616–9630 (2012). DOI: 10.1021/jp301323c
127. D.A. Schmidt, E. Bründermann, M. Havenith  
*Combined far- and near-field chemical nanoscope at ANKA-IR2: Applications and detection schemes*  
*J. Phys.: Conf. Ser.* **359**, 012015 (2012). DOI: 10.1088/1742-6596/359/1/012015
126. S. Funkner, G. Niehues, D.A. Schmidt, M. Heyden, G. Schwaab, K.M. Callahan, D.J. Tobias, M. Havenith  
*Watching the low frequency motions in aqueous salt solutions: The terahertz vibrational signatures of hydrated ions*  
*J. Am. Chem. Soc.* **134**, 1030–1035 (2012). DOI: 10.1021/ja207929u
125. A. Arora, T.Q. Luong, M. Krüger, Y.J. Kim, C.-H. Nam, A. Manz, M. Havenith  
*Terahertz-time domain spectroscopy for the detection of PCR amplified DNA in aqueous solution*  
*Analyst* **137**, 575–579 (2012). DOI: 10.1039/c2an15820e  
(Cover article – <https://pubs.rsc.org/en/content/articlepdf/2012/an/c2an90002e>)
124. M. Havenith  
*Der THz-Tanz des Wassers mit den Proteinen*  
*Biospektrum* **17**, 38–41 (2011). DOI: 10.1007/s12268-011-0008-4
123. T.Q. Luong, P. Verma, R. Mitra, M. Havenith  
*Onset of hydrogen bonded collective network of water in 1,4-dioxane*  
*J. Phys. Chem. A* **115**, 14462–14469 (2011). DOI: 10.1021/jp204927r



- 
122. F. Ballout, H. Krassen, I. Kopf, K. Ataka, E. Bründermann, J. Heberle, M. Havenith  
*Scanning near field IR microscopy of proteins in lipid bilayers*  
Phys. Chem. Chem. Phys. **13**, 21432–21436 (2011). DOI: 10.1039/c1cp21512d
121. T. Poerschke, D. Habig, M. Havenith  
*High resolution IR spectroscopy of the C-H stretch bands of benzene monomer and dimer in helium nanodroplets*  
Z. Phys. Chem. **225**, 1447–1456 (2011). DOI: 10.1524/zpch.2011.0193
120. M. Grossman, B. Born, M. Heyden, D. Tworowski, G.B. Fields, I. Sagi, M. Havenith  
*Correlated structural kinetics and retarded solvent dynamics at the metalloprotease active site*  
Nat. Struct. Mol. Biol. **18**, 1102–1108 (2011). DOI: 10.1038/nsmb.2120  
See also: P. Ball, *More than a bystander*, Nature **478**, 467–468 (2011). DOI: 10.1038/478467a
119. M. Krüger, S. Funkner, E. Bründermann, M. Havenith  
*Uncertainty and ambiguity in terahertz parameter extraction and data analysis*  
J. Infrared Millim. Terahertz Waves **32**, 699–715 (2011). DOI: 10.1007/s10762-010-9669-1
118. G. Niehues, M. Heyden, D.A. Schmidt, M. Havenith  
*Exploring hydrophobicity by THz absorption spectroscopy of solvated amino acids*  
Faraday Discuss. **150**, 193–207 (2011). DOI: 10.1039/c0fd00007h
117. F. Ballout, J.-S. Samson, D.A. Schmidt, E. Bründermann, Y.-L. Mathis, B. Gasharova, A.D. Wieck, M. Havenith  
*Non-invasive nano-imaging of ion implanted and activated copper in silicon*  
J. Appl. Phys. **110**, 024307 (2011). DOI: 10.1063/1.3606415
116. T.Q. Luong, P.K. Verma, R.K. Mitra, M. Havenith  
*Do hydration dynamics follow the structural perturbation during thermal denaturation of a protein: A terahertz absorption study*  
Biophys. J. **101**, 925–933 (2011). DOI: 10.1016/j.bpj.2011.05.011  
(Cover article)
115. M. Filimon, I. Kopf, D.A. Schmidt, E. Bründermann, J. Rühle, S. Santer, M. Havenith  
*Local chemical composition of nanophase-separated polymer brushes*  
Phys. Chem. Chem. Phys. **13**, 11620–11626 (2011). DOI: 10.1039/c0cp02756a
114. M. Krüger, M.-M. Huang, E. Bründermann, H. Weingärtner, M. Havenith  
*Combined THz and microwave dielectric spectroscopy of intermolecular interactions in homologous protic ionic liquids*  
IEEE Trans. Terahertz Sci. Technol. **1**, 313–320 (2011). DOI: 10.1109/TTHZ.2011.2159540
113. A. Metzelthin, E. Sánchez-García, Ö. Birer, G. Schwaab, W. Thiel, W. Sander, M. Havenith  
*Acetylene furan trimer formation at 0.37 K as a model for ultracold aggregation of non- and weakly polar molecules*  
ChemPhysChem **12**, 2009–2017 (2011). DOI: 10.1002/cphc.201001040
112. A. Gutberlet, G. Schwaab, M. Havenith  
*High resolution IR spectroscopy of dimers of HDO with H<sub>2</sub>O in helium nanodroplets*  
J. Phys. Chem. A **115**, 6297–6305 (2011). DOI: 10.1021/jp201018x
111. M. Havenith  
*THz-Spektroskopie und Solvatationsdynamik*  
Nachrichten aus der Chemie **59**, 291–296 (2011). DOI: 10.1002/nadc.201176376

**2006-2010**

110. N. Zotov, M. Bartsch, L. Chernova, D.A. Schmidt, M. Havenith, G. Eggeler  
*Effects of annealing on the microstructure and the mechanical properties of EB-PVD thermal barrier coatings*  
Surf. Coat. Technol. **205**, 452–464 (2010). DOI: 10.1016/j.surfcoat.2010.07.008
109. M. Heyden, S. Ebbinghaus, M. Havenith  
*THz spectroscopy as a tool to study hydration dynamics*  
In: Encyclopedia of Analytical Chemistry: Applications, theory and instrumentation, Editor R.A. Meyers, Wiley-VCH (2010). DOI:10.1002/9780470027318.A9162
108. M. Heyden, M. Havenith  
*Combining THz spectroscopy and MD simulations to study protein-hydration coupling*  
Methods **52**, 74–83 (2010). DOI: 10.1016/j.ymeth.2010.05.007
107. A. Gutberlet, G. Schwaab, M. Havenith  
*High resolution IR spectroscopy of HDO and HDO-(N<sub>2</sub>)<sub>n</sub> in helium nanodroplets*  
J. Chem. Phys. **133**, 154313 (2010). DOI: 10.1063/1.3505054
106. S. Ebbinghaus, K. Meister, B. Born, A.L. DeVries, M. Gruebele, M. Havenith  
*Antifreeze glycoprotein activity correlates with long-range protein-water dynamics*  
J. Am. Chem. Soc. **132**, 12210–12211 (2010). DOI: 10.1021/ja1051632
105. M. Heyden, J. Sun, S. Funkner, G. Mathias, H. Forbert, M. Havenith, D. Marx  
*Dissecting the THz spectrum of liquid water from first principles via correlations in time and space*  
PNAS **107**, 12068–12073 (2010). DOI: 10.1073/pnas.0914885107
104. M.A. Sliem, T. Hikov, Z.-A. Li, M. Spasova, M. Farle, D.A. Schmidt, M. Havenith-Newen, R.A. Fischer  
*Interfacial Cu/ZnO contact by selective photodeposition of copper onto the surface of small ZnO nanoparticles in non-aqueous colloidal solution*  
Phys. Chem. Chem. Phys. **12**, 9858–9866 (2010). DOI: 10.1039/c003861j
103. M. Filimon, I. Kopf, F. Ballout, D.A. Schmidt, E. Bründermann, J. Rühle, S. Santer, M. Havenith  
*Smart polymer surfaces: Mapping chemical landscapes on the nanometre scale*  
Soft Matter **6**, 3764–3768 (2010). DOI: 10.1039/c0sm00098a
102. N. Pérez-Hernández, T.Q. Luong, C. Pérez, J.D. Martín, M. Havenith,  
*Pore size dependent dynamics of confined water probed by FIR spectroscopy*  
Phys. Chem. Chem. Phys. **12**, 6928–6932 (2010). DOI: 10.1039/c000985g
101. M. Krüger, E. Bründermann, S. Funkner, H. Weingärtner, M. Havenith  
*Communications: Polarity fluctuations of the protic ionic liquid ethylammonium nitrate in the terahertz regime*  
J. Chem. Phys. **132**, 101101 (2010). DOI: 10.1063/1.3352585
100. K. Meister, D.A. Schmidt, E. Bründermann, M. Havenith  
*Confocal Raman microscopy as an analytical tool to assess the mitochondrial status in human spermatozoa*  
Analyst **135**, 1370–1374 (2010). DOI: 10.1039/b927012d
099. K. Meister, J. Niesel, U. Schatzschneider, N. Metzler-Nolte, D.A. Schmidt, M. Havenith

- Label-free imaging of metal-carbonyl complexes in live cells by Raman microspectroscopy*  
Angew. Chem. Intl. Ed. **49**, 3310–3312 (2010). DOI: 10.1002/anie.201000097  
(Cover article – <https://onlinelibrary.wiley.com/doi/10.1002/anie.201001495>)  
See also: P. Hildebrandt, *A spectral window to the cell*, Angew. Chem. Intl. Ed. **49**, 4540–4541 (2010). DOI: 10.1002/anie.201001616
098. E. Bründermann, D.A. Schmidt, I. Kopf, M. Havenith  
*Nano-spectroscopy and chemical nanoscopy of biomaterials*  
AIP Conf. Proc. **1214**, 7–9 (2010). DOI: 10.1063/1.3326355
097. S. Kundu, W. Xia, W. Busser, M. Becker, D.A. Schmidt, M. Havenith, M. Muhler  
*The formation of nitrogen-containing functional groups on carbon nanotube surfaces: A quantitative XPS and TPD study*  
Phys. Chem. Chem. Phys. **12**, 4351–4359 (2010). DOI: 10.1039/b923651a
096. I. Kopf, C. Grunwald, E. Bründermann, L. Casalis, G. Scoles, M. Havenith  
*Detection of hybridization on nanografted oligonucleotides using scanning near-field infrared microscopy*  
J. Phys. Chem. C **114**, 1306–1311 (2010). DOI: 10.1021/jp906813f
095. D.A. Schmidt, Ö. Birer, S. Funkner, B. Born, R. Gnanasekaran, G. Schwaab, D.M. Leitner, M. Havenith  
*Rattling in the cage: Ions as probes of sub-picosecond water network dynamics*  
J. Am. Chem. Soc. **131**, 18512–18517 (2009). DOI: 10.1021/ja9083545
094. B. Born, M. Havenith  
*Terahertz dance of proteins and sugars with water*  
J. Infrared Millim. Terahertz Waves **30**, 1245–1254 (2009). DOI: 10.1007/s10762-009-9514-6
093. A. Gutberlet, G. Schwaab, Ö. Birer, M. Masia, A. Kaczmarek, H. Forbert, M. Havenith, D. Marx  
*Aggregation induced dissociation of HCl(H<sub>2</sub>O)<sub>4</sub> below 1 K: The smallest droplet of acid*  
Science **324**, 1545–1548 (2009). DOI: 10.1126/science.1171753  
See also:  
T.S. Zwier, *Perspective: Squeezing the water out of HCl(aq)*  
Science **324**, 1522–1523 (2009). DOI: 10.1126/science.1175387  
Nature research highlights, *Chemistry: The tiniest acid drop*  
Nature **459**, 1036 (2009). DOI: 10.1038/4591036d  
J. Urquhart, *Smallest acid droplet formed*  
<https://www.chemistryworld.com/news/smallest-acid-droplet-formed/3003684.article>
092. J.-S. Samson, R. Meißner, E. Bründermann, M. Böke, J. Winter, M. Havenith  
*Characterization of single diamond-like and polymer-like nanoparticles by mid-infrared nanospectroscopy*  
J. Appl. Phys. **105**, 064908 (2009). DOI: 10.1063/1.3086650
091. Ö. Birer, M. Havenith  
*High resolution infrared spectroscopy of formic acid dimer*  
Annu. Rev. Phys. Chem **60**, 263–275 (2009). DOI: 10.1146/annurev.physchem.040808.090431
090. B. Born, H. Weingärtner, E. Bründermann, M. Havenith  
*Solvation dynamics of model peptides probed by terahertz spectroscopy. Observation of the onset of collective network motions*  
J. Am. Chem. Soc. **131**, 3752–3755 (2009). DOI: 10.1021/ja808997y

089. E. Bründermann, I. Kopf, M. Havenith  
*Chemical nanoscopy of cell-like membranes*  
Proc. SPIE **7188**, 71880I (2009). DOI: 10.1117/12.808276
088. E. Bründermann, B. Born, S. Funkner, M. Krüger, M. Havenith  
*Terahertz spectroscopic techniques for the study of proteins in aqueous solutions*  
Proc. SPIE **7215**, 72150E (2009). DOI: 10.1117/12.808270
087. A.-S. Müller, T. Baumbach, S. Casalbuoni, B. Gasharova, M. Hagelstein, E. Huttel, Y.-L. Mathis, D.A. Moss, A. Plech, R. Rossmanith, E. Bründermann, M. Havenith, S. Hillenbrand, K.G. Sonnad  
*TBONE: Ultra-fast high-power coherent THz to mid-IR radiation facility*  
Proc. **PAC09**, TU5RFP028, 1156–1158 (2009)
086. B. Born, S.J. Kim, S. Ebbinghaus, M. Gruebele, M. Havenith  
*The terahertz dance of water with the proteins: The effect of protein flexibility on the dynamical hydration shell of ubiquitin*  
Faraday Discuss. **141**, 161–173 (2009). DOI: 10.1039/b804734k
085. A. Gutberlet, Ö. Birer, T. Poerschke, M. Havenith  
*High resolution infrared spectroscopy of the asymmetric C-H stretch of 1,2,4,5-Tetracyanobenzene (TCNB) and (TCNB)<sub>2</sub> in superfluid helium nanodroplets*  
J. Chem. Phys. **129**, 174311 (2008). DOI: 10.1063/1.2996356
084. A. Metzethin, Ö. Birer, E. Sánchez-García, M. Havenith  
*High resolution IR-spectroscopy of acetylene-furan in ultracold helium nanodroplets*  
J. Chem. Phys. **129**, 114307 (2008). DOI: 10.1063/1.2976772
083. S.J. Kim, B. Born, M. Havenith, M. Gruebele  
*Echtzeitnachweis von Änderungen im Protein-Wassernetzwerk während der Proteinfaltung mit Hilfe von Terahertz-Absorptionsspektroskopie*  
Angew. Chem. **120**, 6586–6589 (2008). DOI: 10.1002/ange.200802281  
(Cover article – <https://onlinelibrary.wiley.com/doi/10.1002/ange.200890220>)
082. S.J. Kim, B. Born, M. Havenith, M. Gruebele  
*Real-time detection of protein-water dynamics upon protein folding by terahertz absorption Spectroscopy*  
Angew. Chem. Int. Ed. **47**, 6486–6489 (2008). DOI: 10.1002/anie.200802281  
(Cover article – <https://onlinelibrary.wiley.com/doi/10.1002/anie.200890166>)
081. D.M. Leitner, M. Gruebele, M. Havenith  
*Solvation dynamics of biomolecules: Modeling and terahertz experiments*  
HFSP J. **2**, 314–323 (2008). DOI: 10.2976/1.2976661
080. K. Schröck, F. Schröder, M. Heyden, R.A. Fischer, M. Havenith  
*Characterization of interfacial water in MOF-5 (Zn<sub>4</sub>(O)(BDC)<sub>3</sub>)—a combined spectroscopic and theoretical study*  
Phys. Chem. Chem. Phys. **10**, 4732–4739 (2008). DOI: 10.1039/b807458P
079. G. Wollny, E. Bründermann, Z. Arsov, L. Quaroni, M. Havenith  
*Nanoscale depth resolution in scanning near-field infrared microscopy*  
Opt. Express **16**, 7453–7459 (2008). DOI: 10.1364/OE.16.007453
078. M. Heyden, E. Bründermann, U. Heugen, G. Niehues, D.M. Leitner, M. Havenith  
*Long range influence of carbohydrates on the solvation dynamics of water – Answers*

- from THz absorption measurements and molecular modeling simulations*  
J. Am. Chem. Soc. **130**, 5773–5779 (2008). DOI: 10.1021/ja0781083
077. S. Ebbinghaus, S.J. Kim, M. Heyden, X. Yu, M. Gruebele, D.M. Leitner, M. Havenith  
*Protein sequence- and pH-dependent hydration probed by terahertz spectroscopy*  
J. Am. Chem. Soc. **130**, 2374–2375 (2008). DOI: 10.1021/ja0746520
076. E. Bründermann, M. Havenith  
*SNIM: Scanning near-field infrared microscopy*  
Annu. Rep. Prog. Chem., Sect. C: Phys. Chem. **104**, 235–255 (2008). DOI: 10.1039/b703982b  
(Cover article – <https://pubs.rsc.org/en/content/articlepdf/2008/pc/b807901n>)
075. A. Gutberlet, G.W. Schwaab, M. Havenith  
*High resolution IR spectroscopy of the carbonyl stretch of (DCOOD)<sub>2</sub>*  
Chem. Phys. **343**, 158–167 (2008). DOI: 10.1016/j.chemphys.2007.08.025
074. A. Metzelthin, M. Havenith  
*Observation of the R(0.5) <sup>2</sup>Π<sub>1/2</sub> transition in <sup>15</sup>N<sup>18</sup>O in helium nanodroplets*  
Mol. Phys. **105**, 3025–3027 (2007). DOI: 10.1080/00268970701730104
073. S. Ebbinghaus, S.J. Kim, M. Heyden, X. Yu, U. Heugen, M. Gruebele, D.M. Leitner, M. Havenith  
*An extended dynamical solvation shell around proteins*  
PNAS **104**, 20749–20752 (2007). DOI: 10.1073/pnas.0709207104
072. M. Havenith  
*Schwingende Gerüste und tanzende Wassermoleküle*  
Nachrichten aus der Chemie **55**, 1090–1093 (2007). DOI: 10.1002/nadc.200751938
071. M. Ortlieb, Ö. Birer, M. Letzner, G.W. Schwaab, M. Havenith  
*Observation of rovibrational transitions of HCl, (HCl)<sub>2</sub> and H<sub>2</sub>O-HCl in liquid helium nanodroplets*  
J. Phys. Chem. A **111**, 12192–12199 (2007). DOI: 10.1021/jp0759980
070. M. Ortlieb, M. Havenith  
*Proton transfer in (HCOOH)<sub>2</sub>: An IR-high resolution spectroscopic study of the antisymmetric C-O stretch*  
J. Phys. Chem. A **111**, 7355–7363 (2007). DOI: 10.1021/jp070763+
069. M. Havenith, K. Kleinermanns, T. Koop  
*Physikalische Chemie des Wassers*  
Nachrichten aus der Chemie **55**, 285–288 (2007). DOI: 10.1002/nadc.200743720
068. I. Kopf, J.-S. Samson, G. Wollny, Ch. Grunwald, E. Bründermann, M. Havenith  
*Chemical imaging of micro-structured self-assembled monolayers with nanometer resolution*  
J. Phys. Chem. C **111**, 8166–8171 (2007). DOI: 10.1021/jp070201q
067. G.W. Schwaab, K. Schroeck, M. Havenith  
*Amplification of terahertz pulses in gases beyond thermodynamic equilibrium*  
Phys. Rev. A **75**, 032522 (2007). DOI: 10.1103/PhysRevA.75.032522
066. S. Rudolph, G. Wollny, K. von Haeften, M. Havenith  
*Probing collective excitations in helium nanodroplets: Observation of phonon wings in the infrared spectrum of methane*  
J. Chem. Phys. **126**, 124318 (2007). DOI: 10.1063/1.2709887

065. M. Havenith  
*Coherent proton tunneling in hydrogen bonds of isolated molecules: Carboxylic dimers*  
In: Hydrogen-Transfer Reactions, Editors J.T. Hynes, J.P. Klinman, H.-H. Limbach, R.L. Schowen, Wiley-VCH, 33–51 (2006). DOI: 10.1002/9783527611546.ch2
064. D.M. Leitner, M. Havenith M. Gruebele  
*Biomolecule large amplitude motion and solvation dynamics: Modeling and probes from THz to X-rays*  
Int. Rev. Phys. Chem. **25**, 553–582 (2006). DOI: 10.1080/01442350600862117
063. U. Heugen, G. Schwaab, E. Bründermann, M. Heyden, X. Yu, D.M. Leitner, M. Havenith  
*Solute-induced retardation of water dynamics probed directly by terahertz spectroscopy*  
PNAS **103**, 12301–12306 (2006). DOI: 10.1073/pnas.0604897103
062. M. Havenith, M. Ortlieb  
*Gefangen in der Quantenflüssigkeit*  
Physik in unserer Zeit **37**, 59 (2006). DOI: 10.1002/piuz.200690029
061. E. Bründermann, M. Havenith  
*Applications of semiconductor terahertz lasers in biomolecular spectroscopy and imaging*  
Proc. SPIE **6194**, 619406 (2006). DOI: 10.1117/12.673830
060. E. Bründermann, M. Havenith, G. Scalari, M. Giovanni, J. Faist, J. Kunsch, L. Mechold, M. Abraham  
*Turn-key compact high temperature terahertz quantum cascade lasers: Imaging and room temperature detection*  
Opt. Express **14**, 1829–1841 (2006). DOI: 10.1364/OE.14.001829
059. K. von Haeften, S. Rudolph, I. Simanowski, M. Havenith, R.E. Zillich, K.B. Whaley  
*Probing phonon-rotation coupling in Helium nanodroplets: Infrared spectroscopy of CO and its isotopomers*  
Phys. Rev. B **73**, 054502 (2006). DOI: 10.1103/PhysRevB.73.054502
058. J.-S. Samson, G. Wollny, E. Bründermann, A. Bergner, A. Hecker, G. Schwaab, A. D. Wieck, M. Havenith  
*Set-up of a scanning near field microscope (SNIM): Imaging of sub-surface nano-structures in gallium-doped silicon*  
Phys. Chem. Chem. Phys. **8**, 753–758 (2006). DOI: 10.1039/b512780g
057. S. Ebbinghaus, K. Schröck, J.C. Schauer, E. Bründermann, M. Heyden, G. Schwaab, M. Böke, J. Winter, M. Tani, M. Havenith  
*Terahertz time-domain spectroscopy as a new tool for the characterization of dust forming plasmas*  
Plasma Sources Sci. Technol. **15**, 72–77 (2006). DOI: 10.1088/0963-0252/15/1/011

**2001-2005**

056. K. von Haeften, A. Metzelthin, S. Rudolph, V. Staemmler, M. Havenith  
*High resolution spectroscopy of NO in helium droplets: A prototype for open shell molecular interactions in a quantum solvent*  
Phys. Rev. Lett. **95**, 215301 (2005). DOI: 10.1103/PhysRevLett.95.215301
055. M. Havenith, G.W. Schwaab

- Attacking a small beast: Ar-CO, a prototype for intermolecular forces*  
Z. Phys. Chem. **219**, 1053–1088 (2005). DOI: 10.1524/zpch.2005.219.8.1053
054. A. Bergner, U. Heugen, E. Bründermann, G. Schwaab, M. Havenith, D.R. Chamberlin, E.E. Haller  
*New p-Ge THz spectrometer for the study of solutions: THz absorption spectroscopy of water*  
Rev. Sci. Instr. **76**, 063110 (2005). DOI: 10.1063/1.1928427
053. E. Bründermann, U. Heugen, R. Schiwon, B. Born, G.W. Schwaab, S. Ebbinghaus, K. Schröck,  
D.R. Chamberlin, E.E. Haller, M. Havenith  
*Terahertz imaging applications in spectroscopy of biomolecules*  
IEEE MTT-S International Microwave Symposium Digest, 625–628 (2005).  
DOI: 10.1109/MWSYM.2005.1516679
052. R. Schiwon, G. Schwaab, E. Bründermann, M. Havenith  
*Terahertz cavity enhanced attenuated total reflection spectroscopy*  
Appl. Phys. Lett. **86**, 201116 (2005). DOI: 10.1063/1.1929072
051. K. von Haeften, M. Havenith  
*He droplets: A fluid with unusual properties*  
In: Electronic excitations in liquefied rare gases, Editors W.F. Schmidt and E. Illenberger,  
American Scientific Publishers (2005).
050. E. Bründermann, A. Bergner, F. Petrat, R. Schiwon, G. Wollny, I. Kopf, H. de Groot, M. Havenith  
*Fast quantification of water in single living cells by near-infrared microscopy*  
Analyst **129**, 893–896 (2004). DOI: 10.1039/B408954P
049. S. Hoffmann, M. Hofmann, E. Bründermann, M. Havenith, M. Matus, J.V. Moloney, A.S.  
Moskalenko, M. Kira, S.W. Koch, S. Saito, K. Sakai  
*Four-wave mixing and direct terahertz emission with two-color semiconductor lasers*  
Appl. Phys. Lett. **84**, 3585–3587 (2004). DOI: 10.1063/1.1737486
048. R.A. Jockusch, R.T. Kroemer, F.O. Talbot, L.C. Snoek, P. Çarçabal, J.P. Simons, M. Havenith, J.M.  
Bakker, I. Compagnon, G. Meijer, G. von Helden  
*Probing the glycosidic linkage: UV and IR ion-dip spectroscopy of lactoside*  
J. Am. Chem. Soc. **126**, 5709–5714 (2004). DOI: 10.1021/ja031679k
047. F. Madeja, M. Havenith, K. Nauta, R.E. Miller, J. Chocholoušová, P. Hobza  
*Polar isomer of formic acid dimer formed in helium nano-droplets*  
J. Chem. Phys. **120**, 10554–10560 (2004). DOI: 10.1063/1.1709942
046. R. Schiwon, G.W. Schwaab, E. Bründermann, M. Havenith  
*Far-infrared multilayer mirrors*  
Appl. Phys. Lett. **83**, 4119–4121 (2003). DOI: 10.1063/1.1627479
045. M. Havenith  
*Comment on: Theoretical absorption spectrum of the Ar-CO van der Waals complex [J. Chem.  
Phys. 118, 9596 (2003)]*  
J. Chem. Phys. **119**, 7604 (2003). DOI: 10.1063/1.1606671
044. I. Scheele, M. Havenith  
*High-resolution IR spectroscopy of a high lying  $K_a = 0$  mode of the weakly bound van der Waals  
complex Ar-CO*  
Mol. Phys. **101**, 1423–1427 (2003). DOI: 10.1080/0026897031000092265

043. F. Madeja, A. Hecker, S. Ebbinghaus, M. Havenith  
*High resolution spectroscopy of  $\nu_3$  band of the van der Waals complex Ar-DCOOH*  
Mol. Phys. **101**, 1511–1515 (2003). DOI: 10.1080/0026897031000108078
042. A. Hecker, I. Scheele, M. Havenith  
*IR-High resolution spectroscopy of the  $N_2O$  dimer: The torsional mode*  
Phys. Chem. Chem. Phys. **5**, 2333–2336 (2003). DOI: 10.1039/b300733m
041. M. Havenith, B.A. Hess  
*Weakly interacting molecular complexes*  
In: Interactions in molecules: Electronic and steric effects (final report of the Collaborative Research Centre 334), Editor S.D. Peyerimhoff, Wiley-VCH, 110–131 (2003).
040. F. Madeja, A. Hecker, S. Ebbinghaus, M. Havenith  
*High resolution spectroscopy of  $\nu_3$  band of DCOOD*  
Spectrochim. Acta A **59**, 1773–1782 (2003). DOI: 10.1016/S1386-1425(02)00412-2
039. A. Hecker, M. Havenith, C. Braxmaier, U. Strößner, A. Peters  
*High resolution Doppler-free spectroscopy of molecular iodine using a continuous wave optical parametric oscillator*  
Opt. Commun. **218**, 131–134 (2003). DOI: 10.1016/S0030-4018(03)01187-8
038. N. Pörtner, A.F. Vilesov, M. Havenith  
*Spontaneous alignment of tetracene molecules in  $^4He$  droplets*  
Chem. Phys. Lett. **368**, 458–464 (2003). DOI: 10.1016/S0009-2614(02)01903-6
037. G. Gimmler, M. Havenith  
*High-resolution IR-spectroscopy of the  $N_2O$ - $H_2O$  and  $N_2O$ - $D_2O$  van der Waals complexes*  
J. Mol. Spec. **216**, 315–321, (2002). DOI: 10.1006/jmsp.2002.8687
036. F. Madeja, M. Havenith  
*High resolution spectroscopy of carboxylic acid in the gas phase: Observation of proton transfer in  $(DCOOH)_2$*   
J. Chem. Phys. **117**, 7162–7168 (2002). DOI: 10.1063/1.1507581
035. M. Kunze, P. Markwick, N. Pörtner, J. Reuss, M. Havenith  
*IR-MW double resonance spectroscopy of OCS in pure  $^4He$  and mixed  $^4He/^3He$  clusters*  
J. Chem. Phys. **116**, 7473–7485 (2002). DOI: 10.1063/1.1467330
034. F. Madeja, P. Markwick, M. Havenith, K. Nauta, R.E. Miller  
*Rotationally resolved infrared spectroscopy of  $h_2$ - and  $d_1$ -formic acid monomer in liquid He-droplets*  
J. Chem. Phys. **116**, 2870–2878 (2002). DOI: 10.1063/1.1432998
033. M. Havenith  
*Infrared spectroscopy of molecular clusters: An introduction to intermolecular forces*  
Springer Tracts in Modern Physics **176**, Springer-Verlag Berlin Heidelberg (2002).  
DOI: 10.1007/3-540-45457-8
032. N. Pörtner, A.F. Vilesov, M. Havenith  
*The formation of heterogeneous van der Waals complexes in helium droplets*  
Chem. Phys. Lett. **343**, 281–288 (2001). DOI: 10.1016/S0009-2614(01)00648-0
031. G. Gimmler, M. Havenith



*Free-jet infrared diode laser spectroscopy of the  $\nu_2$ -band of the Ar-N<sub>2</sub>O van der Waals complex*  
J. Mol. Struct. **599**, 117–123 (2001). DOI: 10.1016/S0022-2860(01)00840-7

030. I. Scheele, R. Lehnig, M. Havenith  
*IR spectroscopy of van der Waals modes in the intermolecular potential of Ar-CO: The  $K_a = 0$  combination of stretch and bending*  
Mol. Phys. **99**, 197–203 (2001). DOI: 10.1080/00268970010007587
029. I. Scheele, R. Lehnig, M. Havenith  
*Observation of a high lying van der Waals mode in the intermolecular potential of Ar-CO*  
Mol. Phys. **99**, 205–209 (2001). DOI: 10.1080/00268970010008351

### 1988-2000

028. S. Grebenev, M. Havenith, F. Madeja, J.P. Toennies, A.F. Vilesov  
*Microwave-infrared double resonance spectroscopy of OCS molecules inside a <sup>4</sup>He droplet*  
J. Chem. Phys. **113**, 9060–9066 (2000). DOI: 10.1063/1.1286243
027. S. Grebenev, M. Hartmann, M. Havenith, B. Sartakov, J.P. Toennies, A.F. Vilesov  
*The rotational spectrum of single OCS molecules in liquid <sup>4</sup>He droplets*  
J. Chem. Phys. **112**, 4485–4495 (2000). DOI: 10.1063/1.481011
026. U. Merker, P. Engels, F. Madeja, M. Havenith, W. Urban  
*High-resolution CO-laser sideband spectrometer for molecular-beam optothermal spectroscopy in the 5-6.6  $\mu$ m wavelength region*  
Rev. Sci. Instr. **70**, 1933–1938 (1999). DOI: 10.1063/1.1149691
025. C. Schmidt, M. Perić, P. Mürtz, M. Wienkoop, M. Havenith, W. Urban  
*Faraday laser magnetic resonance spectroscopy of vibrationally excited C<sub>2</sub>D*  
J. Mol. Spec. **190**, 112–124 (1998). DOI: 10.1006/jmsp.1998.7563
024. M. Scherer, M. Havenith, R. Mausberger, T.L. Wilson  
*A search for (H<sub>2</sub>O)<sub>2</sub> in the galaxy and toward comet Hale-Bopp*  
Astron. Astrophys. **335**, 1070–1076 (1998).
023. M. Wienkoop, P. Mürtz, P.-C. Schumann, M. Havenith, W. Urban  
*First observation of ro-vibrational transitions of the SiC radical by infrared LMR spectroscopy*  
Chem. Phys. **225**, 17–21 (1997). DOI: 10.1016/S0301-0104(97)00199-7
022. M. Behrens, U. Buck, R. Fröchtenicht, M. Hartmann, M. Havenith  
*The ammonia dimer spectrum in cold helium clusters*  
J. Chem. Phys. **107**, 7179–7186 (1997). DOI: 10.1063/1.474957
021. S. König, M. Havenith  
*Measurement of the  $K_a=1$  ( $\nu_{CO}=1$ ) stretching mode in Ar-CO using a Herriott multipass cell*  
Mol. Phys. **91**, 265–272 (1997). DOI: 10.1080/002689797171571
020. Y. Xu, S. Civiš, R. McKellar, S. König, M. Haverlag, G. Hilpert, M. Havenith  
*High K ("Propeller") states in the infrared spectrum of the Ar-CO complex*  
Mol. Phys. **87**, 1071–1082 (1996). DOI: 10.1080/00268979600100741
019. C. Pfelzer, M. Havenith, M. Perić, P. Mürtz, W. Urban  
*Faraday laser magnetic resonance spectroscopy on vibrational excited C<sub>2</sub>H*  
J. Mol. Spec. **176**, 28–37 (1996). DOI: 10.1006/jmsp.1996.0058

018. S. König, G. Hilpert, M. Havenith  
*Observation of strong Coriolis coupling in the IR spectrum of Ar-CO*  
Mol. Phys. **86**, 1233–1247 (1995). DOI: 10.1080/00268979500102701
017. B. Meyer, S. Saupe, M.H. Wappelhorst, T. George, F. Kühnemann, M. Schneider, M. Havenith, W. Urban, J. Legrand  
*CO laser sideband spectrometer: Sub-Doppler heterodyne frequency measurements around 5  $\mu\text{m}$*   
Appl. Phys. B **61**, 169–173 (1995). DOI: 10.1007/BF01090939
016. H. Linnartz, M. Havenith, W.L. Meerts  
*The ammonia dimer: Complex dynamics with a dynamical complex*  
Com. At. Mol. Phys. **30**, 315–329 (1995).
015. N. Heineking, W. Stahl, E.H.T. Olthof, P.E.S. Wormer, A. van der Avoird, M. Havenith  
*The nuclear quadrupole coupling constants and the structure of the para-para ammonia dimer*  
J. Chem. Phys. **102**, 8693–8703 (1995). DOI: 10.1063/1.468972
014. H. Linnartz, W.L. Meerts, M. Havenith  
*The ammonia dimer: New infrared–far-infrared double resonance results*  
Chem. Phys. **193**, 327–338 (1995). DOI: 10.1016/0301-0104(94)00413-5
013. M. Havenith, M. Petri, C. Lubina, G. Hilpert, W. Urban  
*IR spectroscopy of  $(\text{CO})_2$  using concentration frequency double modulation in a supersonic expansion*  
J. Mol. Spec. **167**, 248–161 (1995). DOI: 10.1006/jmsp.1994.1232
012. G. Hilpert, H. Linnartz, M. Havenith, J.J. ter Meulen, W.L. Meerts  
*Tunable infrared and far-infrared direct absorption spectroscopy of molecular ions in a supersonic jet expansion*  
Chem. Phys. Lett. **219**, 384–388 (1994). DOI: 10.1016/0009-2614(94)00129-4
011. M. Havenith, G. Hilpert, M. Petri, W. Urban  
*Measurement of the first excited bending state of Ar-CO using a new concentration modulation technique in the jet*  
Mol. Phys. **81**, 1003–1010 (1994). DOI: 10.1080/00268979400100661
010. H. Linnartz, A. Kips, W.L. Meerts, M. Havenith  
*The electric dipole moment of  $(\text{NH}_3)_2$  for  $G: ||K||=1$*   
J. Chem. Phys. **99**, 2449–2452 (1993). DOI: 10.1063/1.465208
009. M. Havenith, H. Linnartz, E. Zwart, A. Kips, J.J. ter Meulen, W.L. Meerts  
*An infrared–far-infrared double resonance study on  $(\text{NH}_3)_2$  in a jet*  
Chem. Phys. Lett. **193**, 261–268 (1992). DOI: 10.1016/0009-2614(92)85665-W
008. H. Linnartz, M. Havenith, E. Zwart, W.L. Meerts, J.J. ter Meulen  
*The determination of the electric dipole moment of  $\text{KrH}^+$*   
J. Mol. Spec. **153**, 710–717 (1992). DOI: 10.1016/0022-2852(92)90505-1
007. M. Havenith, M. Schneider, W. Bohle, W. Urban  
*Sub-Doppler Faraday LMR spectroscopy: First applications to NO and  $\text{DBr}^+$*   
Mol. Phys. **72**, 1149–1158 (1991). DOI: 10.1080/00268979100100821
006. M. Havenith, R.C. Cohen, K.L. Busarow, D.-H. Gwo, Y.T. Lee, R.J. Saykally

- 
- Measurement of the intermolecular vibration-rotation-tunneling spectrum of the ammonia dimer by tunable far infrared laser spectroscopy*  
J. Chem. Phys. **94**, 4776–4789 (1991). DOI: 10.1063/1.460562
005. M. Havenith, E. Zwart, W.L. Meerts, J.J. ter Meulen  
*Determination of the dipole moment of  $\text{HN}_2^+$*   
J. Chem. Phys. **93**, 8446–8451 (1990). DOI: 10.1063/1.459282
004. D.-H. Gwo, M. Havenith, K.L. Busarow, R.C. Cohen, Ch.A. Schmuttenmaer, R.J. Saykally  
*Tunable far infrared laser spectroscopy of van der Waals bonds: The  $J_{KC} = 1_0 \leftarrow 0_0 \Sigma$  bending vibration of  $\text{Ar-}^{14}\text{NH}_3$*   
Mol. Phys. **71**, 453–460 (1990). DOI: 10.1080/00268979000101901
003. W. Urban, J.-X. Lin, V.V. Subramaniam, M. Havenith, J.W. Rich  
*Treanor pumping of CO initiated by CO laser excitation*  
Chem. Phys. **130**, 389–399 (1989). DOI: 10.1016/0301-0104(89)87068-5
002. R.C. Cohen, K.L. Busarow, K.B. Laughlin, G.A. Blake, M. Havenith, Y.T. Lee, R.J. Saykally  
*Tunable far infrared laser spectroscopy of van der Waals bonds: Vibration-rotation-tunneling spectra of  $\text{Ar-H}_2\text{O}$*   
J. Chem. Phys. **89**, 4494–4504 (1988). DOI: 10.1063/1.454789
001. M. Havenith, W. Bohle, J. Werner, W. Urban  
*Vibration rotation spectroscopy of excited electronic states: Faraday-L.M.R. spectroscopy of  $\text{CO } a^3\pi$*   
Mol. Phys. **64**, 1073–1088 (1988). DOI: 10.1080/00268978800100723
-