



- modifying the experimental conditions in a controlled sequential manner



| MS: | micrOTOF (Bruker Daltonics, Bremen, Germany) |
|-------------|--|
| Ion Source: | custom nano Electrospray Ionization (nESI) Source [2]; |
| | Bruker CaptiveSpray nanoBooster™ (Bruker Daltonics, Bremen, Germany) |
| Gas Supply: | Nitrogen 5.0 (Messer Industriegase GmbH, Germany). |
| | All gas flows are controlled by mass flow controllers (MKS Instruments, |
| | Germany) |
| Chemicals: | all chemicals were purchased from Sigma Aldrich, Germany, and used without |
| | further purification |

Ion-solvent interactions in nanoESI-MS: Characterization of charge depletion and charge conservation (supercharging) processes

Christine Polaczek; Alexander Haack; Marco Thinius; Walter Wißdorf; Hendrik Kersten; Thorsten Benter

[2] M. Thinius, M. Langner, H. Kersten, T. Benter, Impact of chemical modifiers on the cluster chemistry during electrospray ionization, Proceedings of the 63th ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, USA (2016)

| alculated | ∆G va | ues of | the | reactio | on (| M=metl | hyl | ami | ne) | • |
|-----------|--------|--------------------|--------|---------|------|-----------------------|-----|-----|-----|---|
| | [M(sol | vent) _n | H]+ -: | > M + | (sol | lvent) _n H | + | | | |

| n | ∆G [kJ/mol] MeOH | ΔG [kJ/mol] ACN |
|---|------------------|-----------------|
| 1 | 195.1 | 190.6 |
| 2 | 118.2 | 136.8 |
| 3 | 62 | 157.5 |
| 4 | 51.1 | _ |

• ion-solvent interactions are governing factors on the travel from ion solvation to the ion transfer stages • experimental and computational results are in good agreement regarding the interactions between amines and MeOH or ACN • further experimental and computational investigations with different analytes and solvents are planned



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