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OH···NO! Investigating the interactions between TEMPO and large halogenated alcohols

Tuesday 16 September 2025 15:00 (20 minutes)

Motivated by a large dynamical nuclear polarization effect observed for aminoxyl (NO) radicals combined with halogenated solvents [1] and the investigation of the microsolvation of TEMPO in the gas phase by Brás et. al. [2][3], the present work investigates the interactions between TEMPO and (halogenated) benzyl alcohol derivatives.
The OH stretching vibration of the alcohol is used as a sensitive probe for the presence of a specific heterodimer (1:1) conformation by comparing slit jet FTIR-spectra with the results of harmonic DFT calculations. When TEMPO is combined with benzyl alcohol, two conformers with different ring stacking variants are observed. The preferred stacking can be controlled in subtle ways by introducing a halogen (F, Cl, Br, I) to the *ortho*- or *para*-position of the aromatic system of benzyl alcohol. Variation of the halogen size and substitution position uncovers the interplay between hydrogen bonding and dispersion forces. [4]

[1] G. Liu, M. Levien, N. Karschin, G. Parigi, C. Luchinat, M. Bennati, *Nat. Chem.* 9 (**2017**) 676. [2] E. M. Brás, T. L. Fischer, M. A. Suhm, *Angew. Chem. Int. Ed.* 60 (**2021**) 19013. [3] E. M. Brás, C. Zimmermann, R. Fausto, M. A. Suhm, *Phys. Chem. Chem. Phys.* 26 (**2024**) 5822. [4] E. Sennert, G. Bistoni, M. A. Suhm, *J. Phys. Chem. A* 129 (**2025**) 1648.

Keywords

Hydrogen bond: medium, strong; State of system: gas.

This abstract is submitted for....

Early-career researchers´ workshop

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