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MICROWAVE SPECTROSCOPY OF TERPENOIDS NON-COVALENTLY BONDED TO HYDROGEN SULFIDE

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Biogenic volatile organic compounds (BVOCs) are a class of molecules that have a noticeable effect on atmospheric chemical and physical processes. They are emitted naturally into the atmosphere mainly by plants and forests. An interesting family of this class is the monoterpenes ($C_{10}H_{16}$) and terpenoids (oxygenated terpenes) which are unsaturated hydrocarbons that are formed by the combination of two isoprene units (C_5H_8). These molecules are known to contribute to Secondary Organic Aerosol (SOA) and tropospheric ozone formation,^{a,b} mainly through oxidation pathways. In addition, these molecules can form Hydrogen-bonded complexes with surrounding atmospheric molecules. The synergic combination of quantum chemical calculations and Fourier transform microwave spectroscopy (FTMW) in jet-cooled conditions, is a powerful tool to study the gas phase micro-solvation of atmospheric relevant molecules. Many hydrated complexes were studied using this approach in our group.^{c,d} We present herein a new approach, which employs the same theoretical-experimental approach to characterize complexes of terpenoids, i.e., alcohols and ketones, with H_2S , an atmospheric trace gas. The observed complexes are compared to their analog hydrates.

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^aD. Kotzias, J. L. Hjorth, H. Skov, *Toxicol Environ Chem* 1989, 20–21, 95–99

^bT. Hoffmann, J. R. Odum, F. Bowman, D. Collins, D. Klockow, R. C. Flagan, J. H. Seinfeld, *J. Atmos. Chem.* 1997, 26, 189–222

^cE. M. Neeman, J. R. Avilés Moreno and T. R. Huet, *Phys. Chem. Chem. Phys.* 2021,23, 18137-18144

^dE. M. Neeman, N. Osseiran and T. R. Huet, *J. Chem. Phys.* 2022, doi.org/10.1063/5.0084562

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Competing for Rao Prize? No

Competing for Miller Prize? No