



HAL
open science

MICROWAVE SPECTROSCOPY OF TERPENOIDS NON-COVALENTLY BONDED TO HYDROGEN SULFIDE

Noureddin Osseiran, Elias M. Neeman, Manuel Goubet, Pascal Drean,
Therese R. Huet

► **To cite this version:**

Noureddin Osseiran, Elias M. Neeman, Manuel Goubet, Pascal Drean, Therese R. Huet. MICROWAVE SPECTROSCOPY OF TERPENOIDS NON-COVALENTLY BONDED TO HYDROGEN SULFIDE. 75th International Symposium on Molecular Spectroscopy, Jun 2022, Urbana-Champaign (Illinois), United States. hal-04220213

HAL Id: hal-04220213

<https://hal.science/hal-04220213v1>

Submitted on 27 Sep 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

MICROWAVE SPECTROSCOPY OF TERPENOIDS NON-COVALENTLY BONDED TO HYDROGEN SULFIDE

NOUREDDIN OSSEIRAN, ELIAS M. NEEMAN, MANUEL GOUBET, PASCAL DRÉAN, THERESE R. HUET, UMR 8523 - PhLAM - Physique des Lasers Atomes et Molécules, University of Lille, CNRS, F-59000 Lille, France.

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.

The present work was funded by the ANR Labex CaPPA, by the Regional Council Hauts-de-France, by the European Funds for Regional Economic Development, and by the CPER CLIMIBIO.

^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

NOTE: The horizontal line across the page indicates the maximum allowed length of the abstract including footnotes. If your abstract is close to or exceeds the length limit, it may appear on page 2 of this document.

Time required: 15 min

Session Categories (Keywords) by Relevance: Clusters/Complexes — Non-covalent interactions — Microwave and THz — Atmospheric science

Mini-Symposia Requested: None — None

Competing for Rao Prize? No

Competing for Miller Prize? No