GAS PHASE THz SPECTROSCOPY OF CATECHOL: HIGH-RESOLUTION ANALYSIS OF THE LOW FREQUENCY MODES INVOLVING AN INTRAMOLECULAR HYDROGEN BOND

ARNAUD CUISSET, GUILLAUME DHONT, JONAS BRUCKHUISEN, ATEF JABRI, ANTHONY ROUCOU, HAMDI BAYOUDH, THI THANH TRAN, *Laboratoire de Physico-Chimie de l'Atmosphère, Université du Littoral Côte d'Opale, Dunkerque, France*; MARIE-ALINE MARTIN-DRUMEL, *CNRS, Institut des Sciences Moleculaires d'Orsay, Orsay, France*.

1,2-Benzenediol, commonly known as catechol, is emitted directly from biomass burning as well as produced in the atmosphere through the gas-phase reaction of benzene and phenol with OH radicals.[a] Catechol displays appreciable gas-phase reactivity and its monitoring in the atmosphere via rovibrational spectroscopy has a strong interest. From a molecular point of view, catechol is interesting because its two vicinal hydroxyl groups can act interchangeably as both hydrogen donors and acceptors in internal hydrogen bonding.[b] We performed a rotationally resolved analysis of the low-frequency out of plane bending modes of the intramolecular H-bond of catechol. Using synchrotron-based FT-Far-IR spectroscopy at the AILES beamline of SOLEIL[c] and high level of theory anharmonic quantum chemistry calculations, we have fully resolved and analyzed the rovibrational structures of the -OH acceptor and -OH donor torsional bands. Numerous hot bands involving the lowest vibrational energy modes are observed and an attempt of assignment is performed. Finally, using a versatile millimeter-wave spectrometer,[d] the room temperature Doppler limited rotational spectrum of catechol has been measured in the 70-220 GHz frequency range. Pure rotational lines belonging to the ground and the four lowest energy vibrationally excited states have been assigned and a global fit gathering the far-IR and millimeter-wave data provides the rotational and centrifugal distorsion constants of the different far-IR modes involving the intramolecular hydrogen bond.

[a] Z. Finewax, J. A. de Gouw, P. J. Ziemann, *Environ. Sci. Technol.* **52**, 1981-1989 (2018).

[b] W. Caminati, S. Di Bernardo, *J. Mol. Struct.*, **240**, 263-274 (1990).

[c] J.B. Brubach, L. Manceron, M. Rouzieres, O. Pirali, D. Balcon, F. K. Tchana, V. Boudon, M. Tudorie, T. Huet, A. Cuisset, P. Roy, *AIP Conf. Proc.* **1214**, 81–84 (2009).

[d] G. Mouret, M. Guinet, A. Cuisset, L. Croizé, S. Eliet, R. Bocquet, F. Hindle, *IEEE Sens. J.* **13**, 133-138 (2013).