

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

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1,2-Benzenediol, commonly known as catechol, was investigated, an ortho substituted aromatic volatile organic compound (VOC) with two hydroxyl groups which, due to tunneling between two symmetrically equivalent structures, can interchangeably act as donor and acceptor in a weak hydrogen bond^a. Catechol displays appreciable gas-phase reactivity and its monitoring in the atmosphere via rovibrational spectroscopy has a strong interest. We performed a rotationally resolved analysis of the “free” and “bonded” –OH torsion modes of the intramolecular H-bond using synchrotron-based FT-Far-IR spectroscopy at the AILES beamline of SOLEIL^b. High level of theory anharmonic quantum chemistry calculations were required for the rovibrational assignment. Numerous series of hot bands involving the lowest vibrational energy modes are observed and a set of anharmonic parameters is proposed. Finally, using a millimeter-wave spectrometer,^c 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. Splitting due to the tunneling were resolved for the free –OH torsion state and a global fit gathering the far-IR and millimeter-wave data provides the rotational parameters of the low-energy far-IR modes, especially those involving the intramolecular hydrogen bond.

^aW. Caminati, S. Di Bernardo, *J. Mol. Struct.*, **240**, 263-274 (1990).

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

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