# MICROSOLVATION OF 3-METHYLCATECHOL WITH WATER: A THEORETICAL AND ROTATIONAL SPECTROSCOPIC STUDY

**ARSH S. HAZRAH, ARAN INSAUSTI, JIARUI MA, MOHAMAD H. AL-JABIRI, YUNJIE XU, and WOLFGANG JÄGER**, *Department of Chemistry, University of Alberta, Edmonton, AB, CANADA T6G 2G2*

Biomass burning events, such as forest fires, can influence Earth's climate system by releasing complex mixtures of volatile organic compounds. In a forest fire, lignin, an organic polymer and a major component of wood, undergoes pyrolysis resulting in the direct release of substituted catechols,[1] which contribute to the formation of secondary organic aerosol.[2] An example is 3-methylcatechol (3MC), which can be photo-oxidized or aggregate with other atmospherically relevant molecules, such as water, to form small molecular clusters or hydrates. These hydrates play an important role in the early phases of aerosol particle formation, and their study can provide valuable thermodynamic data for modelling.

We measured rotational spectra of hydrates of 3-methylcatechol with a broadband chirped-pulse Fourier transform microwave spectrometer in the 2-6 GHz range.[3] Grimme's Conformer-Rotamer Ensemble Sampling Tool (CREST)[4] was used to identify possible conformers of the hydrates to aid the spectral assignments. Transitions of several hydrates, 3MC-$(H_2O)_{n=1\text{-}5}$, could be assigned in the experimental spectrum. For the monohydrate and dihydrate, splittings of rotational transitions into quartets were observed. These splittings are a consequence of the methyl internal rotation and the proton exchange motion of the water molecule. Methyl internal rotation splittings are still present for the tri-, tetra-, and pentahydrate, but a splitting attributable to a proton exchange motion is no longer observed.

Interpretation of the results allowed us to identify a preferred solvation pathway which will be described and rationalized with the help of non-covalent interactions analyses.[5]

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