π-System Assisted Micro-Solvation of 3-Methylcatechol Unveiled by Chirped Pulse Microwave Spectroscopy

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3-methylcatechol (3MC), a common substituted catechol, can be released into the atmosphere during biomass burning events. There, it can be photo-oxidized or aggregate with other atmospherically relevant molecules, such as water, to form small molecular clusters, including hydrates. These clusters may lead to the formation of critical nuclei, which can the grow spontaneously to form atmospheric aerosol particles.
To elucidate the conformationally complex 3MC hydrate structures, we analyzed rotational spectra measured with a chirped-pulse Fourier transform microwave spectrometer in the 2-6 GHz range. Two monomer conformers, including their respective ^{13}C isotopologues, were assigned and substitution structures and semi-experimental effective structures were determined. Subsequently, transitions of several hydrates, 3MC-$(H_2O)_{n=1-5}$, were also assigned in the experimental spectrum. For several of the hydrates splitting of rotational transitions into quartets were observed. These splittings are a consequence of the methyl internal rotation (MIR) and the proton exchange of the water molecule. Analysis of the data reveals that water does not aggregate to 3MC in the usual droplet-like fashion. Instead, water molecules cover the aromatic face of 3MC in a surface wetting-like process.