# O-TOLUIC ACID MONOMER AND MONOHYDRATE: ROTATIONAL SPECTRA, STRUCTURES, AND ATMOSPHERIC IMPLICATIONS

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Clusters of carboxylic acids with water, sulfuric acid, and other atmospheric species potentially increase the rate of new particle formation in the troposphere.[a,b] Here, we present high-resolution pure rotational spectra of *o*-toluic acid and its complex with water in the range of 5-14 GHz, measured with a cavity-based molecular beam Fourier-transform microwave spectrometer. In both the monomer and the complex, the carboxylic acid functional group adopts a *syn*- conformation, with the acidic proton oriented away from the aromatic ring. In the complex, water participates in two hydrogen bonds, forming a six-membered intermolecular ring. Despite its large calculated *c*-dipole moment, no *c*-type transitions were observed for the complex, because of a large amplitude "wagging" motion of the unbound hydrogen of water, similar to the case of the benzoic acid-water complex.[c] No methyl internal rotation splittings were observed, consistent with a high barrier (7 kJ $mol^{-1}$) calculated for the monomer at the B3LYP/6-311++G(d,p) level of theory. Using statistical thermodynamics, experimental rotational constants were combined with a theoretical frequency analysis and binding energy to give an estimate of the percentage of hydrated acid in the atmosphere under various conditions.

[a] F. Riccobono, *et al.*, *Science*, **344**, 717 (2014).
[b] R. Zhang, *et al.*, *Science*, **304**, 1487 (2004).
[c] E. G. Schnitzler and W. Jäger, *Phys. Chem. Chem. Phys.*, **16**, 2305 (2014).