

MICROSOLVATION OF α -PINENE OXIDE AS OBSERVED BY BROADBAND ROTATIONAL SPECTROSCOPY

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α -pinene is the most abundant monoterpene in the atmosphere and its oxidation yields to several oxygenated species that play a major role in the formation of secondary organic aerosols. α -pinene oxide ($C_{10}H_{16}O$) is generated from the reaction of ozone with α -pinene and has been shown to contribute to the formation of organosulfates under atmospheric conditions. Thus, understanding its interactions with atmospheric molecules is crucial to explain the first steps of molecular aggregation in the aerosol formation. Here, we present the investigation of the hydrates of α -pinene oxide, $C_{10}H_{16}O \cdots (H_2O)_n$ ($n=1,2$), using two different chirped-pulse Fourier transform microwave spectrometers operating in the 2-18 GHz frequency range,^{1,2} supported by quantum chemical calculations. The hydrates consist of water chains anchored to the oxygen atom of α -pinene oxide by a primary O-H $\cdots$ O hydrogen bond and further stabilized by secondary C-H $\cdots$ O interactions. The structures of these hydrates have been further confirmed by the analysis of the rotational spectra of their ^{18}O water isotopologues and compared with those of related species.

References

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