MICROSOLVATION OF β-PROPIOLACTONE AS REVEALED BY CHIRPED-PULSE FOURIER TRANSFORM MICROWAVE SPECTROSCOPY.

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Microwave spectra of water clusters of β-propiolactone with up to five water molecules attached are presented. Helium or neon carrier gas with 3 atm of backing pressure is flowed over a room-temperature water reservoir, then over a room-temperature sample of β-propiolactone before being expanded into a chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer operating between 6.5 and 18.5 GHz. A very dense spectrum, with approximately 2000 lines with a signal to noise ratio of at least 3:1, was observed, of which 800 have been assigned to a total of 20 species, including isotopomers in natural abundance and clusters with the carrier gas. Due to the complexity of the spectrum, after the first few, all other spectra were assigned with the aid of microwave-microwave double resonance experiments, either performed on the CP-FTMW spectrometer or in a Balle-Flygare-type cavity FTMW spectrometer. In the case of an extremely dense spectrum like this in which many species are present, these double resonance measurements are required to successfully analyze the spectrum. Stark effect measurements and assignments of isotopically substituted species are used to determine the structures of these microsolvated complexes.