GAS PHASE INFRARED SPECTROSCOPY OF ISOMERIC BENZYL AND TROPYLIUM CATIONS

J. PHILIPP WAGNER, Department of Chemistry, University of Georgia, Athens, GA, USA; DAVID C Mc-DONALD, Chemistry, University of Georgia, Athens, GA, USA; MICHAEL A DUNCAN, Department of Chemistry, University of Georgia, Athens, GA, USA.

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The isomeric benzyl and tropylium $C_7H_7^+$ cations have been of great interest to physical organic and gaseous ion chemists for many decades. Still, infrared spectroscopic characterization of these ions in the gas phase could so far only be achieved for their methylated derivatives but not for the $C_7H_7^+$ ions themselves. Thus, we set out to produce both relevant isomers of this elusive ion in a cold molecular beam experiment through ionization of different precursor molecules comprising the preformed 6- and 7-membered rings. We measured their IR spectra via photodissociation with a tunable OPO/OPA laser system in combination with the argon messenger atom technique. The obtained spectra were assigned with the aid of second order vibrational perturbation theory utilizing dispersion-corrected density functional theory.

