INFRARED SPECTROSCOPY OF THE MASS 43 CATION: ACETYL CATION AND PROTONATED KETENE

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The mass 43 cation $[C_2, H_3, O]^+$ is prominent in mass spectra of organic molecules. Theory predicts no less than nine structural isomers, and the acetyl cation CH_3CO^+ is the global minimum. The infrared spectrum of the mass 43 cation from methyl acetate shows vibrations only from the acetyl cation. The effects of the methyl free internal rotor are discussed. The mass 43 cation from acetone shows evidence for both the acetyl cation and the less thermodynamically stable (50 kcal/mol) protonated ketene isomer CH_2COH^+. The effects of varying the kinetic trapping conditions in our ion source on isomeric ratios of the mass 43 cation are discussed.