INFRARED SPECTRA OF TWO C7H7 ISOMERS: TROPYL AND BENZYL

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Infrared(IR) spectroscopy is a powerful tool to learn about the vibrational structure of a molecule. The aim of the present study is learn more about the benzyl and tropyl radicals, two isomers with the composition C_7H_7. These radicals are produced in a discharge source, and subsequently jet-cooled. Resonant UV ionization in combination with infrared depletion spectroscopy is performed on these molecules, and the ion yield on the parent mass channel of the molecule is monitored as a function of IR-wavelength. Intense tunable infrared radiation in the region between 40 and 3300 cm^{-1} is generated by the free electron laser FELIX.
Both the benzyl as well as the tropyl radical posses some degree of symmetry; they belong to the C_{2v} and D_{7h} point groups respectively. Because of its high symmetry and its degenerate ground state, the tropyl molecule is subject to the Jahn-Teller effect, which distorts its molecular frame to lower symmetry and could give rise to interesting effects in the infrared spectra.
In the cationic state, the isomers are seperated only marginally in energy, and by a ring opening reaction of the benzyl molecule, tropyl can be formed. One of the open questions that remains is which of the isomers is more stable. Infrared spectra of both benzyl and tropyl will be presented in the talk in conjunction with quantum chemical calculations on both species.