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Isomerisation studies in ion traps

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The benzylium/ tropylium ion ($C_7H_7^+$) dichotomy is well known in mass spectrometry and could be of interest for larger species such as the 1-methylpyrene fragment ($C_{17}H_{11}^+$) [1].
Common ways of distinguishing isomers are spectroscopy and chemical reactivity. In ion traps, the density of species is too low for conventional absorption spectroscopy and action schemes have to be applied. However, one would like to avoid schemes that introduce considerable internal energy in order not to affect the initial populations.

In this work we present the application of the FELion cryogenic rf ion trap to the spectroscopy of $C_7H_7^+$ and $C_{17}H_{11}^+$. Using tagging spectroscopy and the wavelength coverage of the free electron laser FELIX, we were able to record the mid-IR spectra of tropylium and benzylium ion, and confirm these are the only two stable isomers produced upon electron bombardment of toluene [2]. Using the same electron bombardment for 1-methylpyrene, we found only one isomer, the $PyrCH_2^+$ (pyrene with a mehylene group, analogous to benzylium ion)[3]. This result is consistent with recent calculations on the unimolecular dissociation of 1-methylpyrene ion to $PyrC_7^+$ ion, which is predicted to be extremely unlikely [5].

Using the cryogenic FTICR setup PIRENEA, we are now investigating the ossibility to overcome the barrier between the two isomers. In this experiment, we apply chemical reactivity to probe and isolate isomers. We hope to generalize the benzylium/ tropylium ion dichotomy.

References:

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