Infrared action spectroscopy of doubly charged PAHs in a 22-pole cryogenic ion trap

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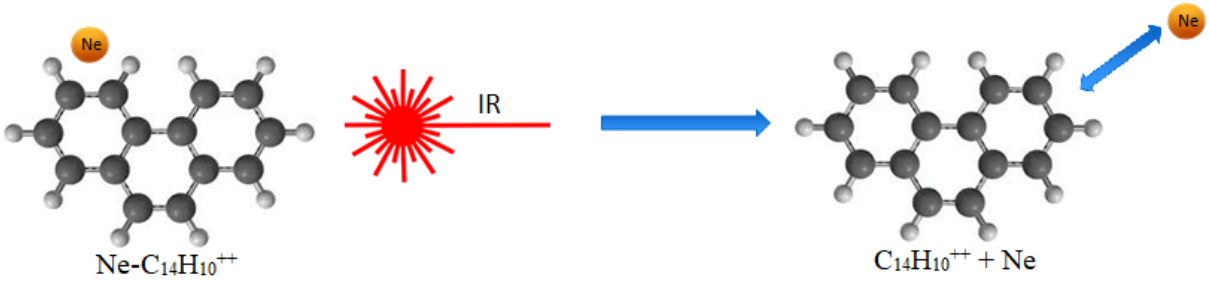
Motivation: PAHs are suspected to be possible carriers of aromatic infrared bands observed in the spectra of galactic and extra galactic sources and that they exist in different charge states in the interstellar medium [1]. To identify these PAHs, laboratory infrared gas phase spectrum is necessary which can be compared with the observed astronomical data. Spectroscopic studies employing IRMPD by utilizing the intense FEL IR radiation at FELIX laboratory have been done for a number of cationic, protonated, anionic PAHs of varying sizes [2,3] and recently for the dication HBC^{++} [4].

Aim: We present here the experimental gas-phase infrared spectra of three different PAH (Polycyclic Aromatic Hydrocarbons) dications (Naphthalene^{++}, $C_{10}H_8^{++}$, Anthracene^{++} and Phenanthrene^{++}, $C_{14}H_{10}^{++}$) in the fingerprint region (500 – 1600) cm^{-1}.

Method: The dications were produced by electron impact ionization of the corresponding vapors with 70 eV electrons and the spectra were obtained by Infrared Predissociation (IRPD) of the mass-selected ions complexed in-situ with Ne in a 22-pole cryogenic ion trap setup (FELion) [5] operated at temperature 15K using the intense and widely tunable free electron infrared lasers at the FELIX Laboratory. We also performed DFT calculations at B3LYP 6-31g level for both singlet and triplet states of all ions in order to compare the vibrational frequencies to the corresponding experimental data.



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References

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