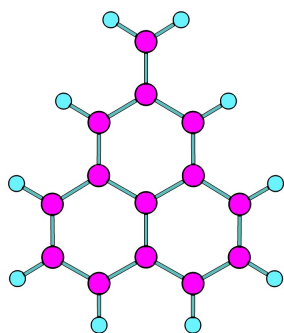


EXTRATERRESTRIAL ISOMER OF PHENANTHRENE DICATION STUDIED BY TAGGING PHOTODISSOCIATION ION SPECTROSCOPY AND DFT CALCULATIONS

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The search for the chemical structures that account for diffuse interstellar bands (DIBs) remains the main challenge in astrochemistry. It relies on experimental verification of structures obtained from stable isomers in laboratory conditions. The actual interstellar medium (ISM), however, is exposed to much harsher conditions. Herein we demonstrate the isomerization of small, doubly charged polyaromatic hydrocarbon phenanthrene obtained by electron ionization at relatively high electron energies. We performed electronic and vibrational tagging photodissociation spectroscopy measurements. Our results show that phenanthrene dication has a minor $C_{14}H_{10}^{2+}$ isomer, originating from the isomerization of phenanthrene dication during the harsh ionization process. Hole-burning spectroscopy experiments provided the IR spectrum of an isomer which could be assigned based on DFT calculations as a fully conjugated system representing the global minimum on the $C_{14}H_{10}^{2+}$ potential energy surface. The found isomer has no neutral closed-shell form and can only exist as a radical or as an ion. Finally, the IR spectrum of this isomer reveals features characteristic for the ISM, suggesting that it can potentially be a candidate for the DIB search. These results open new directions in searching for potential DIB candidates.