Positive ion mass spectrometry for fragmentation of anthracene by low energy electron impact

Positive ion mass spectrometry for fragmentation of anthracene by low energy electron impact

M. Dunne*, M. L. Gradziel*, and P. J. M. van der Burgt* [1]

* Department of Experimental Physics, National University of Ireland Maynooth, Maynooth, Co. Kildare, Ireland

Synopsis. We have studied the fragmentation of anthracene molecules induced by low energy electron impact. A reflectron time-of-flight mass spectrometer has been used to mass resolve and detect positively charged fragments. Using computer controlled data acquisition, mass spectra have been measured as a function of electron impact from 5 to 100 eV. The mass spectra show clear indications of double and triple ionization. Ion yield curves and appearance energies for most of the positive ions have been extracted from the data.

Polycyclic aromatic hydrocarbons have environmental relevance, because they are formed as by-products in the combustion of organic materials. They are believed to be a major component of the interstellar medium, because they are considered to be responsible for the emission features that dominate the infrared spectra of many galactic and extragalactic sources [1].

In order to obtain information about electron-induced fragmentation patterns of anthracene ($C_{14}H_{10}$), we have measured mass spectra of positive ions of anthracene, with electron energies ranging from 5 to 100 eV in steps of 0.5 eV.

A resistively heated oven generates a beam of anthracene molecules. The oven is mounted in an expansion chamber and the forward section of the beam effusing from a capillary in the oven passes through a skimmer into the collision chamber, where the beam is crossed by a pulsed electron beam (0.3 μs, 8 kHz). Positively charged fragments are extracted into a reflectron time-of-flight mass spectrometer. LabVIEW based data acquisition techniques are used to measure mass spectra as a function of electron impact energy. More details about the experiment and the data analysis can be found in [2-4], which present results obtained for electron impact on some of the nucleobases.

Ion yield curves for most fragment ions of anthracene have been obtained by fitting groups of adjacent peaks in the mass spectra with sequences of normalized Gaussians. Appearance energies have been determined by fitting a threshold function of the form $f(E) = c(E - E_0)^p$ (for $E > E_0$) to the ion yield curves. This function is convoluted with a Gaussian to account for the electron beam energy resolution.

We observe clear indications of multiple ionization in the mass spectra. The triply-charged parent is weakly present at 59.3 u, just separated from the 60-65 u group of fragments, and the appearance energy is 45.5 ± 0.5 eV. In the 83-91 u group of fragments, half-integer peaks are clearly present. The threshold for double ionization is not entirely clear. The 89 u ion has an appearance energy of 20.2 ± 0.7 eV and a second onset at 23.6 ± 0.6 eV.

Mass spectra, ion yield curves and appearance energies will be presented at the conference and will be compared with other research on anthracene and other polycyclic aromatic hydrocarbons (eg. [5-7]).

References

[1] A. G. G. M. Tielens 2013 *Rev. Mod. Phys.* **53**, 1021
[2] P. J. M. van der Burgt 2014 *Eur. J. Phys. D* **68**, 135
[3] P. J. M. van der Burgt, F. Mahon, G. Barrett, and M. L. Gradziel 2014 *Eur. J. Phys. D* **68**, 151
[4] P. J. M. van der Burgt, S. Finnegan, and S. Eden 2015 *Eur. J. Phys. D* **69**, 173
[5] S. Denifl, B. Sonnweber, J. Mack, L.T. Scott, P. Scheier, K. Becker and T.D. Märk 2006 *Int. J. Mass Spectrom.* **249–250**, 353
[6] G. Reitsma, H. Zettergren, S. Martin, R. Brédy, L. Chen, J. Bernard, R. Hoekstra and T. Schlathölter 2012 *J. Phys. B: At. Mol. Opt. Phys.* **45**, 215201
[7] R. Brédy, C. Ortéga, M. Ji, J. Bernard, L. Chen, G. Montagne and S. Martin 2013 *Phys. Scr.* **T156**, 014042

[1] E-mail: peter.vanderburgt@nuim.ie