Functional Group Dependence and Site Selectivity in Dissociative Attachment

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It is well known that dissociative electron attachment (DEA) plays an important role in electron induced chemistry. Several experiments have shown that selective fragmentation through DEA enables chemical control. It has been found that this selectivity emerges from two aspects. The first one is purely based on threshold energy and arises from the differences in the electron affinity of the fragments and the bond dissociation energies [1, 2]. The second one originates from functional group dependence [3, 4]. This is mostly seen in core or valence excited resonances. Here, the selectivity is more versatile in that it is independent of the threshold energy and has a broader energy range in which the selectivity is displayed. The optical absorption bands shown by these molecules have common features, characteristic to the functional groups present. It appears that these very features are displayed in the formation of core excited resonances, giving rise to the observed selectivity in braking the O-H, C-H or N-H bonds in molecules through DEA. Such selectivity observed in alcohols, carboxylic acids and amines [3, 4]. The site/bond selectivity observed in bigger molecules like Thymine [5] and higher alcohols [6] can also be interpreted based on the functional groups.

We have been continuing the investigation of the functional group dependence in organic molecules on a wider scale, including aromatics, in terms of the mass spectra, ion yield curves, absolute cross sections and momentum distributions. In this talk I would briefly review the role of functional group dependence in DEA and summarize our new findings.

References

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