Using Dissociative Electron Attachment as a Fingerprinting Tool to Detect Explosives

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In recent years, the need for detection of explosives and the need to distinguish them among several other similar, yet unperilous substances has increased. One of the core problems in this field is the similarity of nitrogen-dioxide-containing compounds, which have a range of applications including explosives and cosmetic products.

Very recently we extended the investigations of applying dissociative electron attachment (DEA) as a tool to unambiguously assign explosives to HMX ($C_4H_8N_8O_8$). This highly powerful explosive can be found in the chemical classification of nitramines.

Capture of low energy electrons by HMX leads to the formation of a variety of DEA fragments at virtually no electron energy, reflecting the explosive character of HMX. Some of the fragments are the same as in DEA processes of compounds like RDX or TNT. The resonance positions of the fragments are similar for several compounds, therefore aggravating the distinction of parent substances. However, due to differences in the relative intensities of the fragment formation at several electron energies, one can assign a fragment to its parent molecule, hence fingerprinting the individual substances.

To support the measurements of DEA resonances, we performed quantum chemical calculations utilizing Møller-Plesset perturbation theory truncated at the second order for geometry optimizations, visualization of the molecular orbitals, and calculation of energetics together with the 6-311++G(2d,p) basis set.

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References:

[1] J. Postler et. al, J. Am. Soc. Mass. Spectrom. (2013).