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Fragmentation of acetonitrile in collisions with H^- and O^- ions

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Synopsis. Relative cross sections for the production of negatively charged fragments have been determined as a function of ion impact energy in low-energy (0.5 - 5.5 keV) collisions of H^- and O^- with acetonitrile molecules. The most abundantly produced negative ions from fragmentation by H^- and O^- impact are CH_3CN^-, CH_2CN^- and CN^-. Notably, the parent negative ion CH_3CN^- is produced abundantly.

Acetonitrile (CH_3CN) is the simplest organic molecule which has both methyl and cyano groups. It is an important precursor molecule in the study of the origins of life, and it has also been detected in interstellar space and in planetary atmospheres. For these reasons it is important to study fragmentation patterns of acetonitrile in low-energy collisions with ions. Of interest is the comparison of the H^- induced fragmentation with that of equivelocity electrons.

We have studied molecular dissociation patterns following impact of negative ions on acetonitrile. Beams of H^-, O^- and OH^- ions with energies in the range 0.5 - 5.5 keV were generated at Queen's University Belfast using a Cs sputter source attached to a low energy (1-10 keV) ion accelerator. The negative ion beam was crossed at right angles by an effusive jet of the target molecules.

The effusive beams of acetonitrile were generated by evaporating liquid samples from a small glass reservoir. The liquids were purified using several cycles of freeze-drying. Both positive and negative ionized fragments were detected using a Hiden quadrupole mass spectrometer (1-300 amu) mounted at right angles to both the ion beam and the molecular beam.

All ion yields were normalized for small variations in ion current and target gas density, and were corrected for the mass sensitivity of the quadrupole. In this manner, total relative cross sections for the production of negatively charged fragments have been determined as a function of ion impact energy.

Figure 1 shows the results obtained for O^- impact. All cross sections at all impact energies are relative to the cross section for the production of CH_2CN^- (40 u), which is set to 100 at 2 keV. With the exception of CH_3CN^- (41 u), all cross sections decrease as the ion impact energy is increased. The relative cross section for the production of H^- is very small and is not included in the graph.

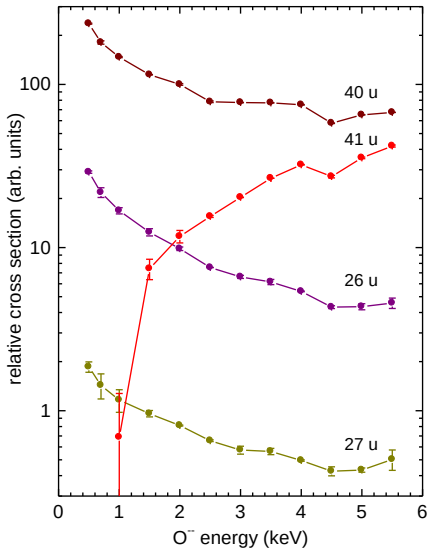

Figure 1. Relative cross sections for the production of negative fragment ions in O^- impact on acetonitrile.

For comparison, measurements of dissociative electron attachment using a trochoidal monochromator have also been performed.

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