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Dissociative electron attachment to carbonyl fluoride, F_2CO

Low energy electron attachment to gas phase carbonyl fluoride, F_2CO, has been performed by means of a crossed electron-molecular beam experiment in an electron energy range from 0 to 30 eV with an energy resolution of ~0.5 eV. F_2CO has been suggested as a suitable candidate for replacement feed gas to the traditional highly global warming SF_6 and other perfluorocarbons used in the plasma semiconductor industry. F_2CO has been, therefore, extensively used as a cleaning agent in chemical vapour deposition equipment, as well.

In present study, the excitation function of the electron attachment to F_2CO was measured as a function of incident electron energy by using a tuneable electron source assembled directly at the entrance of a quadrupole mass spectrometer (Hiden Analytical Ltd. EPIC).

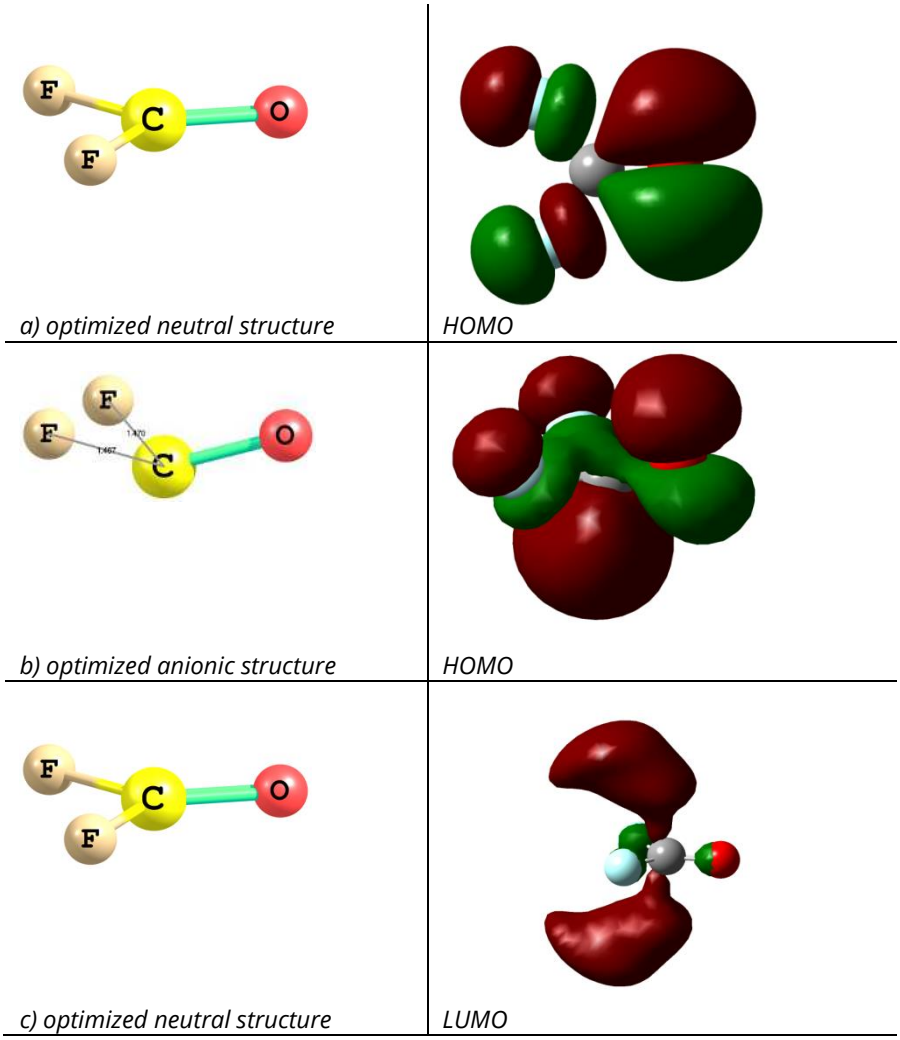


*Figure 1: Optimized structures of F_2CO as neutral (a) and negatively charged (b) molecule. Highest occupied molecular orbital of the neutral molecule (a) and of the anion (b). The lowest unoccupied molecular orbital is shown in (c). All results obtained at HF/6-311++G** level*

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The most intense signal is observed at 19 amu due to F^- and two other anionic species with lower intensities at 38 and 47 amu assigned to F_2^- and COF^-, respectively. Product anions (F^- and COF^-) are observed mainly in the low energy region arising from simple bond breaking, while F_2^- is being produced from two bond cleavages with further structural and electronic rearrangement. Quantum chemical calculations on the electronic properties of F_2CO have been performed in order to complement the experimental results. It was found that in the present gas phase system the LUMO wave function showed an extended profile from the carbon site to the fluorines. The mechanism yielding F_2^- formation proceeds through the attachment of the extra electron and two C–F bond ruptures. Such configuration may imply considerable geometry change in the temporary negative ion, which is supported by the calculations.

References:

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