

Low energy elastic cross section of fluoroacetylene by electron impact

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Synopsis Electron impact low energy cross sections for fluoroacetylene is investigated for which there are no reported results in the literature. We have used various target models to compute accurate target properties and the best target model is used for the final scattering calculation. The fluorination effect in the cross section is studied by comparing the results with difluoroacetylene and acetylene.

Fluoroacetylene (HCCF) is a simple linear structure molecule similar to acetylene (HCCH) and difluoroacetylene (FCCF) and offers a very good opportunity to study the effect of fluorination by replacing the hydrogen atom in HCCH with fluorine atom and by replacing the fluorine atom in the case of FCCF with hydrogen atom in the scattering cross sections. Recently we have investigated FCCF [1] and compared its cross section with HCCH [2] and obtained interesting results in terms of cross section and resonances. Hence it is of great interest to study HCCF with respect to HCCH and FCCF for various cross sections and resonance along with fluorination effect.

The R-matrix method [3] is used for the present study at low energies. The cc-pVTZ basis set is used for the representation of the target wave function with 16 target states included in the calculation. The calculations are done in the C_{2v} point group symmetry. The absolute value of the ground state energy estimated is -175.75 Hartree. The present target model predicts the dipole moment of 0.285 *au* which is in very good agreement with the experimental value of 0.283 *au* [4]. The first excitation energy of 7.09 eV is also in reasonable agreement with the recent calculation of Khiri *et al.* [5] at 6.326 eV. The target properties are listed in Table 1 with available comparison.

Table 1. Target properties for HCCF.

Properties	Present	Others
Absolute Ground state energy (Hartree)	-175.75	-
Dipole moment (au)	0.285	0.283[4]
First excitation energy (eV)	7.09	6.326[5]

The scattering calculations are carried out further with this model and the sample result for

elastic cross section (Q_{el}) of HCCF along with comparison of FCCF by us [1] and HCCH by Gauf *et al.* [2] is presented in Figure 1. The π^* resonance is predicted at 5.30 eV for HCCF due to (2B_1 , 2B_2) states. The π^* resonances for HCCH and FCCF is detected at 2.5 eV by Gauf *et al.* and 5.86 eV by us. It is clearly observed that by replacing the hydrogen atom with fluorine atom shifts the resonance to the higher energy side as seen in the case of HCCH, HCCF and FCCF in Figure 1. In addition to π^* resonance we have also detected another resonance at 3.17 eV due to 2A_1 state for HCCF.

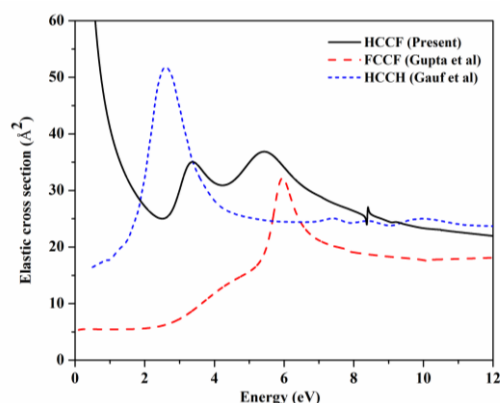


Figure 1. Q_{el} for HCCF, FCCF [1] and HCCH [2].

At low energies below 3 eV, the cross section for HCCF shows sharp rise unlike HCCH and FCCF which is due to dipole moment of the molecule as given in Table 1. The experimental investigations will be useful for further understanding and to verify the present results.

References

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