

Positive and Negative Photoion Spectroscopy Study of Monochlorothiophenes

Yun-Feng Xu,¹ Shan Xi Tian,^{1,a)} Liuli Chen,¹ Fu-Yi Liu,² and Liusi Sheng²

¹*Hefei National Laboratory for Physical Sciences at the Microscale and Department of Chemical Physics, University of Science and Technology of China, Hefei, Anhui 230026, China*

²*National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, China*

a) Corresponding author. E-mail: sxtian@ustc.edu.cn

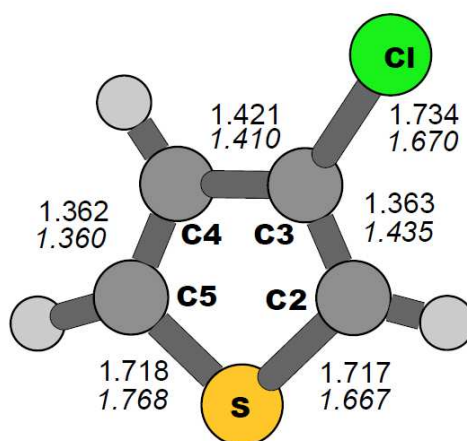
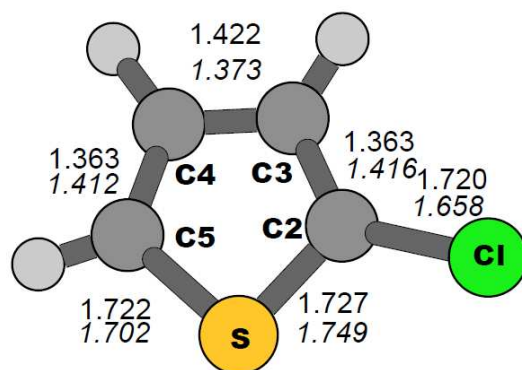
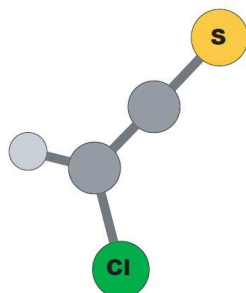
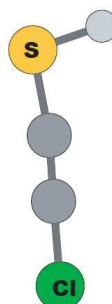


Figure S1. Optimized geometrical parameters (bond lengths in angstrom) and energies (in Hartree) of the neutral (normal) and cationic (italic) monochlorothiophenes.

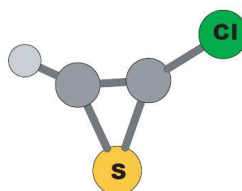
$m/z=92$



C_2HCIS^+ (1)
($C_s, ^2A''$: -934.897312H)

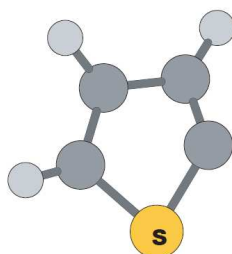


C_2HCIS^+ (2)
($C_s, ^2A''$: -934.865311H)

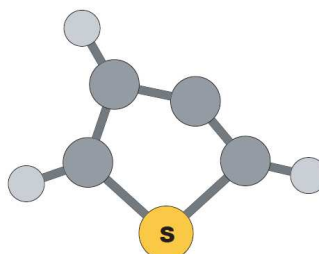


C_2HCIS^+ (3)
($C_s, ^2A''$: -934.870208H)

$m/z=83$



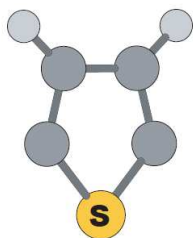
$2-C_4H_3S^+$
($C_1, ^1A'$: -552.009095H)



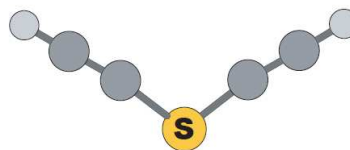
$3-C_4H_3S^+$
($C_s, ^1A'$: -552.026326H)

Figure S2. Optimized geometries of some predominant daughter cations with $m/z = 92$ and 83 (the total energies in Hartree).

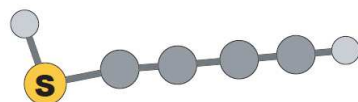
$m/z=82$



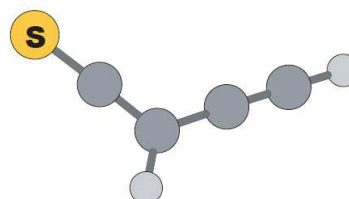
C₄H₂S⁺ (1)
(C_{2v}, ²A₂: -551.337845H)



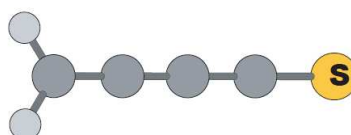
C₄H₂S⁺ (2)
(C_{2v}, ²B₁: -551.384220H)



C₄H₂S⁺ (3)
(C_S, ²A⁺: -551.416934H)



C₄H₂S⁺ (4)
(C_S, ²A⁺: -551.441709H)



C₄H₂S⁺ (5)
(C_{2v}, ²B₁: -551.459417H)

Figure S3. Optimized geometries of some predominant daughter cations with $m/z = 82$ (the total energies in Hartree).

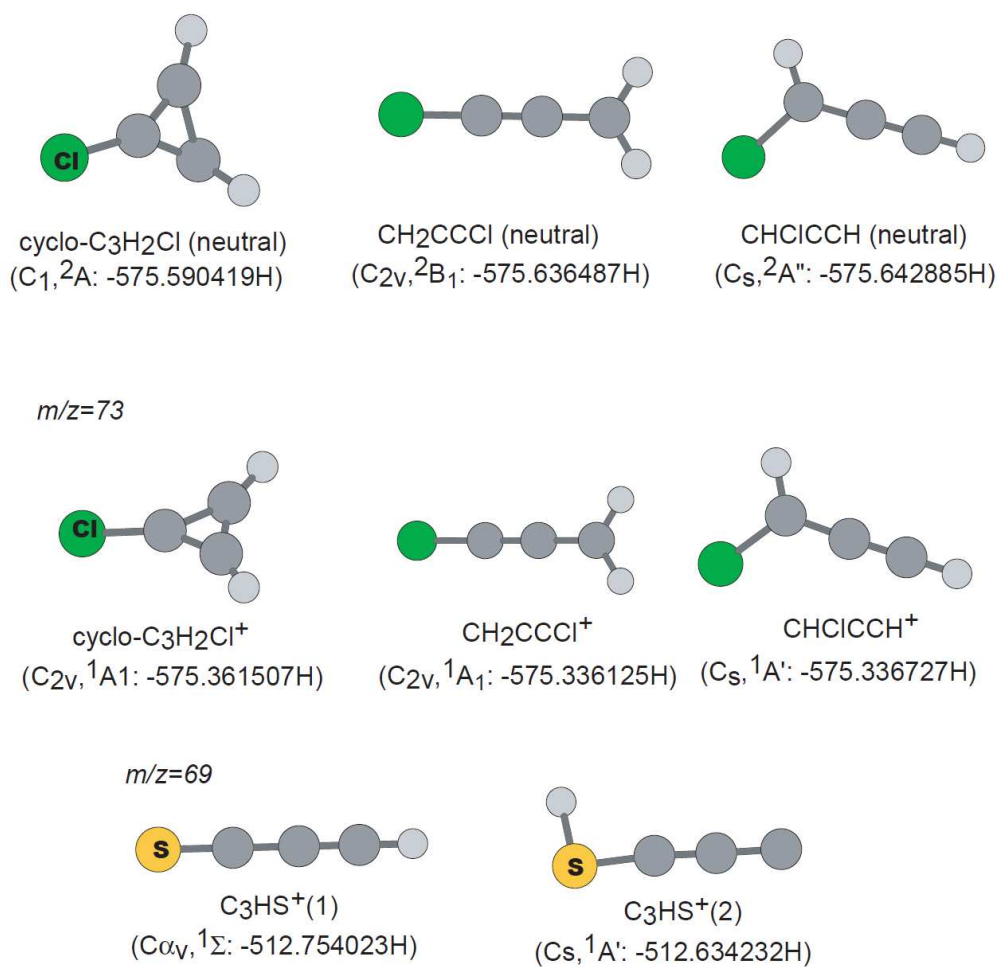
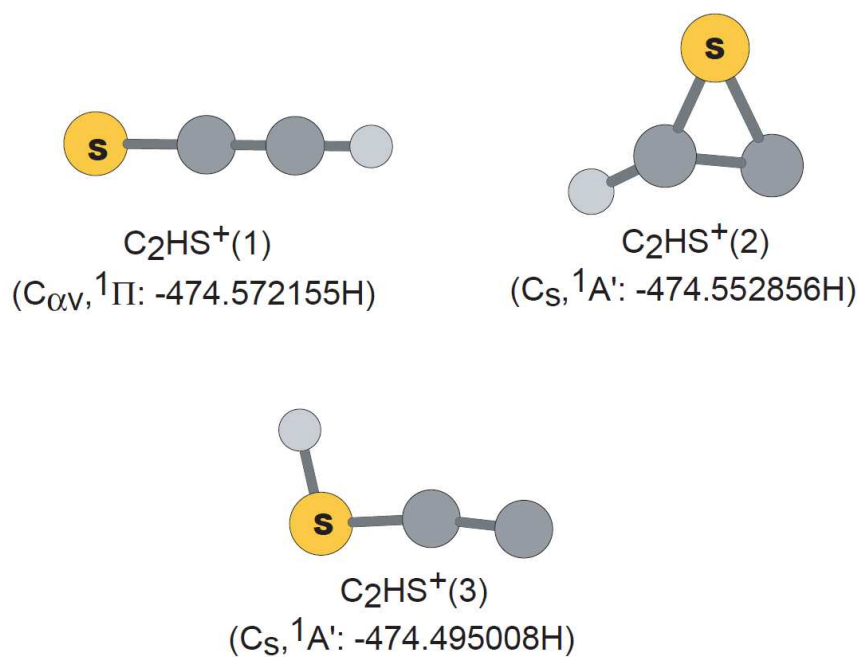


Figure S4. Optimized geometries of some predominant daughter cations with m/z =73 and 69 and the neutral fragments (at the top panels), all energies in Hartree.

$m/z=57$



$m/z=39$

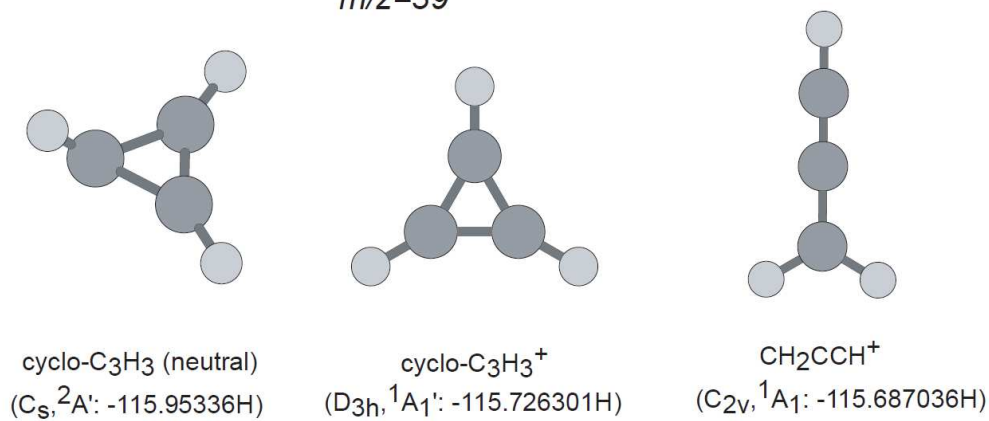


Figure S5. Optimized geometries of some predominant daughter cations with $m/z = 57$ and 39 and the neutral fragment cyclo- C_3H_3 , all energies in Hartree