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Mechanistic insight into the kinetic fragmentation of norpinonic acid in the gas phase: an experimental and density functional theory (DFT) study

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S1. Synthesis of investigated compound

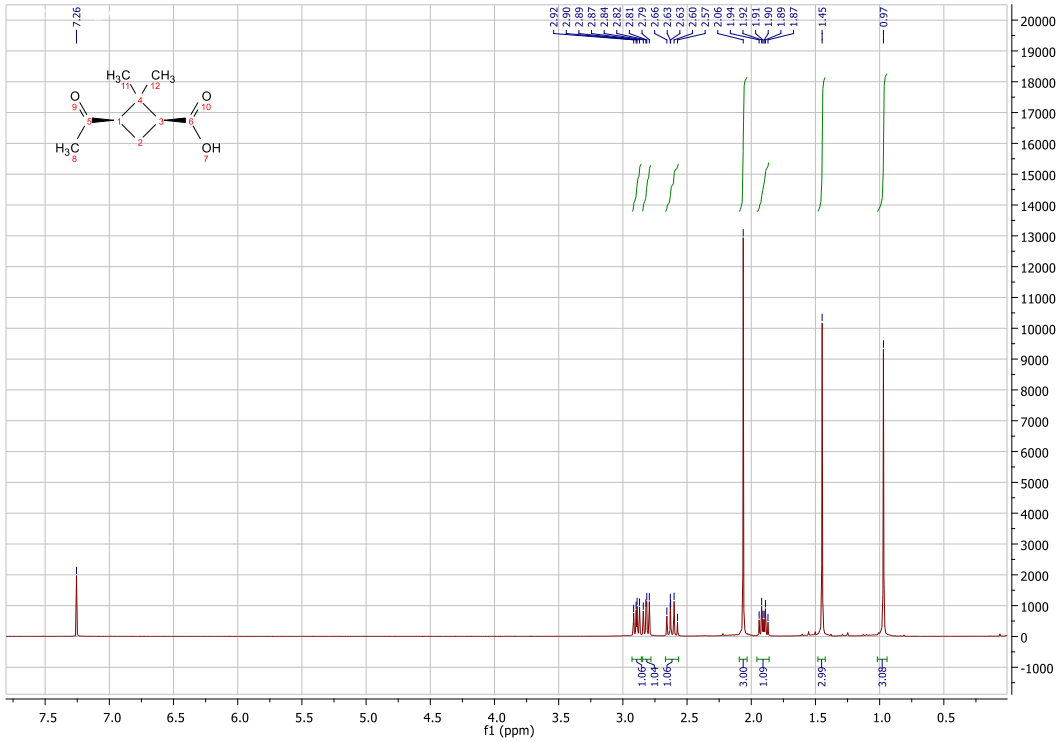
S1.1 Synthesis protocol

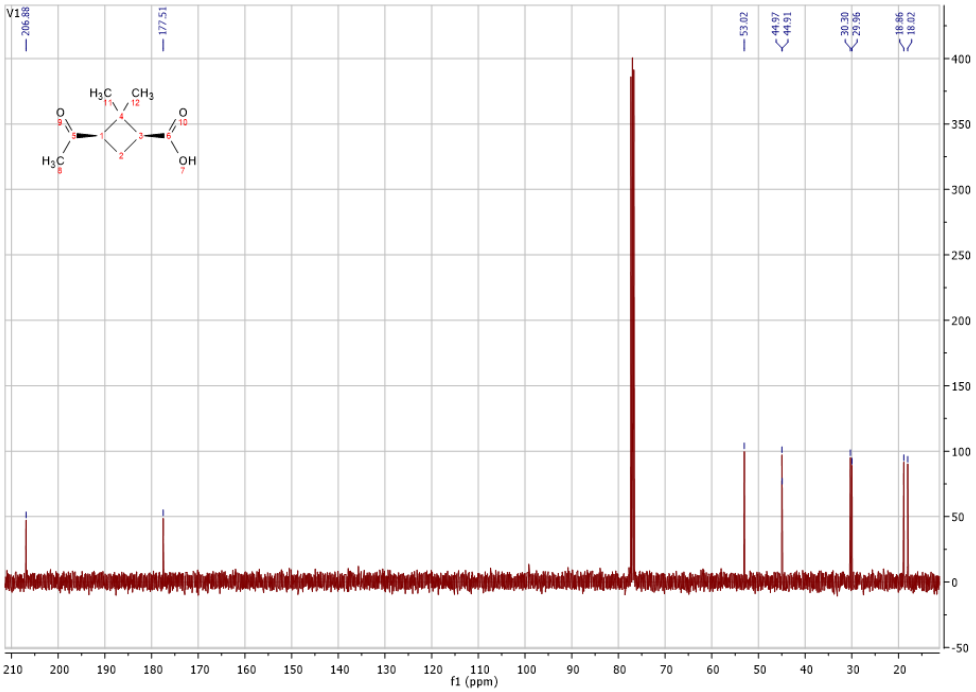
The commercially available (1S)-(-)-verbenone (CAS Registry No. 1196-01-6, ≥ 94%, Sigma-Aldrich) was used as starting material. The protocol for the synthesis of norpinonic acid covered one step - the oxidative cleavage of the double C=C bond using $RuCl_3$×H2O (CAS Registry No. 14898-67-0, Sigma-Aldrich, ≥99.98%). Other chemicals used in cis-norpinonic acid synthesis were as follows: sodium periodate (CAS Registry No. 7790-28-5, Sigma-Aldrich, ≥ 99.8%), carbon tetrachloride (CAS Registry No. 56-23-5, Sigma-Aldrich, ≥ 99.5%), acetonitrile (CAS Registry No. 75-05-8, POCH, ≥ 99.9%), hexane (CAS Registry No. 110-54-3, POCH, ≥ 99.9%), ethyl acetate (CAS Registry No. 60-29-7, POCH, ≥ 99.9%), magnesium sulfate (CAS Registry No. 7487-88-9, POCH, ≥ 98.5%).

To the stirred solution of (1S)-(-)-verbenone (2.5 mL, 16 mmol) in 2:2:3 carbon tetrachloride-acetonitrile-water (130 mL), catalytic $RuCl_3$ hydrate (120 mg) and $NaIO_4$ (13.4 g, 63 mmol) were added. The resulting mixture was stirred overnight at the room temperature, then diethyl ether (100 mL) was added and stirring for the next 5 min. Then mixture was extracted with diethyl ether (3×100 mL). The combined organic extracts were dried ($MgSO_4$) and concentrated under reduced pressure. Norpinonic acid was isolated as white crystals after crystallization from diethyl ether (yield: 80%).

The structural identification of the final product based on IR, ESI-HR-MS, ^1H , ^{13}C and 2D NMR analytical spectra proved the presence of cis-norpinonic acid stereoisomeric form.

S1.2 Copies of 1H and 13C NMR spectra of isolated compound





S2. Experimental procedures

S2.1 Breakdown Curves

Collision spectra were recorded by varying the collision energy in incremental steps. Collision mass spectra were recorded with an energy resolution of 8–30 eV in the lab frame and 2-10 minutes of collection time at each step. Creation of the total breakdown curves was performed using absolute peak heights. Breakdown curves at five different argon pressures are presented in.

S2.2 Extrapolation Procedure

To determine the onset/threshold energies (at each gas pressure) to enable a comparison of the energetics of the observed processes, we used a simple extrapolation procedure. By performing a linear fit of the approximately linearly rising section of the breakdown curve, we define the onset energy at each gas pressure by calculation of the energy (X value) at zero intensity (Y = 0).To compare the experimental and theoretical energy values, we opted also for gas pressure extrapolation. We used the energies taken from extrapolation at five different gas pressures to define the onset energy by calculation of the energy (Y value) at zero gas pressure (X = 0). Summaries are presented in Tables.

S2.3 Bimolecular reaction

To perform the gas-phase reactions, we introduce neutral reagent vapors into the collision cell by attaching a flask filled with each reagent to the gas inlet system. The results of these experiments for reaction between methyl thiocyanate (CH_3SCN) or dimethyl disulfide (CH_3SSCH_3) and all ions are presented in Figures.

S3. Experimental results

S3.1 Fragment ion mass spectra

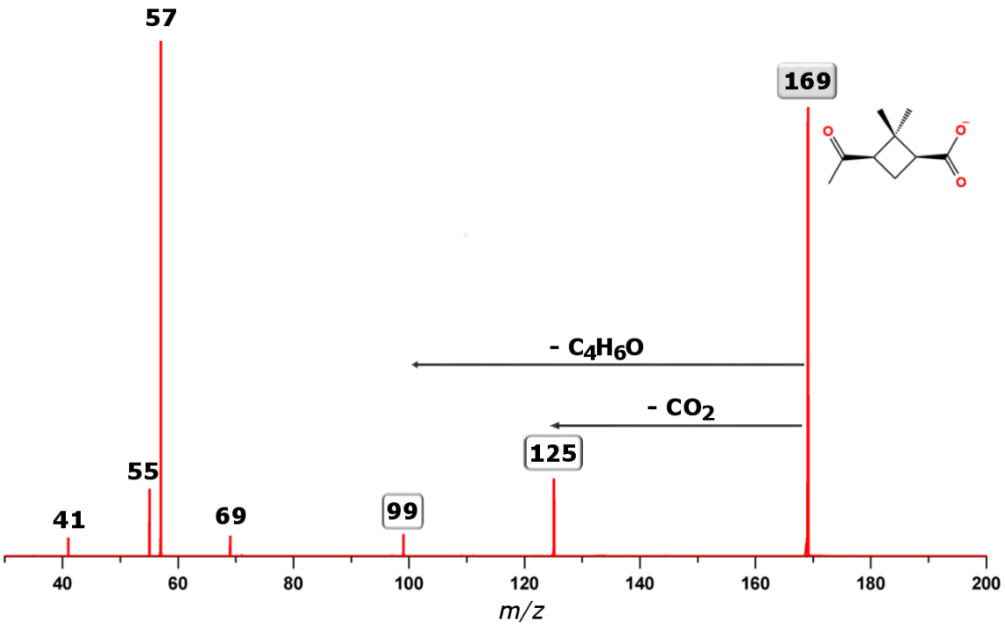


Figure S1. Fragment ion mass spectrum of $C_9H_{13}O_3^-$ (*m/z* 169) recorded with a ToF voltage of 3kV, taken at a collision energy of 3.8 eV (CM) with argon collision gas at nominal pressure of 3.54 $\times 10^{-4}$ mBar.

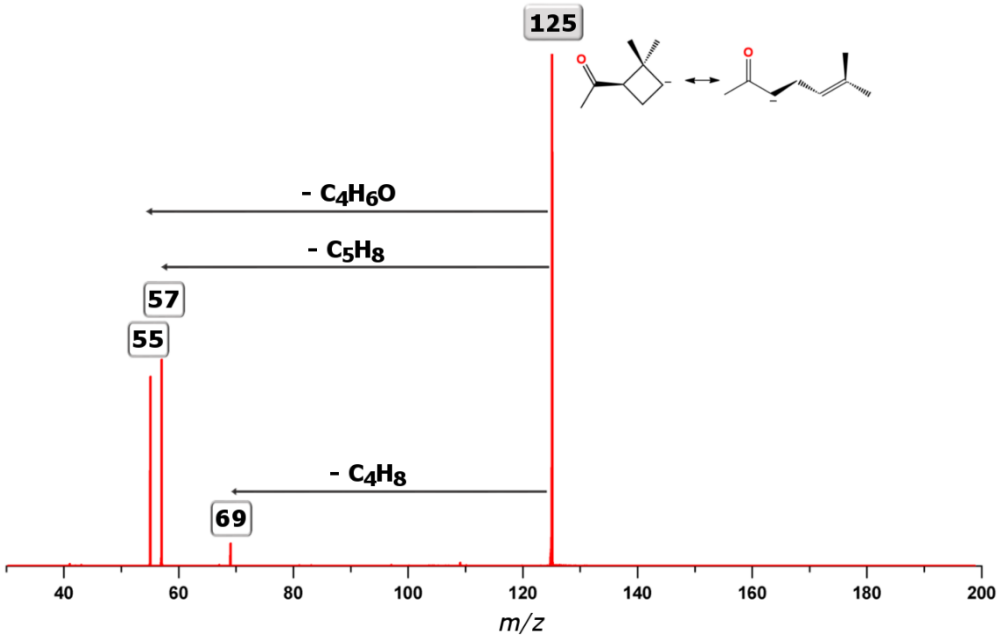


Figure S2. Fragment ion mass spectrum of $C_8H_{13}O^-$ (*m/z* 125) recorded with a ToF voltage of 3kV, taken at a collision energy of 4.1 eV (CM) with argon collision gas at nominal pressure of 3.54 $\times 10^{-4}$ mBar.

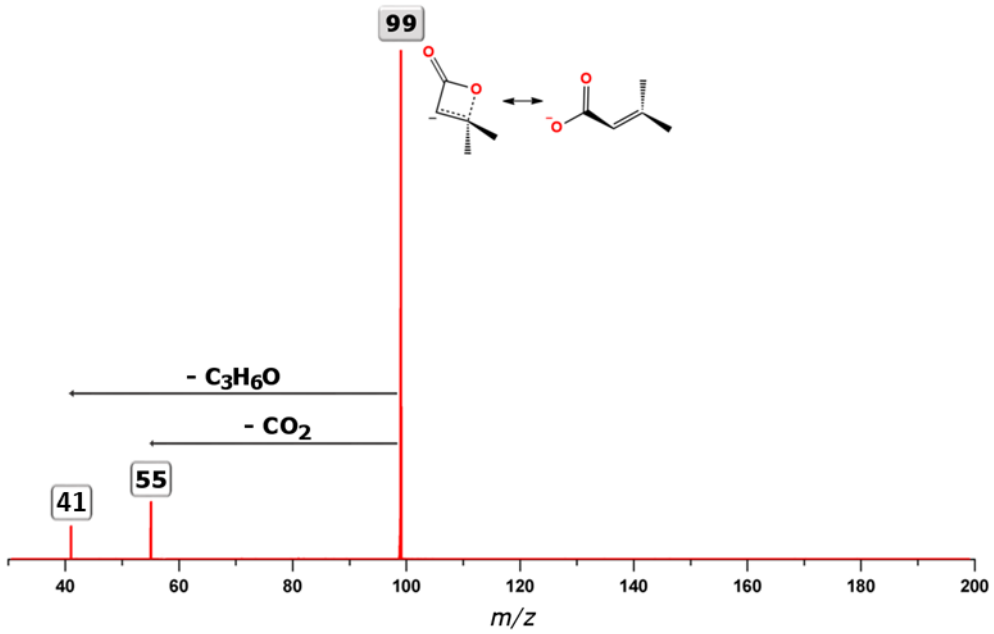


Figure S3. Fragment ion mass spectrum of $C_5H_7O_2^-$ (*m/z* 99) recorded with a ToF voltage of 3kV, taken at a collision energy of 4.3 eV (CM) with argon collision gas at nominal pressure of 3.54 ×10^{-4} mBar.

S3.2 Breakdown curves and extrapolation results

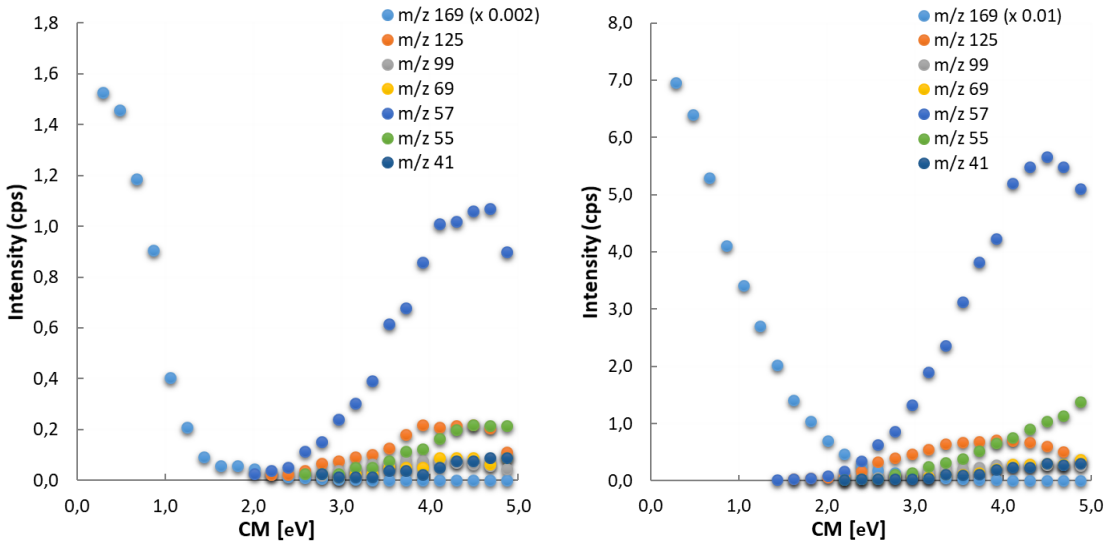


Figure S4. Breakdown curves for $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 1.06 × 10^{-4} mbar (left) and 2.08 × 10^{-4} mbar (right). The intensity of the *m/z* 169 anion have been multiplied by a scaling factor for readability.

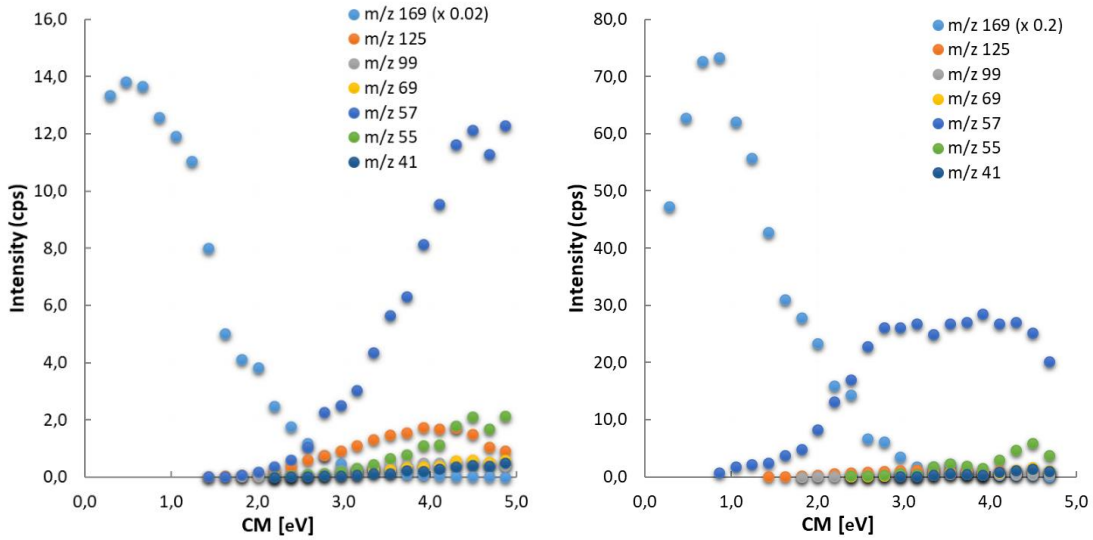


Figure S5. Breakdown curves for $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 3.04 × 10^{-4} mbar (left) and 4.18 × 10^{-4} mbar (right). The intensity of the *m/z* 169 anion have been multiplied by a scaling factor for readability.

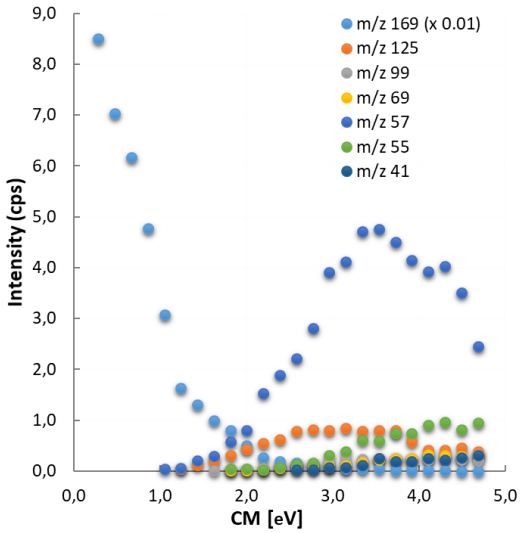


Figure S6. Breakdown curve for $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 5.09 × 10^{-4} mbar. The intensity of the *m/z* 169 anion have been multiplied by a scaling factor for readability.

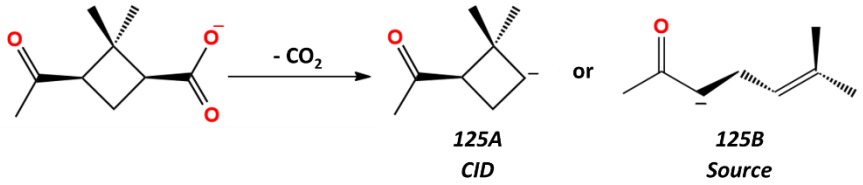


Figure S7. Decarboxylation of $C_9H_{13}O_3^-$ (*m/z* 169) ion leading to the formation of $C_8H_{13}O^-$ (*m/z* 125) ion. *Comment: From computational and experimental study is known that cyclic structure of m/z 125 (125A) is formed in collision-induced dissociation (CID) experiment, while linear structure of m/z 125 (125B) is formed in an ion source during ionization process.*

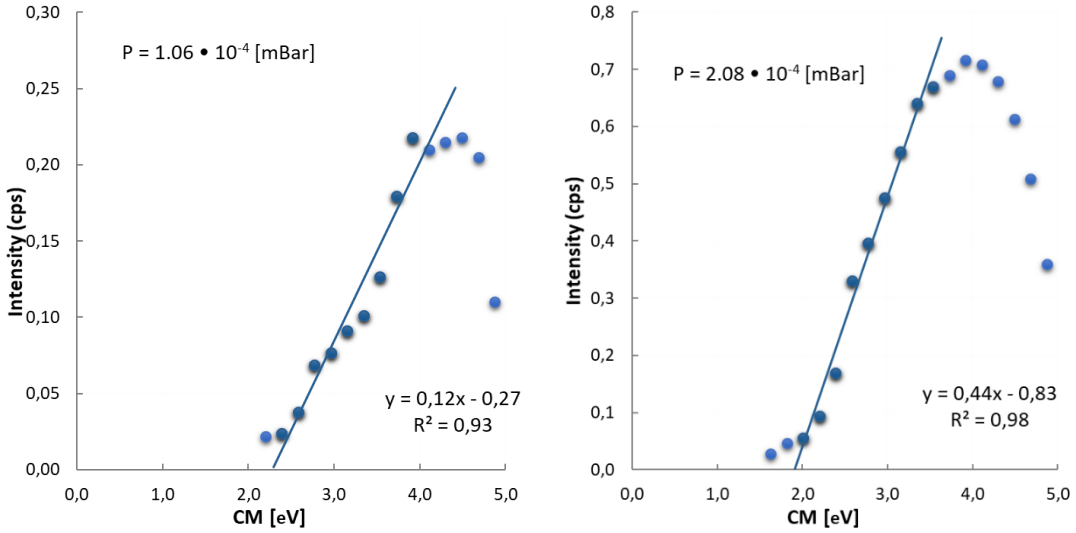


Figure S8. Extrapolation procedure for the decarboxylation of $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 1.06×10^{-4} mbar (left) and 2.08×10^{-4} mbar (right).

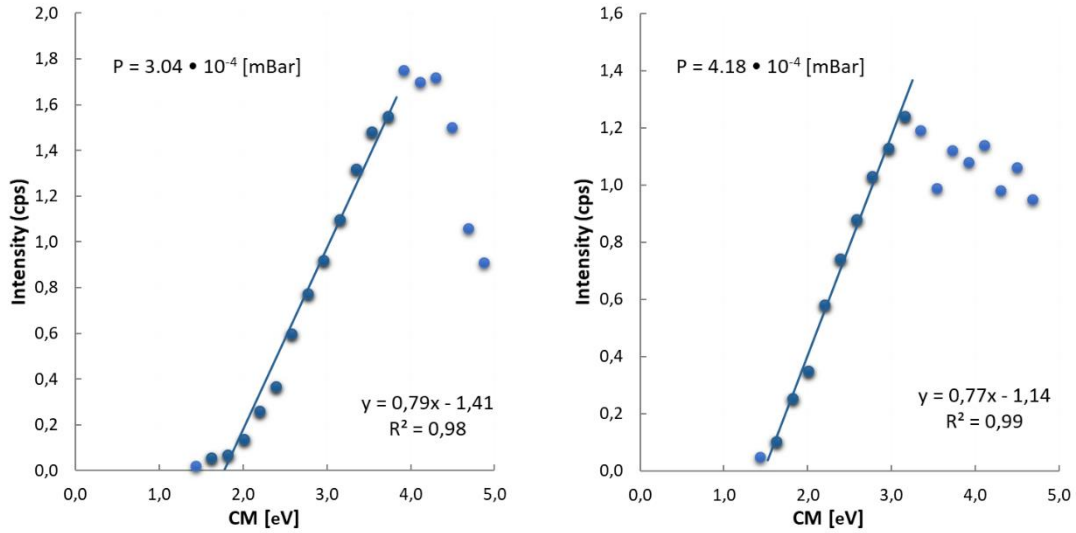


Figure S9. Extrapolation procedure for the decarboxylation of $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 3.04×10^{-4} mbar (left) and 4.18×10^{-4} mbar (right).

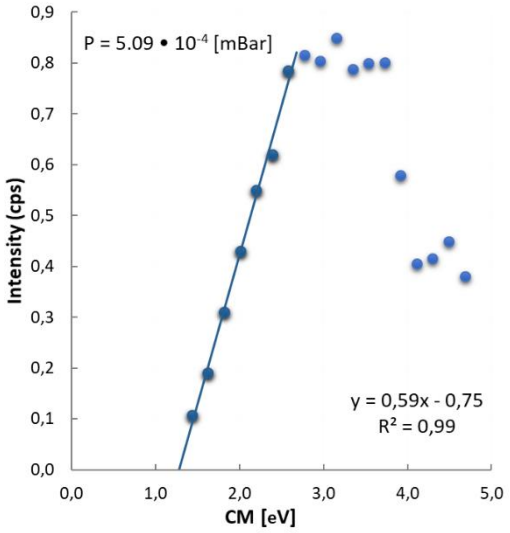


Figure S10. Extrapolation procedure for the decarboxylation of $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 5.09×10^{-4} mbar.

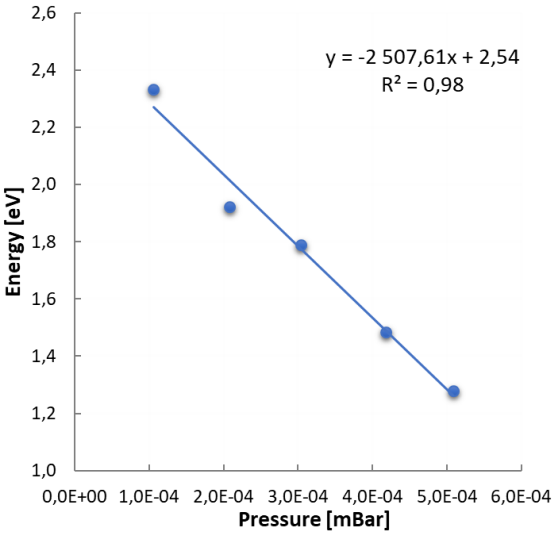


Figure S11. Extrapolation procedure for the decarboxylation of $C_9H_{13}O_3^-$ (*m/z* 169) at a gas pressure of 0 mbar.

Table S1. Summary of the values from the extrapolation procedure for decarboxylation of $C_9H_{13}O_3^-$ (*m/z* 169).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \cdot 10^{-4}$	-0.27	0.12	2,33	225
$2.08 \cdot 10^{-4}$	-0.83	0.44	1,92	186
$3.04 \cdot 10^{-4}$	-1.41	0.79	1,79	173
$4.18 \cdot 10^{-4}$	-1.12	0.77	1,49	143
$5.09 \cdot 10^{-4}$	-0.75	0.59	1,28	124
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-2507,61	2,54	2,54	245

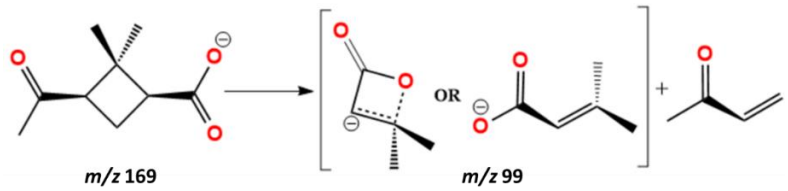


Figure S12. Elimination of C_4H_6O from $C_9H_{13}O_3^-$ (*m/z* 169) leading to the formation of $C_5H_7O_2^-$ (*m/z* 99) an ion, which can have two possible structure.

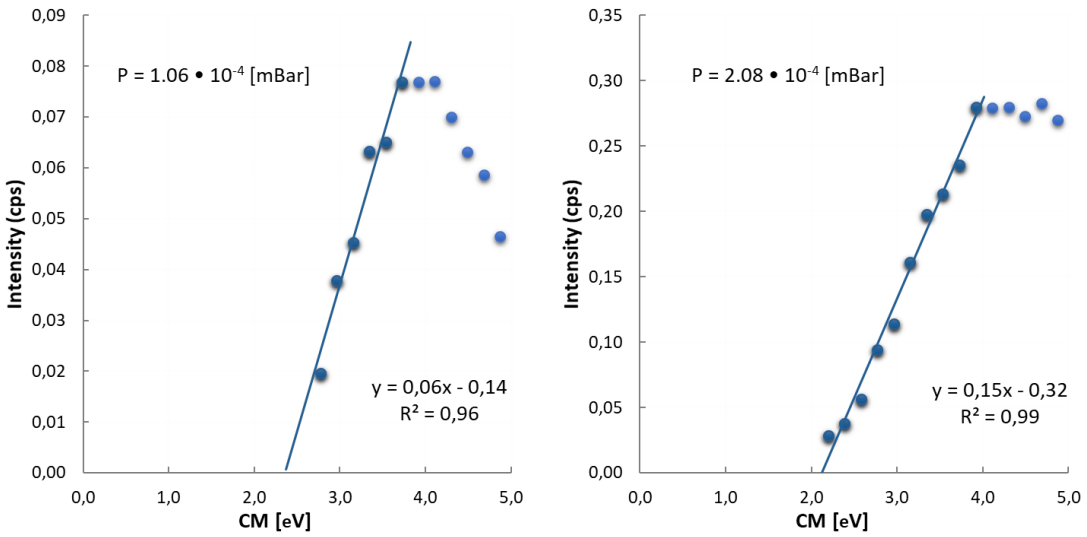


Figure S13. Extrapolation procedure for the elimination of C_4H_6O from $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 1.06×10^{-4} mbar (left) and 2.08×10^{-4} mbar (right).

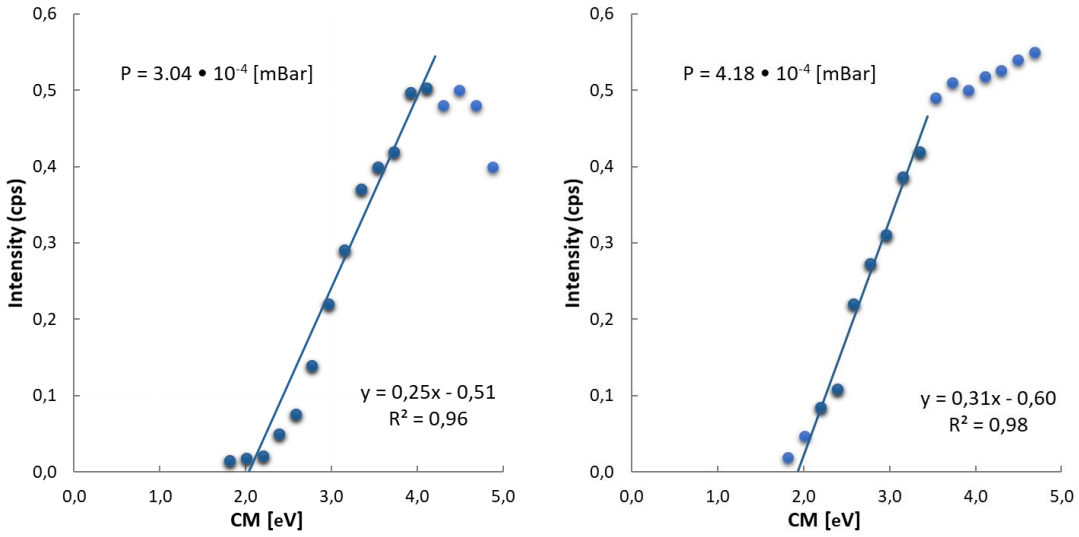


Figure S14. Extrapolation procedure for the elimination of C_4H_6O from $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 3.04×10^{-4} mbar (left) and 4.18×10^{-4} mbar (right).

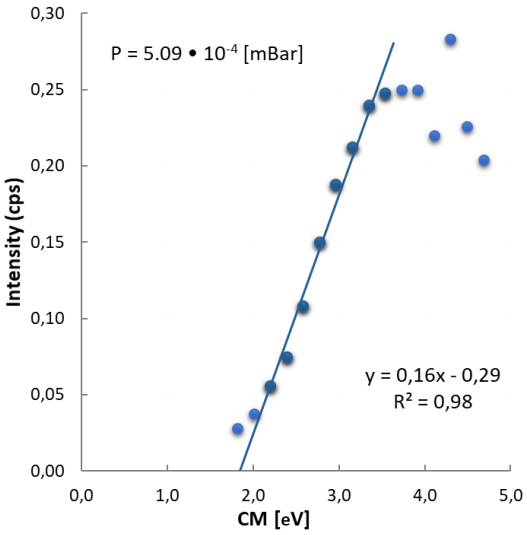


Figure S15. Extrapolation procedure for the elimination of C_4H_6O from $C_9H_{13}O_3^-$ (*m/z* 169) recorded at an argon collision gas pressure of 5.09×10^{-4} mbar.

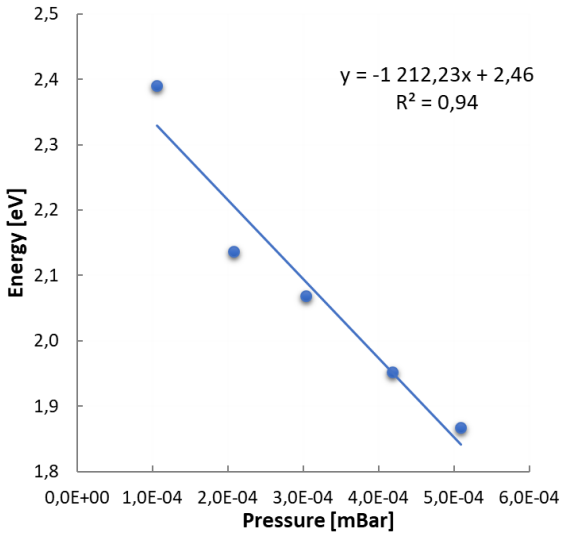


Figure S16. Extrapolation procedure for the elimination of C_4H_6O from $C_9H_{13}O_3^-$ (*m/z* 169) at a gas pressure of 0 mbar.

Table S2. Summary of the values from the extrapolation procedure for the elimination of C_4H_6O from $C_9H_{13}O_3^-$ (*m/z* 169).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \cdot 10^{-4}$	-0.14	0.06	2,39	231
$2.08 \cdot 10^{-4}$	-0.32	0.15	2,14	206
$3.04 \cdot 10^{-4}$	-0.51	0.25	2,07	200
$4.18 \cdot 10^{-4}$	-0.60	0.31	1,95	188
$5.09 \cdot 10^{-4}$	-0.29	0.16	1,87	180
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-1212,23	2,46	2,46	237

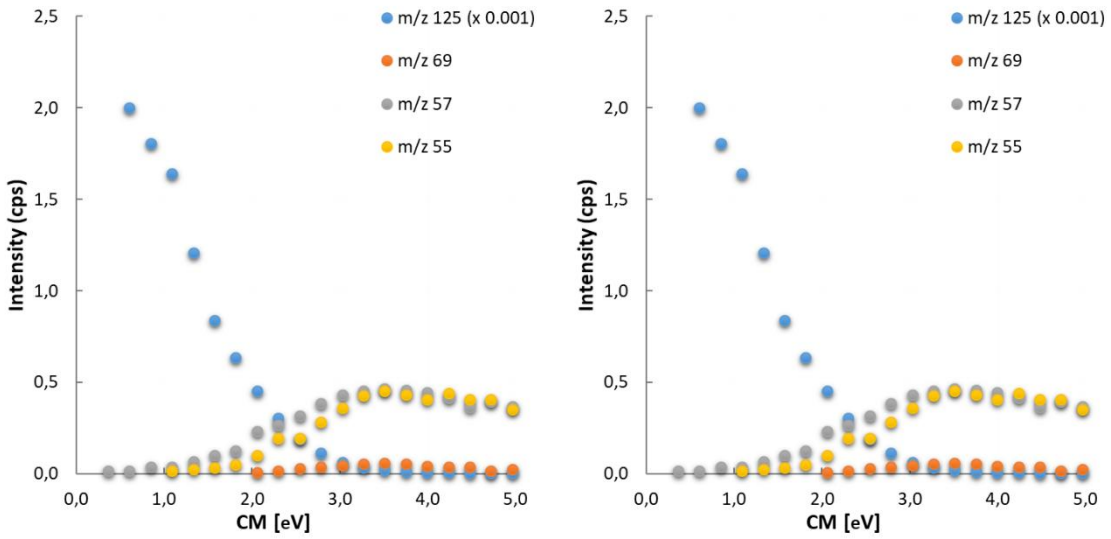


Figure S17. Breakdown curves for $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure of 1.06×10^{-4} mbar (left) and 2.05×10^{-4} mbar (right). The intensity of the *m/z* 125 anion have been multiplied by a scaling factor for readability.

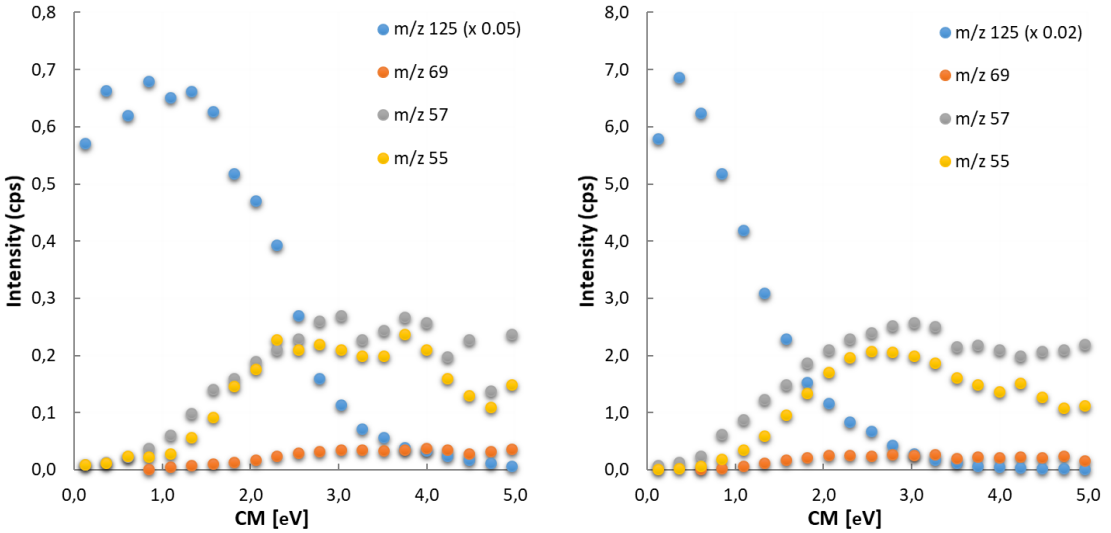


Figure S18. Breakdown curves for $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure of 3.17×10^{-4} mbar (left) and 4.14×10^{-4} mbar (right). The intensity of the *m/z* 125 anion have been multiplied by a scaling factor for readability.

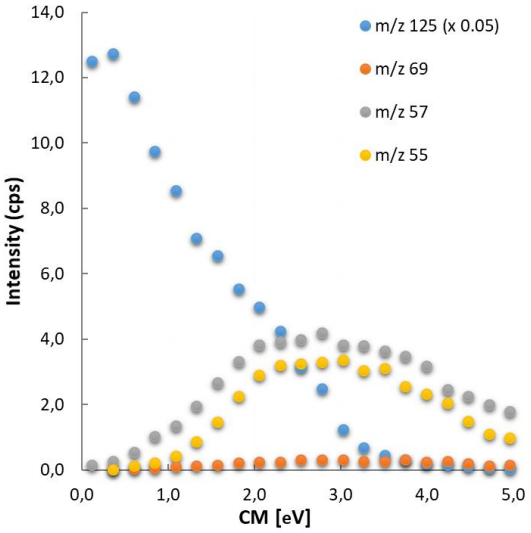


Figure S19. Breakdown curve for $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure of 5.07 × 10^{-4} mbar. The intensity of the *m/z* 125 anion have been multiplied by a scaling factor for readability.

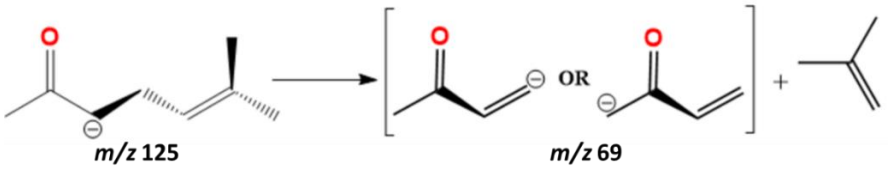


Figure S20. Elimination reaction of C_4H_8 from $C_8H_{13}O^-$ (*m/z* 125) leading to the formation of $C_4H_5O^-$ (*m/z* 69) an ion, which can have two possible structure.

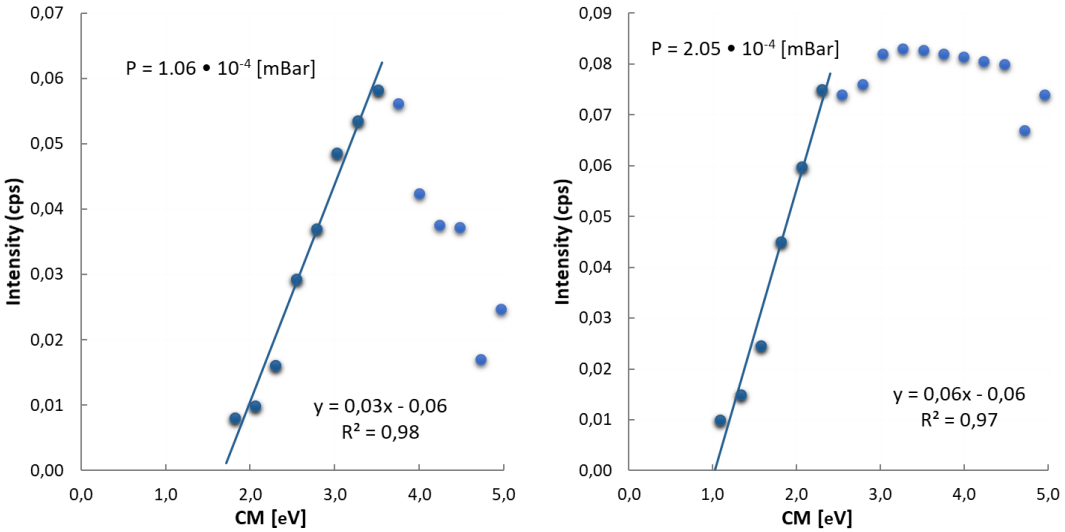


Figure S21. Extrapolation procedure for the elimination of C_4H_8 from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure gas pressure of 1.06 × 10^{-4} mbar (left) and 2.05 × 10^{-4} mbar (right).

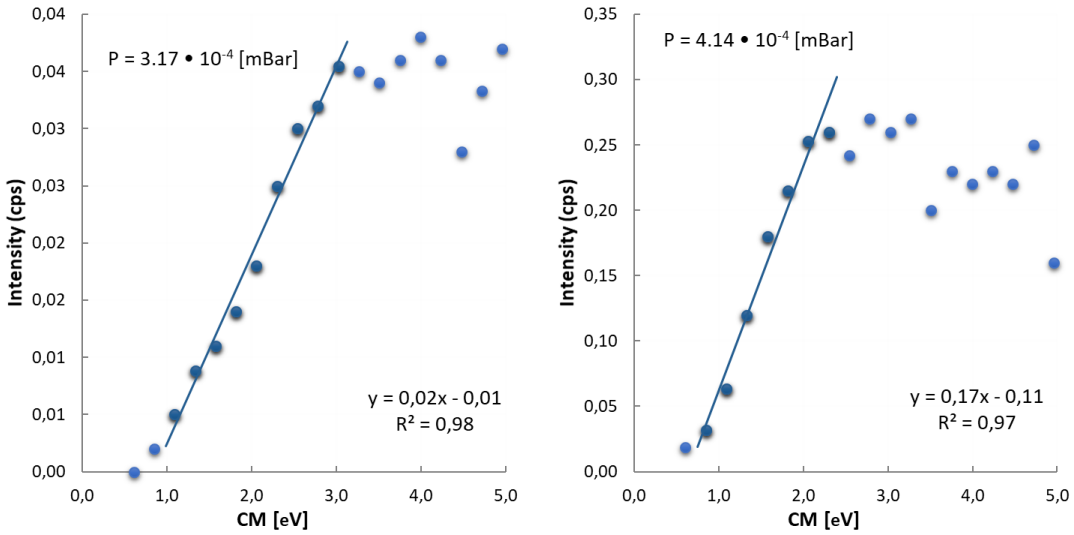


Figure S22. Extrapolation procedure for the elimination of C_4H_8 from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure 3.17×10^{-4} mbar (left) and 4.14×10^{-4} mbar (right).

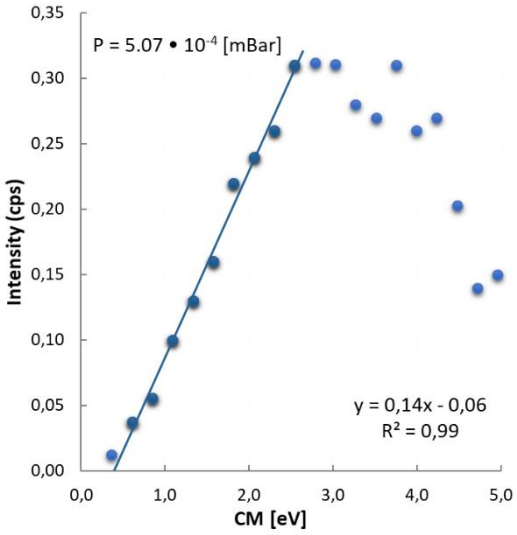


Figure S23. Extrapolation procedure the elimination of C_4H_8 from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure of 5.07×10^{-4} mbar.

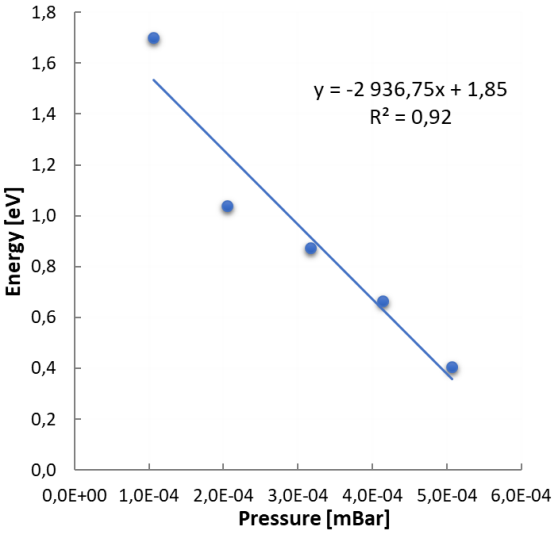


Figure S24. Extrapolation procedure for the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125) at a gas pressure of 0 mbar.

Table S3. Summary of the values from the extrapolation procedure for the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \bullet 10^{-4}$	-0.06	0.03	1,70	164
$2.05 \bullet 10^{-4}$	-0.06	0.06	1,04	100
$3.17 \bullet 10^{-4}$	-0.01	0.02	0,87	84
$4.14 \bullet 10^{-4}$	-0.11	0.17	0,66	64
$5.07 \bullet 10^{-4}$	-0.06	0.14	0,40	39
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-2936,75	1,85	1,85	178

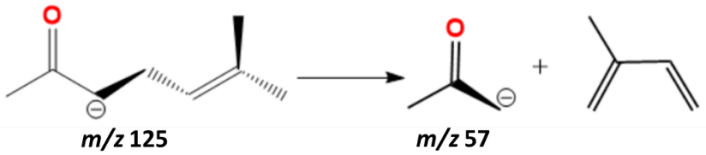


Figure S25. Elimination reaction of C_5H_8 from $C_8H_{13}O^-$ (*m/z* 125) leading to the formation of $C_3H_5O^-$ (*m/z* 57) an ion.

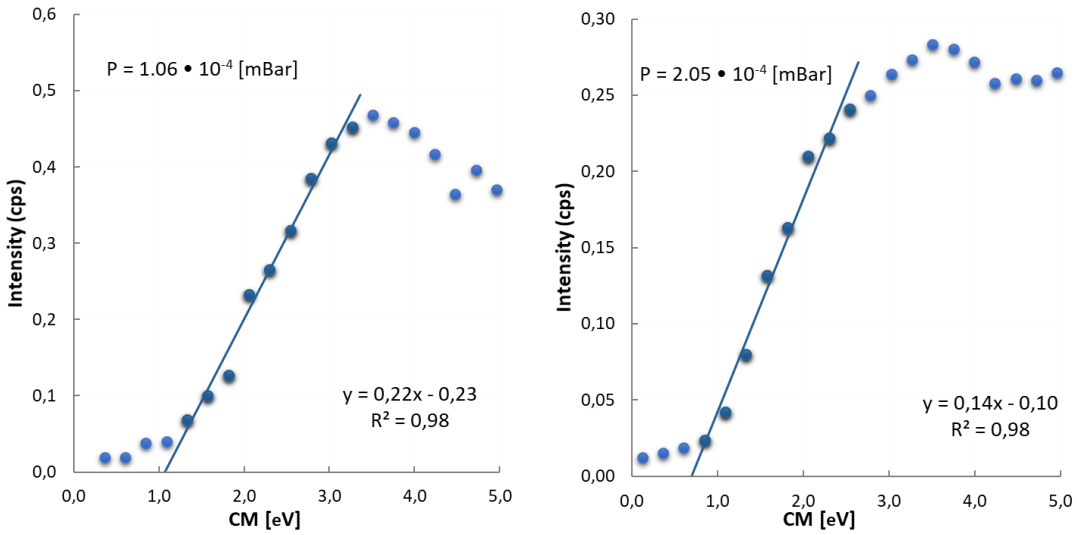


Figure S26. Extrapolation procedure for the elimination of C_5H_8 from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure gas pressure of 1.06×10^{-4} mbar (left) and 2.05×10^{-4} mbar (right).

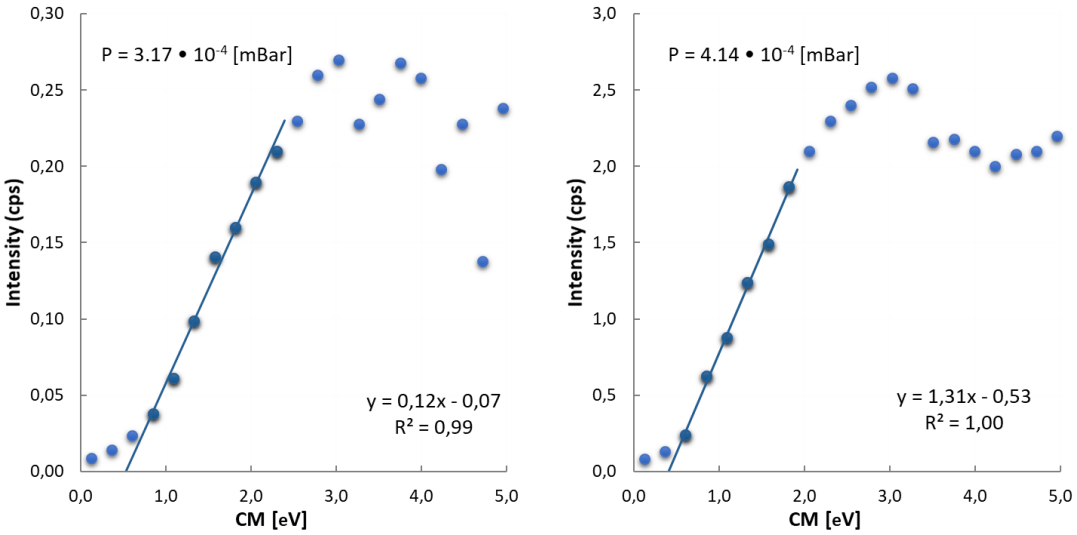


Figure S27. Extrapolation procedure for the elimination of C_5H_8 from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure 3.17×10^{-4} mbar (left) and 4.14×10^{-4} mbar (right).

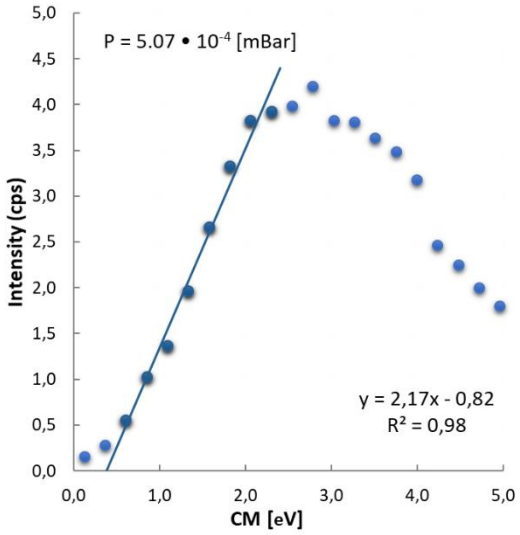


Figure S28. Extrapolation procedure the elimination of C_5H_8 from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure of 5.07×10^{-4} mbar.

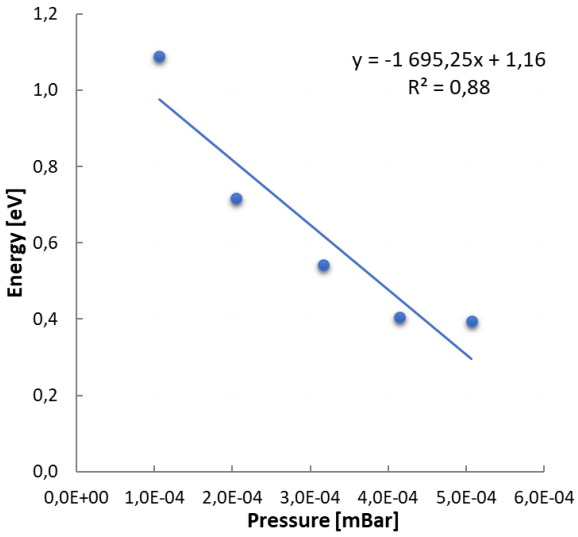


Figure S29. Extrapolation procedure for the elimination of C_5H_8 from $C_8H_{13}O^-$ (*m/z* 125) at a gas pressure of 0 mbar.

Table S4. Summary of the values from the extrapolation procedure for the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \cdot 10^{-4}$	-0.06	0.03	1,09	105
$2.05 \cdot 10^{-4}$	-0.06	0.06	0,72	69
$3.17 \cdot 10^{-4}$	-0.01	0.02	0,54	52
$4.14 \cdot 10^{-4}$	-0.11	0.17	0,41	39
$5.07 \cdot 10^{-4}$	-0.06	0.14	0,39	38
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-1695,25	1,16	1,16	111

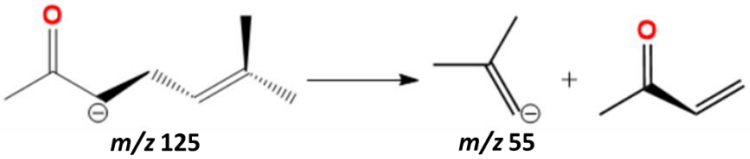


Figure S30. Elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125) leading to the formation of $C_4H_7^-$ (*m/z* 55) a ion.

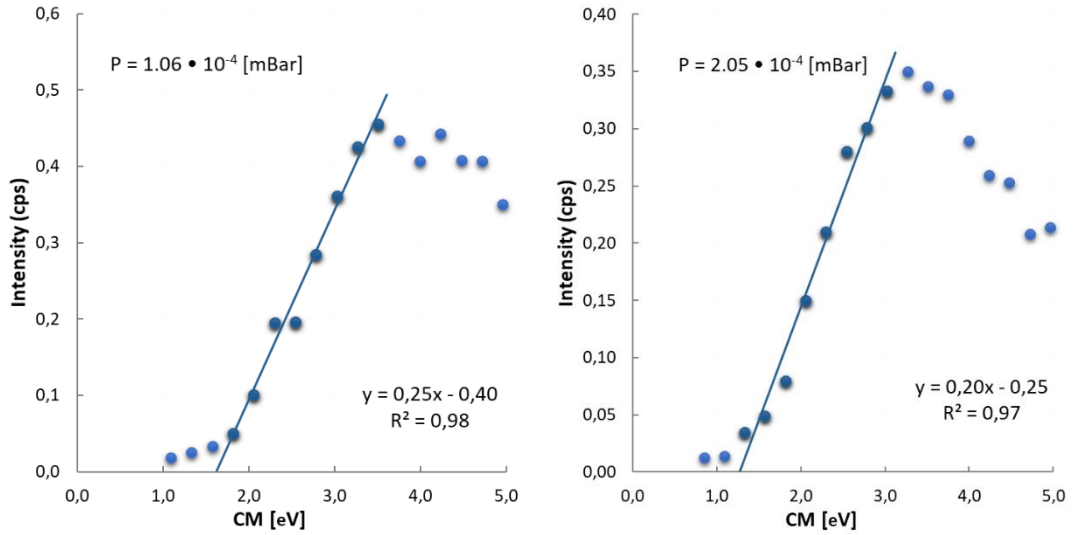


Figure S31. Extrapolation procedure for the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure gas pressure of 1.06×10^{-4} mbar (left) and 2.05×10^{-4} mbar (right).

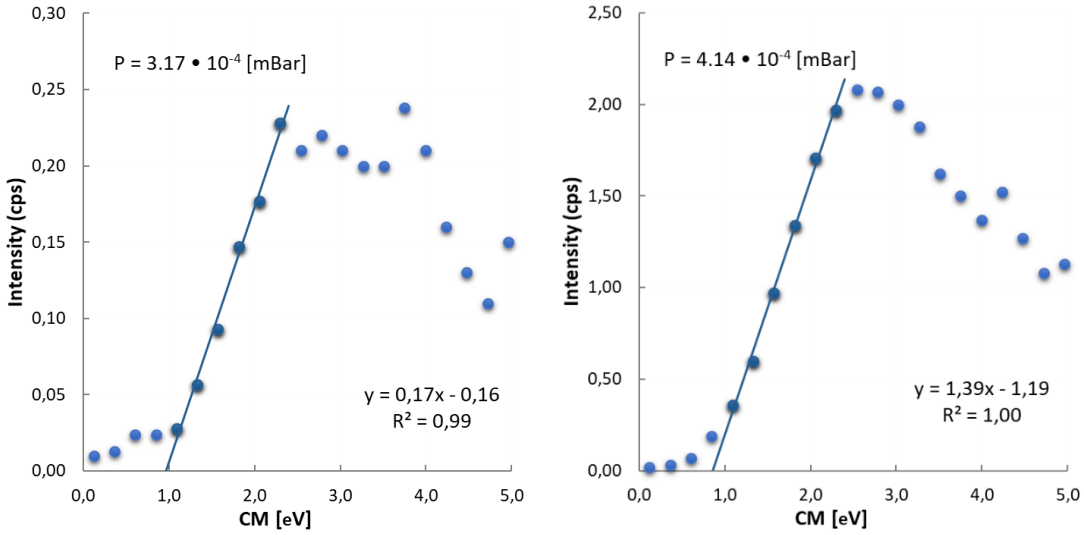


Figure S32. Extrapolation procedure for the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure 3.17×10^{-4} mbar (left) and 4.14×10^{-4} mbar (right).

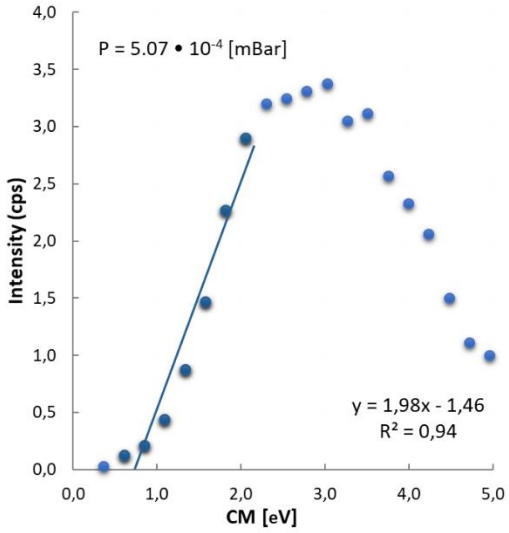


Figure S33. Extrapolation procedure the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125) recorded at an argon collision gas pressure of 5.07×10^{-4} mbar.

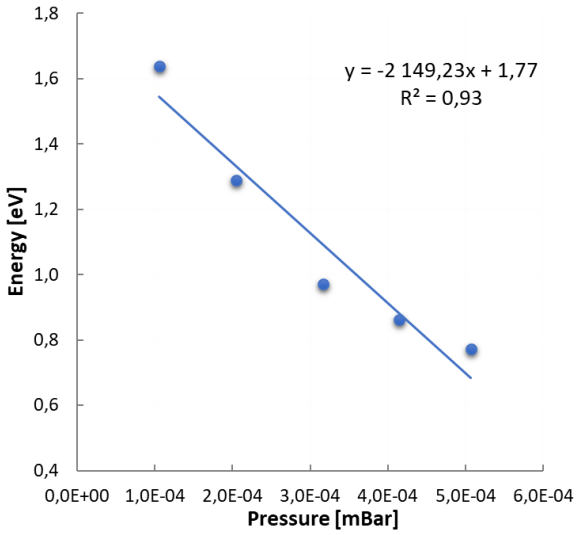


Figure S34. Extrapolation procedure for the elimination of C_5H_8 from $C_8H_{13}O^-$ (*m/z* 125) at a gas pressure of 0 mbar.

Table S5. Summary of the values from the extrapolation procedure for the elimination of C_4H_6O from $C_8H_{13}O^-$ (*m/z* 125).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \cdot 10^{-4}$	-0.40	0.17	1,64	158,03
$2.05 \cdot 10^{-4}$	-0.25	0.20	1,29	124,44
$3.17 \cdot 10^{-4}$	-0.16	0.17	0,97	93,79
$4.14 \cdot 10^{-4}$	-1.19	1.39	0,86	83,23
$5.07 \cdot 10^{-4}$	-1.46	1.98	0,77	74,46
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-2149,233	1,773	1,77	171

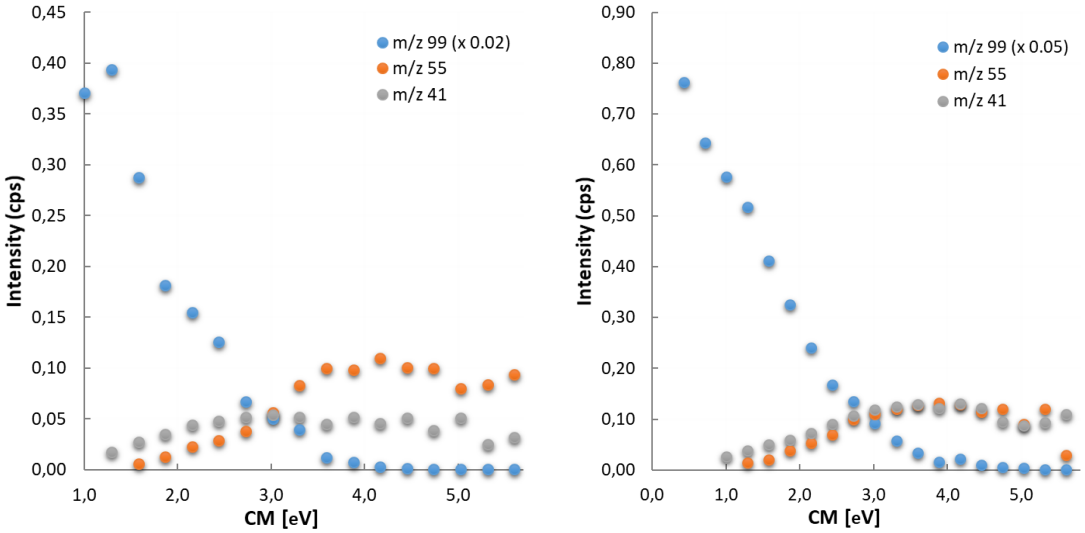


Figure S35. Breakdown curves for $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure of 1.06 × 10^{-4} mbar (left) and 2.06 × 10^{-4} mbar (right). The intensity of the *m/z* 99 anion have been multiplied by a scaling factor for readability.

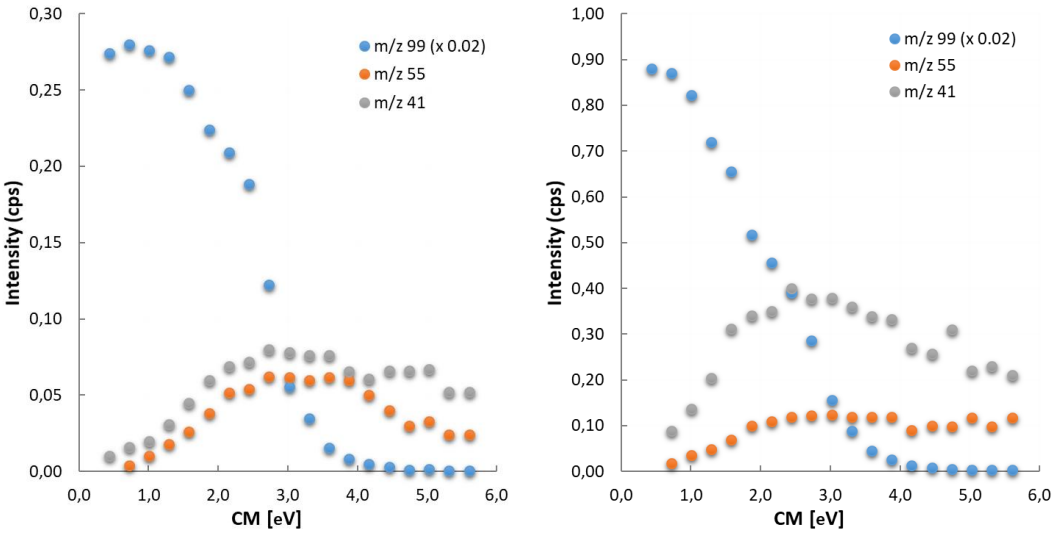


Figure S36. Breakdown curves for $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure of 3.20×10^{-4} mbar (left) and 4.16×10^{-4} mbar (right). The intensity of the *m/z* 99 anion have been multiplied by a scaling factor for readability.

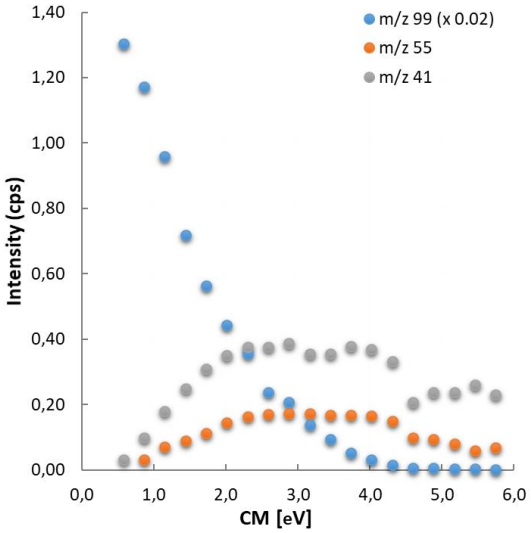


Figure S37. Breakdown curve for $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure of 5.11×10^{-4} mbar. The intensity of the *m/z* 99 anion have been multiplied by a scaling factor for readability.

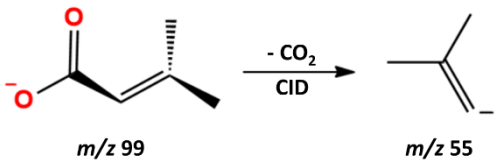


Figure S38. Decarboxylation reaction of $C_5H_7O_2^-$ (*m/z* 99) leading to the formation of $C_4H_7^-$ (*m/z* 55) an ion.

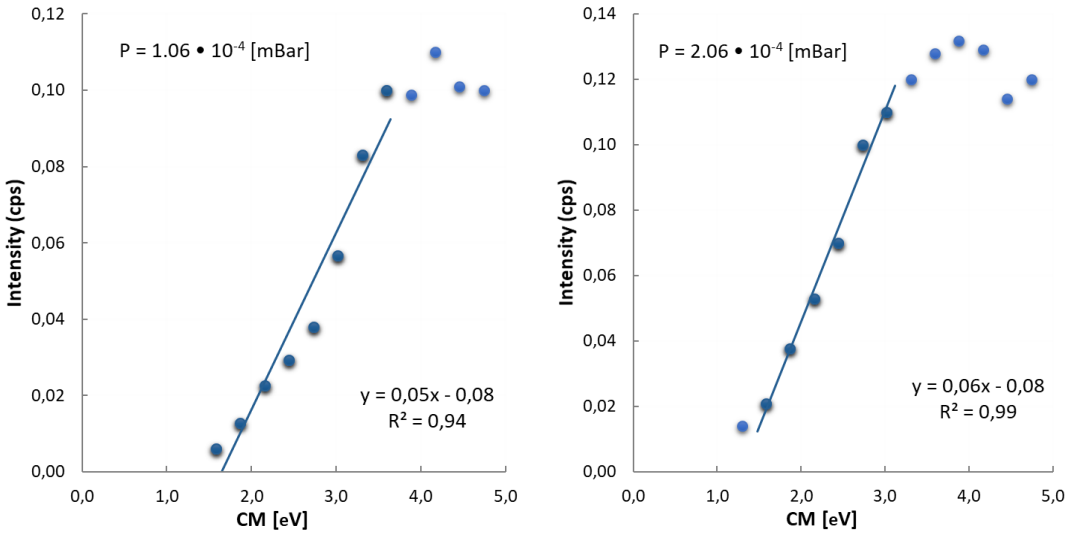


Figure S39. Extrapolation procedure for the decarboxylation of $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure gas pressure of 1.06×10^{-4} mbar (left) and 2.06×10^{-4} mbar (right).

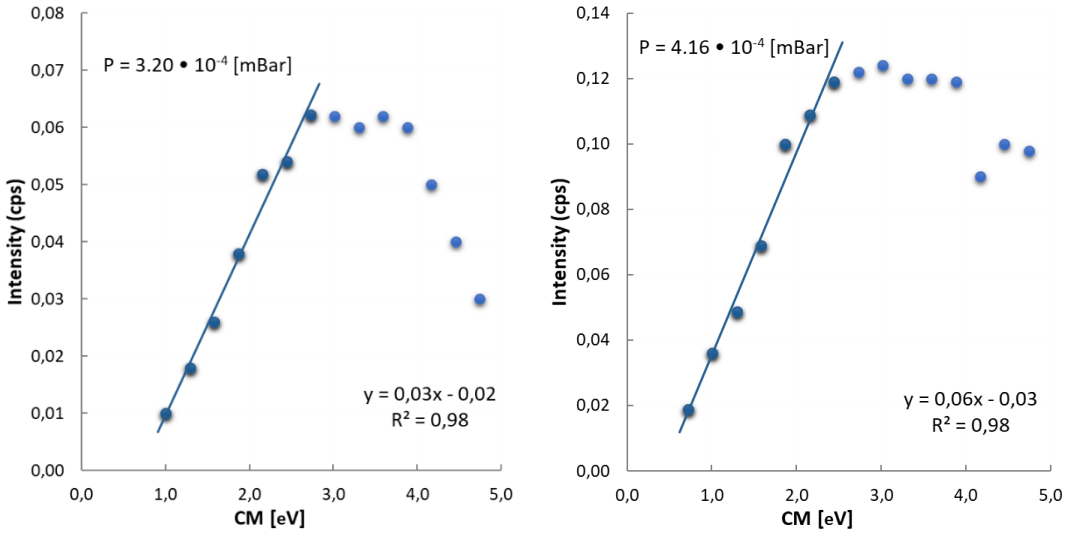


Figure S40. Extrapolation procedure for the decarboxylation of $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure gas pressure of 3.20×10^{-4} mbar (left) and 4.16×10^{-4} mbar (right).

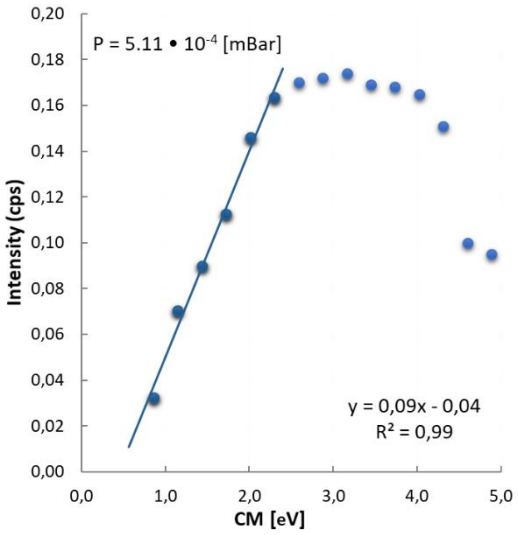


Figure S41. Extrapolation procedure for the decarboxylation of $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure gas pressure of 5.11×10^{-4} mbar.

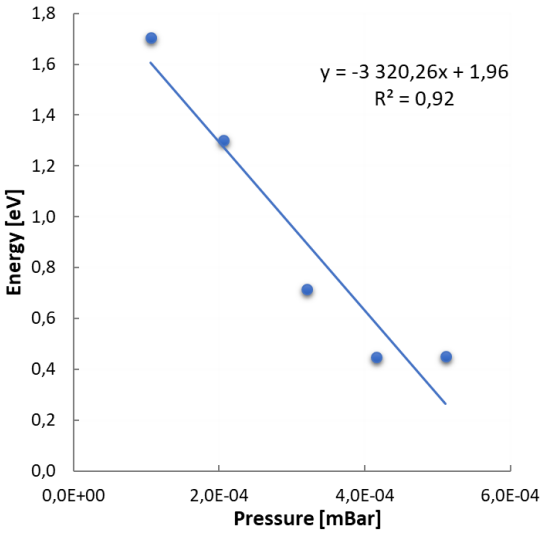


Figure S42. Extrapolation procedure for the decarboxylation of $C_5H_7O_2^-$ (*m/z* 99) at a gas pressure of 0 mbar.

Table S6. Summary of the values from the extrapolation procedure for the decarboxylation of $C_5H_7O_2^-$ (*m/z* 99).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \cdot 10^{-4}$	-0.27	0.12	1,70	164
$2.06 \cdot 10^{-4}$	-0.83	0.44	1,30	126
$3.20 \cdot 10^{-4}$	-1.41	0.79	0,72	69
$4.16 \cdot 10^{-4}$	-1.12	0.77	0,45	43
$5.11 \cdot 10^{-4}$	-0.75	0.59	0,45	44
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-3320,26	1,96	1,96	189

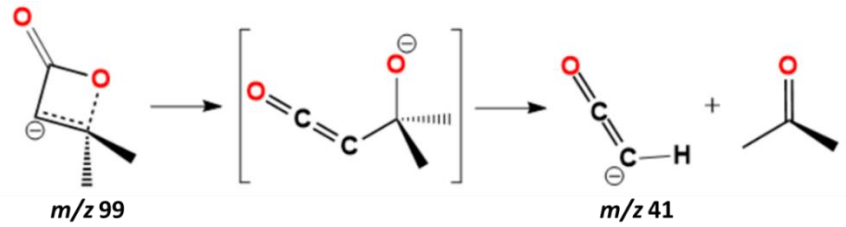


Figure S43. Elimination reaction of C_3H_6O from $C_5H_7O_2^-$ (*m/z* 99) leading to the formation of C_2HO^- (*m/z* 41) an ion.

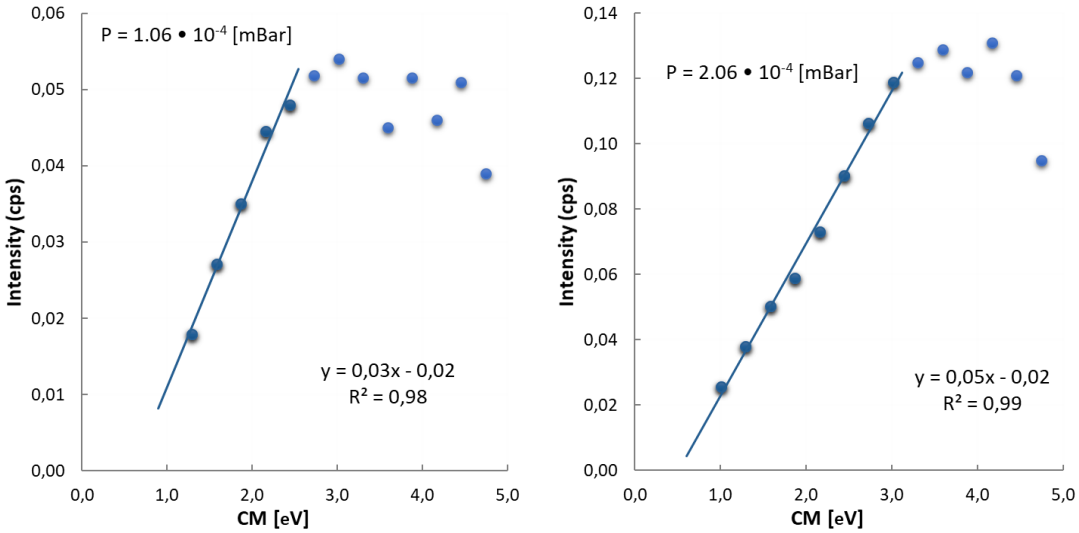


Figure S44. Extrapolation procedure for elimination of C_3H_6O from $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure gas pressure of 1.06×10^{-4} mbar (left) and 2.06×10^{-4} mbar (right).

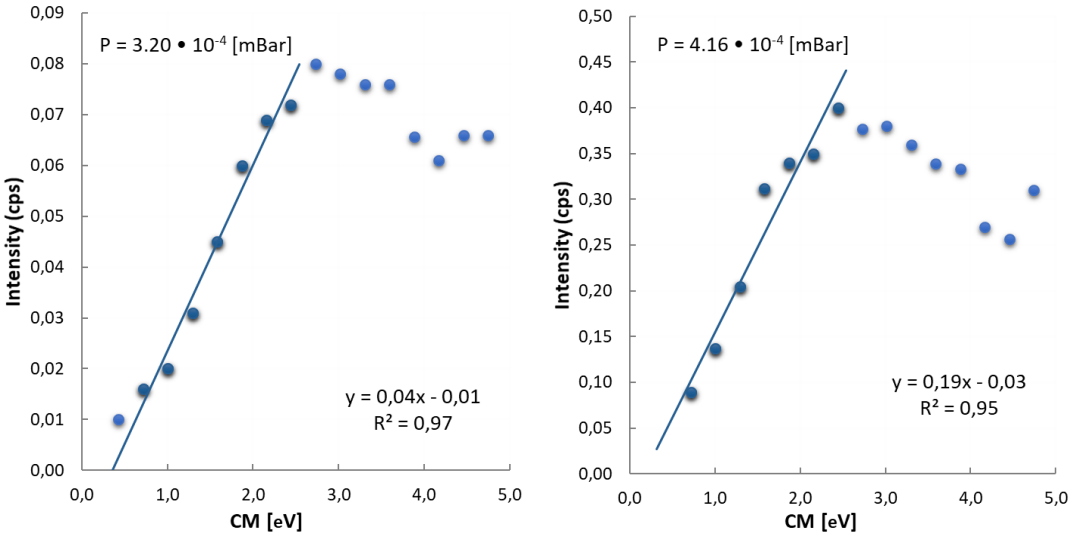


Figure S45. Extrapolation procedure for elimination of C_3H_6O from $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure gas pressure of 3.20×10^{-4} mbar (left) and 4.16×10^{-4} mbar (right).

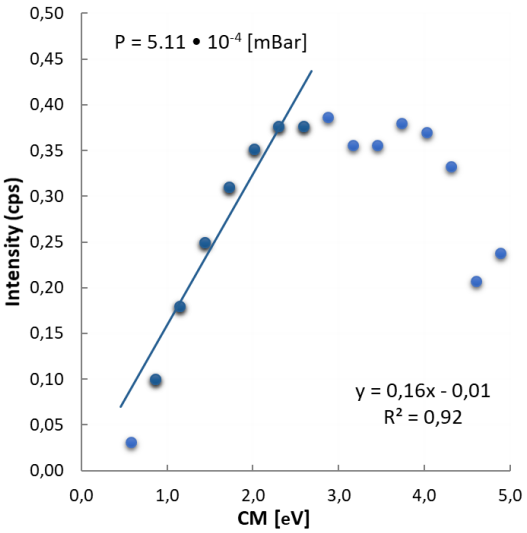


Figure S46. Extrapolation procedure for elimination of C_3H_6O from $C_5H_7O_2^-$ (*m/z* 99) recorded at an argon collision gas pressure gas pressure of 5.11×10^{-4} mbar.

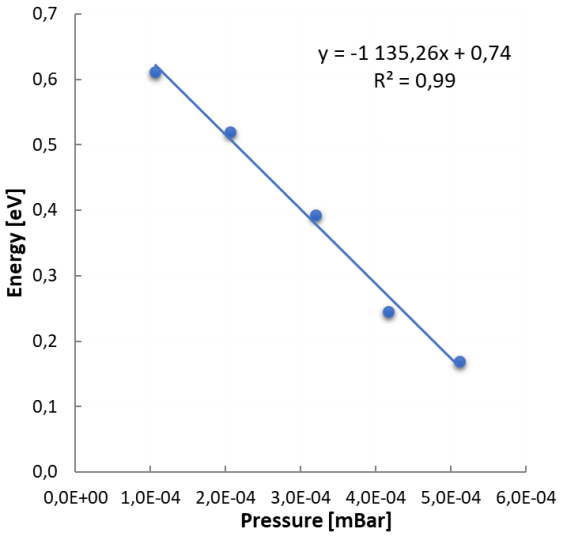


Figure S47. Extrapolation procedure for elimination of C_3H_6O from $C_5H_7O_2^-$ (*m/z* 99) at a gas pressure of 0 mbar.

Table S7. Summary of the values from the extrapolation procedure for elimination of C_3H_6O from $C_5H_7O_2^-$ (*m/z* 99).

Pressure [mBar]:	Intercept	Slope	X at Y=0 [eV]	[kJ/mol]
$1.06 \cdot 10^{-4}$	-0.02	0.03	0,61	59
$2.06 \cdot 10^{-4}$	-0.02	0.05	0,52	50
$3.20 \cdot 10^{-4}$	-0.01	0.04	0,39	38
$4.16 \cdot 10^{-4}$	-0.03	0.19	0,25	24
$5.11 \cdot 10^{-4}$	-0.01	0.16	0,17	16
Extrapolated pressure [mBar]:	Intercept	Slope	Y at X=0 [eV]	[kJ/mol]
0	-1135,26	0,74	0,74	72

S3.3 Reactions with dimethyl disulfide (CH_3SSCH_3)

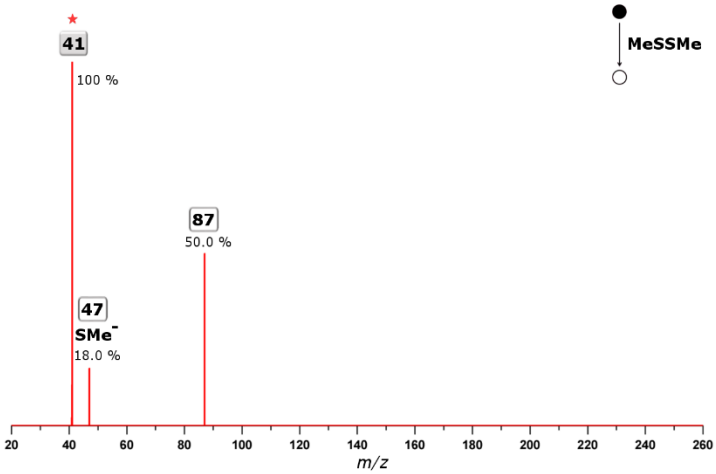


Figure S48. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and C_2HO^- (*m/z* 41) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.7 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar.

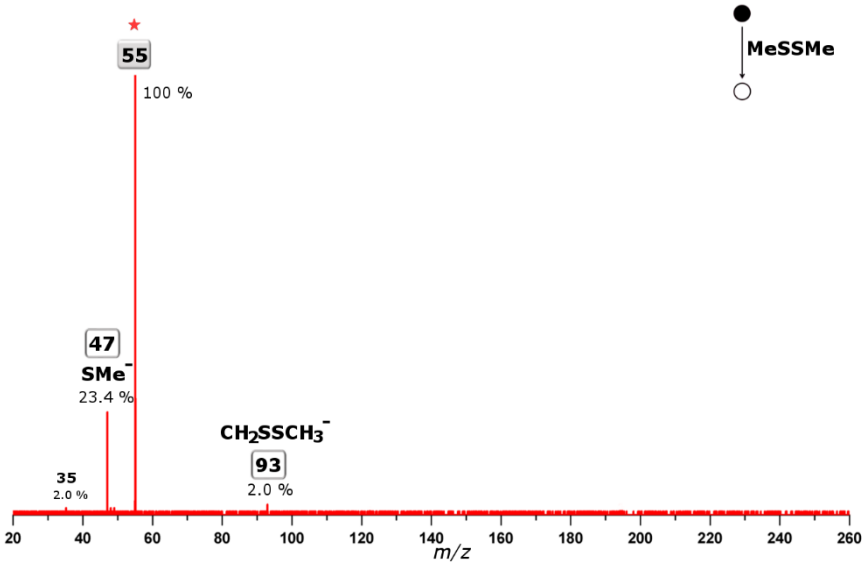


Figure S49. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and $C_4H_7^-$ (*m/z* 55) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.63 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar.

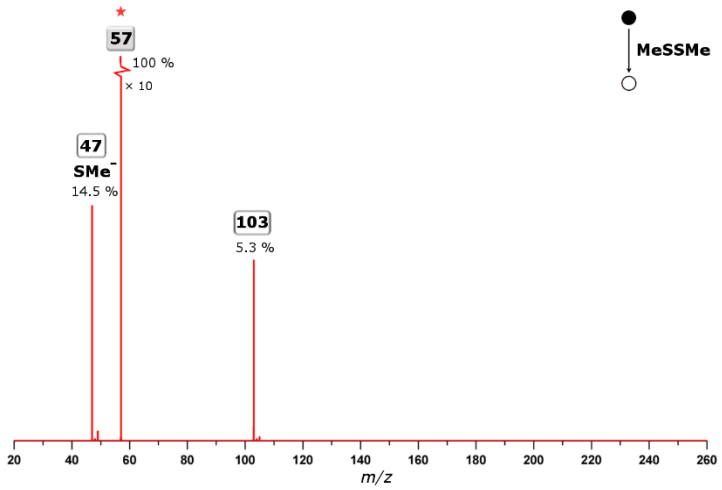


Figure S50. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and $C_3H_5O^-$ (*m/z* 57) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.62 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar.

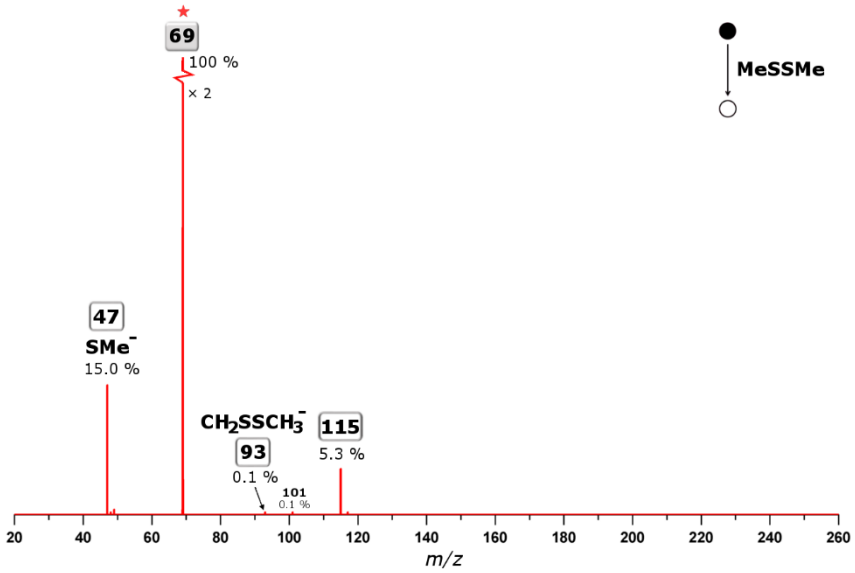


Figure S51. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and $C_4H_5O^-$ (*m/z* 69B) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.62 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar.

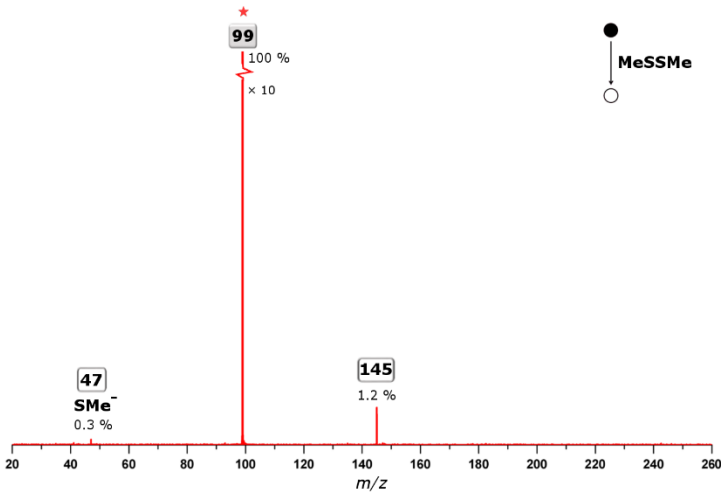


Figure S52. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and $C_5H_6O_2^-$ (*m/z* 99) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.49 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar.

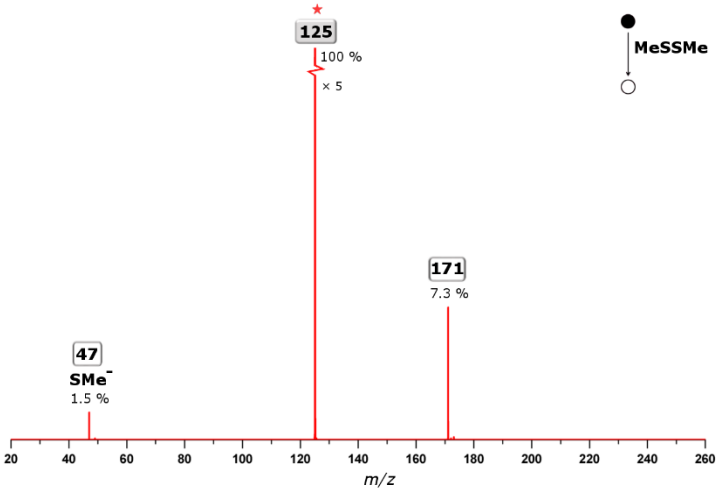


Figure S53. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and $C_8H_{13}O^-$ (*m/z* 125) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.43 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar.

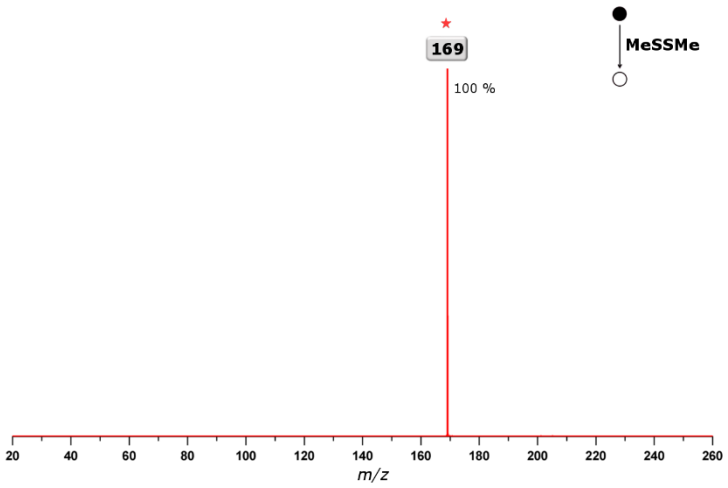


Figure S54. Mass spectrum of the reaction between dimethyl disulfide (CH_3SSCH_3) and $C_9H_{13}O_3^-$ (*m/z* 169) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.36 eV (CM) with reagent vapors at nominal pressures of 3.43×10^{-4} mBar. Please note the lack of the product in this reaction.

S3.4 Reactions with methyl thiocyanate (CH_3SCN)

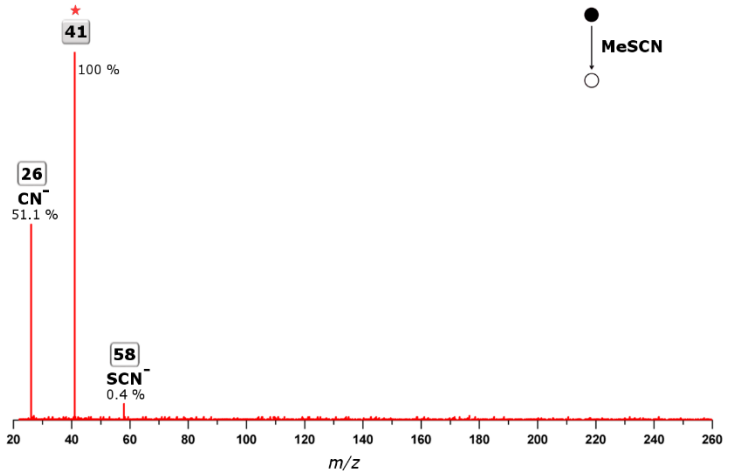


Figure S55. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and C_2HO^- (*m/z* 41) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.64 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

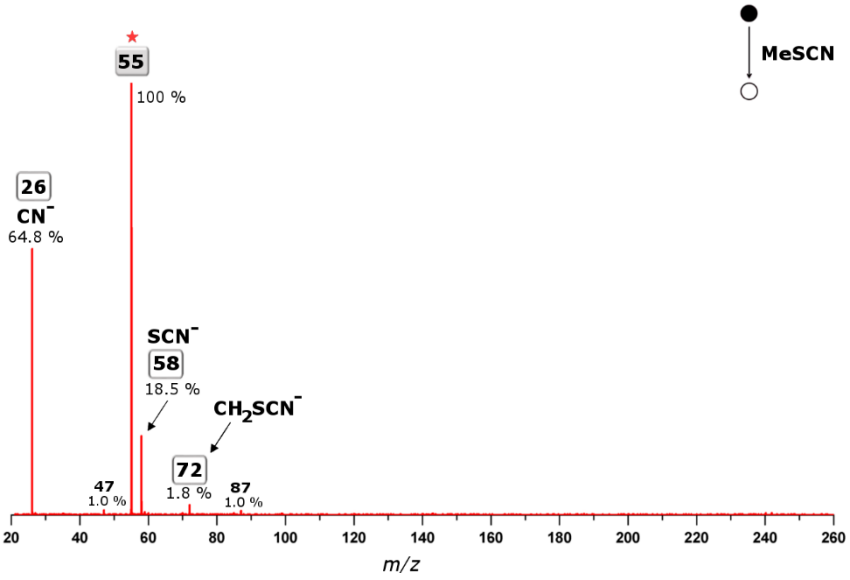


Figure S56. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and $C_4H_7^-$ (*m/z* 55) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.57 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

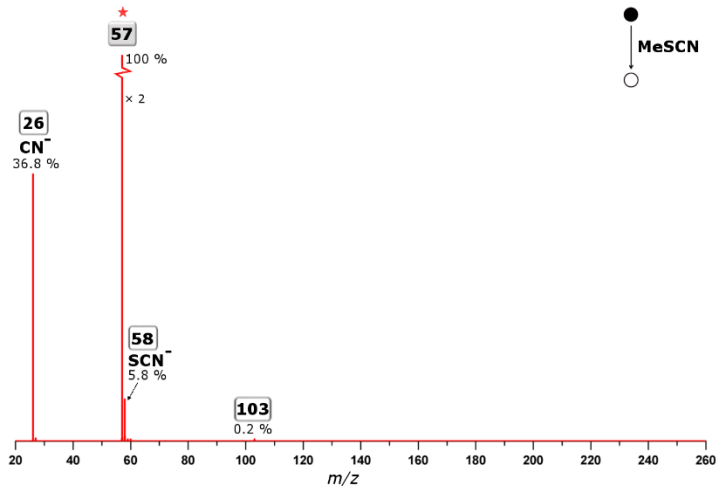


Figure S57. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and $C_3H_5O^-$ (*m/z* 57) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.56 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

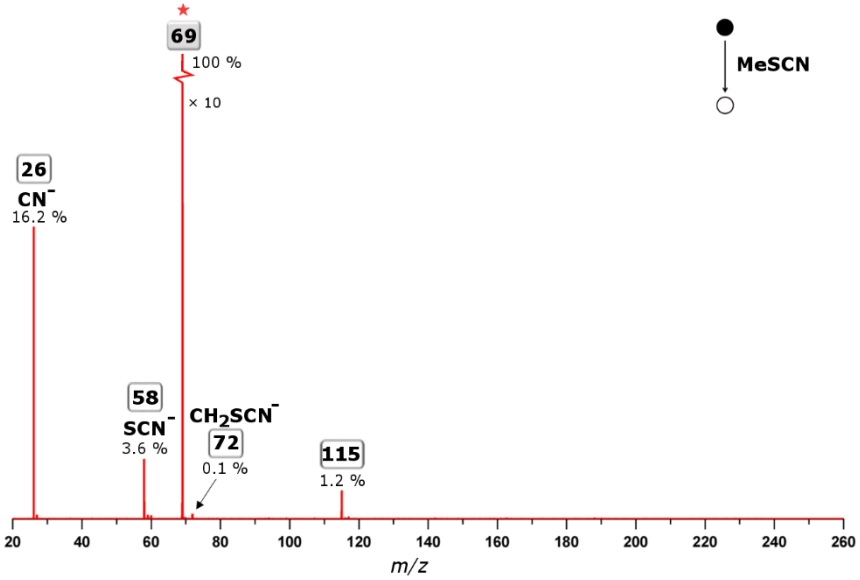


Figure S58. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and $C_4H_5O^-$ (*m/z* 69B) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.51 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

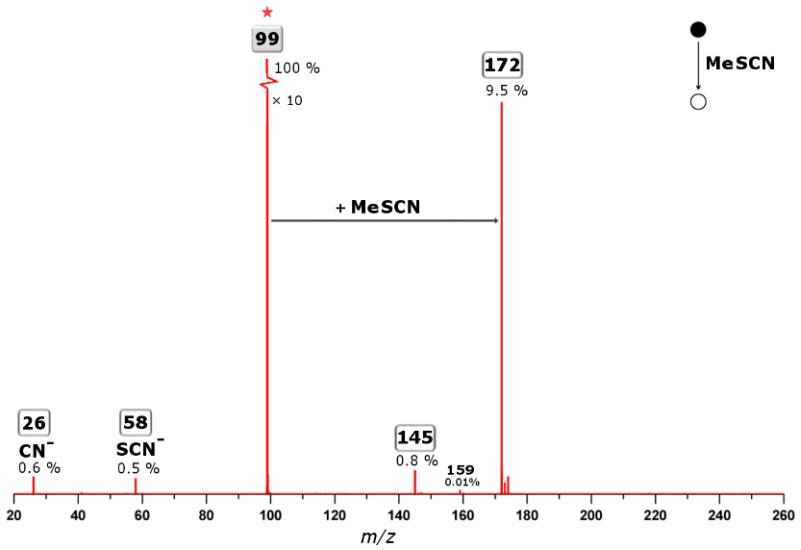


Figure S59. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and $C_5H_6O_2^-$ (*m/z* 99) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.42 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

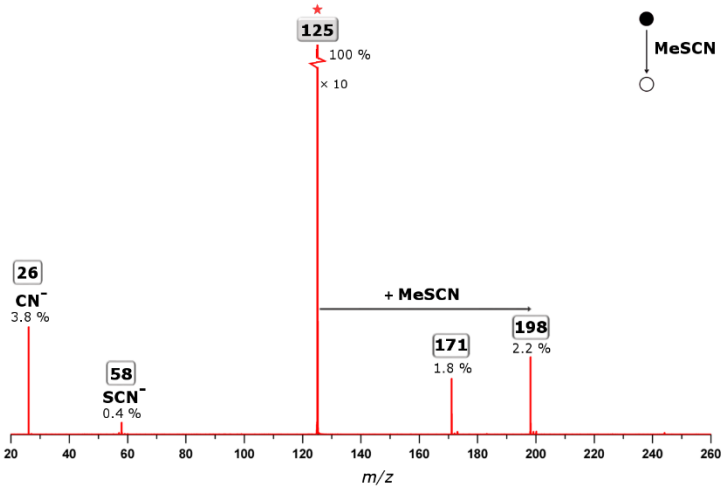


Figure S60. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and $C_8H_{13}O^-$ (*m/z* 125) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.37 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

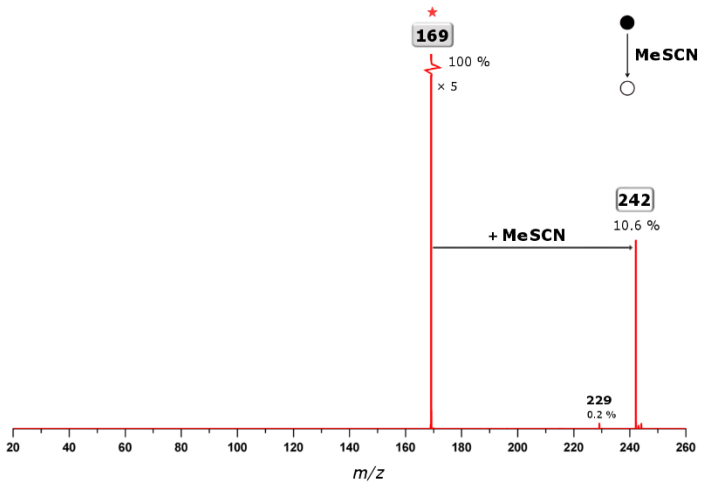


Figure S61. Mass spectrum of the reaction between methyl thiocyanate (CH_3SCN) and $C_9H_{13}O_3^-$ (*m/z* 169) recorded with a ToF voltage of 3kV, taken at a collision energy of 0.30 eV (CM) with reagent vapors at nominal pressures of 1.53×10^{-4} mBar.

S4. Computed data for norpinonic acid

The mathematical models used for calculations in Gaussian 09 are called FEM (Final Element Method) and Symplex. These methods cut an N-dimensional space into small subsystems that can be described by N linear equations. The equations can be solved when the solution of at least one of them is known. Therefore, the programme guesses the solution of one and then recursively solves all the others. Once all solutions are obtained, the initial guess can be modified and the calculation repeated. This process is performed until the new solution gives the same result as the previous iteration, which is called convergence. Among other things, the chosen basis set influences the quality of the guesswork, while the theoretical model influences the type of calculations the matrixes will undergo *(Tomberg, A., 2013, Gaussian 09W Tutorial, an Introduction to Computational Chemistry Using G09W and Avogadro Software).*

Because density functional methods are best regarded as approximations to the resolving for the electron density in a molecular system and the exact exchange correlation function is not known, comparative analysis of different DFT models in terms of performance is an important part of computational chemistry. Quite often, one particular set of functionals and functional bases works very well for a particular application, so for the study of structures not precisely described by quantum chemistry, calculations should be carried out with various functionals to get closer to experimental results.

CAM-B3LYP (Becke Three-Parameter Hybrid Functionals) long-range-corrected version of B3LYP, uses the non-local correlation provided by the LYP expression, which contains both local and non-local terms *(Axel D. Becke; Density-functional thermochemistry. III. The role of exact exchange. J. Chem. Phys. 1 April 1993; 98 (7): 5648–5652. https://doi.org/10.1063/1.464913; T. Yanai, D. Tew, and N. Handy, "A new hybrid exchange-correlation functional using the Coulomb-attenuating method (CAM-B3LYP)," Chem. Phys. Lett., 393 (2004) 51-57. https://doi.org/10.1016/j.cplett.2004.06.011).*

ωB97XD is the latest functional from Chai and Head-Gordon includes long-range exact exchange, a small fraction of short-range exact exchange, a modified exchange density functional for short-range interaction, the correlation density functional and empirical dispersion corrections. *(J.-D. Chai and M. Head-Gordon, "Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections," Phys. Chem. Chem. Phys., 10 (2008) 6615-20. https://doi.org/10.1039/B810189B).*

PBE1PBE Perdew, Burke and Ernzerhof's 1996 basic function, transformed into a hybrid function by Adamo. This function uses 25% exact exchange and 75% DFT exchange *(J. P. Perdew, K. Burke, and*

M. Ernzerhof, "Generalized gradient approximation made simple," Phys. Rev. Lett., 77 (1996) 3865-68. https://doi.org/10.1103/PhysRevLett.77.3865; C. Adamo and V. Barone, "Toward reliable density functional methods without adjustable parameters: The PBE0 model," J. Chem. Phys., 110 (1999) 6158-69. DOI: 10.1063/1.478522).

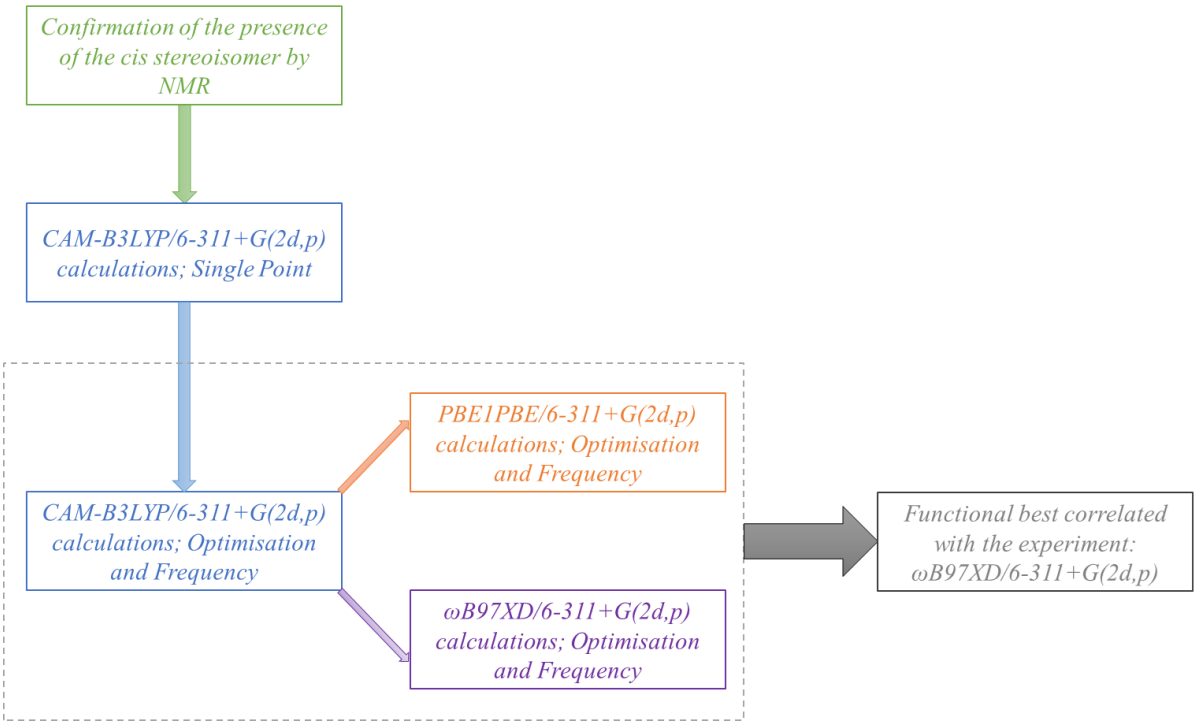


Figure S62. A schematic representation of the strategy used to determine the functional.

S4.1 Computated fragmentation pathways

Table S8. Calculated electron energy values in kJ/mol for fragmentation reaction *of m/z* 169 anion.

	Theoretical method		
Structure	**CAM-B3LYP/ 6-311+G(2d,p)**	**PBE1PBE/ 6-311+G(2d,p)**	**ωB97XD/ 6-311+G(2d,p)**
TS_1	307	300	322
TS_2	266	287	301
TS_3	247	241	274
TS_4	176	172	197
TS_5	279	290	304
TS_6	273	294	304
TS_7	256	278	289
TS_8	170	181	201
TS_9	177	164	187
TS_10	178	171	198
TS_11	264	288	304
TS_12	302	318	341
TS_13	275	285	304
CX_99	158	169	187
CX_125B	254	280	288

IC_125B	119	103	143
IC_125C	100	96	120
IC_169	82	79	90

Table S9. Calculated electron energy values and experimental values in kJ/mol for fragmentation reaction of *m/z* 169 anion.

		Theoretical method			
		CAM-B3LYP/ 6-311+G(2d,p)	**PBE1PBE/ 6-311+G(2d,p)**	**ωB97XD/ 6-311+G(2d,p)**	**Experimental energy**
Fragmentation reaction	169 → 99	200	205	216	245
	99 → 55	246	246	252	189
	99 → 41	75	67	91	72
	169 → 125	265	272	272	237
	125 → 69	183	185	200	178
	125 → 57	103	93	97	111
	125 → 55	258	262	257	187

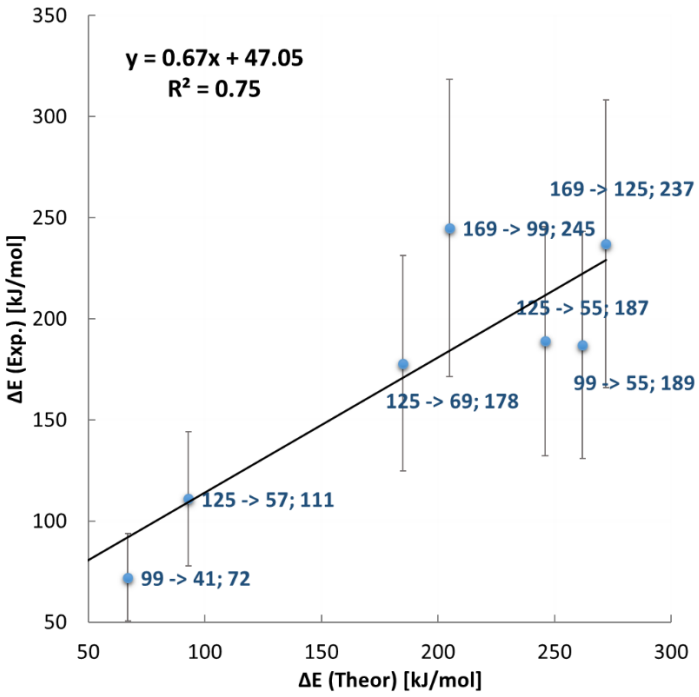


Figure S63. A correlation between the theoretical and the experimental results obtained with PBE1PBE/6-311+g(2d,p) level of theory. Experimental threshold energies as a function of the theoretical threshold energies (kJ/mol).

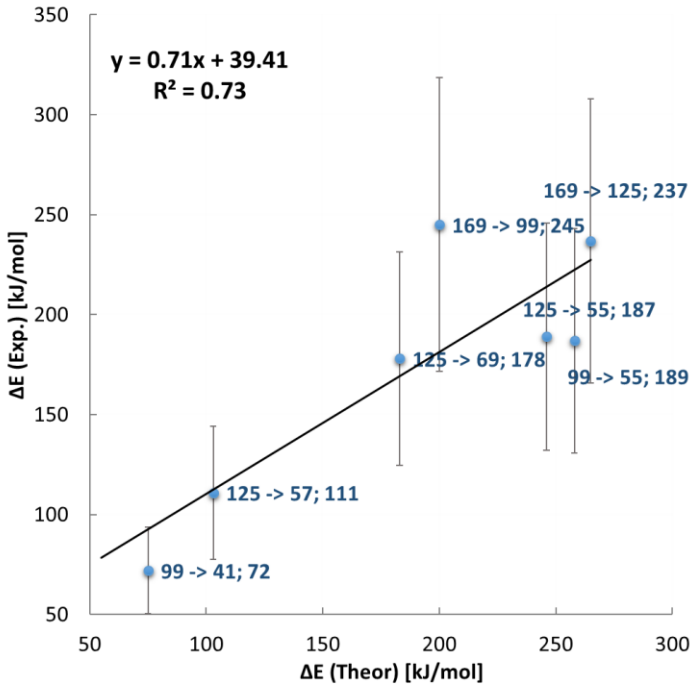


Figure S64. A correlation between the theoretical and the experimental results obtained with CAM-B3LYP/6-311+g(2d,p) level of theory. Experimental threshold energies as a function of the theoretical threshold energies (kJ/mol).

S4.2 Proton affinity calculation

Table S10. Calculated proton affinity values in kJ/mol for anions and reagents.

		Theoretical method		
	Structure	**CAM-B3LYP/ 6-311+G(2d,p)**	**PBE1PBE/ 6-311+G(2d,p)**	**ω/ 6-311+G(2d,p)**
Anions	**P_41**	1527	1535	1542
	P_55	1709	1714	1719
	P_57	1540	1545	1555
	P_69A	1611	1618	1621
	P_69B	1530	1532	1542
	P_99A	1560	1545	1557
	P_99B	1434	1445	1449
	IC_125A	1539	1540	1558
	P_125	1703	1701	1719
	S_169	1378	1422	1430
Neutral reagents	**CH_2Cl_2**	1569	1578	1581
	$CHCl_3$	1496	1501	1505
	$CHBr_3$	1467	1465	1479
	CH_3SSCH_3	1525	1550	1565
	CH_3SCN	1548	1551	1561
	CH_3NO_2	1478	1478	1497

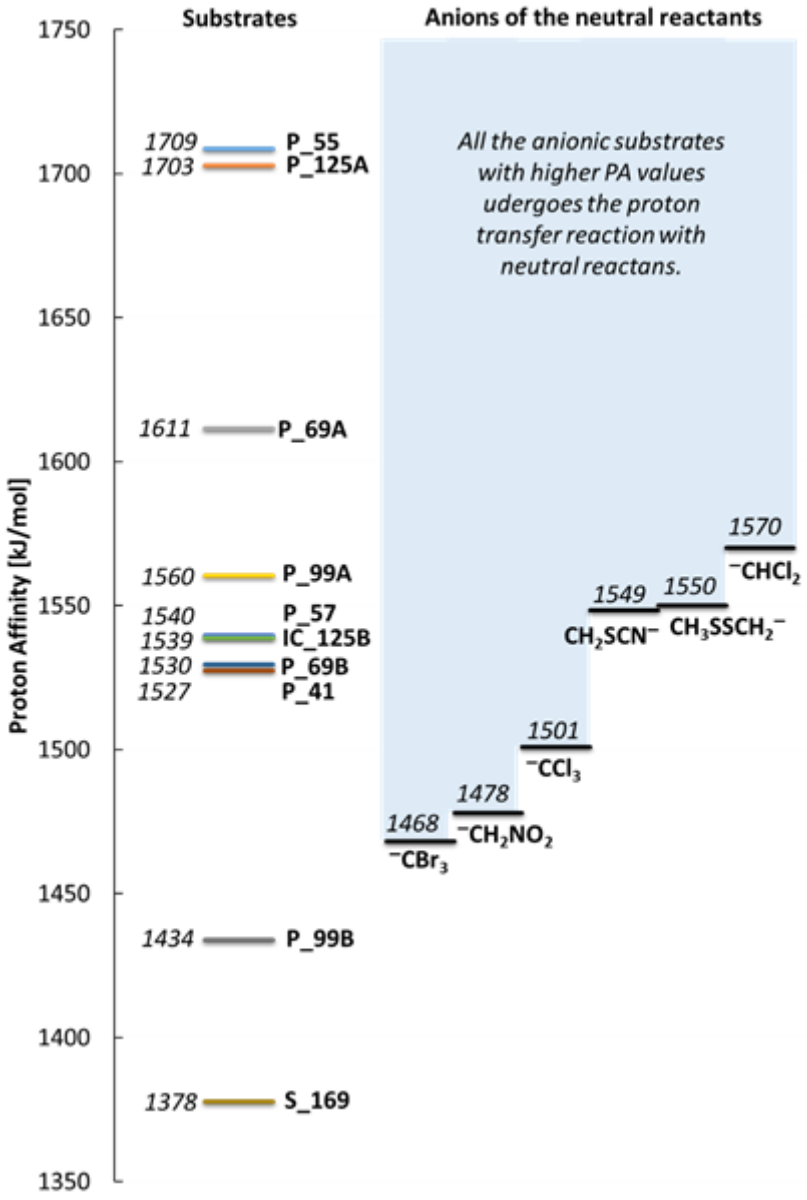
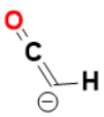
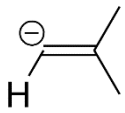
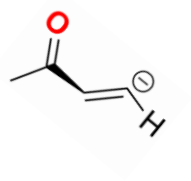
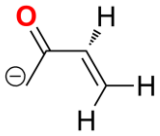


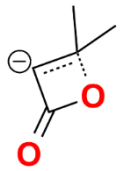
Figure S65. Proton affinity of the anionic fragment structures, compared with proton affinities of appropriate deprotonated reagents used in gas phase reactions obtained by theoretical calculation.

S5. Geometries

S5.1 Anions/neutral structures/fragmentation structures

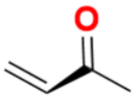
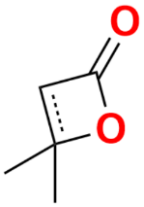
Anions				
P_41	C	1.24478300	-0.09751100	-0.00000200
	H	2.19261000	0.38814900	0.00000800
	C	0.00642700	0.01585900	0.00000500
	O	-1.21248300	0.01272000	-0.00000300
	O	-1.21248300	0.01272000	-0.00000300
P_55	C	0.24376500	1.55782800	0.00003400

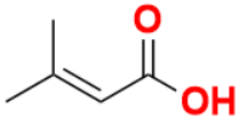
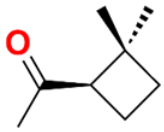
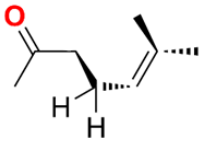
	C	0.02515300	0.22458800	-0.00003900
	H	1.34443700	1.73932000	-0.00006500
	C	1.08186300	-0.87834400	0.00000600
	H	0.99449700	-1.53854700	0.88110600
	H	0.99333700	-1.53975800	-0.88009400
	H	2.09050900	-0.45194100	-0.00096900
	C	-1.38018400	-0.35289400	0.00002400
	H	-1.57067800	-0.98994900	-0.88219300
	H	-1.57041200	-0.99079200	0.88165500
	H	-2.10527300	0.46460100	0.00041700
P_57	C	-1.19319300	-0.77858400	0.00004900
	H	-1.03374800	-1.85325400	0.00017500
	H	-2.21505300	-0.40827000	-0.00048800
	C	-0.13229300	0.10904100	0.00004700
	O	-0.18258700	1.38160900	0.00001000
	C	1.28538000	-0.48928900	-0.00003900
	H	1.82736500	-0.12622300	-0.88144300
	H	1.82726800	-0.12644800	0.88151700
	H	1.29549400	-1.58568100	-0.00019200
P_69A	C	1.96937200	0.35995400	0.00002100
	H	2.93105200	-0.19685000	0.00000500
	C	-0.45944500	-0.19496800	0.00000000
	O	-1.36657600	-1.04027100	0.00001300
	C	-0.83760000	1.27643800	-0.00000500
	H	0.05850300	1.89847100	0.00001300
	H	-1.45304200	1.48136600	-0.88279100
	H	-1.45308000	1.48137800	0.88275000
	C	0.95550200	-0.55665300	-0.00002400
	H	1.08220100	-1.65082600	-0.00003100
P_69B	C	0.61300900	-0.04131300	0.00319000
	O	1.47823900	-0.94403900	-0.01960700
	C	0.81063800	1.30716300	0.01133600
	H	1.82155400	1.70395000	-0.00709300
	H	-0.02133500	2.01009600	0.03836000
	C	-0.79635200	-0.56439300	0.02442800
	H	-0.80960000	-1.65218700	0.07270600
	C	-1.94913300	0.09050500	-0.01790800
	H	-2.89297300	-0.43672200	0.00148000
	H	-1.99253100	1.17540400	-0.07486700
P_99A	C	0.38682800	-0.00073600	1.10999500
	C	-0.70638800	-0.00012400	0.07593600
	H	0.42126000	0.00352900	2.18965400

	C	-1.56291600	-1.25796600	-0.04602200
	H	-2.24665600	-1.34056600	0.80849500
	H	-2.16359700	-1.24935100	-0.96596100
	H	-0.91279200	-2.13585300	-0.05458700
	C	-1.56053000	1.25950500	-0.04690800
	H	-2.16049900	1.25158200	-0.96729700
	H	-2.24478700	1.34355900	0.80706400
	H	-0.90862500	2.13603400	-0.05530000
	C	1.33062400	-0.00051800	0.09372100
	O	0.32253900	-0.00123100	-0.96462700
	O	2.53871000	-0.00000700	-0.14567400
P_99B	C	-0.08253100	-0.68656500	-0.00050700
	C	1.12021300	-0.09474800	0.00014100
	H	-0.11111300	-1.77612600	-0.00128800
	C	2.38525100	-0.91919700	-0.00058300
	H	2.17073300	-1.99191300	-0.00192200
	H	3.00369000	-0.69149400	-0.88016300
	H	3.00317600	-0.69358700	0.87988600
	C	1.34089100	1.39419500	0.00128500
	H	1.92554300	1.69370300	0.88326300
	H	1.92584800	1.69509700	-0.88007100
	H	0.37736500	1.90672900	0.00178400
	C	-1.48365000	-0.06824100	-0.00022100
	O	-1.59094900	1.18592700	-0.00178600
	O	-2.40608600	-0.92281100	0.00151300
P_125	C	-1.72308000	1.27461800	-0.07010100
	C	-0.28699100	1.73925700	-0.48081400
	C	0.13927700	0.27251500	-0.68314600
	C	-1.14439000	-0.15552700	0.14258300
	H	-2.34487800	1.25154300	-0.98280900
	H	0.26681200	2.23598200	0.33085200
	H	-0.17867400	2.37991800	-1.37053700
	H	-0.03582200	-0.03900200	-1.71828500
	C	-1.91696400	-1.33237500	-0.44144100
	H	-1.39773700	-2.29057700	-0.29786300
	H	-2.89844200	-1.39806000	0.04665400
	H	-2.08782400	-1.19137400	-1.51426400
	C	-0.84646900	-0.44511300	1.61887000
	H	-1.79909100	-0.57786800	2.14351400
	H	-0.23090800	-1.34733400	1.76535000
	H	-0.35208900	0.40747000	2.09280400
	C	1.48021700	-0.28821500	-0.29767800
	O	1.86613800	-1.37887100	-0.70637600
	C	2.36516900	0.50894700	0.63901000

	H	3.25780000	-0.07026100	0.88373000
	H	2.64971800	1.45139800	0.15887100
	H	1.82141900	0.77449900	1.54929300
IC_125A	C	-0.99836500	-0.89971200	-0.10591900
	C	0.15277700	-0.80105900	-1.07376800
	C	1.50823200	-0.95947500	-0.42720600
	C	-2.03495400	-0.08325700	0.07368200
	H	-0.92010300	-1.75238600	0.56634100
	H	0.08105900	0.12711400	-1.64643800
	H	0.02464100	-1.60177300	-1.81609100
	H	1.91559400	-1.96616100	-0.38747900
	C	-3.04633900	-0.33321100	1.15938600
	H	-3.07373800	0.49861900	1.87315700
	H	-4.05948600	-0.42659600	0.75024400
	H	-2.81869900	-1.24410600	1.71415100
	C	-2.29945200	1.15644000	-0.73360600
	H	-3.26612800	1.08911000	-1.24654700
	H	-2.35025500	2.03812100	-0.08487100
	H	-1.53398500	1.33686800	-1.48456700
	C	2.26804100	0.02559500	0.16475300
	O	3.39666700	-0.13683200	0.72132100
	C	1.75830000	1.47177700	0.17517900
	H	1.68396600	1.80247700	1.21429200
	H	2.50381600	2.10659000	-0.31146900
	H	0.79054400	1.62418900	-0.30630400
IC_125B	C	-1.36203200	1.03394700	-0.13722400
	C	0.07145800	1.42244000	-0.45248000
	C	1.08119700	0.39391800	-0.85889000
	C	-1.96784800	-0.13954900	0.03304400
	H	-2.00961700	1.90826400	-0.03088100
	H	0.42526100	1.99160700	0.41546200
	H	-0.01946100	2.18988600	-1.24044900
	H	0.97359000	-0.01487000	-1.86138300
	C	-3.44260000	-0.19048500	0.34136000
	H	-3.98254000	-0.76471800	-0.42041800
	H	-3.62692700	-0.69503600	1.29670800
	H	-3.88381500	0.80651700	0.39220600
	C	-1.32018200	-1.49314500	-0.04282600
	H	-1.44163100	-2.02176500	0.91001400
	H	-1.81366600	-2.10811900	-0.80497900
	H	-0.26063100	-1.42007900	-0.27444400
	C	2.10492700	-0.14296700	-0.11257000
	O	2.90357700	-1.05183300	-0.50313100
	C	2.35046000	0.32952100	1.32469000

	H	2.20369600	-0.51984900	1.99793400
	H	3.39799000	0.62873100	1.41177900
	H	1.71685200	1.15201000	1.66288200
S_169	C	1.12197900	0.02007100	-0.78957800
	C	0.00096400	-0.95644900	-1.17254900
	C	-1.04272000	0.10561000	-0.77881500
	C	0.08658300	0.86845900	0.01460100
	H	1.47635400	0.59725200	-1.64642100
	H	0.03819900	-1.81573900	-0.50454900
	H	-0.03346800	-1.31594400	-2.20253600
	H	-1.32732600	0.72502600	-1.63190400
	C	0.12700400	2.36845500	-0.20378800
	H	-0.71673800	2.86413500	0.28604400
	H	1.05741700	2.76996500	0.20355400
	H	0.09210100	2.61214100	-1.26833200
	C	0.11657100	0.55571800	1.50504100
	H	1.01913300	0.98785700	1.93879500
	H	-0.75844000	0.97157100	2.01408700
	H	0.16585800	-0.51666600	1.69526400
	C	-2.31733700	-0.23079100	-0.06047600
	C	2.34901800	-0.49417300	-0.00982100
	O	3.16352400	0.39902800	0.30975400
	O	-3.21895000	0.57955300	0.02216000
	O	2.38325700	-1.71580100	0.24526000
	C	-2.46727800	-1.59713600	0.56026600
	H	-3.42132900	-1.65730900	1.08016200
	H	-2.41668500	-2.36132300	-0.21904100
	H	-1.64642000	-1.80178200	1.24820200
Neutral fragments				
P_41N	C	0.00642700	0.01585900	0.00000500
	O	-1.21236721	0.01398374	0.01699319
	C	1.20262468	-0.09365146	-0.00000176
	H	1.64977607	0.87843683	-0.00001276
	H	1.51182613	-0.62846311	0.87365204
P_55N	C	0.02468900	0.22379100	-0.00001300
	C	1.07677400	-0.87793800	-0.00006700
	H	0.98789200	-1.53687900	0.87836400
	H	0.98771800	-1.53696000	-0.87841900
	H	2.08174300	-0.45147600	-0.00018600
	C	-1.38141400	-0.34424400	0.00015700
	H	-1.57346400	-0.97910700	-0.87960100
	H	-1.57329200	-0.97900600	0.88002400
	H	-2.10062500	0.47440300	0.00018100

	C	0.25549253	1.55919235	-0.00010088
	H	-0.18247085	1.99689927	0.87253921
	H	1.31030199	1.73883973	0.00184921
P_57N	C	-0.00530100	0.17565700	-0.00006300
	O	0.01888100	1.37695300	0.00001200
	C	1.27887300	-0.62246700	-0.00036700
	H	1.87467900	-0.33223100	-0.86655200
	H	1.85406700	-0.36289300	0.88951900
	H	1.11120700	-1.69818900	-0.01961800
	C	-1.29960500	-0.59186100	0.00032000
	H	-1.35224900	-1.22776100	-0.88711200
	H	-1.33864300	-1.25556800	0.86767200
	H	-2.14390900	0.09304200	0.01665800
P_69N	C	0.60330900	-0.05462800	0.03333200
	O	1.38490200	-1.03163500	-0.19398200
	C	-0.82685400	-0.46160200	0.27541500
	H	-0.91419000	-1.38893900	0.83889300
	C	-1.92752100	0.11394900	-0.19480200
	H	-2.91352300	-0.29634300	0.00370000
	H	-1.87418300	1.01203700	-0.79992900
	C	0.90405158	1.26541297	0.09343831
	H	0.59370825	1.74351661	-0.81210237
	H	0.39570955	1.70959274	0.92361462
	H	1.96018860	1.38536926	0.21625968
P_99AN	C	-0.70478600	-0.00001500	0.07386900
	C	-1.55944900	-1.25461900	-0.04357300
	H	-2.23953800	-1.33612400	0.81060800
	H	-2.16193900	-1.24624100	-0.95923400
	H	-0.91088900	-2.13007800	-0.05370500
	C	-1.55756500	1.25575900	-0.04478300
	H	-2.16041800	1.24722700	-0.96020300
	H	-2.23723500	1.33934100	0.80953700
	H	-0.90770200	2.13024400	-0.05624000
	C	1.33087000	-0.00033100	0.09454500
	O	0.32146700	-0.00133100	-0.96605500
	O	2.53014900	-0.00003000	-0.14320000
	C	0.38769400	-0.00028800	1.10368900
	H	0.43288296	-0.87400880	1.71970030
	H	0.43273601	0.87329384	1.71990810
P_99BN	C	-0.07963900	-0.68279700	-0.00052400
	C	1.11525000	-0.09423500	-0.00003900
	H	-0.10713900	-1.76979100	-0.00100900

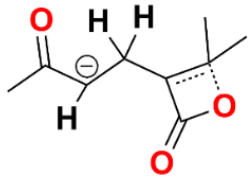
	C	2.37750300	-0.91548300	-0.00024500
	H	2.16300800	-1.98513100	-0.00093700
	H	2.99419000	-0.68811600	-0.87779900
	H	2.99377300	-0.68918300	0.87787700
	C	1.33496300	1.39078800	0.00080000
	H	1.91859900	1.68964200	0.88036700
	H	1.91927400	1.69053400	-0.87801600
	H	0.37467700	1.90290500	0.00065900
	C	-1.47943500	-0.06801000	-0.00017300
	O	-2.39454300	-0.92078300	0.00102900
	O	-1.58954238	1.18556336	-0.00104038
	H	-2.51904623	1.42560831	-0.00204427
P_125N	C	-0.28011600	1.74391200	-0.46002100
	C	0.13927300	0.28078300	-0.68274900
	C	-1.13841100	-0.15559700	0.14351000
	H	0.28506300	2.23438700	0.34352900
	H	-0.18950100	2.38815800	-1.34452800
	H	-0.03948700	-0.01742100	-1.71781200
	C	-1.92606700	-1.30532700	-0.46095600
	H	-1.41984100	-2.27077800	-0.34198300
	H	-2.90301300	-1.37042900	0.03042300
	H	-2.10072300	-1.13800200	-1.52629900
	C	-0.83219800	-0.48050000	1.60634900
	H	-1.77886000	-0.62129300	2.13433800
	H	-0.22241500	-1.38722200	1.72667400
	H	-0.33006900	0.35585200	2.09435100
	C	1.47225000	-0.29076400	-0.30191200
	O	1.84214800	-1.38140000	-0.70106500
	C	2.36764200	0.50345900	0.62223500
	H	3.25339200	-0.08160600	0.86604600
	H	2.65726200	1.43689400	0.13350400
	H	1.83158500	0.78051500	1.53028100
	C	-1.70813400	1.28085400	-0.03165600
	H	-2.06131974	1.74169394	0.86711337
	H	-2.45850732	1.35772012	-0.79055750
IC_125AN	C	-0.99836500	-0.89971200	-0.10591900
	C	0.15277700	-0.80105900	-1.07376800
	C	-2.03495400	-0.08325700	0.07368200
	H	-0.92010300	-1.75238600	0.56634100
	H	0.08105900	0.12711400	-1.64643800
	H	0.02464100	-1.60177300	-1.81609100
	C	-3.04633900	-0.33321100	1.15938600
	H	-3.07373800	0.49861900	1.87315700
	H	-4.05948600	-0.42659600	0.75024400

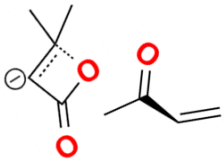
	H	-2.81869900	-1.24410600	1.71415100
	C	-2.29945200	1.15644000	-0.73360600
	H	-3.26612800	1.08911000	-1.24654700
	H	-2.35025500	2.03812100	-0.08487100
	H	-1.53398500	1.33686800	-1.48456700
	C	2.26804100	0.02559500	0.16475300
	O	3.39666700	-0.13683200	0.72132100
	C	1.75830000	1.47177700	0.17517900
	H	1.68396600	1.80247700	1.21429200
	H	2.50381600	2.10659000	-0.31146900
	H	0.79054400	1.62418900	-0.30630400
	C	1.50823200	-0.95947500	-0.42720600
	H	1.53034391	-1.60437696	0.42632345
	H	2.05640284	-1.40936892	-1.22845764
IC_125BN	C	-1.36203200	1.03394700	-0.13722400
	C	0.07145800	1.42244000	-0.45248000
	C	-1.96784800	-0.13954900	0.03304400
	H	-2.00961700	1.90826400	-0.03088100
	H	0.42526100	1.99160700	0.41546200
	H	-0.01946100	2.18988600	-1.24044900
	C	-3.44260000	-0.19048500	0.34136000
	H	-3.98254000	-0.76471800	-0.42041800
	H	-3.62692700	-0.69503600	1.29670800
	H	-3.88381500	0.80651700	0.39220600
	C	-1.32018200	-1.49314500	-0.04282600
	H	-1.44163100	-2.02176500	0.91001400
	H	-1.81366600	-2.10811900	-0.80497900
	H	-0.26063100	-1.42007900	-0.27444400
	C	2.10492700	-0.14296700	-0.11257000
	O	2.90357700	-1.05183300	-0.50313100
	C	2.35046000	0.32952100	1.32469000
	H	2.20369600	-0.51984900	1.99793400
	H	3.39799000	0.62873100	1.41177900
	H	1.71685200	1.15201000	1.66288200
	C	1.08119700	0.39391800	-0.85889000
	H	1.28846018	0.92973418	-1.76157655
	H	0.86014124	-0.62657551	-1.09261494
S_169N	C	1.06869600	-0.14685800	-0.76648300
	C	-0.07856200	-1.16918700	-0.84959300
	C	-1.06647900	0.00860600	-0.69117600
	C	0.08265300	0.88552500	-0.10202900
	H	1.35671800	0.22251700	-1.75419100
	H	-0.07932100	-1.83580800	0.01469700
	H	-0.14242500	-1.77073700	-1.75862600

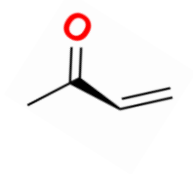
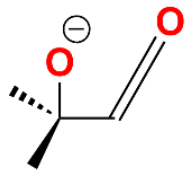
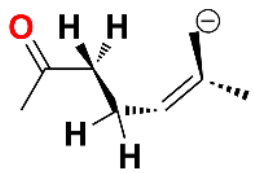
	H	-1.33987000	0.39663700	-1.68210300
	C	0.18363800	2.31354800	-0.61323000
	H	-0.63894200	2.91669800	-0.21757300
	H	1.12822500	2.76864700	-0.29897000
	H	0.13894600	2.35065700	-1.70647600
	C	0.14243300	0.85266500	1.42459900
	H	1.08279900	1.29187400	1.77238600
	H	-0.68442700	1.42802600	1.84475500
	H	0.08026600	-0.16508500	1.82190900
	C	-2.36905500	-0.14861300	0.05849400
	C	2.34050000	-0.45019400	-0.03276900
	O	3.31790700	0.26376900	-0.03901800
	O	-2.84971000	0.78280400	0.67510600
	O	2.30263900	-1.59651500	0.67950600
	H	3.15971100	-1.67873500	1.12844200
	C	-3.06312600	-1.48650300	-0.02258100
	H	-4.07129700	-1.40417500	0.38358900
	H	-3.09916600	-1.84421800	-1.05657600
	H	-2.50210300	-2.23069900	0.55258100

5.2 Products of the CID experiments

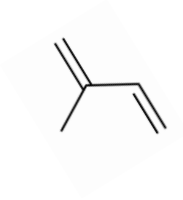
IC_169	C	0.91118400	-0.45462200	-0.60549700
	C	-0.36076500	-1.24471000	-0.28481400
	C	-1.57722500	-0.58244700	-0.85806000
	C	1.20173900	0.90575700	0.06676000
	H	1.00282100	-0.37735500	-1.69161400
	H	-0.44274900	-1.37410500	0.79517600
	H	-0.19054200	-2.25656200	-0.68354900
	H	-1.55383300	-0.39795400	-1.93098500
	C	1.42564300	2.06401300	-0.87317700
	H	0.46774100	2.36920000	-1.29742400
	H	1.86402500	2.91422200	-0.34566800



	H	2.09295500	1.77873400	-1.68787700
	C	0.36676300	1.28192400	1.26370300
	H	0.81394500	2.13825600	1.77393900
	H	-0.64248200	1.53400100	0.93895000
	H	0.29899200	0.45676100	1.97087400
	C	-2.72711800	-0.17482700	-0.21572500
	C	2.24075100	-0.86027600	-0.00896800
	O	2.51324400	0.36090400	0.52671100
	O	-3.70665900	0.41003200	-0.76879800
	O	2.92810100	-1.83360600	0.05992200
	C	-2.91302800	-0.41707900	1.28679000
	H	-3.82111600	-1.00894900	1.42228900
	H	-2.08969800	-0.92672100	1.79072400
	H	-3.08522000	0.54542100	1.77641400
CX_99	C	1.70999700	0.11981700	0.89271600
	C	-1.70134500	0.71428000	-0.14612100
	C	-2.99880100	0.87284100	0.09613700
	C	2.83899600	-0.50813000	0.12164100
	H	1.35818700	0.03509200	1.90830400
	H	-1.27814900	-0.25816800	-0.36647800
	H	-0.97692400	1.52519800	-0.13400100
	H	-3.41507200	1.84775800	0.32737500
	C	4.23057400	-0.41699500	0.72846200
	H	4.31736900	-1.08962600	1.58757200
	H	5.00319700	-0.69164300	0.00212600
	H	4.41161600	0.60244400	1.06790400
	C	2.59608300	-1.87418800	-0.49976700
	H	3.37513500	-2.12742000	-1.22702400
	H	2.58584100	-2.64856200	0.27325300
	H	1.62921100	-1.87554500	-1.00207000
	C	-3.98836000	-0.21590200	0.08509600
	C	1.63963400	1.11460100	-0.06337500
	O	2.67179300	0.53393900	-0.89489200
	O	-5.16358500	0.00881700	0.31167600
	O	1.04742600	2.14645800	-0.36751500
	C	-3.52964400	-1.62577700	-0.21064300
	H	-4.38855300	-2.29098200	-0.15922600
	H	-3.07895700	-1.68233200	-1.20272700
	H	-2.77076400	-1.94321400	0.50597100
P^{o}_70	C	1.92426400	0.17849900	-0.00018500
	C	0.87638900	-0.63128100	0.00029500
	H	1.81877600	1.25609900	-0.00070000
	H	2.93440800	-0.21067700	-0.00009800
	H	0.99772400	-1.70856400	0.00078100

	C	-0.53974600	-0.18798800	-0.00007100
	O	-1.41985300	-1.01938700	-0.00020100
	C	-0.85822300	1.28507300	0.00014400
	H	-1.93775600	1.40978100	0.00033700
	H	-0.43502400	1.77124100	0.88092400
	H	-0.43540000	1.77139700	-0.88073200
IC_99	C	-0.53957400	-0.00012200	-0.81326000
	C	0.72445400	0.00000900	0.14288000
	H	-0.46860500	-0.00017600	-1.89520000
	C	1.54826200	-1.25702600	-0.25544500
	H	1.80491800	-1.29643600	-1.32263100
	H	2.47064400	-1.26057400	0.33202100
	H	0.97158300	-2.14566300	0.00557500
	C	1.54811400	1.25710300	-0.25557000
	H	2.47049500	1.26082400	0.33189900
	H	1.80476900	1.29643600	-1.32275900
	H	0.97132700	2.14569600	0.00535800
	C	-1.72973000	-0.00011400	-0.29502900
	O	0.38761800	0.00004800	1.42349400
	O	-2.80440400	0.00005200	0.16704200
IC_125B	C	0.84785200	-0.35330100	0.40201800
	C	-0.13744500	0.50217600	0.90714600
	C	2.08600600	-0.07578200	-0.11704200
	H	0.59221300	-1.41606100	0.44630800
	H	0.01677700	1.57567400	0.91006600
	C	3.08960700	-1.15517300	-0.38270000
	H	3.56043400	-1.06429800	-1.37502400
	H	3.92831200	-1.16745100	0.33977000
	H	2.62266500	-2.14343100	-0.33531100
	C	2.57107200	1.33492300	-0.22463600
	H	2.98623900	1.73505400	0.72039500
	H	3.36410300	1.43266700	-0.97732100
	H	1.76030600	2.01563500	-0.50977900
	C	-2.24195000	-0.22582800	-0.08000400
	O	-2.53366800	-1.33545900	-0.49739900
	C	-2.53975500	0.98613200	-0.94323800
	H	-1.97906800	0.91539100	-1.87611300
	H	-3.60466900	0.97630500	-1.19226900
	H	-2.27475200	1.92087300	-0.45111200
	C	-1.52511800	0.00418000	1.22072900
	H	-1.52898900	-0.94404600	1.77026700
	H	-2.07584500	0.74339800	1.81567200
CX_125B	C	-1.52656200	0.22838400	-0.73896500

	C	1.37698000	1.68552300	0.25799300
	C	2.56401800	1.09439500	0.17092700
	C	-2.68933600	-0.02070400	-0.11871200
	H	-1.72093400	0.44937900	-1.80991000
	H	0.41977800	1.15610900	0.12518700
	H	1.32677600	2.76142200	0.40104700
	H	3.49357400	1.65464400	0.22617000
	C	-4.06939200	-0.00975800	-0.75661000
	H	-4.57448200	-0.98282500	-0.66171200
	H	-4.73745600	0.72366700	-0.28036500
	H	-4.00298500	0.23389300	-1.81836400
	C	-2.75281300	-0.35741700	1.35780500
	H	-3.36443300	0.36439100	1.91981800
	H	-3.20597900	-1.34398600	1.53693100
	H	-1.74890300	-0.35996700	1.78267400
	C	2.75278800	-0.35340100	-0.07092100
	O	3.86143800	-0.76973200	-0.36874400
	C	1.57528500	-1.26837800	0.07873700
	H	1.81438100	-2.23475500	-0.36318400
	H	1.37995800	-1.40664500	1.14654900
	H	0.64338600	-0.84932500	-0.33640300
IC_125C	C	-0.90564900	-0.07593300	-0.90452800
	C	0.16871700	-1.10180300	-0.81436900
	C	1.19765700	-0.96671800	0.36739800
	C	-1.96979400	-0.03204300	-0.01259800
	H	-0.89811400	0.60393200	-1.74946500
	H	0.74650500	-1.14582300	-1.74366000
	H	-0.26836900	-2.10318700	-0.67463400
	H	1.79006000	-1.88182400	0.43539900
	C	-3.04579500	0.99752100	-0.30487600
	H	-3.87271000	0.54459600	-0.86046600
	H	-3.45788300	1.41167400	0.61913000
	H	-2.65356100	1.82243000	-0.90484300
	C	-2.17610900	-0.83920300	1.09437800
	H	-3.06722300	-0.72505700	1.70034300
	H	-1.50893800	-1.65224800	1.35237800
	H	0.61804300	-0.83295100	1.28367700
	C	2.14145500	0.17702300	0.18346500
	O	3.27204800	0.02760800	-0.24833400
	C	1.60061800	1.53784800	0.51127400
	H	1.39905700	1.60316000	1.58361500
	H	2.30233800	2.31555100	0.21165500
	H	0.62781600	1.63872400	0.01267700
P^{O}_69	C	0.85592800	-0.53275900	-0.27176500

	C	2.01113500	-0.09946300	0.21080500
	C	-0.45397700	0.11176700	-0.06523500
	H	0.84189000	-1.45592800	-0.84665600
	H	2.93630200	-0.62373600	0.00884700
	H	2.06818700	0.78646500	0.83185600
	C	-1.61039400	-0.82181700	0.15404100
	H	-1.44948300	-1.43989200	1.04076000
	H	-2.54554400	-0.27713400	0.27731200
	H	-1.72036100	-1.50443600	-0.69291400
	C	-0.60204200	1.43123400	-0.09352900
	H	-1.56757200	1.89218400	0.07446000
	H	0.23267800	2.08869600	-0.29957000
TS_1	C	-1.72949000	1.20055800	-0.18635200
	C	-0.29789500	1.71574900	-0.42062100
	C	0.33046800	0.36217900	-0.79552300
	C	-1.35619100	-0.13100000	0.18879000
	H	-2.29421500	1.21108700	-1.12403700
	H	0.16962400	2.15342600	0.47146500
	H	-0.22040400	2.48674500	-1.20071500
	H	0.00565500	-0.00873900	-1.76595200
	C	-2.06874000	-1.34302100	-0.36183300
	H	-1.35445600	-2.16330400	-0.48081800
	H	-2.85366400	-1.67932400	0.32730900
	H	-2.52099400	-1.12892400	-1.33211100
	C	-0.82476400	-0.39195500	1.58450500
	H	-1.67902200	-0.59034400	2.24645400
	H	-0.15491400	-1.25743200	1.61095100
	H	-0.30182400	0.47674700	1.98324400
	C	1.55041000	-0.23331700	-0.36360800
	O	1.96629500	-1.32924400	-0.79371800
	C	2.35225800	0.40264900	0.76961000
	H	2.60597200	-0.36838900	1.50219100
	H	3.29112300	0.78389500	0.35512800
	H	1.84042800	1.22746400	1.26683500
TS_2	C	-1.27697700	-0.14758100	-0.03688900
	C	1.06917100	1.52520900	-0.40738400
	C	2.11824200	0.79798200	-0.81104800
	C	-2.61449500	-0.16091200	-0.01620800
	H	-0.87565100	-1.00028000	-0.62110700
	H	0.63015500	1.44121900	0.57175800
	H	0.59613600	2.23911300	-1.07005300
	H	2.51733500	0.88448400	-1.81621800
	C	-3.50519900	-1.19780100	-0.68111100
	H	-4.14981800	-1.71158700	0.04716900

	H	-4.18376100	-0.74250600	-1.41760000
	H	-2.90668500	-1.95199900	-1.19405500
	C	-3.41611400	0.90279400	0.70465500
	H	-4.08829100	1.44385300	0.02235400
	H	-4.05768200	0.47304500	1.48809000
	H	-2.74268200	1.62306900	1.16889100
	C	2.75027200	-0.22442400	0.01725200
	O	3.73585400	-0.84081400	-0.37019800
	C	2.12138800	-0.52908200	1.35281500
	H	2.57691500	-1.42824100	1.76376800
	H	2.28375100	0.30262200	2.04326400
	H	1.03571600	-0.64337800	1.24282600
TS_3	C	-1.19777000	-0.67018400	0.08896100
	C	0.12848600	-0.07626800	0.05528600
	C	1.32004000	-0.75445300	-0.15473900
	C	-2.41055300	-0.07145200	-0.28938500
	H	-1.18203100	-1.75845300	0.14692800
	H	-0.72943400	-0.34809700	1.30719200
	H	0.13905600	1.00557500	0.11503200
	H	1.29466300	-1.81672400	-0.37521400
	C	-3.66031000	-0.72033300	0.22781600
	H	-3.89461300	-0.43819800	1.27948300
	H	-4.54341000	-0.44839300	-0.36270500
	H	-3.58314400	-1.81225800	0.21150500
	C	-2.45840600	1.42211100	-0.32517600
	H	-3.41152300	1.78341600	-0.72477800
	H	-2.35087200	1.88082700	0.68719800
	H	-1.66294000	1.85515700	-0.94051500
	C	2.60972700	-0.17616200	-0.04536900
	O	3.66388700	-0.80424700	-0.23225800
	C	2.72500600	1.30170900	0.32131600
	H	3.77963600	1.57129500	0.31533200
	H	2.18768100	1.93615300	-0.38700100
	H	2.30852800	1.49387200	1.31334400
TS_4	C	1.15456500	0.06181000	1.08283000
	C	-0.07527700	-0.75827600	1.37763300
	C	-0.99985000	-0.91940500	0.15813400
	C	1.82732600	-0.06278400	-0.08028900
	H	1.43605400	0.83982000	1.78772000
	H	-0.61003800	-0.31769300	2.22712000
	H	0.20102900	-1.77018400	1.70533500
	H	-1.44285800	-1.91039000	0.05745800
	C	2.88859600	0.93924200	-0.45888300
	H	3.86759900	0.46119300	-0.56644700

	H	2.65277000	1.39331100	-1.42725800
	H	2.97314300	1.74144600	0.27930800
	C	1.44608200	-1.07605500	-1.04591900
	H	1.91281600	-0.98868400	-2.02880300
	H	1.47111000	-2.10642500	-0.68692900
	H	-0.02654000	-0.95280900	-0.77778400
	C	-1.94401700	0.09203100	-0.20036100
	O	-2.98708700	-0.13245300	-0.83681900
	C	-1.61923000	1.54625800	0.10797500
	H	-1.01317000	1.95414700	-0.70561900
	H	-2.55226500	2.10868300	0.15882300
	H	-1.04212800	1.67028600	1.02491900
TS_5	C	-1.45228500	-0.04566300	-0.89297500
	C	0.93313900	1.44598700	-0.30483700
	C	2.22794200	1.10728800	-0.20171800
	C	-2.52872800	-0.04565400	-0.10331700
	H	-1.64168900	-0.49694800	-1.88164900
	H	-0.17699200	0.66792200	-0.50556900
	H	0.77067900	2.51477400	-0.50069800
	H	3.05762000	1.81161500	-0.30381200
	C	-3.89149300	-0.59688500	-0.46671100
	H	-4.20437300	-1.39250500	0.22344500
	H	-4.66958000	0.17718800	-0.41281100
	H	-3.89028100	-1.00663300	-1.47811500
	C	-2.47631800	0.53304000	1.29387700
	H	-3.21030900	1.33958800	1.42636400
	H	-2.71177500	-0.22390100	2.05420900
	H	-1.48540700	0.93346700	1.50687100
	C	2.68666100	-0.26482000	0.04255400
	O	3.87730600	-0.55356300	0.02859200
	C	1.65621300	-1.32545000	0.34765300
	H	2.09124800	-2.30780800	0.16518500
	H	1.38872700	-1.25250000	1.40531800
	H	0.73289200	-1.18281900	-0.21462500
TS_6	C	0.15733900	-0.82413500	-0.76570200
	C	1.77164900	0.03139000	0.19415000
	H	0.70081900	-1.72313500	-1.07903600
	C	1.18692400	1.20295500	0.94337800
	H	1.98587500	1.73862100	1.46943100
	H	0.69435600	1.90265700	0.27015100
	H	0.45916400	0.86938400	1.68379400
	C	2.59933800	0.42563000	-1.00637700
	H	2.89459300	-0.45674300	-1.57659500
	H	2.03609900	1.08377200	-1.66946000

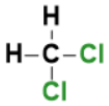
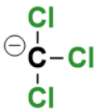
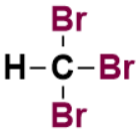
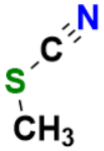
	H	3.51381900	0.94009100	-0.68396400
	C	-2.13871200	-0.12456700	-0.03208900
	O	-3.23391600	-0.44701000	0.43574900
	C	-1.92230500	1.34224200	-0.36053000
	H	-1.02980100	1.49404800	-0.96212400
	H	-2.80685700	1.69750200	-0.89242700
	H	-1.84128600	1.91673100	0.56427600
	C	-1.11373000	-1.09314400	-0.34480100
	H	-1.48828000	-2.11445300	-0.23461100
	C	2.16998000	-1.06612300	0.91940700
	H	2.77881000	-1.84056700	0.46699100
	H	1.71112100	-1.29732000	1.87295300
TS_7	C	-1.24510300	-0.04273400	-0.75923700
	C	1.64083800	1.85553600	0.36759200
	C	2.62106800	0.99851800	0.11457000
	C	-2.44214500	-0.05397800	-0.16588400
	H	-1.30922500	0.23113400	-1.82675700
	H	0.61539600	1.51953100	0.48380900
	H	1.82845000	2.92358200	0.40581400
	H	3.63351600	1.34083800	-0.08164100
	C	-3.76458000	0.26635300	-0.83710800
	H	-4.46369400	-0.58030600	-0.78388200
	H	-4.27339900	1.11198300	-0.35292900
	H	-3.61666400	0.51737100	-1.88850200
	C	-2.60663200	-0.40664700	1.29748900
	H	-3.05681400	0.41837700	1.86728400
	H	-3.27065600	-1.27135800	1.43506700
	H	-1.64232200	-0.64436000	1.74564900
	C	2.42440200	-0.47249000	-0.04831400
	O	3.24683000	-1.08164000	-0.73667300
	C	1.22311200	-1.05237600	0.52557800
	H	1.22538200	-2.13946500	0.45716700
	H	1.03333600	-0.70926600	1.54339800
	H	0.21630000	-0.61803600	-0.07921100
TS_8	C	-0.97973300	-0.01688800	-0.88331400
	C	-0.02131400	-1.00450600	-0.93381900
	C	-2.12954600	-0.03615200	-0.02083100
	H	-0.82250700	0.88678200	-1.46462500
	H	0.73417200	-0.96643500	-1.70756400
	H	-0.28824200	-2.00165700	-0.60406700
	C	-3.13600700	1.06547000	-0.25664000
	H	-3.52986200	1.02166700	-1.27610200
	H	-3.97250100	1.00154700	0.44102900
	H	-2.66660700	2.04644200	-0.13859600

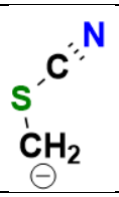
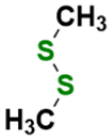
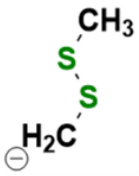
	C	-2.36662700	-0.93503900	0.95799900
	H	-3.28046600	-0.89853200	1.53912400
	H	-1.65720600	-1.71558900	1.20042500
	C	2.28965100	0.10435200	0.21297200
	O	3.21713100	0.12279900	-0.62215600
	C	1.77310800	1.42684000	0.75536100
	H	1.62634000	1.39590700	1.83721300
	H	2.46431000	2.22809300	0.49480400
	H	0.79342400	1.62641900	0.30281700
	C	1.56138200	-1.03849100	0.59205600
	H	1.97947800	-2.00512200	0.33371300
	H	0.93713000	-0.99542900	1.47637700
TS_9	C	1.04978200	-0.39108900	-0.68162800
	C	-0.09854100	-1.38383000	-0.68246500
	C	-1.24306300	-0.42871100	-0.92580900
	C	0.53875100	0.83553000	0.04799700
	H	1.24707100	-0.10470300	-1.71912000
	H	-0.17697900	-1.88431000	0.28290800
	H	0.02619300	-2.16823300	-1.43605300
	H	-1.20012100	0.12319300	-1.86069900
	C	0.44732900	2.17674600	-0.59526000
	H	-0.60567900	2.45629000	-0.68721200
	H	0.94768900	2.92092700	0.02852700
	H	0.90430700	2.18244900	-1.58364400
	C	0.05925600	0.77691600	1.46533600
	H	0.73242500	1.37370700	2.08340500
	H	-0.94617600	1.19396600	1.54167600
	H	0.05275100	-0.23803700	1.85682100
	C	-2.41976500	-0.23881900	-0.19870200
	C	2.39903400	-0.47775000	0.00572700
	O	2.51981700	0.69205600	0.53908400
	O	-3.25713700	0.65852400	-0.45768100
	O	3.18189600	-1.41266500	0.02212700
	C	-2.73328700	-1.10738600	1.01475700
	H	-2.01501700	-1.90509800	1.20182800
	H	-2.80079000	-0.47302200	1.90203800
	H	-3.71925900	-1.55009300	0.86157000
TS_10	C	0.94633200	0.39057300	0.60210500
	C	-0.96636600	1.19430300	-0.41413000
	C	-2.13274400	1.07805400	0.29761100
	C	1.72266600	-0.83219200	0.14311300
	H	0.56335400	0.56748500	1.59649600
	H	-0.79438600	0.58653800	-1.29099400
	H	-0.40984500	2.12038700	-0.39267400

	H	-2.35697400	1.79393100	1.08126200
	C	2.54054900	-1.54289300	1.20671600
	H	1.88204700	-2.09711000	1.88095400
	H	3.24446800	-2.25038200	0.75764000
	H	3.10198800	-0.81550300	1.79300700
	C	1.03850200	-1.81868900	-0.78130800
	H	1.76804500	-2.49620900	-1.23467300
	H	0.31360100	-2.41838800	-0.22601400
	H	0.51369000	-1.29233000	-1.57666100
	C	-3.08802900	0.02273700	0.15875000
	C	1.93033800	1.16982400	-0.06542200
	O	2.59274200	0.06105300	-0.64127200
	O	-4.11254500	-0.04874500	0.84477500
	O	2.22576200	2.32490900	-0.27584600
	C	-2.84467400	-1.06102000	-0.88140700
	H	-3.72258400	-1.70324000	-0.91978000
	H	-2.65919800	-0.63731500	-1.87009800
	H	-1.97132400	-1.65979200	-0.61589000
TS_11	C	-0.27218600	-0.61350000	-0.88094500
	C	0.83914400	-0.08632100	-0.18463800
	H	-0.30826800	-1.65771200	-1.17379100
	C	1.86521200	-1.02086700	0.40381000
	H	1.90243900	-1.94542700	-0.17618800
	H	2.86979300	-0.59206200	0.47272200
	H	1.53383400	-1.27798100	1.41227200
	C	1.33943100	1.31934500	-0.39567300
	H	1.74992800	1.74739300	0.52322700
	H	2.14321600	1.28670500	-1.14466900
	H	0.54176500	1.95672000	-0.76813600
	C	-1.30816600	-0.06171100	-0.01449800
	O	-0.61786100	0.52231400	0.97237200
	O	-2.53380300	-0.11472900	-0.06159400
TS_12	C	0.47683900	0.00000000	-0.89937100
	C	-0.69581200	0.00000000	0.08642900
	H	0.46325200	0.00000000	-1.98596000
	C	-1.56992200	1.25263000	-0.16466300
	H	-1.97927600	1.30025000	-1.18291000
	H	-2.39904000	1.25019900	0.54870400
	H	-0.96430900	2.14192200	0.01673400
	C	-1.56992200	-1.25263000	-0.16466300
	H	-2.39904000	-1.25019800	0.54870400
	H	-1.97927500	-1.30025000	-1.18291000
	H	-0.96430900	-2.14192200	0.01673500
	C	1.63117900	0.00000000	-0.27503300

	O	-0.15027700	0.00000000	1.32693400
	O	2.72375500	0.00000000	0.13865500

5.3 Proton transfer (PR) reaction

CH_2Cl_2	C	0.00000000	0.00000000	0.76311300
	H	-0.89885900	0.00000000	1.37081900
	H	0.89885900	0.00000000	1.37081900
	Cl	0.00000000	1.47460800	-0.21530300
	Cl	0.00000000	-1.47460800	-0.21530300
$CHCl_2$	C	-0.02636900	0.95405500	0.00000000
	H	1.05476000	1.18343600	0.00000000
	Cl	-0.02636900	-0.20317000	1.50771100
	Cl	-0.02636900	-0.20317000	-1.50771100
$CHCl_3$	C	0.00000000	0.00000000	0.45285000
	H	0.00000000	0.00000000	1.53642700
	Cl	0.00000000	1.68170700	-0.08340200
	Cl	1.45640100	-0.84085300	-0.08340200
	Cl	-1.45640100	-0.84085300	-0.08340200
CCl_3	C	0.00000000	0.00000000	0.72425900
	Cl	0.00000000	1.70640500	-0.08520700
	Cl	1.47779000	-0.85320300	-0.08520700
	Cl	-1.47779000	-0.85320300	-0.08520700
$CHBr_3$	C	-0.00020600	-0.00002200	0.52270800
	H	-0.00021800	-0.00004800	1.60455900
	Br	0.43287100	1.79169500	-0.04514600
	Br	1.33543800	-1.27066100	-0.04514400
	Br	-1.76826800	-0.52102800	-0.04516200
CBr_3	C	0.00000000	0.00000000	0.81761900
	Br	0.00000000	1.87698300	-0.04672100
	Br	-1.62551500	-0.93849200	-0.04672100
	Br	1.62551500	-0.93849200	-0.04672100
CH_3SCN	C	-1.48350600	0.80496100	0.00000400
	H	-2.51383700	0.44797700	-0.00003800
	H	-1.29544800	1.38932400	-0.89813500
	H	-1.29551300	1.38926300	0.89819600
	S	-0.46277500	-0.69990700	-0.00001800
	C	1.07262400	0.00209800	-0.00018700
	N	2.13921200	0.44708400	0.00019400
CH_2SCN	C	-1.69524200	0.69300900	0.00004000
	H	-1.67518900	1.29592700	0.91025600
	H	-1.67581000	1.29530800	-0.91060500

	S	-0.55025900	-0.59283600	0.00004700
	C	1.13319900	-0.01565600	-0.00016800
	N	2.21820000	0.40428900	0.00005200
CH_3SSCH_3	S	0.90023900	0.49001000	-0.49082300
	S	-0.90024600	0.49002000	0.49081600
	C	-1.84888700	-0.78922200	-0.37651800
	H	-2.84597000	-0.77622000	0.07064200
	H	-1.92460200	-0.55383000	-1.43711900
	H	-1.40732800	-1.77493600	-0.23300000
	C	1.84889700	-0.78920500	0.37652900
	H	1.40751300	-1.77495800	0.23276400
	H	2.84606700	-0.77599500	-0.07043000
	H	1.92436800	-0.55397400	1.43718300
CH_3SSCH_2	S	0.97985200	-0.13747200	-0.00000100
	C	2.41222043	-0.79885926	-0.86913272
	H	2.47021033	-0.75823899	-1.98671794
	H	3.38215629	-0.35335769	-0.55106438
	H	2.62502582	-1.86894963	-0.64545271
	C	-0.78806600	0.74601200	0.00000500
	H	-0.59134407	1.68900827	0.50579855
	H	-1.39627571	0.07828002	0.60662141
	S	-1.58733886	1.04793285	-1.55770227