Supporting Information for

Nucleophilic substitution reactions of cyclic thiosulfinates are accelerated by hyperconjugative interactions

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Supplementary Table 1. Reactant and Transition Structure S_1–S_2 Bond Lengths.

	1	2	3	4	5	6	7	8
S_1-S_2 react.	2.12	2.17	2.14	2.13	2.15	2.14	2.13	2.13
S_1-S_2 TS	2.27	2.32	2.46	2.48	2.43	2.41	2.4	2.44
S_1-S_2 react.	2.10	2.14	2.13	2.08	2.07	2.08	2.08	2.08
S_1-S_2 TS	2.27	2.38	2.38	2.47	2.5	2.42	2.49	2.46

Supplementary Figure 1. Coordinates of optimized stationary points of reactants **(3—10)a** and **(3—10)b** using M06-2X/6-311++G(d,p) IEF-PCM^{H2O}.

Methyl_Thiolate

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	CH3S(1-)
Number of Basis Functions	73
Electronic Energy (Eh)	-438.209663176
Sum of electronic and zero-point Energies (Eh)	-438.17273
Sum of electronic and thermal Energies (Eh)	-438.169681
Sum of electronic and enthalpy Energies (Eh)	-438.168737
Sum of electronic and thermal Free Energies (Eh)	-438.195294
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	13

__Molecular Geometry in Cartesian Coordinates__

```xyz
C          -0.000000        0.000000       -1.130787
H          -0.000000        1.017917       -1.525484
H           0.881542       -0.508958       -1.525484
S           0.000000        0.000000        0.710073
H          -0.881542       -0.508958       -1.525484
```

__Frequencies__ (Top 10 out of 9)

```
  1.     710.5292 cm-1 (Symmetry: ?A)
  2.     953.9094 cm-1 (Symmetry: ?A)
  3.     957.4586 cm-1 (Symmetry: ?A)
  4.    1347.5282 cm-1 (Symmetry: ?A)
  5.    1479.6620 cm-1 (Symmetry: ?A)
  6.    1481.2514 cm-1 (Symmetry: ?A)
  7.    3047.4960 cm-1 (Symmetry: A1)
  8.    3116.8720 cm-1 (Symmetry: E)
  9.    3117.2872 cm-1 (Symmetry: E)
```

***

3a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	CH2OS2
Number of Basis Functions	118
Electronic Energy (Eh)	-910.82939738
Sum of electronic and zero-point Energies (Eh)	-910.796407
Sum of electronic and thermal Energies (Eh)	-910.792152
Sum of electronic and enthalpy Energies (Eh)	-910.791207
Sum of electronic and thermal Free Energies (Eh)	-910.824074
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	24

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.697029        0.014477       -0.482443
C           0.524109        1.143479        0.201047
S           1.281392       -0.489006        0.083583
O          -1.706161       -0.330171        0.556929
H           0.255186        1.473649        1.198529
H           0.899634        1.899313       -0.478490
```

__Frequencies__ (Top 10 out of 12)

```
  1.     281.1701 cm-1 (Symmetry: A)
  2.     361.0781 cm-1 (Symmetry: A)
  3.     457.5815 cm-1 (Symmetry: A)
  4.     599.7161 cm-1 (Symmetry: A)
  5.     851.1966 cm-1 (Symmetry: A)
  6.     926.3478 cm-1 (Symmetry: A)
  7.     973.2585 cm-1 (Symmetry: A)
  8.    1078.8131 cm-1 (Symmetry: A)
  9.    1104.7904 cm-1 (Symmetry: A)
 10.    1441.6020 cm-1 (Symmetry: A)
```
***
3b_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	CH2S2
Number of Basis Functions	96
Electronic Energy (Eh)	-835.642981205
Sum of electronic and zero-point Energies (Eh)	-835.613489
Sum of electronic and thermal Energies (Eh)	-835.610123
Sum of electronic and enthalpy Energies (Eh)	-835.609179
Sum of electronic and thermal Free Energies (Eh)	-835.639689
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	20

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           1.048985       -0.319729       -0.000002
C           0.000272        1.135841       -0.000001
S          -1.049193       -0.319383        0.000001
H           0.000812        1.705396       -0.920385
H           0.000877        1.705358        0.920408
```

__Frequencies__ (Top 10 out of 9)

```
```

```
  1.     517.4562 cm-1 (Symmetry: A)
  2.     621.3439 cm-1 (Symmetry: A)
  3.     885.1527 cm-1 (Symmetry: A)
  4.     954.4319 cm-1 (Symmetry: A)
  5.     976.6701 cm-1 (Symmetry: A)
  6.    1091.5116 cm-1 (Symmetry: A)
  7.    1466.6299 cm-1 (Symmetry: A)
  8.    3163.3494 cm-1 (Symmetry: A)
  9.    3269.0906 cm-1 (Symmetry: A)
```

***

4a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C2H4OS2
Number of Basis Functions	154
Electronic Energy (Eh)	-950.134114061
Sum of electronic and zero-point Energies (Eh)	-950.071859
Sum of electronic and thermal Energies (Eh)	-950.066522
Sum of electronic and enthalpy Energies (Eh)	-950.065577
Sum of electronic and thermal Free Energies (Eh)	-950.101209
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	28

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.908539       -0.153788       -0.452626
C           0.095676        1.386595       -0.302780
C           1.272123        0.823468        0.483601
S           1.071627       -0.930374       -0.044131
O          -1.758881       -0.235500        0.779846
H          -0.496324        2.163033        0.179520
H           0.375030        1.682599       -1.313583
H           1.133552        0.902004        1.558928
H           2.242584        1.222568        0.199541
```

__Frequencies__ (Top 10 out of 21)

```
  1.     131.0597 cm-1 (Symmetry: A)
  2.     269.1548 cm-1 (Symmetry: A)
  3.     326.6100 cm-1 (Symmetry: A)
  4.     445.8414 cm-1 (Symmetry: A)
  5.     500.7762 cm-1 (Symmetry: A)
  6.     661.3069 cm-1 (Symmetry: A)
  7.     722.2829 cm-1 (Symmetry: A)
  8.     830.3837 cm-1 (Symmetry: A)
  9.     955.5185 cm-1 (Symmetry: A)
 10.    1008.8409 cm-1 (Symmetry: A)
```
***
4b_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C2H4S2
Number of Basis Functions	132
Electronic Energy (Eh)	-874.944257737
Sum of electronic and zero-point Energies (Eh)	-874.885459
Sum of electronic and thermal Energies (Eh)	-874.881144
Sum of electronic and enthalpy Energies (Eh)	-874.8802
Sum of electronic and thermal Free Energies (Eh)	-874.913265
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	24

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.065536       -0.628113        0.098579
C          -0.724146        1.151847       -0.242721
C           0.724142        1.151849        0.242721
S           1.065538       -0.628110       -0.098578
H          -1.399529        1.814332        0.293974
H          -0.788312        1.324364       -1.316056
H           0.788307        1.324367        1.316056
H           1.399522        1.814337       -0.293975
```

__Frequencies__ (Top 10 out of 18)

```
  1.     203.2265 cm-1 (Symmetry: A)
  2.     449.4764 cm-1 (Symmetry: A)
  3.     500.8979 cm-1 (Symmetry: A)
  4.     688.9446 cm-1 (Symmetry: A)
  5.     722.4384 cm-1 (Symmetry: A)
  6.     862.4175 cm-1 (Symmetry: A)
  7.     959.5563 cm-1 (Symmetry: A)
  8.    1001.3543 cm-1 (Symmetry: A)
  9.    1103.3037 cm-1 (Symmetry: A)
 10.    1203.5006 cm-1 (Symmetry: A)
```
***

5a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C3H6OS2
Number of Basis Functions	190
Electronic Energy (Eh)	-989.463257447
Sum of electronic and zero-point Energies (Eh)	-989.371538
Sum of electronic and thermal Energies (Eh)	-989.365319
Sum of electronic and enthalpy Energies (Eh)	-989.364375
Sum of electronic and thermal Free Energies (Eh)	-989.402099
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	32

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.118444       -0.204409       -0.378651
C          -0.171055        1.331011       -0.653462
C           0.927916        1.376635        0.394215
C           1.791309        0.131295        0.235773
S           0.686109       -1.308666       -0.078074
O          -1.818753       -0.007892        0.940355
H           0.226733        1.282645       -1.669147
H          -0.897022        2.139243       -0.570288
H           0.480844        1.409207        1.389676
H           1.537628        2.272399        0.262396
```

```
H           2.369455       -0.083973        1.132163
H           2.460724        0.219173       -0.619194
```

__Frequencies__ (Top 10 out of 30)

```
  1.     111.0170 cm-1 (Symmetry: A)
  2.     234.5875 cm-1 (Symmetry: A)
  3.     277.5966 cm-1 (Symmetry: A)
  4.     349.2926 cm-1 (Symmetry: A)
  5.     438.2524 cm-1 (Symmetry: A)
  6.     461.6862 cm-1 (Symmetry: A)
  7.     531.6345 cm-1 (Symmetry: A)
  8.     646.0792 cm-1 (Symmetry: A)
  9.     678.9954 cm-1 (Symmetry: A)
 10.     861.3629 cm-1 (Symmetry: A)
```

***

5b_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C3H6S2
Number of Basis Functions	168
Electronic Energy (Eh)	-914.274851982
Sum of electronic and zero-point Energies (Eh)	-914.187119
Sum of electronic and thermal Energies (Eh)	-914.181634
Sum of electronic and enthalpy Energies (Eh)	-914.18069
Sum of electronic and thermal Free Energies (Eh)	-914.217647
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	28

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.794440       -1.145606        0.033144
C          -1.450254        0.574913        0.104834
C          -0.358070        1.543236       -0.332327
C           0.947180        1.139178        0.337753
S           1.259188       -0.601180       -0.106884
```

```
H          -2.319754        0.618340       -0.549154
H          -1.756897        0.769422        1.131581
H          -0.634582        2.559582       -0.040990
H          -0.239081        1.513190       -1.416886
H           0.881933        1.232637        1.422428
H           1.799263        1.711459       -0.028699
```

__Frequencies__ (Top 10 out of 27)

```
  1.      27.9747 cm-1 (Symmetry: A)
  2.     300.6580 cm-1 (Symmetry: A)
  3.     389.6149 cm-1 (Symmetry: A)
  4.     473.4817 cm-1 (Symmetry: A)
  5.     517.9033 cm-1 (Symmetry: A)
  6.     672.5491 cm-1 (Symmetry: A)
  7.     693.6922 cm-1 (Symmetry: A)
  8.     853.5899 cm-1 (Symmetry: A)
  9.     894.9561 cm-1 (Symmetry: A)
 10.     925.3759 cm-1 (Symmetry: A)
```
***

6a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H8OS2
Number of Basis Functions	226
Electronic Energy (Eh)	-1028.76825423
Sum of electronic and zero-point Energies (Eh)	-1028.647575
Sum of electronic and thermal Energies (Eh)	-1028.64031
Sum of electronic and enthalpy Energies (Eh)	-1028.639366
Sum of electronic and thermal Free Energies (Eh)	-1028.679333
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	36

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.003174       -1.557261       -0.422972
```

```
S          -1.354357        0.077652       -0.206397
C          -0.231419        1.387405       -0.807450
C           0.995449        1.574763        0.075053
C           1.959603        0.387741        0.066585
C           1.341855       -0.889988        0.619955
O          -1.522116        0.356887        1.268299
H          -0.855018        2.283295       -0.817520
H           0.022043        1.117163       -1.834152
H           1.514705        2.468510       -0.278028
H           0.667466        1.779466        1.098044
H           2.825145        0.636721        0.686593
H           2.326934        0.207137       -0.947970
H           2.069235       -1.700697        0.670965
H           0.933972       -0.732471        1.620726
```

__Frequencies__ (Top 10 out of 39)

```
  1.     112.5043 cm-1 (Symmetry: A)
  2.     194.7829 cm-1 (Symmetry: A)
  3.     243.4699 cm-1 (Symmetry: A)
  4.     304.8492 cm-1 (Symmetry: A)
  5.     338.0509 cm-1 (Symmetry: A)
  6.     359.4040 cm-1 (Symmetry: A)
  7.     427.8570 cm-1 (Symmetry: A)
  8.     445.8754 cm-1 (Symmetry: A)
  9.     524.8572 cm-1 (Symmetry: A)
 10.     634.6410 cm-1 (Symmetry: A)
```

***

6b_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C4H8S2
Number of Basis Functions	204
Electronic Energy (Eh)	-953.586417106
Sum of electronic and zero-point Energies (Eh)	-953.469429
Sum of electronic and thermal Energies (Eh)	-953.463207
Sum of electronic and enthalpy Energies (Eh)	-953.462263
Sum of electronic and thermal Free Energies (Eh)	-953.499787

| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 32
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           1.122019        0.991363        0.315756
S           1.118852       -0.994616       -0.315754
C          -0.466961       -1.507778        0.427439
C          -1.659119       -0.749097       -0.149176
C          -1.656574        0.753807        0.149154
C          -0.462201        1.509185       -0.427493
H          -0.393912       -1.374164        1.508784
H          -0.544181       -2.575210        0.212722
H          -1.693884       -0.909540       -1.231320
H          -2.570048       -1.185778        0.270275
H          -2.566060        1.193581       -0.270152
H          -1.690995        0.914410        1.231302
H          -0.389377        1.375232       -1.508748
H          -0.536357        2.576808       -0.212443
```

__Frequencies__ (Top 10 out of 36)

```
  1.     181.6062 cm-1 (Symmetry: A)
  2.     231.8222 cm-1 (Symmetry: A)
  3.     293.4102 cm-1 (Symmetry: A)
  4.     349.9327 cm-1 (Symmetry: A)
  5.     370.1472 cm-1 (Symmetry: A)
  6.     491.1524 cm-1 (Symmetry: A)
  7.     508.6505 cm-1 (Symmetry: A)
  8.     667.2621 cm-1 (Symmetry: A)
  9.     676.1891 cm-1 (Symmetry: A)
 10.     803.6331 cm-1 (Symmetry: A)
```

***

7a_Reactant

Run with Gaussian 16revisionA.03.

| Datum | Value
|
|:---|---:|
| Charge | 0
|
| Multiplicity | 1
|
| Stoichiometry | C5H10OS2
|
| Number of Basis Functions | 262
|
| Electronic Energy (Eh) | -1068.06759181
|

| Sum of electronic and zero-point Energies (Eh) | -1067.917889
|
| Sum of electronic and thermal Energies (Eh) | -1067.909519
|
| Sum of electronic and enthalpy Energies (Eh) | -1067.908574
|
| Sum of electronic and thermal Free Energies (Eh) | -1067.950925
|
| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 40
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.583325        0.080075       -0.178060
C          -0.604704        1.566874       -0.564854
C           0.702452        1.737841        0.203435
C           1.881818        0.921981       -0.353932
C           2.180520       -0.388474        0.379040
C           0.965214       -1.259222        0.684843
S          -0.201680       -1.478674       -0.699179
O          -1.699000        0.083640        1.328210
H          -1.308256        2.369914       -0.330068
H          -0.450283        1.546509       -1.645870
H           0.943530        2.801657        0.146738
H           0.534131        1.524125        1.264041
H           1.698744        0.711006       -1.411443
H           2.786340        1.532945       -0.317535
H           2.657124       -0.167232        1.340105
H           2.904113       -0.960905       -0.206592
H           0.369603       -0.855793        1.509462
H           1.265230       -2.267775        0.970112
```

__Frequencies__ (Top 10 out of 48)

```
  1.     118.8111 cm-1 (Symmetry: A)
  2.     169.3134 cm-1 (Symmetry: A)
  3.     211.8459 cm-1 (Symmetry: A)
  4.     226.1384 cm-1 (Symmetry: A)
  5.     260.1081 cm-1 (Symmetry: A)
  6.     321.8407 cm-1 (Symmetry: A)
  7.     342.4044 cm-1 (Symmetry: A)
  8.     394.5000 cm-1 (Symmetry: A)
  9.     426.5671 cm-1 (Symmetry: A)
 10.     494.4263 cm-1 (Symmetry: A)
```

***

7b_Reactant

Run with Gaussian 16revisionA.03.

| Datum | Value
|

|:---|-----------------------:|
Charge	0
Multiplicity	1
Stoichiometry	C5H10S2
Number of Basis Functions	240
Electronic Energy (Eh)	-992.887077713
Sum of electronic and zero-point Energies (Eh)	-992.741301
Sum of electronic and thermal Energies (Eh)	-992.733819
Sum of electronic and enthalpy Energies (Eh)	-992.732875
Sum of electronic and thermal Free Energies (Eh)	-992.773288
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	36

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.301573       -1.466776        0.559343
C           1.266325       -1.263625       -0.362844
C           2.032026        0.020002       -0.069701
C           1.303546        1.334701       -0.381932
C           0.192989        1.704261        0.618775
C          -1.236837        1.448040        0.154244
S          -1.551573       -0.226844       -0.527781
H           1.863353       -2.133789       -0.079577
H           1.022518       -1.348604       -1.423259
H           2.950679       -0.020963       -0.664562
H           2.340040        0.024712        0.980725
H           2.054461        2.127766       -0.372964
H           0.899865        1.304523       -1.399880
H           0.359642        1.177079        1.561356
H           0.247201        2.771017        0.854340
H          -1.939167        1.631082        0.967371
H          -1.496564        2.104827       -0.679803
```

__Frequencies__ (Top 10 out of 45)

```
  1.     130.0263 cm-1 (Symmetry: A)
  2.     182.4703 cm-1 (Symmetry: A)
  3.     220.2901 cm-1 (Symmetry: A)
  4.     262.3870 cm-1 (Symmetry: A)
  5.     278.8449 cm-1 (Symmetry: A)
  6.     346.8667 cm-1 (Symmetry: A)
  7.     457.6359 cm-1 (Symmetry: A)
  8.     469.8397 cm-1 (Symmetry: A)
```

```
  9.     513.8968 cm-1 (Symmetry: A)
 10.     651.3520 cm-1 (Symmetry: A)
```
***
8a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C6H12OS2
Number of Basis Functions	298
Electronic Energy (Eh)	-1107.36736296
Sum of electronic and zero-point Energies (Eh)	-1107.188603
Sum of electronic and thermal Energies (Eh)	-1107.179109
Sum of electronic and enthalpy Energies (Eh)	-1107.178165
Sum of electronic and thermal Free Energies (Eh)	-1107.223028
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	44

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.745677        0.286387       -0.287685
C          -0.488794        1.571639       -0.650162
C           0.567126        1.767915        0.441575
C           1.989010        1.376833        0.022467
C           2.184478       -0.027304       -0.551229
C           1.944690       -1.196937        0.404453
C           0.497238       -1.492234        0.808457
S          -0.685745       -1.544313       -0.585077
O          -2.006330        0.418023        1.194177
H          -1.114837        2.458567       -0.768090
H          -0.075116        1.322380       -1.628866
H           0.258638        1.245595        1.349102
H           0.574851        2.825251        0.713928
H           2.644400        1.500948        0.890892
H           2.331869        2.095836       -0.728538
H           1.565883       -0.162391       -1.444409
H           3.219501       -0.097231       -0.897061
H           2.513336       -1.038655        1.328157
H           2.350907       -2.100061       -0.058852
H           0.087565       -0.787527        1.534532
```

```
H           0.433907       -2.479559        1.266623
```

__Frequencies__ (Top 10 out of 57)

```
  1.     104.5385 cm-1 (Symmetry: A)
  2.     139.1307 cm-1 (Symmetry: A)
  3.     185.9257 cm-1 (Symmetry: A)
  4.     193.8756 cm-1 (Symmetry: A)
  5.     229.3645 cm-1 (Symmetry: A)
  6.     288.6110 cm-1 (Symmetry: A)
  7.     316.3881 cm-1 (Symmetry: A)
  8.     339.7632 cm-1 (Symmetry: A)
  9.     356.9698 cm-1 (Symmetry: A)
 10.     415.7173 cm-1 (Symmetry: A)
```

***

8b_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C6H12S2
Number of Basis Functions	276
Electronic Energy (Eh)	-1032.18848046
Sum of electronic and zero-point Energies (Eh)	-1032.013568
Sum of electronic and thermal Energies (Eh)	-1032.005061
Sum of electronic and enthalpy Energies (Eh)	-1032.004117
Sum of electronic and thermal Free Energies (Eh)	-1032.046681
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	40

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.961776       -1.445563       -0.394620
C          -1.862865       -0.169977        0.565598
C          -1.898460        1.221470       -0.072625
C          -0.544181        1.754274       -0.544537
C           0.544313        1.754251        0.544531
C           1.898552        1.221338        0.072630
```

```
C           1.862847       -0.170104       -0.565598
S           0.961670       -1.445628        0.394621
H          -1.424744       -0.163226        1.563502
H          -2.876621       -0.563985        0.661398
H          -2.330414        1.902479        0.669757
H          -2.588105        1.203757       -0.921045
H          -0.223796        1.151286       -1.397544
H          -0.683814        2.765788       -0.933474
H           0.684018        2.765766        0.933440
H           0.223887        1.151310        1.397555
H           2.588190        1.203569        0.921054
H           2.330564        1.902312       -0.669750
H           2.876572       -0.564189       -0.661408
H           1.424717       -0.163316       -1.563498
```

__Frequencies__ (Top 10 out of 54)

```
  1.     155.3572 cm-1 (Symmetry: A)
  2.     175.0785 cm-1 (Symmetry: A)
  3.     194.2543 cm-1 (Symmetry: A)
  4.     196.6446 cm-1 (Symmetry: A)
  5.     269.8353 cm-1 (Symmetry: A)
  6.     288.4424 cm-1 (Symmetry: A)
  7.     353.1223 cm-1 (Symmetry: A)
  8.     354.8649 cm-1 (Symmetry: A)
  9.     463.0481 cm-1 (Symmetry: A)
 10.     481.1488 cm-1 (Symmetry: A)
```

***

9a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C7H14OS2
Number of Basis Functions	334
Electronic Energy (Eh)	-1146.66826856
Sum of electronic and zero-point Energies (Eh)	-1146.460733
Sum of electronic and thermal Energies (Eh)	-1146.450038
Sum of electronic and enthalpy Energies (Eh)	-1146.449094
Sum of electronic and thermal Free Energies (Eh)	-1146.496473

| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 48
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           1.474502       -0.205271       -0.538855
C           1.028763       -1.721912        0.387142
C          -0.446408       -1.822586        0.755779
C          -1.445393        1.408886       -0.765261
C          -0.300845        2.207932       -0.142227
S           0.851170        1.230244        0.903731
C          -2.316215        0.638056        0.244160
C          -1.411407       -1.693706       -0.441612
C          -2.634893       -0.806512       -0.170379
O           2.984843       -0.229192       -0.585290
H           1.683899       -1.733976        1.260547
H           1.335420       -2.516943       -0.297577
H          -0.665286       -1.069016        1.512752
H          -0.583433       -2.789931        1.245187
H          -2.057527        2.121528       -1.325352
H          -1.027082        0.734496       -1.515207
H          -0.680784        2.954389        0.559532
H           0.280299        2.725877       -0.904662
H          -3.258952        1.170200        0.391868
H          -1.823532        0.634661        1.219728
H          -1.760231       -2.686786       -0.734160
H          -0.876887       -1.312785       -1.316469
H          -3.242870       -1.266114        0.615872
H          -3.254139       -0.792578       -1.073370
```

__Frequencies__ (Top 10 out of 66)

```
  1.     108.0713 cm-1 (Symmetry: A)
  2.     140.2451 cm-1 (Symmetry: A)
  3.     146.5121 cm-1 (Symmetry: A)
  4.     167.7579 cm-1 (Symmetry: A)
  5.     234.2927 cm-1 (Symmetry: A)
  6.     257.7856 cm-1 (Symmetry: A)
  7.     262.6891 cm-1 (Symmetry: A)
  8.     285.9254 cm-1 (Symmetry: A)
  9.     312.2245 cm-1 (Symmetry: A)
 10.     333.7029 cm-1 (Symmetry: A)
```

***

9b_Reactant

Run with Gaussian 16revisionA.03.

| Datum | Value
|
|:----------|----------:|

Charge	0
Multiplicity	1
Stoichiometry	C7H14S2
Number of Basis Functions	312
Electronic Energy (Eh)	-1071.49052658
Sum of electronic and zero-point Energies (Eh)	-1071.286773
Sum of electronic and thermal Energies (Eh)	-1071.277036
Sum of electronic and enthalpy Energies (Eh)	-1071.276092
Sum of electronic and thermal Free Energies (Eh)	-1071.32146
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	44

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.594583        0.781227        0.686665
C          -0.627073        2.100196       -0.156323
C           0.743332        1.697573       -0.683038
C           0.744965       -1.696734        0.683195
C          -0.625044       -2.100655        0.156454
S          -1.593628       -0.782655       -0.686817
C           1.728436       -1.226154       -0.400266
C           1.727078        1.227412        0.400372
C           2.558914        0.001139       -0.000130
H          -0.545538        2.863096        0.623671
H          -1.248212        2.500953       -0.957245
H           1.150083        2.563888       -1.213247
H           0.597828        0.926528       -1.441790
H           1.152372       -2.562508        1.213783
H           0.598739       -0.925499        1.441625
H          -1.245891       -2.501807        0.957405
H          -0.542788       -2.863623       -0.623399
H           1.173814       -1.006492       -1.316303
H           2.408928       -2.042747       -0.655490
H           1.172521        1.006770        1.316220
H           2.406707        2.044570        0.656088
H           3.214870       -0.263816        0.836088
H           3.214296        0.266872       -0.836553
```

__Frequencies__ (Top 10 out of 63)

```
  1.     122.7262 cm-1 (Symmetry: A)
  2.     144.8838 cm-1 (Symmetry: A)
  3.     145.4642 cm-1 (Symmetry: A)
```

```
  4.     167.0791 cm-1 (Symmetry: A)
  5.     249.8331 cm-1 (Symmetry: A)
  6.     262.4500 cm-1 (Symmetry: A)
  7.     286.3590 cm-1 (Symmetry: A)
  8.     317.2203 cm-1 (Symmetry: A)
  9.     355.2039 cm-1 (Symmetry: A)
 10.     399.4279 cm-1 (Symmetry: A)
```
***

10a_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C8H16OS2
Number of Basis Functions	370
Electronic Energy (Eh)	-1185.97367104
Sum of electronic and zero-point Energies (Eh)	-1185.737491
Sum of electronic and thermal Energies (Eh)	-1185.725512
Sum of electronic and enthalpy Energies (Eh)	-1185.724568
Sum of electronic and thermal Free Energies (Eh)	-1185.774973
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	52

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.578471        0.167425       -0.550594
C          -1.370536        1.749588        0.347958
C           0.066463        2.076976        0.729203
C           1.049279        2.091664       -0.458402
C           1.938293       -0.929647       -0.751133
C           1.459515       -2.271358       -0.171860
C          -0.058303       -2.403345       -0.060728
S          -0.876796       -1.129177        0.983916
C           2.411885        0.054232        0.328338
C           2.431537        1.521719       -0.113372
O          -3.073667        0.024344       -0.696684
H          -1.781112        2.470978       -0.363288
H          -2.037594        1.690209        1.210391
H           0.391396        1.370874        1.493730
H           0.051492        3.057826        1.211414
```

```
H           1.163910        3.117039       -0.818440
H           0.632437        1.534307       -1.301870
H           2.757371       -1.098814       -1.455289
H           1.127071       -0.495018       -1.343453
H           1.912913       -2.436979        0.810303
H           1.787738       -3.099885       -0.806659
H          -0.526636       -2.362270       -1.046508
H          -0.335236       -3.355121        0.393439
H           1.781874       -0.057011        1.213852
H           3.418760       -0.237114        0.644022
H           2.876175        2.125754        0.684943
H           3.084240        1.629523       -0.986289
```

__Frequencies__ (Top 10 out of 75)

```
  1.      77.3679 cm-1 (Symmetry: A)
  2.     104.2078 cm-1 (Symmetry: A)
  3.     129.5450 cm-1 (Symmetry: A)
  4.     155.4657 cm-1 (Symmetry: A)
  5.     195.8908 cm-1 (Symmetry: A)
  6.     218.9618 cm-1 (Symmetry: A)
  7.     245.1579 cm-1 (Symmetry: A)
  8.     272.5575 cm-1 (Symmetry: A)
  9.     281.6402 cm-1 (Symmetry: A)
 10.     299.3065 cm-1 (Symmetry: A)
```

***

10b_Reactant

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	0
Multiplicity	1
Stoichiometry	C8H16S2
Number of Basis Functions	348
Electronic Energy (Eh)	-1110.79310363
Sum of electronic and zero-point Energies (Eh)	-1110.560655
Sum of electronic and thermal Energies (Eh)	-1110.549605
Sum of electronic and enthalpy Energies (Eh)	-1110.548661
Sum of electronic and thermal Free Energies (Eh)	-1110.597147

| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 48
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           1.906687       -0.780468        0.689798
C           0.944689       -2.086856       -0.178015
C          -0.428510       -1.670812       -0.678030
C          -1.515799       -1.541530        0.393174
C          -1.515858        1.541493       -0.393169
C          -0.428582        1.670812        0.678043
C           0.944612        2.086878        0.178034
S           1.906621        0.780519       -0.689815
C          -2.741168        0.760300        0.114576
C          -2.741136       -0.760386       -0.114580
H           1.564675       -2.443657       -1.000093
H           0.881387       -2.883982        0.568534
H          -0.754005       -2.416347       -1.411655
H          -0.318468       -0.740341       -1.236200
H          -1.824176       -2.550115        0.684908
H          -1.114960       -1.080158        1.300097
H          -1.824271        2.550067       -0.684902
H          -1.114997        1.080138       -1.300090
H          -0.318524        0.740349        1.236222
H          -0.754100        2.416346        1.411658
H           1.564596        2.443670        1.000117
H           0.881298        2.884018       -0.568499
H          -2.851484        0.956044        1.188286
H          -3.644000        1.158110       -0.357607
H          -3.643956       -1.158232        0.357594
H          -2.851436       -0.956133       -1.188292
```

__Frequencies__ (Top 10 out of 72)

```
  1.      89.1305 cm-1 (Symmetry: A)
  2.      99.5591 cm-1 (Symmetry: A)
  3.     126.2113 cm-1 (Symmetry: A)
  4.     177.8482 cm-1 (Symmetry: A)
  5.     208.2965 cm-1 (Symmetry: A)
  6.     238.7385 cm-1 (Symmetry: A)
  7.     261.7031 cm-1 (Symmetry: A)
  8.     268.7878 cm-1 (Symmetry: A)
  9.     290.9594 cm-1 (Symmetry: A)
 10.     301.0285 cm-1 (Symmetry: A)
```
***

Supplementary Figure 2. Coordinates of optimized stationary points of methyl thiolate substitution products of **(3—10)a** and **(3—10)b** using M06-2X/6-311++G(d,p) IEF-PCM^{H2O}.

3a_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C2H5OS3(1-)
Number of Basis Functions	191
Electronic Energy (Eh)	-1349.07448786
Sum of electronic and zero-point Energies (Eh)	-1349.003117
Sum of electronic and thermal Energies (Eh)	-1348.994473
Sum of electronic and enthalpy Energies (Eh)	-1348.993528
Sum of electronic and thermal Free Energies (Eh)	-1349.038314
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	37

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -2.402657        0.572171        0.098779
C          -0.688139        0.588164       -0.453738
S           0.347313       -0.441353        0.665333
O          -2.953669       -0.874662       -0.318591
S           2.145439       -0.616758       -0.363438
C           2.969735        0.948346        0.059368
H          -0.335874        1.620183       -0.425104
H          -0.608933        0.185781       -1.464773
H           2.398819        1.795090       -0.317348
H           3.098157        1.025951        1.137197
H           3.946076        0.926272       -0.425804
```

__Frequencies__ (Top 10 out of 27)

```
  1.      48.6967 cm-1 (Symmetry: A)
  2.      67.5728 cm-1 (Symmetry: A)
```

```
  3.     113.9681 cm-1 (Symmetry: A)
  4.     138.8533 cm-1 (Symmetry: A)
  5.     183.0317 cm-1 (Symmetry: A)
  6.     218.0819 cm-1 (Symmetry: A)
  7.     261.1068 cm-1 (Symmetry: A)
  8.     341.6703 cm-1 (Symmetry: A)
  9.     498.3396 cm-1 (Symmetry: A)
 10.     684.3605 cm-1 (Symmetry: A)
```

***

3b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C2H5S3(1-)
Number of Basis Functions	169
Electronic Energy (Eh)	-1273.89740381
Sum of electronic and zero-point Energies (Eh)	-1273.828595
Sum of electronic and thermal Energies (Eh)	-1273.821256
Sum of electronic and enthalpy Energies (Eh)	-1273.820312
Sum of electronic and thermal Free Energies (Eh)	-1273.861537
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	33

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           2.776835        0.228587       -0.065032
C           1.094066        0.342604        0.600225
S          -0.003382       -0.672442       -0.469967
S          -1.884408       -0.445625        0.398914
C          -2.459285        1.106427       -0.356556
H           1.018416       -0.055266        1.611650
H           0.715768        1.364670        0.588397
H          -3.455466        1.298885        0.042962
H          -1.798533        1.929161       -0.089445
H          -2.513587        1.000028       -1.438226
```

__Frequencies__ (Top 10 out of 24)

```
  1.      73.8157 cm-1 (Symmetry: A)
  2.     100.9252 cm-1 (Symmetry: A)
  3.     136.0659 cm-1 (Symmetry: A)
  4.     183.6063 cm-1 (Symmetry: A)
  5.     224.0376 cm-1 (Symmetry: A)
  6.     271.6557 cm-1 (Symmetry: A)
  7.     490.0227 cm-1 (Symmetry: A)
  8.     698.4814 cm-1 (Symmetry: A)
  9.     716.6399 cm-1 (Symmetry: A)
 10.     747.6444 cm-1 (Symmetry: A)
```
***

4a_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C3H7OS3(1-)
Number of Basis Functions	227
Electronic Energy (Eh)	-1388.37856381
Sum of electronic and zero-point Energies (Eh)	-1388.278216
Sum of electronic and thermal Energies (Eh)	-1388.268412
Sum of electronic and enthalpy Energies (Eh)	-1388.267468
Sum of electronic and thermal Free Energies (Eh)	-1388.315193
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	41

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -2.762062       -0.770304       -0.056688
C          -1.145459       -0.171146       -0.633016
C          -0.358190        0.470039        0.494914
S           1.205406        1.258352       -0.035971
O          -3.518838        0.580591        0.408004
S           2.336258       -0.374040       -0.633962
C           3.028001       -0.936602        0.950308
H          -0.615402       -1.039012       -1.034967
H          -1.302168        0.550359       -1.440163
H          -0.137063       -0.253799        1.281256
```

```
H          -0.934814        1.288395        0.933314
H           3.653851       -1.800243        0.723231
H           3.634369       -0.151022        1.396556
H           2.232194       -1.237284        1.629458
```

__Frequencies__ (Top 10 out of 36)

```
  1.      49.2465 cm-1 (Symmetry: A)
  2.      63.2115 cm-1 (Symmetry: A)
  3.      79.1492 cm-1 (Symmetry: A)
  4.     117.9007 cm-1 (Symmetry: A)
  5.     177.0455 cm-1 (Symmetry: A)
  6.     188.4146 cm-1 (Symmetry: A)
  7.     224.2425 cm-1 (Symmetry: A)
  8.     263.9557 cm-1 (Symmetry: A)
  9.     314.1532 cm-1 (Symmetry: A)
 10.     374.6532 cm-1 (Symmetry: A)
```

***

4b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C3H7S3(1-)
Number of Basis Functions	205
Electronic Energy (Eh)	-1313.19822735
Sum of electronic and zero-point Energies (Eh)	-1313.100563
Sum of electronic and thermal Energies (Eh)	-1313.092039
Sum of electronic and enthalpy Energies (Eh)	-1313.091095
Sum of electronic and thermal Free Energies (Eh)	-1313.13548
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	37

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -3.182433       -0.559828        0.055467
C          -1.611713        0.201972       -0.515501
C          -0.681317        0.499000        0.648440
```

```
S           0.918150        1.248545        0.147572
S           1.895130       -0.358003       -0.728584
C           2.635471       -1.164014        0.723109
H          -1.816392        1.133470       -1.048452
H          -1.103784       -0.469753       -1.211135
H          -0.469532       -0.402867        1.225488
H          -1.123493        1.236515        1.322863
H           3.322852       -0.483918        1.222119
H           1.860251       -1.495826        1.411641
H           3.181898       -2.030785        0.349920
```

__Frequencies__ (Top 10 out of 33)

```
  1.      56.7985 cm-1 (Symmetry: A)
  2.      86.7607 cm-1 (Symmetry: A)
  3.     101.4925 cm-1 (Symmetry: A)
  4.     173.1689 cm-1 (Symmetry: A)
  5.     196.4587 cm-1 (Symmetry: A)
  6.     241.3492 cm-1 (Symmetry: A)
  7.     269.6668 cm-1 (Symmetry: A)
  8.     333.4416 cm-1 (Symmetry: A)
  9.     505.4995 cm-1 (Symmetry: A)
 10.     689.7437 cm-1 (Symmetry: A)
```

***

5a_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C4H9OS3(1-)
Number of Basis Functions	263
Electronic Energy (Eh)	-1427.67913295
Sum of electronic and zero-point Energies (Eh)	-1427.550319
Sum of electronic and thermal Energies (Eh)	-1427.538988
Sum of electronic and enthalpy Energies (Eh)	-1427.538044
Sum of electronic and thermal Free Energies (Eh)	-1427.592097
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	45

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -3.153489       -0.523330        0.400608
C          -1.727293        0.501126       -0.085248
C          -0.616785        0.401001        0.952761
C           0.589547        1.276183        0.634844
S           1.514071        0.783615       -0.866053
O          -4.190738       -0.342419       -0.829429
S           2.365134       -1.011734       -0.276571
C           3.855783       -0.438866        0.592676
H          -2.061001        1.539014       -0.186440
H          -1.377799        0.156144       -1.061751
H          -0.289418       -0.638172        1.057401
H          -1.001194        0.710507        1.930758
H           1.293514        1.295251        1.467997
H           0.285024        2.306164        0.429339
H           4.491585        0.127528       -0.084678
H           3.586221        0.164131        1.457990
H           4.380021       -1.334712        0.926875
```

__Frequencies__ (Top 10 out of 45)

```
  1.       5.4341 cm-1 (Symmetry: A)
  2.      29.6709 cm-1 (Symmetry: A)
  3.      56.0951 cm-1 (Symmetry: A)
  4.      90.1877 cm-1 (Symmetry: A)
  5.     116.4181 cm-1 (Symmetry: A)
  6.     156.0177 cm-1 (Symmetry: A)
  7.     179.0582 cm-1 (Symmetry: A)
  8.     190.3076 cm-1 (Symmetry: A)
  9.     256.9552 cm-1 (Symmetry: A)
 10.     303.1657 cm-1 (Symmetry: A)
```

***

5b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C4H9S3(1-)
Number of Basis Functions	241
Electronic Energy (Eh)	-1352.49836192
Sum of electronic and zero-point Energies (Eh)	-1352.372247

| Sum of electronic and thermal Energies (Eh) | -1352.362271
|
| Sum of electronic and enthalpy Energies (Eh) | -1352.361327
|
| Sum of electronic and thermal Free Energies (Eh) | -1352.411014
|
| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 41
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -3.419128       -0.882703       -0.308123
C          -2.707589        0.437746        0.756203
C          -1.431924        1.083080        0.206197
C          -0.272821        0.097047        0.137104
S           1.217298        0.968328       -0.467651
S           2.610279       -0.562961       -0.556562
C           3.203569       -0.624665        1.160961
H          -3.451151        1.226159        0.893358
H          -2.490986        0.030452        1.748761
H          -1.152590        1.924073        0.852333
H          -1.631085        1.486555       -0.791776
H          -0.498065       -0.717778       -0.549099
H          -0.058995       -0.312615        1.126896
H           3.962544       -1.406885        1.195902
H           2.390619       -0.880682        1.837958
H           3.647119        0.328850        1.440248
```

__Frequencies__ (Top 10 out of 42)

```
  1.       9.7218 cm-1 (Symmetry: A)
  2.      56.2627 cm-1 (Symmetry: A)
  3.      74.8331 cm-1 (Symmetry: A)
  4.     121.1486 cm-1 (Symmetry: A)
  5.     152.1403 cm-1 (Symmetry: A)
  6.     181.5714 cm-1 (Symmetry: A)
  7.     230.9692 cm-1 (Symmetry: A)
  8.     255.6603 cm-1 (Symmetry: A)
  9.     295.2209 cm-1 (Symmetry: A)
 10.     416.2393 cm-1 (Symmetry: A)
```

***

6a_Product

Run with Gaussian 16revisionA.03.

| Datum | Value
|
|:---|---:|
| Charge | -1
|

Multiplicity	1
Stoichiometry	C5H11OS3(1-)
Number of Basis Functions	299
Electronic Energy (Eh)	-1466.98296679
Sum of electronic and zero-point Energies (Eh)	-1466.825447
Sum of electronic and thermal Energies (Eh)	-1466.812842
Sum of electronic and enthalpy Energies (Eh)	-1466.811898
Sum of electronic and thermal Free Energies (Eh)	-1466.867597
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	49

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           2.017382        0.561516       -0.985460
S          -3.773548       -0.104364       -0.537671
C          -2.383130       -0.071894        0.639296
C          -1.175273        0.635424        0.036147
C           0.009071        0.674416        0.999900
C           1.227019        1.396492        0.439358
O          -4.946507       -0.873589        0.272590
S           2.829694       -1.126810       -0.099438
C           4.401879       -0.479768        0.544961
H          -2.131058       -1.104144        0.902310
H          -2.715950        0.439554        1.548072
H          -1.449647        1.660819       -0.237206
H          -0.877584        0.129063       -0.887350
H           0.294167       -0.342600        1.288304
H          -0.287925        1.189138        1.920218
H           0.953683        2.380236        0.046904
H           1.990840        1.542810        1.204215
H           4.220871        0.296957        1.285849
H           4.908015       -1.320378        1.020692
H           5.012802       -0.096247       -0.269617
```

__Frequencies__ (Top 10 out of 54)

```
  1.      24.3712 cm-1 (Symmetry: A)
  2.      41.2416 cm-1 (Symmetry: A)
  3.      49.0159 cm-1 (Symmetry: A)
  4.      81.3338 cm-1 (Symmetry: A)
  5.      96.1229 cm-1 (Symmetry: A)
  6.     105.8812 cm-1 (Symmetry: A)
  7.     152.3208 cm-1 (Symmetry: A)
  8.     162.3434 cm-1 (Symmetry: A)
```

```
  9.     193.5904 cm-1 (Symmetry: A)
 10.     248.6267 cm-1 (Symmetry: A)
```

***

6b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C5H11S3(1-)
Number of Basis Functions	277
Electronic Energy (Eh)	-1391.80218709
Sum of electronic and zero-point Energies (Eh)	-1391.647356
Sum of electronic and thermal Energies (Eh)	-1391.636267
Sum of electronic and enthalpy Energies (Eh)	-1391.635323
Sum of electronic and thermal Free Energies (Eh)	-1391.687008
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	45

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           4.070420       -0.550114        0.314734
S          -1.712490        1.148013       -0.130010
C          -0.463813        0.614001        1.100312
C           0.729446       -0.130329        0.518504
C           1.620642        0.731650       -0.368522
C           2.824476       -0.021847       -0.936303
S          -2.539925       -0.659255       -0.717174
C          -3.772756       -0.937959        0.589942
H          -0.149391        1.549547        1.572481
H          -0.980780        0.018215        1.854054
H           0.373628       -1.001433       -0.043906
H           1.323534       -0.517021        1.351477
H           1.972985        1.597720        0.204429
H           1.024222        1.121342       -1.202256
H           2.460530       -0.902516       -1.475853
H           3.317855        0.616541       -1.673045
H          -4.272572       -1.876119        0.346535
H          -4.498496       -0.127346        0.601627
H          -3.287570       -1.030321        1.560052
```

__Frequencies__ (Top 10 out of 51)

```
  1.      30.8690 cm-1 (Symmetry: A)
  2.      34.5233 cm-1 (Symmetry: A)
  3.      54.9304 cm-1 (Symmetry: A)
  4.     102.2761 cm-1 (Symmetry: A)
  5.     135.4149 cm-1 (Symmetry: A)
  6.     163.3771 cm-1 (Symmetry: A)
  7.     195.0853 cm-1 (Symmetry: A)
  8.     247.5786 cm-1 (Symmetry: A)
  9.     255.3627 cm-1 (Symmetry: A)
 10.     301.9241 cm-1 (Symmetry: A)
```

***

7a_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C6H13OS3(1-)
Number of Basis Functions	335
Electronic Energy (Eh)	-1506.28743208
Sum of electronic and zero-point Energies (Eh)	-1506.101034
Sum of electronic and thermal Energies (Eh)	-1506.087302
Sum of electronic and enthalpy Energies (Eh)	-1506.086357
Sum of electronic and thermal Free Energies (Eh)	-1506.144352
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	53

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -4.117024        0.291203       -0.398047
C          -2.600143       -0.250003        0.453758
C          -1.483416       -0.540500       -0.541785
C          -0.198792       -1.005281        0.143459
C           0.918227       -1.288598       -0.856596
```

```
C           2.236516       -1.715260       -0.225608
S           2.997242       -0.483643        0.896830
O          -5.161537        0.563780        0.810563
S           3.289299        1.151560       -0.342218
C           1.769764        2.119575       -0.083144
H          -2.297193        0.540208        1.148122
H          -2.834712       -1.145183        1.038202
H          -1.814177       -1.306191       -1.252639
H          -1.274537        0.362037       -1.128701
H          -0.400313       -1.911186        0.726822
H           0.126873       -0.242505        0.858502
H           1.092540       -0.412049       -1.490572
H           0.604412       -2.091047       -1.533340
H           2.972998       -1.966312       -0.989112
H           2.100630       -2.589316        0.418278
H           0.902503        1.612402       -0.502014
H           1.923531        3.066074       -0.602593
H           1.624553        2.307310        0.978982
```

__Frequencies__ (Top 10 out of 63)

```
  1.      20.5013 cm-1 (Symmetry: A)
  2.      49.7737 cm-1 (Symmetry: A)
  3.      58.2384 cm-1 (Symmetry: A)
  4.      78.7160 cm-1 (Symmetry: A)
  5.     100.7071 cm-1 (Symmetry: A)
  6.     112.8763 cm-1 (Symmetry: A)
  7.     124.6027 cm-1 (Symmetry: A)
  8.     159.7509 cm-1 (Symmetry: A)
  9.     183.0915 cm-1 (Symmetry: A)
 10.     207.3232 cm-1 (Symmetry: A)
```

***

7b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C6H13S3(1-)
Number of Basis Functions	313
Electronic Energy (Eh)	-1431.10553117
Sum of electronic and zero-point Energies (Eh)	-1430.922107
Sum of electronic and thermal Energies (Eh)	-1430.909629

| Sum of electronic and enthalpy Energies (Eh) | -1430.908685
|
| Sum of electronic and thermal Free Energies (Eh) | -1430.963696
|
| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 49
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -2.548460       -1.224760       -0.276514
C          -0.909065       -0.888626        0.458475
C           0.077461       -0.231436       -0.494190
C           1.419198        0.048287        0.182030
C           2.422997        0.704977       -0.761130
C           3.764368        1.037403       -0.106089
S           4.763790       -0.425831        0.398313
S          -3.330974        0.683398       -0.486922
C          -4.027619        0.972804        1.167133
H          -0.555294       -1.874539        0.772795
H          -1.056599       -0.286213        1.357648
H           0.227990       -0.882434       -1.361560
H          -0.351204        0.705452       -0.864900
H           1.260874        0.702595        1.048815
H           1.842861       -0.885093        0.564903
H           1.982844        1.633087       -1.150106
H           2.595463        0.050296       -1.623302
H           3.577251        1.665468        0.771264
H           4.353103        1.638315       -0.803551
H          -4.790670        0.229726        1.389502
H          -3.242861        0.952162        1.921284
H          -4.477505        1.965809        1.141803
```

__Frequencies__ (Top 10 out of 60)

```
  1.      31.6487 cm-1 (Symmetry: A)
  2.      33.9339 cm-1 (Symmetry: A)
  3.      57.4893 cm-1 (Symmetry: A)
  4.      91.0928 cm-1 (Symmetry: A)
  5.     116.0681 cm-1 (Symmetry: A)
  6.     118.9348 cm-1 (Symmetry: A)
  7.     166.3499 cm-1 (Symmetry: A)
  8.     171.9884 cm-1 (Symmetry: A)
  9.     204.6876 cm-1 (Symmetry: A)
 10.     254.6644 cm-1 (Symmetry: A)
```

***

8a_Product

Run with Gaussian 16revisionA.03.

| Datum | Value
|

|:---|-----------------------:|
Charge	-1
Multiplicity	1
Stoichiometry	C7H15OS3(1-)
Number of Basis Functions	371
Electronic Energy (Eh)	-1545.59017696
Sum of electronic and zero-point Energies (Eh)	-1545.375524
Sum of electronic and thermal Energies (Eh)	-1545.360211
Sum of electronic and enthalpy Energies (Eh)	-1545.359267
Sum of electronic and thermal Free Energies (Eh)	-1545.421977
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	57

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -5.161393       -0.211100       -0.590520
C          -3.712330       -0.202843        0.514173
C          -2.469318        0.305973       -0.206677
C          -1.241037        0.339071        0.702533
C           0.008354        0.852956       -0.008629
C           1.224769        0.902809        0.911328
C           2.483220        1.435718        0.240060
S           3.156800        0.357516       -1.077634
O          -6.360353       -0.763904        0.349498
S           3.853491       -1.264706        0.007820
C           5.493749       -0.678443        0.529137
H          -3.553155       -1.222349        0.879666
H          -3.942149        0.434339        1.374148
H          -2.658191        1.313650       -0.594133
H          -2.260783       -0.331347       -1.073515
H          -1.451661        0.973434        1.571540
H          -1.049025       -0.668226        1.090332
H          -0.185762        1.857635       -0.403486
H           0.225600        0.213357       -0.870487
H           1.429138       -0.092426        1.320443
H           1.005090        1.551421        1.766872
H           3.279798        1.610506        0.964495
H           2.284262        2.381186       -0.272840
H           5.942050       -1.490434        1.102572
H           6.109086       -0.459808       -0.341142
H           5.401707        0.201491        1.163342
```

__Frequencies__ (Top 10 out of 72)

```
  1.      19.3105 cm-1 (Symmetry: A)
  2.      33.6616 cm-1 (Symmetry: A)
  3.      45.1472 cm-1 (Symmetry: A)
  4.      62.8575 cm-1 (Symmetry: A)
  5.      66.6797 cm-1 (Symmetry: A)
  6.      82.5897 cm-1 (Symmetry: A)
  7.     108.0032 cm-1 (Symmetry: A)
  8.     129.4748 cm-1 (Symmetry: A)
  9.     143.1579 cm-1 (Symmetry: A)
 10.     162.0832 cm-1 (Symmetry: A)
```
***
8b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C7H15S3(1-)
Number of Basis Functions	349
Electronic Energy (Eh)	-1470.4088502
Sum of electronic and zero-point Energies (Eh)	-1470.196886
Sum of electronic and thermal Energies (Eh)	-1470.183047
Sum of electronic and enthalpy Energies (Eh)	-1470.182103
Sum of electronic and thermal Free Energies (Eh)	-1470.240784
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	53

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           4.816171        1.423425       -0.215256
C           4.609658       -0.399561       -0.038440
C           3.308874       -0.836928        0.637134
C           2.055953       -0.561749       -0.189002
C           0.775206       -1.023713        0.502638
C          -0.475671       -0.750004       -0.331945
C          -1.740070       -1.216550        0.372471
S          -3.277800       -0.895743       -0.561640
S          -3.431419        1.168694       -0.452273
C          -4.252983        1.385546        1.154866
```

```
H           5.451865       -0.790979        0.537502
H           4.661394       -0.864784       -1.028456
H           3.222727       -0.336844        1.609119
H           3.364320       -1.915245        0.839524
H           2.147672       -1.068719       -1.158267
H           1.991236        0.509887       -0.400432
H           0.841291       -2.096960        0.718460
H           0.683655       -0.516421        1.470533
H          -0.551232        0.323230       -0.534174
H          -0.394328       -1.256089       -1.299262
H          -1.839037       -0.758490        1.359134
H          -1.737337       -2.301777        0.507940
H          -4.387355        2.459349        1.288961
H          -5.222631        0.891951        1.151544
H          -3.629271        0.997624        1.958253
```

__Frequencies__ (Top 10 out of 69)

```
  1.      19.7217 cm-1 (Symmetry: A)
  2.      39.9138 cm-1 (Symmetry: A)
  3.      52.8828 cm-1 (Symmetry: A)
  4.      79.7781 cm-1 (Symmetry: A)
  5.      90.6647 cm-1 (Symmetry: A)
  6.     106.8085 cm-1 (Symmetry: A)
  7.     136.5199 cm-1 (Symmetry: A)
  8.     157.2468 cm-1 (Symmetry: A)
  9.     173.5441 cm-1 (Symmetry: A)
 10.     191.1347 cm-1 (Symmetry: A)
```

***

9a_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C8H17OS3(1-)
Number of Basis Functions	407
Electronic Energy (Eh)	-1584.8937175
Sum of electronic and zero-point Energies (Eh)	-1584.650517
Sum of electronic and thermal Energies (Eh)	-1584.633767
Sum of electronic and enthalpy Energies (Eh)	-1584.632823
Sum of electronic and thermal Free Energies (Eh)	-1584.699022

| Number of Imaginary Frequencies | 0
|
| Mean of alpha and beta Electrons | 61
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           6.015254        0.501134       -0.518010
C           4.600536       -0.071001        0.477596
C           3.303171        0.017353       -0.318010
C          -1.735735       -0.654470       -0.303944
C          -2.947924       -1.066931        0.516283
S          -4.531123       -0.957980       -0.389847
C          -0.443160       -0.740589        0.506833
C           2.081759       -0.408242        0.496392
C           0.783905       -0.330477       -0.304043
O           7.286894        0.323843        0.470828
S          -4.788374        1.091262       -0.568639
C          -5.570699        1.496513        1.021584
H           4.792047       -1.103527        0.786667
H           4.540691        0.548387        1.378234
H           3.379217       -0.612697       -1.211450
H           3.159795        1.045718       -0.669334
H          -1.874788        0.371233       -0.660410
H          -1.662912       -1.296755       -1.187345
H          -3.035045       -0.470568        1.427220
H          -2.884861       -2.118268        0.810745
H          -0.309865       -1.764635        0.875018
H          -0.524822       -0.097933        1.391258
H           1.998696        0.228282        1.385109
H           2.224553       -1.433360        0.857988
H           0.864737       -0.973136       -1.188741
H           0.647245        0.692813       -0.673638
H          -4.904700        1.254101        1.847808
H          -5.753930        2.571401        1.009127
H          -6.514448        0.964621        1.122904
```

__Frequencies__ (Top 10 out of 81)

```
  1.      20.4944 cm-1 (Symmetry: A)
  2.      36.4071 cm-1 (Symmetry: A)
  3.      41.9245 cm-1 (Symmetry: A)
  4.      47.3515 cm-1 (Symmetry: A)
  5.      69.6060 cm-1 (Symmetry: A)
  6.      74.9370 cm-1 (Symmetry: A)
  7.     100.2665 cm-1 (Symmetry: A)
  8.     113.3858 cm-1 (Symmetry: A)
  9.     127.0768 cm-1 (Symmetry: A)
 10.     147.9526 cm-1 (Symmetry: A)
```

***

9b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C8H17S3(1-)
Number of Basis Functions	385
Electronic Energy (Eh)	-1509.71233777
Sum of electronic and zero-point Energies (Eh)	-1509.471795
Sum of electronic and thermal Energies (Eh)	-1509.456598
Sum of electronic and enthalpy Energies (Eh)	-1509.455654
Sum of electronic and thermal Free Energies (Eh)	-1509.517747
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	57

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           3.813256       -1.136263       -0.358948
C           2.172463       -1.063035        0.442404
C           1.082554       -0.459100       -0.429354
C          -3.822777        0.869689       -0.698114
C          -5.172103        0.980354        0.013596
S          -5.975434       -0.631664        0.404416
C          -2.712107        0.275084        0.162538
C          -0.258593       -0.393167        0.300505
C          -1.370209        0.200570       -0.562037
S           4.352620        0.864246       -0.426811
C           5.068906        1.101612        1.227187
H           2.277620       -0.519212        1.383800
H           1.950777       -2.106425        0.683591
H           0.979617       -1.054825       -1.341948
H           1.382267        0.549012       -0.733421
H          -3.514907        1.872642       -1.023982
H          -3.944320        0.265693       -1.605164
H          -5.851409        1.564674       -0.611919
H          -5.032107        1.545932        0.940854
H          -2.600306        0.880864        1.071318
H          -3.008283       -0.726711        0.488436
H          -0.147184        0.206569        1.211590
H          -0.549078       -1.400014        0.623027
H          -1.074524        1.204395       -0.890904
H          -1.482802       -0.402719       -1.471107
H           5.397183        2.140448        1.273727
H           4.319625        0.925853        1.997054
```

```
H           5.921960        0.440682        1.366193
```

__Frequencies__ (Top 10 out of 78)

```
  1.      22.4756 cm-1 (Symmetry: A)
  2.      29.1806 cm-1 (Symmetry: A)
  3.      49.5016 cm-1 (Symmetry: A)
  4.      64.2626 cm-1 (Symmetry: A)
  5.      78.7083 cm-1 (Symmetry: A)
  6.      83.3491 cm-1 (Symmetry: A)
  7.     130.0298 cm-1 (Symmetry: A)
  8.     140.3116 cm-1 (Symmetry: A)
  9.     144.6659 cm-1 (Symmetry: A)
 10.     176.0329 cm-1 (Symmetry: A)
```
***

10a_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C9H19OS3(1-)
Number of Basis Functions	443
Electronic Energy (Eh)	-1624.19685346
Sum of electronic and zero-point Energies (Eh)	-1623.925064
Sum of electronic and thermal Energies (Eh)	-1623.90717
Sum of electronic and enthalpy Energies (Eh)	-1623.906226
Sum of electronic and thermal Free Energies (Eh)	-1623.975604
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	65

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -5.547008        1.160959        0.015212
C          -5.297416       -0.629611       -0.234263
C          -3.902690       -0.951828       -0.763053
C          -2.771455       -0.529959        0.174797
C           1.097556       -1.106477        0.167643
C           2.228928       -0.688137        1.102158
```

```
C           3.596806       -1.209208        0.682842
S           4.233158       -0.499931       -0.880547
C          -0.265508       -0.597054        0.629506
C          -1.404851       -1.023626       -0.292792
O          -7.136963        1.275584        0.310617
S           4.647393        1.453921       -0.327038
C           6.302743        1.280901        0.405043
H          -5.472845       -1.147432        0.714977
H          -6.062218       -0.956244       -0.944321
H          -3.838844       -2.033195       -0.930607
H          -3.762297       -0.474623       -1.739711
H          -2.751005        0.561784        0.263202
H          -2.975830       -0.918555        1.180495
H           1.300774       -0.736310       -0.842818
H           1.072307       -2.201087        0.101551
H           2.024363       -1.066322        2.110179
H           2.268543        0.403561        1.181960
H           3.563809       -2.285019        0.487628
H           4.346929       -1.033122        1.454951
H          -0.465762       -0.962963        1.643856
H          -0.240868        0.497447        0.693572
H          -1.421320       -2.118040       -0.364854
H          -1.210833       -0.649159       -1.305412
H           7.002367        0.896715       -0.334398
H           6.269505        0.628051        1.275534
H           6.607562        2.280646        0.715978
```

__Frequencies__ (Top 10 out of 90)

```
  1.      17.0446 cm-1 (Symmetry: A)
  2.      22.9816 cm-1 (Symmetry: A)
  3.      38.5886 cm-1 (Symmetry: A)
  4.      47.8199 cm-1 (Symmetry: A)
  5.      61.9716 cm-1 (Symmetry: A)
  6.      75.2526 cm-1 (Symmetry: A)
  7.      81.4318 cm-1 (Symmetry: A)
  8.      88.8408 cm-1 (Symmetry: A)
  9.     117.1148 cm-1 (Symmetry: A)
 10.     143.2411 cm-1 (Symmetry: A)
```

***

10b_Product

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C9H19S3(1-)

Number of Basis Functions	421
Electronic Energy (Eh)	-1549.0158641
Sum of electronic and zero-point Energies (Eh)	-1548.746522
Sum of electronic and thermal Energies (Eh)	-1548.730191
Sum of electronic and enthalpy Energies (Eh)	-1548.729247
Sum of electronic and thermal Free Energies (Eh)	-1548.794938
Number of Imaginary Frequencies	0
Mean of alpha and beta Electrons	61

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -2.671946       -1.120379        0.245807
C          -2.425982        0.309409        1.362054
C          -2.065201        1.620194        0.671338
C          -0.859151        1.548422       -0.264985
C           2.905103        0.562580        0.135922
C           4.124999        0.664738       -0.775029
C           5.432006        0.201905       -0.129590
S           5.526874       -1.603307        0.230176
C           1.631660        1.100616       -0.512456
C           0.407251        1.007084        0.395273
S          -4.195452       -0.470069       -0.999145
C          -5.666394       -0.770018        0.026895
H          -1.625166       -0.029431        2.024239
H          -3.325232        0.427443        1.968130
H          -1.870191        2.352238        1.463344
H          -2.937253        1.981429        0.119874
H          -0.661700        2.555404       -0.647325
H          -1.105217        0.928907       -1.134255
H           3.102494        1.119509        1.061430
H           2.756676       -0.482177        0.426022
H           3.948648        0.083391       -1.687854
H           4.242002        1.712308       -1.084896
H           5.577889        0.761475        0.800453
H           6.261091        0.468572       -0.789829
H           1.435099        0.547488       -1.439489
H           1.784779        2.146987       -0.804240
H           0.259660       -0.040913        0.681290
H           0.598334        1.560013        1.324085
H          -5.634618       -0.159769        0.927793
H          -5.738488       -1.825404        0.281777
H          -6.526161       -0.476956       -0.576500
```

__Frequencies__ (Top 10 out of 87)

```
  1.      16.4352 cm-1 (Symmetry: A)
```

```
  2.      19.5902 cm-1 (Symmetry: A)
  3.      29.1608 cm-1 (Symmetry: A)
  4.      51.3798 cm-1 (Symmetry: A)
  5.      65.6468 cm-1 (Symmetry: A)
  6.      81.6052 cm-1 (Symmetry: A)
  7.     105.3403 cm-1 (Symmetry: A)
  8.     129.4932 cm-1 (Symmetry: A)
  9.     147.7672 cm-1 (Symmetry: A)
 10.     162.8538 cm-1 (Symmetry: A)
```
***

Supplementary Figure 3. Coordinates of optimized transition structures of methyl thiolate substitution towards **(3—10)a** and **(3—10)b** using M06-2X/6-311++G(d,p) IEF-PCM^{H2O}.

TS–3a (Constrained Optimization, M06-2X/6-311++G(d,p))

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C2H5OS3(1-)
Number of Basis Functions	191
Electronic Energy (Eh)	-1349.04764193
Sum of electronic and zero-point Energies (Eh)	-1348.977288
Sum of electronic and thermal Energies (Eh)	-1348.96886
Sum of electronic and enthalpy Energies (Eh)	-1348.967916
Sum of electronic and thermal Free Energies (Eh)	-1349.012752
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	37

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -2.233212       -0.269267        0.091731
C          -0.727342        0.035259        1.055998
S          -0.074712       -0.657033       -0.447712
O          -2.732963        1.070448       -0.446820
H          -0.574454        1.101371        1.197464
H          -0.617797       -0.566066        1.953184
C           2.532822        1.343897       -0.056470
H           1.867179        1.741925        0.711827
H           3.526733        1.763576        0.105091
S           2.598967       -0.483469        0.021029
H           2.172456        1.676981       -1.030952
```

__Frequencies__ (Top 10 out of 27)

```
  1.    -147.2093 cm-1 (Symmetry: A)  *
  2.      47.6565 cm-1 (Symmetry: A)
```

```
  3.      71.1399 cm-1 (Symmetry: A)
  4.      86.8871 cm-1 (Symmetry: A)
  5.     111.6082 cm-1 (Symmetry: A)
  6.     155.3225 cm-1 (Symmetry: A)
  7.     219.3794 cm-1 (Symmetry: A)
  8.     317.0194 cm-1 (Symmetry: A)
  9.     361.6671 cm-1 (Symmetry: A)
 10.     629.6306 cm-1 (Symmetry: A)
```
***

TS-3b (Constrained Optimization, M06-2X/6-311++G(d,p))

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C2H5S3(1-)
Number of Basis Functions	169
Electronic Energy (Eh)	-1273.86401613
Sum of electronic and zero-point Energies (Eh)	-1273.79692
Sum of electronic and thermal Energies (Eh)	-1273.789451
Sum of electronic and enthalpy Energies (Eh)	-1273.788507
Sum of electronic and thermal Free Energies (Eh)	-1273.831214
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	33

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           2.613341        0.151315       -0.142204
C           1.154511        0.523109        0.858310
S           0.484670       -0.563266       -0.375126
H           0.812841        1.550923        0.798490
H           1.173426        0.116306        1.863509
C          -2.504461        1.100174       -0.408638
H          -3.526893        1.427621       -0.213212
H          -1.822710        1.822206        0.044001
H          -2.342821        1.104269       -1.487430
S          -2.235144       -0.573113        0.285869
```

__Frequencies__ (Top 10 out of 24)

```
  1.    -181.9612 cm-1 (Symmetry: A)  *
  2.      42.5536 cm-1 (Symmetry: A)
  3.      77.5611 cm-1 (Symmetry: A)
  4.      83.4860 cm-1 (Symmetry: A)
  5.     124.8252 cm-1 (Symmetry: A)
  6.     173.1423 cm-1 (Symmetry: A)
  7.     286.2374 cm-1 (Symmetry: A)
  8.     663.5008 cm-1 (Symmetry: A)
  9.     725.6141 cm-1 (Symmetry: A)
 10.     873.8017 cm-1 (Symmetry: A)
```
***

TS-4a (Constrained Optimization, M06-2X/6-311++G(d,p))

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C3H7OS3(1-)
Number of Basis Functions	227
Electronic Energy (Eh)	-1388.35318226
Sum of electronic and zero-point Energies (Eh)	-1388.25345
Sum of electronic and thermal Energies (Eh)	-1388.244127
Sum of electronic and enthalpy Energies (Eh)	-1388.243183
Sum of electronic and thermal Free Energies (Eh)	-1388.289539
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	41

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           0.049285       -0.630670       -0.340675
C          -0.140262        0.841843        0.751987
C          -1.424040        1.424638        0.177609
S          -2.196658       -0.072475       -0.529966
H           0.724369        1.495967        0.671479
H          -0.253016        0.510175        1.782613
H          -1.224468        2.102574       -0.653192
H          -2.102574        1.891839        0.890851
C           3.093955        0.887084       -0.453146
```

```
H           3.104406        1.700231        0.274701
H           4.087732        0.811950       -0.896223
S           2.623086       -0.699696        0.327445
H           2.385324        1.139813       -1.245759
O          -2.938889       -0.766058        0.625996
```

__Frequencies__ (Top 10 out of 36)

```
  1.    -126.9990 cm-1 (Symmetry: A)  *
  2.      58.9859 cm-1 (Symmetry: A)
  3.      74.1594 cm-1 (Symmetry: A)
  4.     106.3819 cm-1 (Symmetry: A)
  5.     131.7314 cm-1 (Symmetry: A)
  6.     151.6912 cm-1 (Symmetry: A)
  7.     164.1087 cm-1 (Symmetry: A)
  8.     243.1360 cm-1 (Symmetry: A)
  9.     299.3939 cm-1 (Symmetry: A)
 10.     336.0194 cm-1 (Symmetry: A)
```
***

TS-4b (Constrained Optimization, M06-2X/6-311++G(d,p))

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C3H7S3(1-)
Number of Basis Functions	205
Electronic Energy (Eh)	-1313.16651405
Sum of electronic and zero-point Energies (Eh)	-1313.070113
Sum of electronic and thermal Energies (Eh)	-1313.061829
Sum of electronic and enthalpy Energies (Eh)	-1313.060884
Sum of electronic and thermal Free Energies (Eh)	-1313.104882
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	37

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           2.513636       -0.412027        0.394544
```

```
C           0.475103        1.039683       -0.241062
S           0.197187       -0.767852       -0.012663
H          -0.175226        1.425994       -1.024159
H           0.262768        1.544127        0.702546
C          -2.699454        0.698105        0.909298
H          -2.296620        1.695723        0.727582
H          -3.773350        0.785851        1.080291
H          -2.236982        0.295082        1.812019
S          -2.387289       -0.405640       -0.513905
C           1.963531        1.056463       -0.555485
H           2.137215        0.887008       -1.618769
H           2.470563        1.969015       -0.243633
```

__Frequencies__ (Top 10 out of 33)

```
  1.    -185.3353 cm-1 (Symmetry: A)  *
  2.      48.7141 cm-1 (Symmetry: A)
  3.      81.5742 cm-1 (Symmetry: A)
  4.     129.8703 cm-1 (Symmetry: A)
  5.     154.4063 cm-1 (Symmetry: A)
  6.     174.9251 cm-1 (Symmetry: A)
  7.     213.5210 cm-1 (Symmetry: A)
  8.     250.8046 cm-1 (Symmetry: A)
  9.     446.9031 cm-1 (Symmetry: A)
 10.     709.3480 cm-1 (Symmetry: A)
```
***

TS-5a

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C4H9OS3(1-)
Number of Basis Functions	263
Electronic Energy (Eh)	-1427.66986652
Sum of electronic and zero-point Energies (Eh)	-1427.541148
Sum of electronic and thermal Energies (Eh)	-1427.530778
Sum of electronic and enthalpy Energies (Eh)	-1427.529834
Sum of electronic and thermal Free Energies (Eh)	-1427.578566
Number of Imaginary Frequencies	1

| Mean of alpha and beta Electrons | 45
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -2.046690       -0.769728       -0.378073
C          -2.315783        1.021487       -0.269595
C          -1.221953        1.597289        0.612862
C           0.142014        1.342978       -0.009621
S           0.381469       -0.425487       -0.517106
O          -2.356247       -1.308806        1.054149
H          -2.255634        1.412204       -1.289553
H          -3.319739        1.189081        0.123654
H          -1.279858        1.131667        1.600189
H          -1.356641        2.675244        0.742413
H           0.935744        1.573832        0.697103
H           0.282866        1.955631       -0.901379
S           2.807678       -0.086014       -0.572654
C           3.083226       -0.290493        1.217930
H           2.746317       -1.274136        1.546872
H           4.147014       -0.192939        1.437496
H           2.545554        0.471962        1.785880
```

__Frequencies__ (Top 10 out of 45)

```
  1.    -185.4293 cm-1 (Symmetry: A)  *
  2.      52.3649 cm-1 (Symmetry: A)
  3.      60.6178 cm-1 (Symmetry: A)
  4.     105.4183 cm-1 (Symmetry: A)
  5.     124.2395 cm-1 (Symmetry: A)
  6.     148.4073 cm-1 (Symmetry: A)
  7.     187.0192 cm-1 (Symmetry: A)
  8.     198.6764 cm-1 (Symmetry: A)
  9.     247.0361 cm-1 (Symmetry: A)
 10.     294.9943 cm-1 (Symmetry: A)
```
***

TS-5b

Run with Gaussian 16revisionA.03.

| Datum | Value
|
|:---|---:|
| Charge | -1
|
| Multiplicity | 1
|
| Stoichiometry | C4H9S3(1-)
|
| Number of Basis Functions | 241
|

Electronic Energy (Eh)	-1352.4839797
Sum of electronic and zero-point Energies (Eh)	-1352.358616
Sum of electronic and thermal Energies (Eh)	-1352.34925
Sum of electronic and enthalpy Energies (Eh)	-1352.348306
Sum of electronic and thermal Free Energies (Eh)	-1352.394952
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	41

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           0.123220       -0.771624       -0.062631
C          -0.274788        0.864241       -0.803026
C          -1.346553        1.573077        0.010875
C          -2.632815        0.757008       -0.000437
S          -2.212466       -0.997962        0.321154
H           0.654941        1.427326       -0.819830
H          -0.612320        0.707091       -1.830077
H          -1.528846        2.566103       -0.412885
H          -0.992386        1.703584        1.037324
H          -3.117585        0.831349       -0.975369
H          -3.331111        1.106225        0.760791
S           2.635346       -0.413299       -0.424423
C           2.842362        0.743074        0.974830
H           3.878161        1.080038        1.036087
H           2.204684        1.621825        0.849298
H           2.577619        0.258231        1.915617
```

__Frequencies__ (Top 10 out of 42)

```
  1.    -172.9265 cm-1 (Symmetry: A)  *
  2.      46.1997 cm-1 (Symmetry: A)
  3.      64.6655 cm-1 (Symmetry: A)
  4.     107.6796 cm-1 (Symmetry: A)
  5.     115.5643 cm-1 (Symmetry: A)
  6.     166.1406 cm-1 (Symmetry: A)
  7.     192.6900 cm-1 (Symmetry: A)
  8.     247.6802 cm-1 (Symmetry: A)
  9.     309.3249 cm-1 (Symmetry: A)
 10.     352.7081 cm-1 (Symmetry: A)
```

***

TS-6a

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C5H11OS3(1-)
Number of Basis Functions	299
Electronic Energy (Eh)	-1466.97427923
Sum of electronic and zero-point Energies (Eh)	-1466.816172
Sum of electronic and thermal Energies (Eh)	-1466.805003
Sum of electronic and enthalpy Energies (Eh)	-1466.804059
Sum of electronic and thermal Free Energies (Eh)	-1466.853808
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	49

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           0.534432       -0.878094       -0.141467
S          -1.923343       -0.985448       -0.444601
C          -2.118866        0.736999       -1.016951
C          -1.756957        1.759956        0.052765
C          -0.284966        1.758545        0.468196
C           0.183937        0.442326        1.088645
O          -2.628538       -1.029629        0.953155
H          -3.159319        0.858615       -1.327611
H          -1.479445        0.824171       -1.900042
H          -2.026604        2.752435       -0.320111
H          -2.378432        1.570826        0.933350
H          -0.140362        2.548428        1.213165
H           0.348767        2.007632       -0.388689
H           1.110864        0.574437        1.643699
H          -0.579122        0.051293        1.766799
S           2.933971       -0.708560        0.098110
C           3.146905        0.995800       -0.512708
H           4.209701        1.202932       -0.642870
H           2.643215        1.121360       -1.472852
H           2.737761        1.716794        0.197581
```

__Frequencies__ (Top 10 out of 54)

```
  1.    -172.9773 cm-1 (Symmetry: A)  *
  2.      64.7493 cm-1 (Symmetry: A)
  3.      76.2458 cm-1 (Symmetry: A)
```

```
  4.     128.1021 cm-1 (Symmetry: A)
  5.     147.3807 cm-1 (Symmetry: A)
  6.     166.8054 cm-1 (Symmetry: A)
  7.     178.3716 cm-1 (Symmetry: A)
  8.     196.9073 cm-1 (Symmetry: A)
  9.     238.3199 cm-1 (Symmetry: A)
 10.     259.9207 cm-1 (Symmetry: A)
```
***

TS-6b

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C5H11S3(1-)
Number of Basis Functions	277
Electronic Energy (Eh)	-1391.78841963
Sum of electronic and zero-point Energies (Eh)	-1391.633823
Sum of electronic and thermal Energies (Eh)	-1391.623683
Sum of electronic and enthalpy Energies (Eh)	-1391.622739
Sum of electronic and thermal Free Energies (Eh)	-1391.670279
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	45

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           2.066795       -1.308671       -0.065290
S          -0.374716       -0.936611        0.084899
C          -0.018530        0.538843        1.133142
C           0.649897        1.692423        0.387055
C           2.133161        1.495040        0.068634
C           2.431695        0.306947       -0.840958
H           0.605714        0.202529        1.961886
H          -0.983768        0.852087        1.527985
H           0.097568        1.887722       -0.538069
H           0.548186        2.587782        1.010606
H           2.506003        2.406423       -0.412396
H           2.691903        1.376518        1.003491
H           1.844984        0.389834       -1.761275
H           3.487044        0.311007       -1.121621
```

```
S          -2.753877       -0.536767        0.095535
C          -2.773263        1.036315       -0.825050
H          -3.799420        1.283732       -1.099448
H          -2.371387        1.848230       -0.215842
H          -2.175820        0.949512       -1.734569
```

__Frequencies__ (Top 10 out of 51)

```
  1.    -198.8287 cm-1 (Symmetry: A)  *
  2.      67.6196 cm-1 (Symmetry: A)
  3.      74.3616 cm-1 (Symmetry: A)
  4.     130.4167 cm-1 (Symmetry: A)
  5.     161.8667 cm-1 (Symmetry: A)
  6.     176.8240 cm-1 (Symmetry: A)
  7.     210.2201 cm-1 (Symmetry: A)
  8.     231.6656 cm-1 (Symmetry: A)
  9.     257.4465 cm-1 (Symmetry: A)
 10.     289.1762 cm-1 (Symmetry: A)
```
***

TS-7a

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C6H13OS3(1-)
Number of Basis Functions	335
Electronic Energy (Eh)	-1506.2765748
Sum of electronic and zero-point Energies (Eh)	-1506.08957
Sum of electronic and thermal Energies (Eh)	-1506.077191
Sum of electronic and enthalpy Energies (Eh)	-1506.076247
Sum of electronic and thermal Free Energies (Eh)	-1506.128855
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	53

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.859668       -1.154428       -0.502262
```

```
C          -2.223929        0.524592       -1.113304
C          -1.927376        1.673833       -0.149986
C          -0.444859        2.079984       -0.050356
C           0.297067        1.534529        1.172097
C           0.158059        0.033534        1.391892
S           0.531468       -0.976711       -0.087891
O          -2.624666       -1.245157        0.853871
H          -3.288899        0.503562       -1.359914
H          -1.661665        0.626689       -2.045951
H          -2.509994        2.530027       -0.500824
H          -2.327595        1.420309        0.837997
H           0.076136        1.760694       -0.958137
H          -0.373803        3.170540       -0.021999
H          -0.080664        2.030776        2.074220
H           1.358410        1.788431        1.092143
H          -0.860068       -0.234578        1.688462
H           0.835548       -0.302995        2.174992
S           2.975487       -0.658013        0.189379
C           3.134410        0.604415       -1.119959
H           2.701809        1.554699       -0.802797
H           4.188541        0.759722       -1.353431
H           2.622752        0.274499       -2.025657
```

__Frequencies__ (Top 10 out of 63)

```
  1.    -169.2664 cm-1 (Symmetry: A)  *
  2.      49.4183 cm-1 (Symmetry: A)
  3.      77.2824 cm-1 (Symmetry: A)
  4.     111.7186 cm-1 (Symmetry: A)
  5.     119.8444 cm-1 (Symmetry: A)
  6.     138.6142 cm-1 (Symmetry: A)
  7.     161.4785 cm-1 (Symmetry: A)
  8.     182.0178 cm-1 (Symmetry: A)
  9.     188.6954 cm-1 (Symmetry: A)
 10.     236.7629 cm-1 (Symmetry: A)
```
***

TS-7b

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C6H13S3(1-)
Number of Basis Functions	313
Electronic Energy (Eh)	-1431.08442835

| Sum of electronic and zero-point Energies (Eh) | -1430.901155
|
| Sum of electronic and thermal Energies (Eh) | -1430.889713
|
| Sum of electronic and enthalpy Energies (Eh) | -1430.888769
|
| Sum of electronic and thermal Free Energies (Eh) | -1430.939458
|
| Number of Imaginary Frequencies | 1
|
| Mean of alpha and beta Electrons | 49
|

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           1.809883       -1.536993        0.077260
C           2.225198       -0.292692       -1.200591
C           2.465308        1.122470       -0.681928
C           1.263675        1.793442       -0.004022
C           0.910965        1.222754        1.382502
C          -0.371427        0.396453        1.452353
S          -0.609984       -0.929622        0.172565
H           3.118042       -0.642024       -1.724850
H           1.404180       -0.279389       -1.924513
H           2.772282        1.739050       -1.535420
H           3.308827        1.113973        0.017646
H           1.493570        2.857307        0.099264
H           0.391651        1.728614       -0.665189
H           1.749681        0.639690        1.762340
H           0.758193        2.046881        2.088435
H          -0.462813       -0.071247        2.434059
H          -1.229310        1.052736        1.316775
S          -2.934371       -0.415152       -0.058894
C          -2.736047        1.061169       -1.106976
H          -2.151942        0.818927       -1.996069
H          -3.717779        1.422578       -1.415241
H          -2.229068        1.859600       -0.560173
```

__Frequencies__ (Top 10 out of 60)

```
  1.    -207.4044 cm-1 (Symmetry: A)  *
  2.      40.6747 cm-1 (Symmetry: A)
  3.      69.0615 cm-1 (Symmetry: A)
  4.     124.2846 cm-1 (Symmetry: A)
  5.     145.4820 cm-1 (Symmetry: A)
  6.     159.6536 cm-1 (Symmetry: A)
  7.     197.3744 cm-1 (Symmetry: A)
  8.     209.9390 cm-1 (Symmetry: A)
  9.     223.4529 cm-1 (Symmetry: A)
 10.     235.5937 cm-1 (Symmetry: A)
```

***

TS-8a

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C7H15OS3(1-)
Number of Basis Functions	371
Electronic Energy (Eh)	-1545.57554356
Sum of electronic and zero-point Energies (Eh)	-1545.359876
Sum of electronic and thermal Energies (Eh)	-1545.346172
Sum of electronic and enthalpy Energies (Eh)	-1545.345228
Sum of electronic and thermal Free Energies (Eh)	-1545.401245
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	57

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.201355       -1.746536       -0.387323
C          -2.559881       -0.569757       -0.760123
C          -2.860759        0.436523        0.356712
C          -2.482016        1.884374        0.027545
C          -1.033126        2.144256       -0.390064
C           0.034682        1.912167        0.681971
C           0.415478        0.462657        0.984659
S           0.871587       -0.516477       -0.497275
O          -1.432894       -2.146766        1.100443
H          -3.424331       -1.208234       -0.953441
H          -2.285851       -0.089967       -1.703810
H          -2.384382        0.101153        1.280776
H          -3.934241        0.411365        0.561171
H          -2.715403        2.507665        0.898185
H          -3.134149        2.230691       -0.782053
H          -0.782573        1.551725       -1.275702
H          -0.967039        3.190788       -0.702630
H          -0.286519        2.376233        1.623220
H           0.949816        2.426031        0.374332
H          -0.374289       -0.099330        1.484794
H           1.287987        0.446242        1.637987
S           3.134133        0.533975       -0.545223
C           3.896784       -0.654773        0.611436
H           4.949179       -0.406408        0.755079
```

```
H           3.399855       -0.621476        1.583291
H           3.828280       -1.670418        0.219589
```

__Frequencies__ (Top 10 out of 72)

```
  1.    -179.9281 cm-1 (Symmetry: A)  *
  2.      44.6575 cm-1 (Symmetry: A)
  3.      48.6534 cm-1 (Symmetry: A)
  4.      99.4035 cm-1 (Symmetry: A)
  5.     106.6649 cm-1 (Symmetry: A)
  6.     120.5401 cm-1 (Symmetry: A)
  7.     127.0503 cm-1 (Symmetry: A)
  8.     145.8202 cm-1 (Symmetry: A)
  9.     193.5953 cm-1 (Symmetry: A)
 10.     199.6678 cm-1 (Symmetry: A)
```
***

TS-8b

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C7H15S3(1-)
Number of Basis Functions	349
Electronic Energy (Eh)	-1470.39216415
Sum of electronic and zero-point Energies (Eh)	-1470.179661
Sum of electronic and thermal Energies (Eh)	-1470.167242
Sum of electronic and enthalpy Energies (Eh)	-1470.166298
Sum of electronic and thermal Free Energies (Eh)	-1470.218923
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	53

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           0.697925       -1.028941       -0.322126
C           0.428552        0.321839       -1.550584
C           0.309041        1.722109       -0.948017
C          -0.717219        1.847014        0.179882
```

```
C          -2.151209        1.480742       -0.246648
C          -2.906402        0.606451        0.757366
C          -2.205946       -0.706790        1.127889
S          -1.626764       -1.713710       -0.286705
H          -0.470420        0.038232       -2.093874
H           1.270101        0.285216       -2.240764
H           0.045678        2.405430       -1.765408
H           1.293982        2.030013       -0.585288
H          -0.391506        1.202483        1.000086
H          -0.692644        2.869066        0.568702
H          -2.729411        2.392068       -0.424984
H          -2.126727        0.946521       -1.199105
H          -3.895197        0.376079        0.347425
H          -3.074265        1.167335        1.685718
H          -2.889757       -1.323083        1.715461
H          -1.332140       -0.517204        1.757127
S           3.046188       -0.301388       -0.014106
C           2.750051        0.522466        1.586676
H           2.193540        1.451797        1.451874
H           2.176551       -0.132485        2.245265
H           3.703424        0.750177        2.065361
```

__Frequencies__ (Top 10 out of 69)

```
  1.    -209.8984 cm-1 (Symmetry: A)  *
  2.      43.6417 cm-1 (Symmetry: A)
  3.      77.5194 cm-1 (Symmetry: A)
  4.     110.7186 cm-1 (Symmetry: A)
  5.     129.8310 cm-1 (Symmetry: A)
  6.     143.1309 cm-1 (Symmetry: A)
  7.     170.5801 cm-1 (Symmetry: A)
  8.     191.9914 cm-1 (Symmetry: A)
  9.     217.9300 cm-1 (Symmetry: A)
 10.     225.1364 cm-1 (Symmetry: A)
```
***

TS-9a

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C8H17OS3(1-)
Number of Basis Functions	407
Electronic Energy (Eh)	-1584.87501531

Sum of electronic and zero-point Energies (Eh)	-1584.63049
Sum of electronic and thermal Energies (Eh)	-1584.615586
Sum of electronic and enthalpy Energies (Eh)	-1584.614642
Sum of electronic and thermal Free Energies (Eh)	-1584.67308
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	61

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.015147       -1.830067        0.085800
C          -2.230652       -1.073556       -1.095364
C          -3.180721       -0.042604       -0.479078
C           0.383867        1.719399        1.247980
C           0.907652        0.286125        1.282262
S           0.989553       -0.579750       -0.332104
C          -1.119018        1.809089        0.955575
C          -2.884188        1.414528       -0.855006
C          -1.458417        1.863529       -0.538759
O          -1.564176       -1.591319        1.515847
H          -1.630304       -0.667714       -1.913984
H          -2.787382       -1.928346       -1.481271
H          -3.170497       -0.170607        0.606833
H          -4.197047       -0.281644       -0.801915
H           0.587914        2.146958        2.236009
H           0.960795        2.306962        0.526014
H           0.260939       -0.324527        1.919809
H           1.921264        0.252191        1.679283
H          -1.542546        2.692547        1.444038
H          -1.596961        0.938790        1.416328
H          -3.598964        2.058072       -0.329285
H          -3.071755        1.549205       -1.925818
H          -1.308689        2.885092       -0.904436
H          -0.756890        1.237958       -1.093847
S           3.222263        0.575669       -0.859780
C           4.237875       -0.635823        0.056556
H           3.947177       -0.667584        1.109200
H           4.119408       -1.635312       -0.364141
H           5.291847       -0.359231        0.002769
```

__Frequencies__ (Top 10 out of 81)

```
  1.    -155.7149 cm-1 (Symmetry: A)  *
  2.      49.7966 cm-1 (Symmetry: A)
  3.      58.6524 cm-1 (Symmetry: A)
  4.      72.0721 cm-1 (Symmetry: A)
  5.      96.4392 cm-1 (Symmetry: A)
  6.     112.0144 cm-1 (Symmetry: A)
  7.     127.2042 cm-1 (Symmetry: A)
```

```
  8.     139.1976 cm-1 (Symmetry: A)
  9.     177.2006 cm-1 (Symmetry: A)
 10.     193.3493 cm-1 (Symmetry: A)
```
***

TS-9b

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C8H17S3(1-)
Number of Basis Functions	385
Electronic Energy (Eh)	-1509.68763285
Sum of electronic and zero-point Energies (Eh)	-1509.446582
Sum of electronic and thermal Energies (Eh)	-1509.432763
Sum of electronic and enthalpy Energies (Eh)	-1509.431818
Sum of electronic and thermal Free Energies (Eh)	-1509.487641
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	57

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -1.065607       -1.894287        0.819368
C          -2.132544       -1.762024       -0.676173
C          -2.302561       -0.350013       -1.243188
C          -0.456357        1.385895        1.350026
C           0.827140        0.556593        1.315210
S           0.951249       -0.703923       -0.040286
C          -0.830840        2.074493        0.028450
C          -2.968699        0.645762       -0.278941
C          -2.337732        2.047520       -0.275789
H          -3.106733       -2.171446       -0.392537
H          -1.723139       -2.413413       -1.451698
H          -2.892444       -0.426601       -2.163638
H          -1.316853        0.009280       -1.540906
H          -0.327966        2.134501        2.139889
H          -1.262113        0.730486        1.675104
H           0.945556        0.022474        2.258960
H           1.697624        1.195187        1.170822
H          -0.289412        1.594267       -0.789832
```

```
H          -0.493998        3.115453        0.040431
H          -2.933858        0.230395        0.730959
H          -4.030183        0.744105       -0.526241
H          -2.865721        2.664792        0.460253
H          -2.504043        2.520718       -1.250362
S           2.885539        0.354037       -1.039809
C           4.132324       -0.147848        0.192834
H           4.167845       -1.234538        0.277985
H           5.114455        0.214198       -0.114025
H           3.897708        0.274644        1.171897
```

__Frequencies__ (Top 10 out of 78)

```
  1.    -207.4766 cm-1 (Symmetry: A)  *
  2.      51.5361 cm-1 (Symmetry: A)
  3.      61.3006 cm-1 (Symmetry: A)
  4.      86.8857 cm-1 (Symmetry: A)
  5.     114.6180 cm-1 (Symmetry: A)
  6.     136.5495 cm-1 (Symmetry: A)
  7.     140.9816 cm-1 (Symmetry: A)
  8.     159.8054 cm-1 (Symmetry: A)
  9.     190.1707 cm-1 (Symmetry: A)
 10.     203.4153 cm-1 (Symmetry: A)
```
***

TS-10a

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C9H19OS3(1-)
Number of Basis Functions	443
Electronic Energy (Eh)	-1624.18113886
Sum of electronic and zero-point Energies (Eh)	-1623.907889
Sum of electronic and thermal Energies (Eh)	-1623.89175
Sum of electronic and enthalpy Energies (Eh)	-1623.890806
Sum of electronic and thermal Free Energies (Eh)	-1623.951918
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	65

__Molecular Geometry in Cartesian Coordinates__

```xyz
S          -0.898201        1.713500        0.710722
C          -1.805050        1.822434       -0.871752
C          -2.237547        0.470077       -1.432932
C          -3.093574       -0.382523       -0.476529
C          -0.947142       -1.945266        1.220664
C           0.576416       -1.892015        1.428087
C           1.160971       -0.481942        1.424049
S           0.989583        0.438243       -0.167969
C          -1.353579       -2.265756       -0.223860
C          -2.797850       -1.885890       -0.574004
O          -0.373284        3.170706        0.926146
H          -2.658835        2.476852       -0.675140
H          -1.127747        2.337433       -1.559688
H          -1.338213       -0.075020       -1.719817
H          -2.792261        0.653721       -2.357821
H          -4.153474       -0.212207       -0.685507
H          -2.942624       -0.052495        0.554313
H          -1.388752       -2.696056        1.883113
H          -1.370949       -0.985957        1.532473
H           1.084275       -2.490878        0.664985
H           0.838018       -2.333252        2.395694
H           0.679791        0.125809        2.192486
H           2.228144       -0.510613        1.639690
H          -0.661581       -1.763290       -0.903030
H          -1.215504       -3.338781       -0.394888
H          -3.016197       -2.227131       -1.592348
H          -3.484629       -2.425265        0.088122
S           2.953163       -0.712105       -1.074495
C           4.198928        0.420931       -0.373025
H           4.028911        1.440371       -0.721174
H           4.160451        0.411263        0.718146
H           5.195283        0.105347       -0.685099
```

__Frequencies__ (Top 10 out of 90)

```
  1.    -187.9722 cm-1 (Symmetry: A)  *
  2.      47.6070 cm-1 (Symmetry: A)
  3.      52.0603 cm-1 (Symmetry: A)
  4.      81.6039 cm-1 (Symmetry: A)
  5.      91.8693 cm-1 (Symmetry: A)
  6.     108.1707 cm-1 (Symmetry: A)
  7.     111.7646 cm-1 (Symmetry: A)
  8.     127.5650 cm-1 (Symmetry: A)
  9.     146.1626 cm-1 (Symmetry: A)
 10.     179.6252 cm-1 (Symmetry: A)
```

***

TS-10b

Run with Gaussian 16revisionA.03.

Datum	Value
Charge	-1
Multiplicity	1
Stoichiometry	C9H19S3(1-)
Number of Basis Functions	421
Electronic Energy (Eh)	-1548.99240144
Sum of electronic and zero-point Energies (Eh)	-1548.722665
Sum of electronic and thermal Energies (Eh)	-1548.70755
Sum of electronic and enthalpy Energies (Eh)	-1548.706606
Sum of electronic and thermal Free Energies (Eh)	-1548.765562
Number of Imaginary Frequencies	1
Mean of alpha and beta Electrons	61

__Molecular Geometry in Cartesian Coordinates__

```xyz
S           0.527426        2.215441        0.827071
C           1.609976        2.203433       -0.660268
C           2.026053        0.817075       -1.147176
C           3.075398        0.090140       -0.299587
C           0.734988       -2.037842        0.244155
C           0.385949       -1.092894        1.396575
C          -0.984703       -0.434024        1.346930
S          -1.238613        0.745044       -0.058290
C           2.241612       -2.355099        0.205586
C           3.139013       -1.415565       -0.620554
H           1.081527        2.722282       -1.463198
H           2.490407        2.804112       -0.413104
H           2.425502        0.916394       -2.164379
H           1.126724        0.208130       -1.234591
H           4.052417        0.542203       -0.500533
H           2.886601        0.248443        0.765665
H           0.170371       -2.967885        0.369440
H           0.409092       -1.614887       -0.710476
H           1.129272       -0.301949        1.471889
H           0.443884       -1.658628        2.335114
H          -1.154074        0.132921        2.263192
H          -1.777869       -1.174326        1.247214
H           2.612993       -2.378480        1.237915
H           2.388019       -3.365435       -0.188717
H           4.167751       -1.768153       -0.497525
H           2.901371       -1.547920       -1.683659
S          -2.972582       -0.658245       -1.084660
```

```
C          -4.326020       -0.278935        0.078561
H          -4.070500       -0.607894        1.088034
H          -4.522292        0.793831        0.099317
H          -5.234479       -0.796337       -0.232864
```

__Frequencies__ (Top 10 out of 87)

```
  1.    -210.6581 cm-1 (Symmetry: A)  *
  2.      46.0430 cm-1 (Symmetry: A)
  3.      51.6250 cm-1 (Symmetry: A)
  4.      75.9915 cm-1 (Symmetry: A)
  5.     100.5276 cm-1 (Symmetry: A)
  6.     116.6576 cm-1 (Symmetry: A)
  7.     122.3534 cm-1 (Symmetry: A)
  8.     130.4428 cm-1 (Symmetry: A)
  9.     178.3091 cm-1 (Symmetry: A)
 10.     212.2311 cm-1 (Symmetry: A)
```
***