

Supporting Information

Experimental and theoretical study of the reaction of F₂ with thiirane

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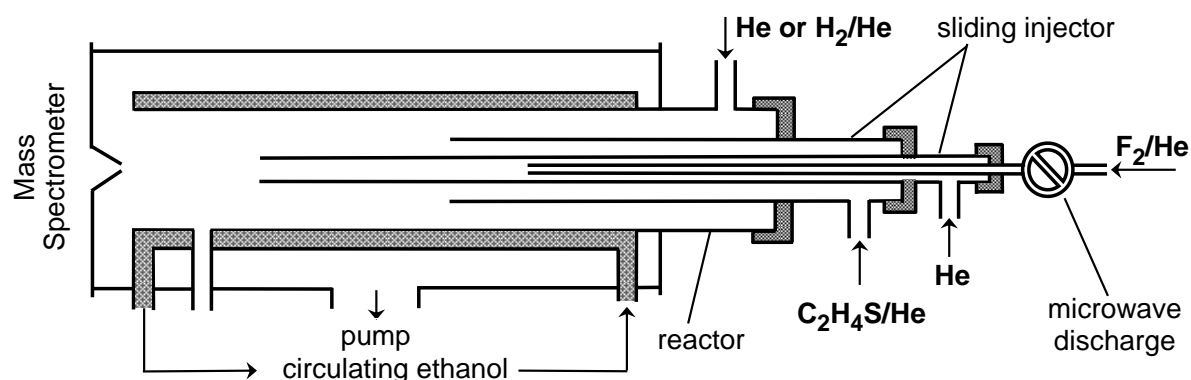


Figure S1. Configuration of the low temperature flow reactor used in the study of reaction (1).

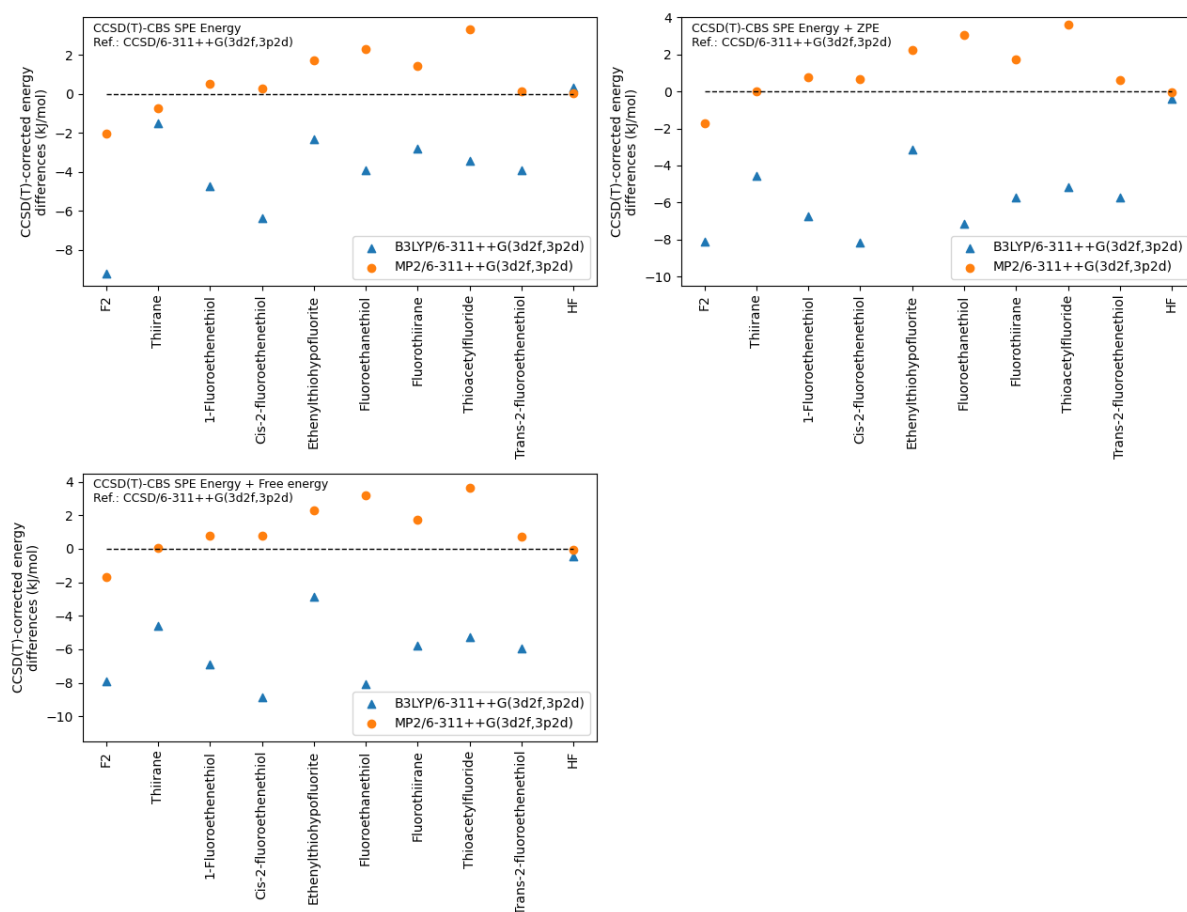


Figure S2. Top left: CCSD(T)-CBS/(aug-cc-pVTZ:aug-cc-pVQZ) single point energy (SPE) differences between B3LYP, MP2 and CCSD (reference) for every molecule. Top right: CCSD(T)-CBS/(aug-cc-pVTZ:aug-cc-pVQZ) single point energy (SPE) + Zero Point Energy (ZPE) differences between B3LYP, MP2 and CCSD (reference) for every molecule. Bottom left: CCSD(T)-CBS/(aug-cc-pVTZ:aug-cc-pVQZ) single point energy (SPE) + thermal free energy differences between B3LYP, MP2 and CCSD (reference) for every molecule. The geometry optimization has been performed at (B3LYP, MP2 or CCSD)/6-311++G(3d2f,3p2d) level in all cases.

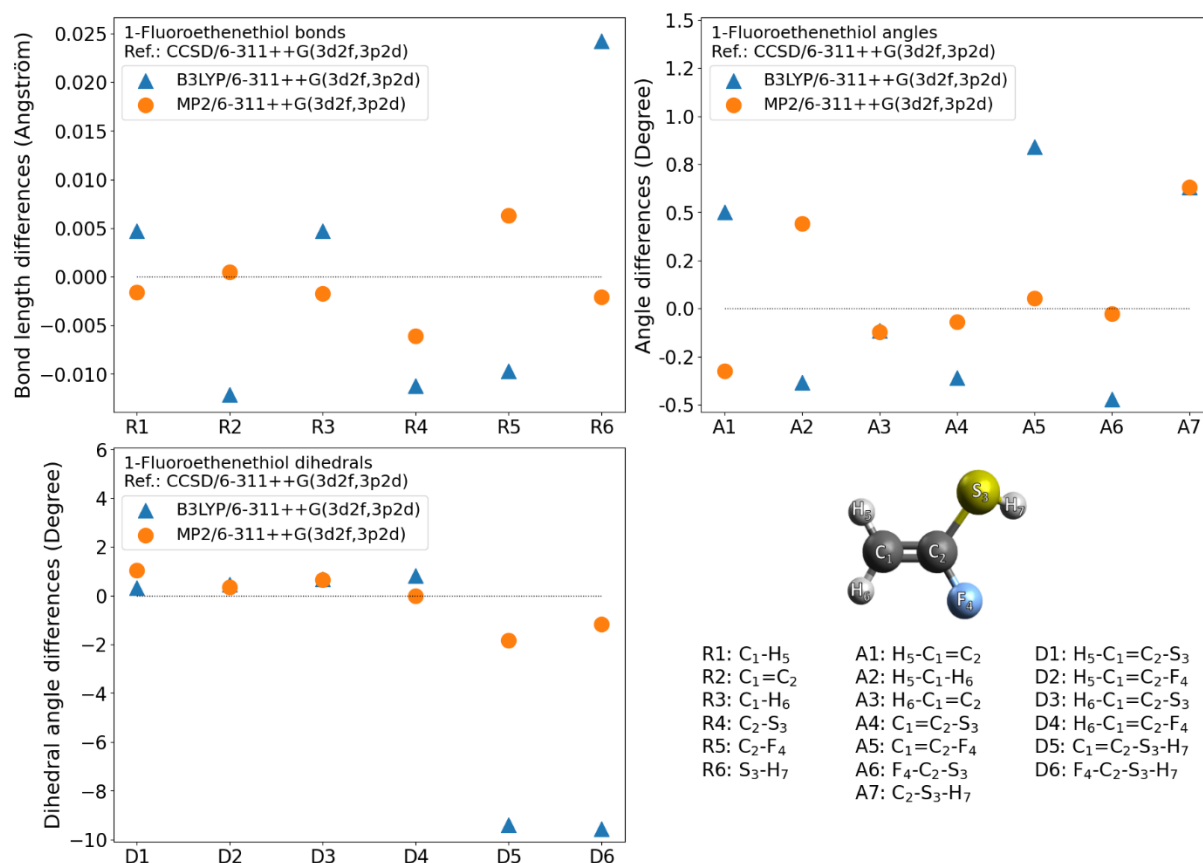


Figure S3. Top left: bond length differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of 1-Fluoroethenethiol. Top right: angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of 1-Fluoroethenethiol. Bottom left: dihedral angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of 1-Fluoroethenethiol.

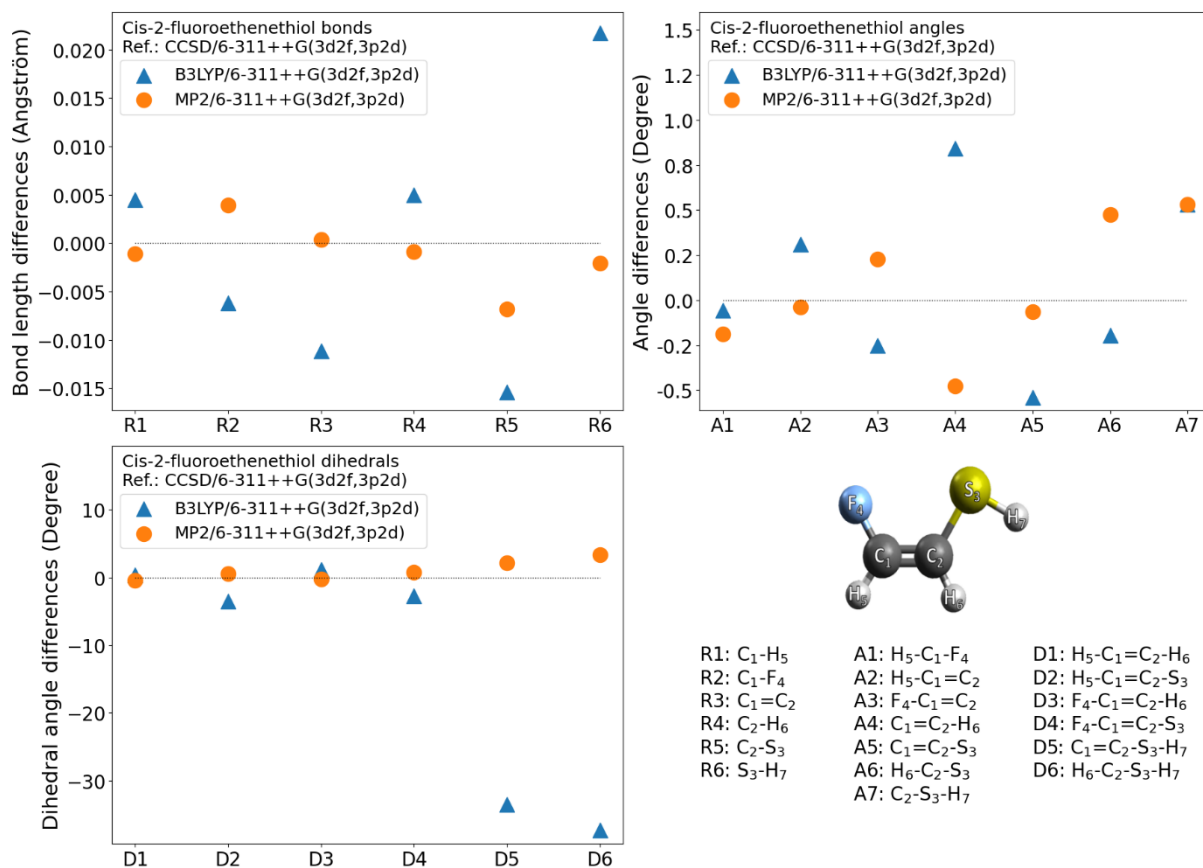


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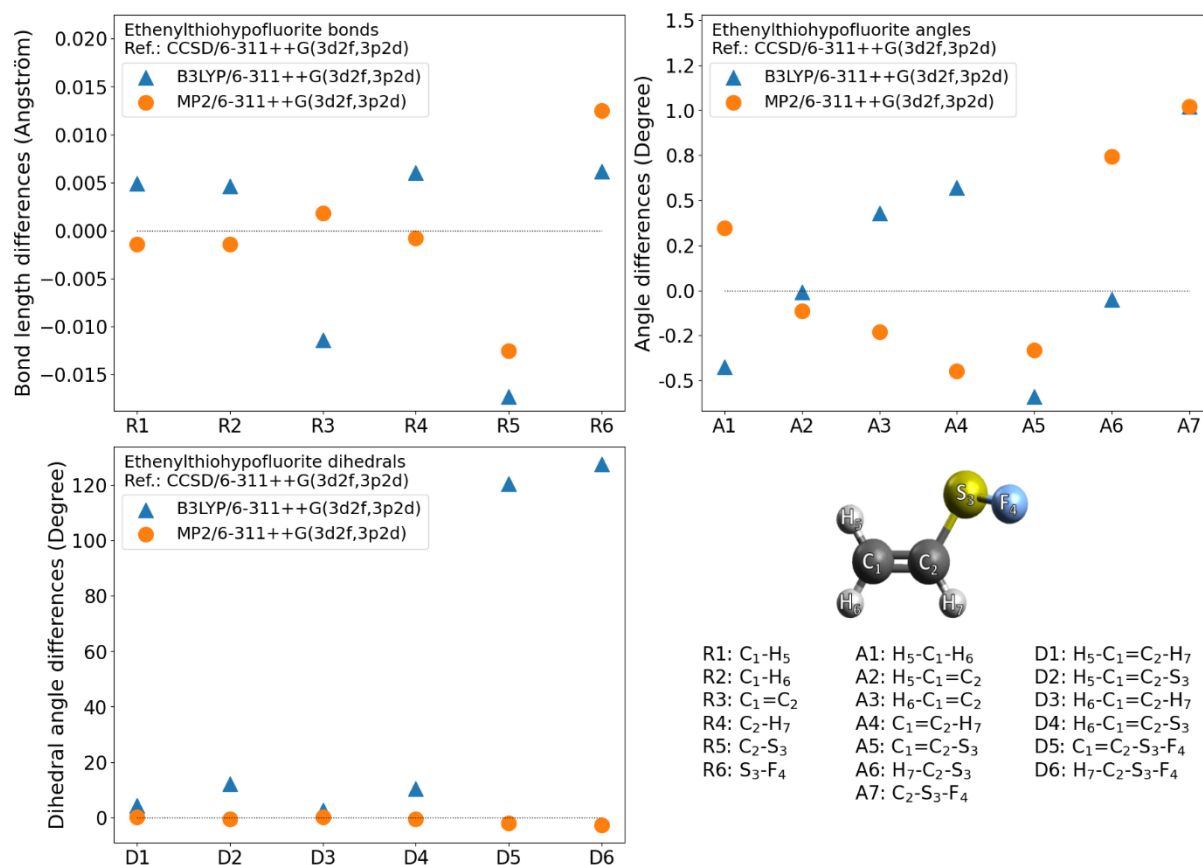


Figure S5. Top left: bond length differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Ethenylthiohypofluorite. Top right: angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Ethenylthiohypofluorite. Bottom left: dihedral angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Ethenylthiohypofluorite.

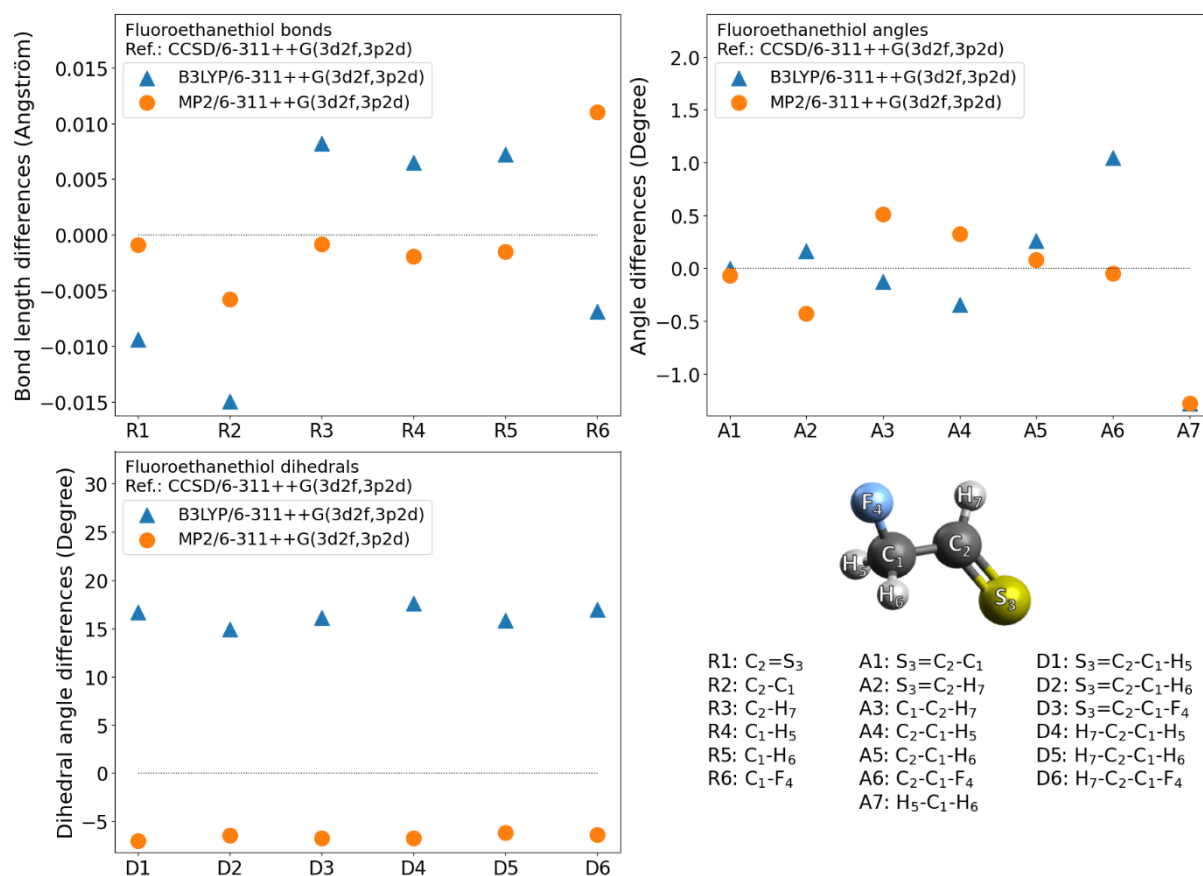


Figure S6. Top left: bond length differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Fluoroethanethiol. Top right: angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Fluoroethanethiol. Bottom left: dihedral angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Fluoroethanethiol.

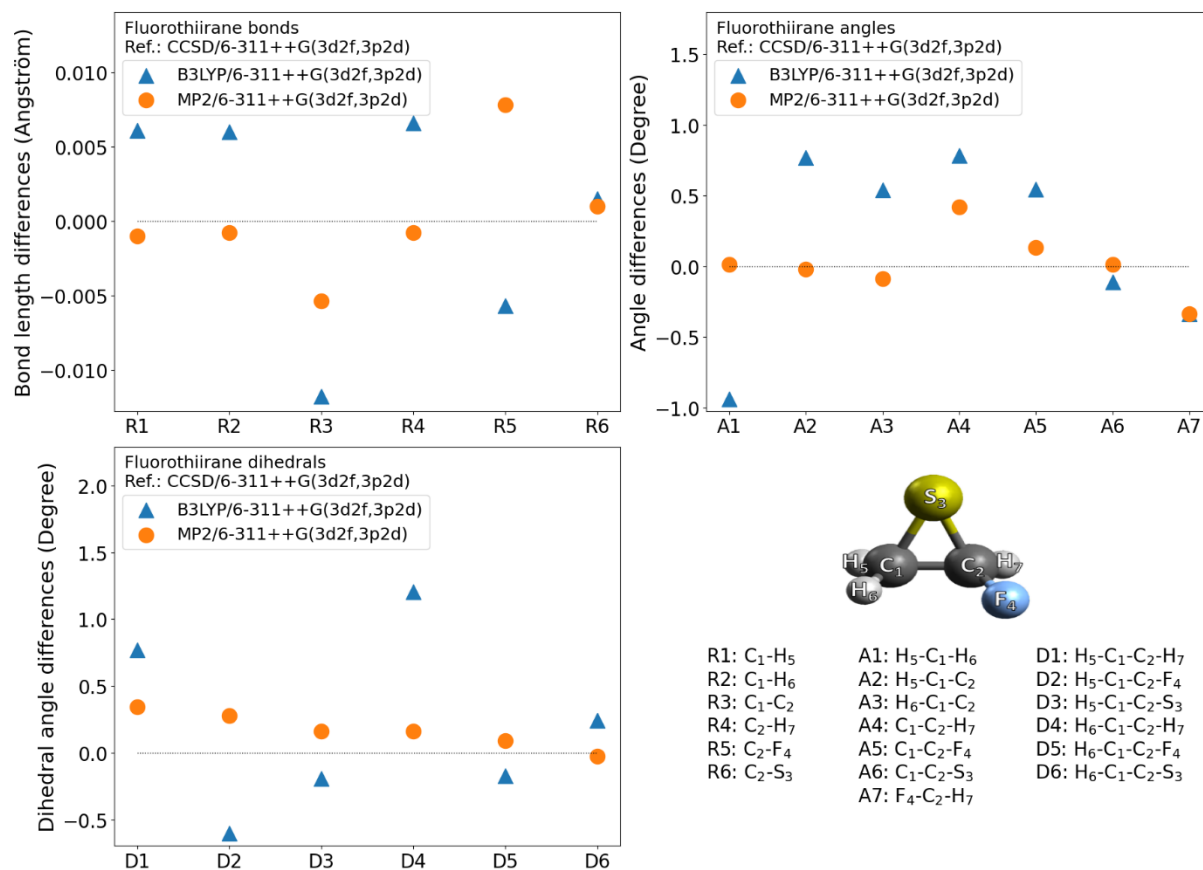


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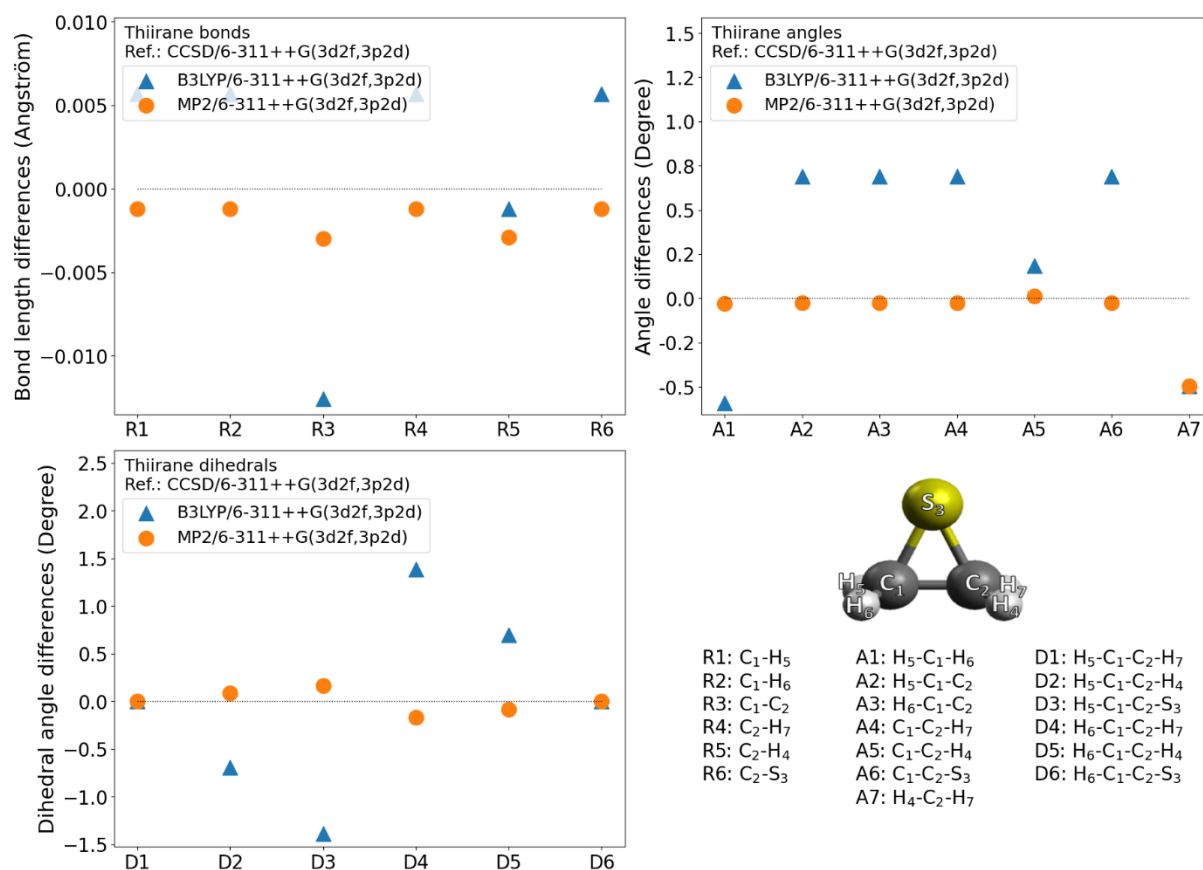


Figure S8. Top left: bond length differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Thiirane. Top right: angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Thiirane. Bottom left: dihedral angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Thiirane.

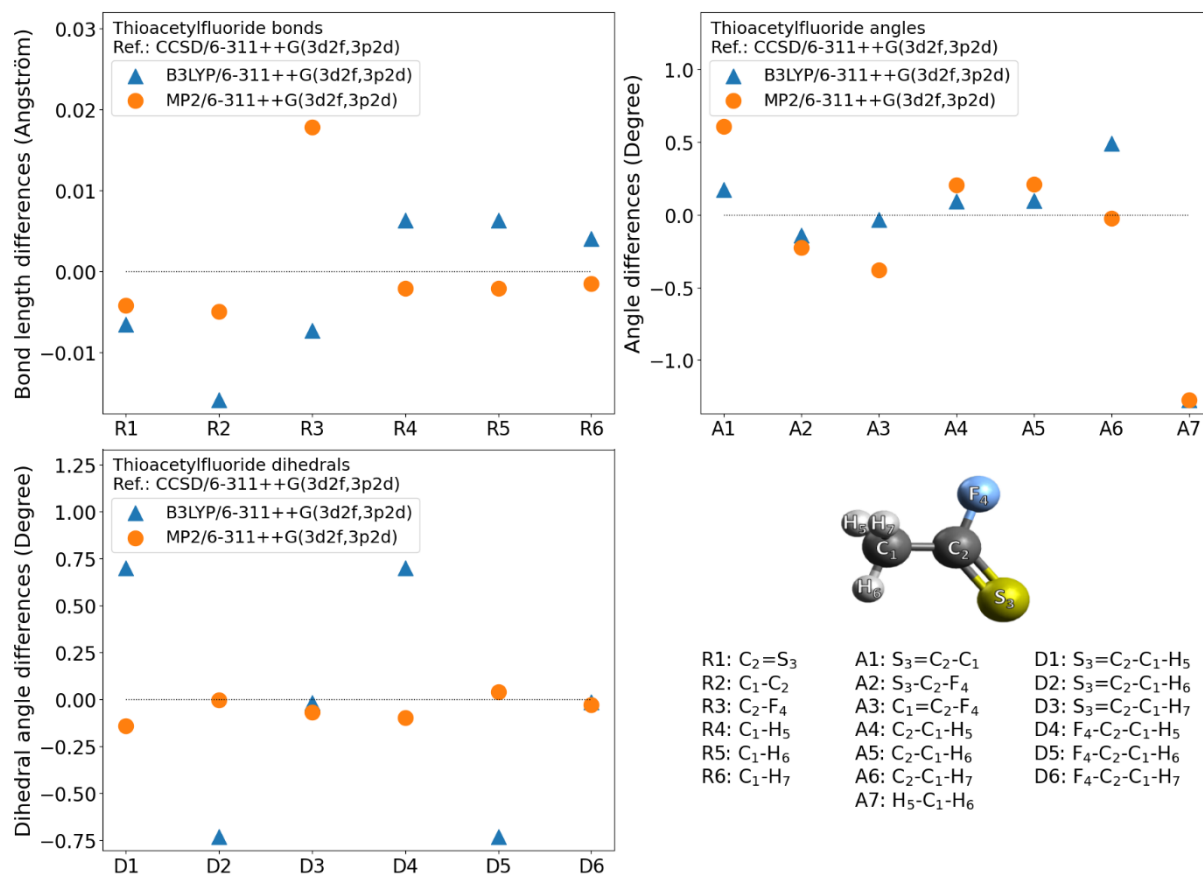


Figure S9. Top left: bond length differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Thioacetylfluoride. Top right: angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Thioacetylfluoride. Bottom left: dihedral angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Thioacetylfluoride.

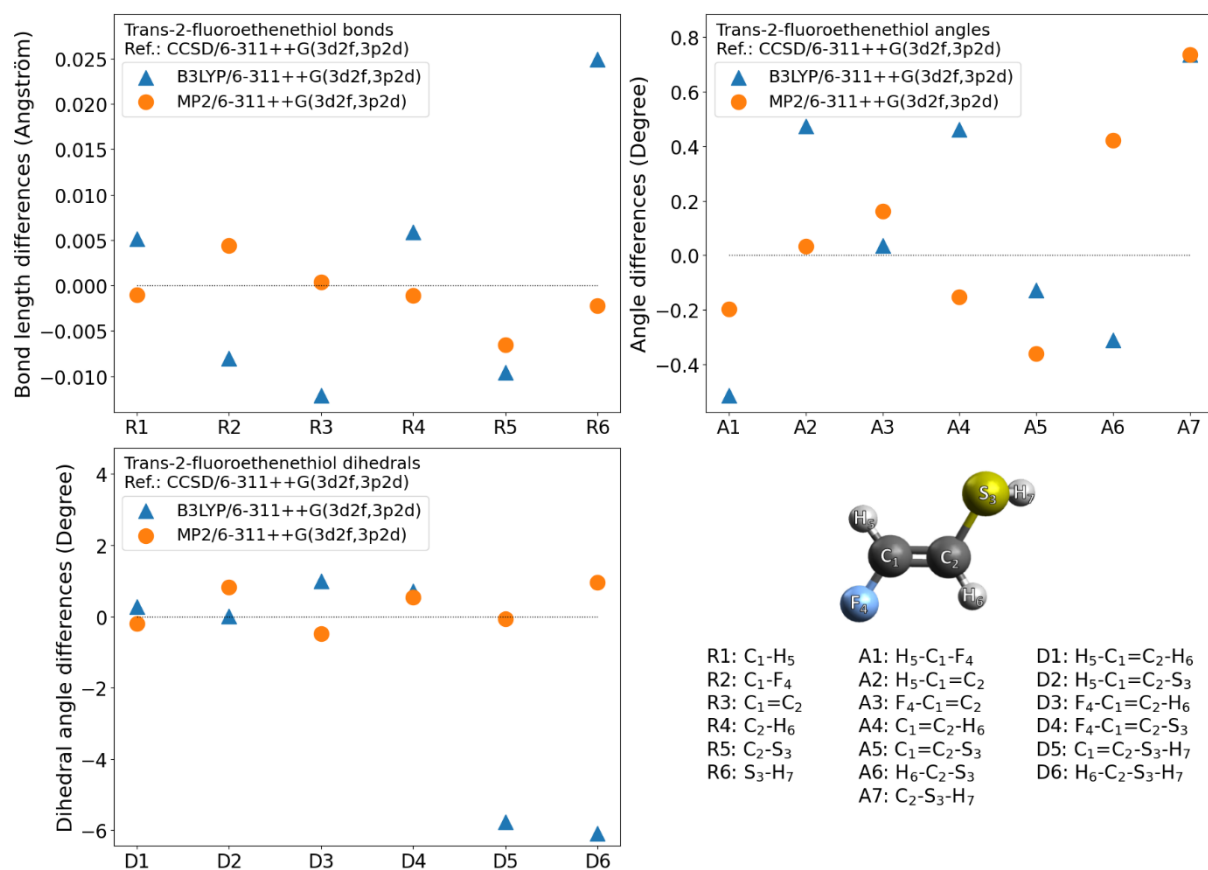


Figure S10. Top left: bond length differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Trans-2-fluoroethenethiol. Top right: angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Trans-2-fluoroethenethiol. Bottom left: dihedral angle differences between MP2/6-311++G(3d2f,3p2d) (Blue) and B3LYP/6-311++G(3d2f,3p2d) (Orange) with CCSD /6-311++G(3d2f,3p2d) level of theory in the case of Trans-2-fluoroethenethiol.

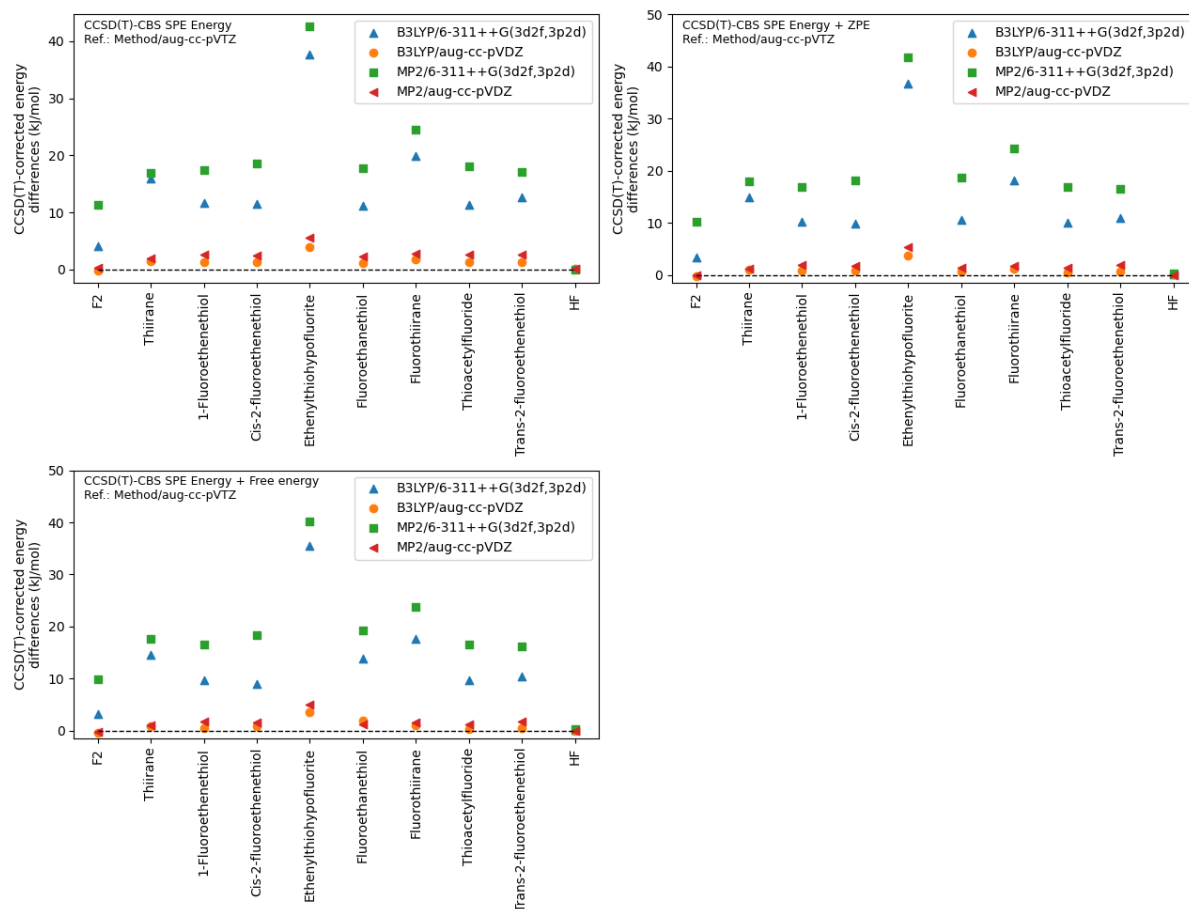


Figure S11. Top left: CCSD(T)-CBS/(aug-cc-pVTZ:aug-cc-pVQZ) single point energy (SPE) differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d), (B3LYP or MP2)/aug-cc-pVDZ and (B3LYP or MP2)/aug-cc-pVTZ (reference) for every molecule. Top right: CCSD(T)-CBS/(aug-cc-pVTZ:aug-cc-pVQZ) single point energy (SPE) + Zero Point Energy (ZPE) differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d), (B3LYP or MP2)/aug-cc-pVDZ and (B3LYP or MP2)/aug-cc-pVTZ (reference) for every molecule. Bottom left: CCSD(T)-CBS/(aug-cc-pVTZ:aug-cc-pVQZ) single point energy (SPE) + thermal free energy differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d), (B3LYP or MP2)/aug-cc-pVDZ and (B3LYP or MP2)/aug-cc-pVTZ (reference) for every molecule. The geometry optimization has been performed at (B3LYP, MP2 or CCSD)/6-311++G(3d2f,3p2d) level in all cases.

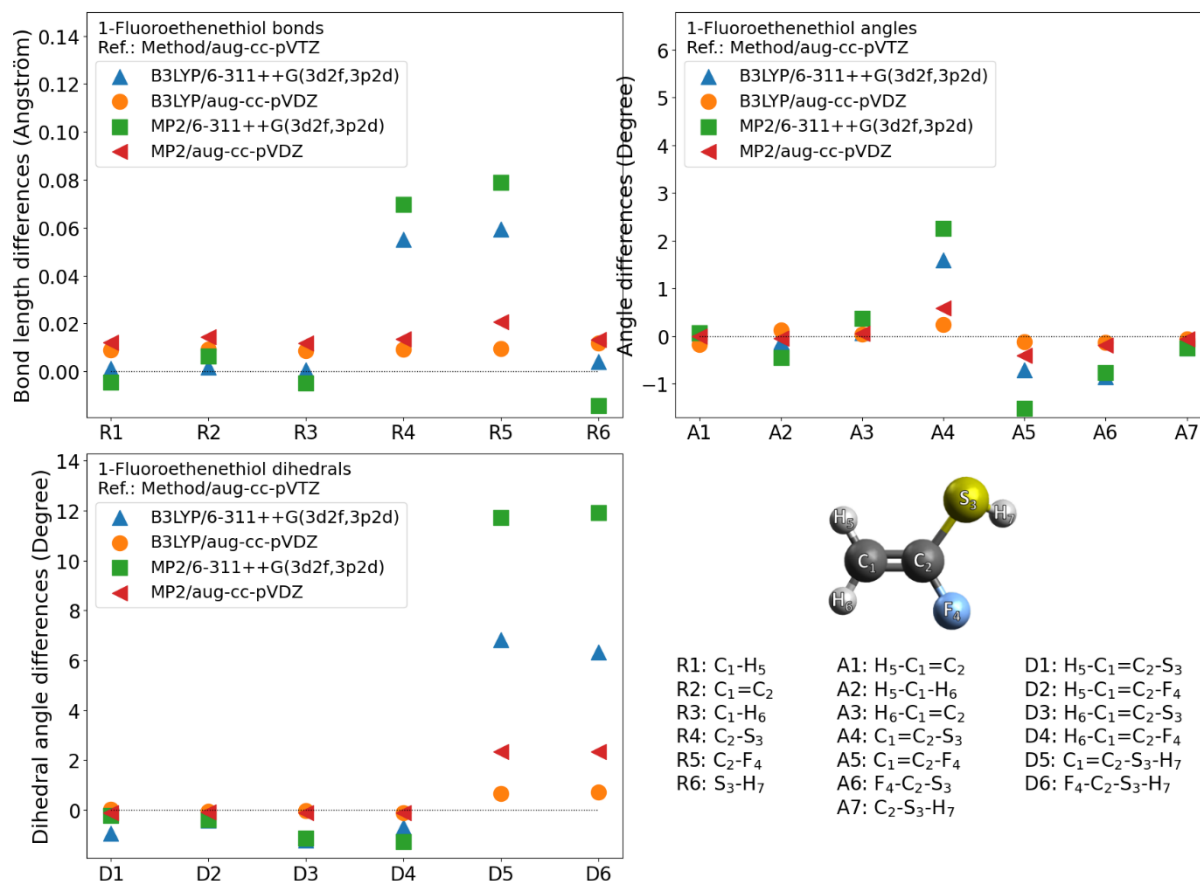


Figure S12. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of 1-Fluoroethenethiol. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of 1-Fluoroethenethiol. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of 1-Fluoroethenethiol.

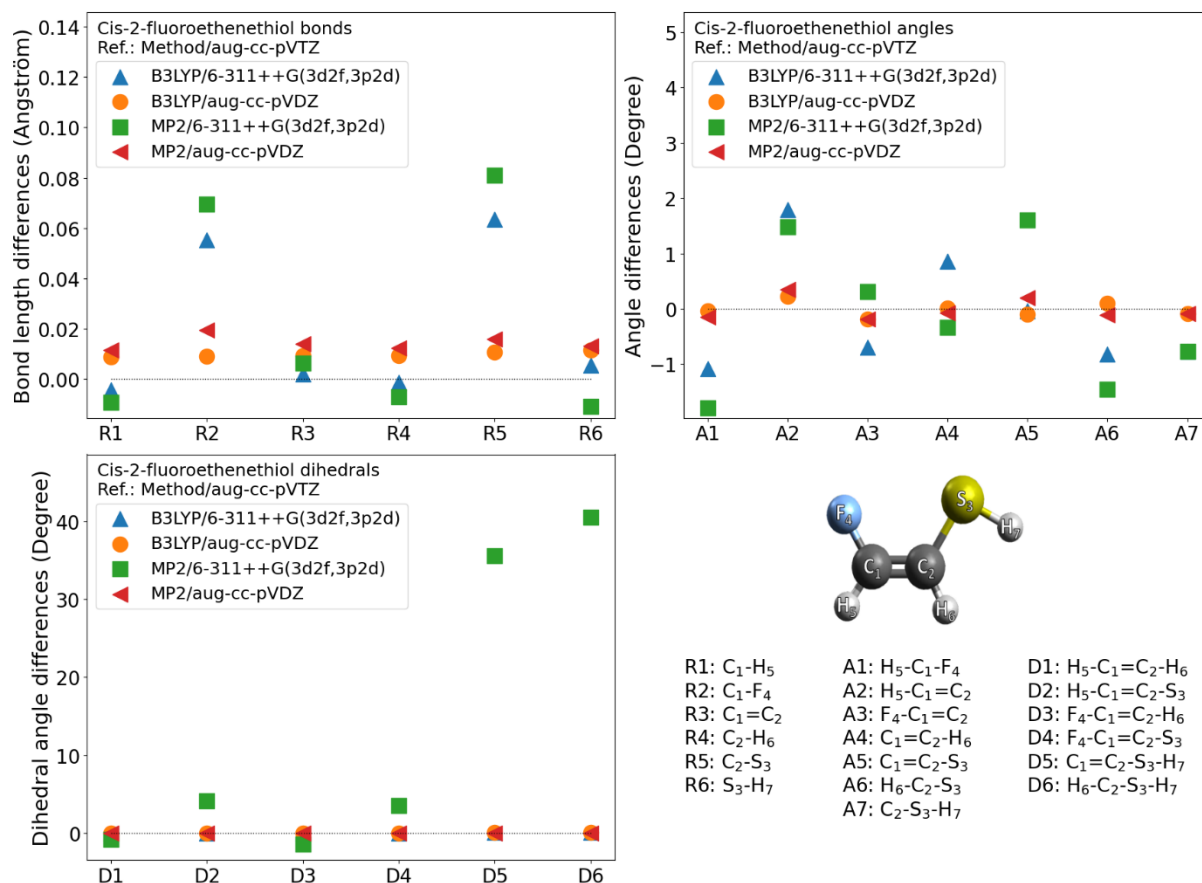


Figure S13. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Cis-2-fluoroethenethiol. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Cis-2-fluoroethenethiol. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Cis-2-fluoroethenethiol.

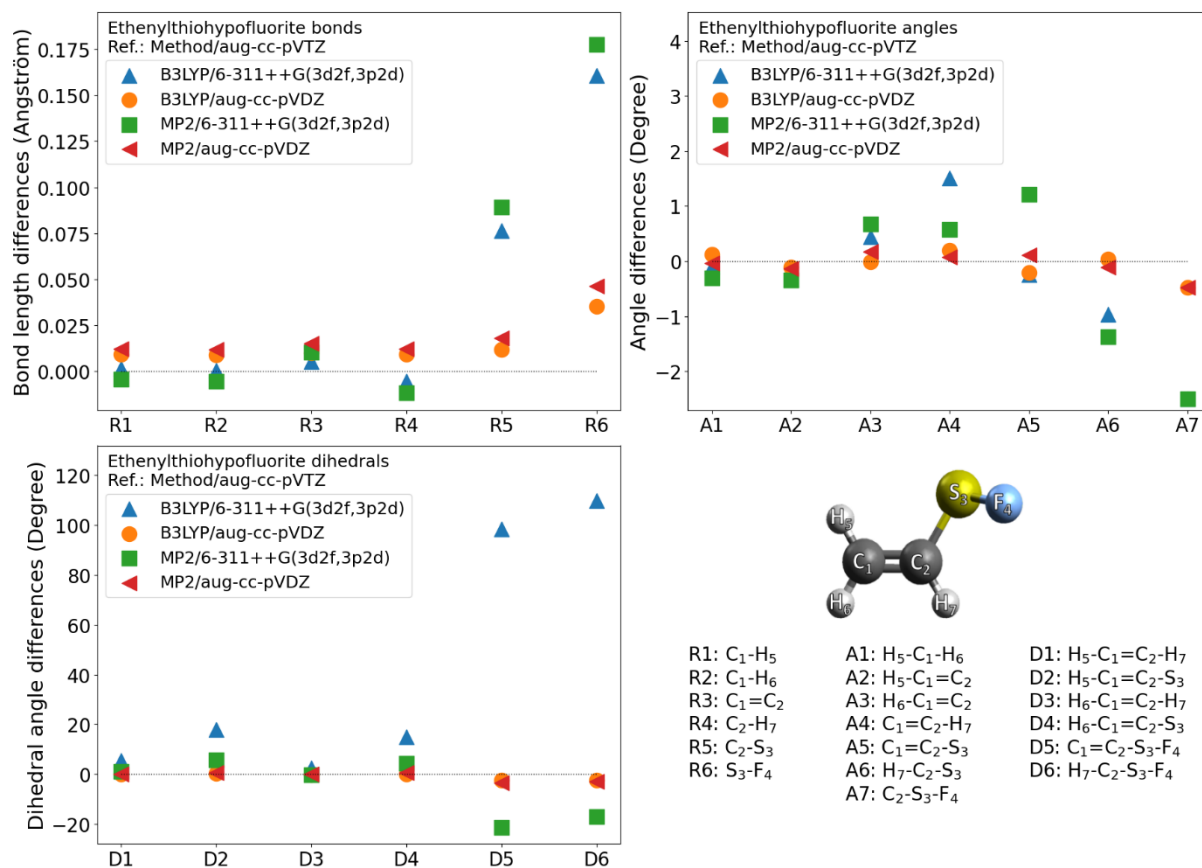


Figure S14. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Ethenylthiohypofluorite. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Ethenylthiohypofluorite. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Ethenylthiohypofluorite.

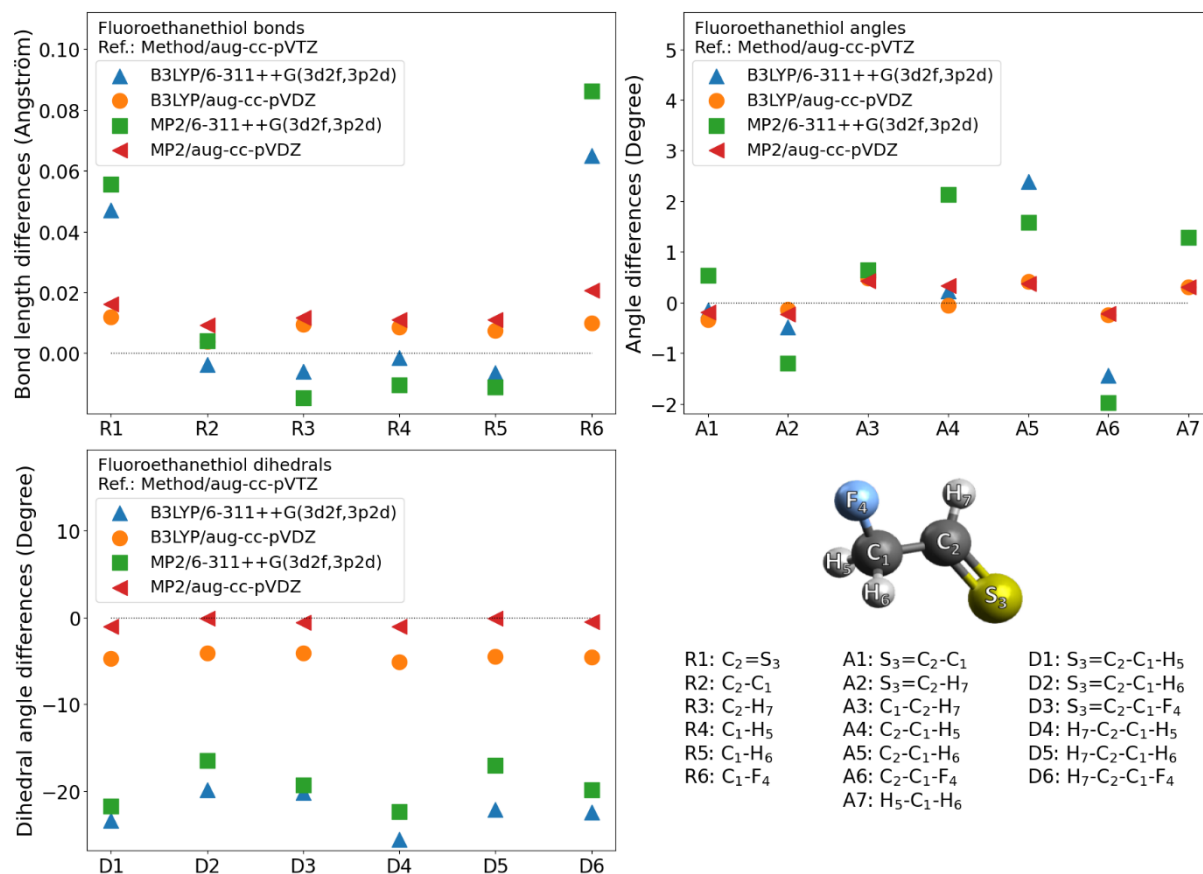


Figure S15. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Fluoroethanethiol. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Fluoroethanethiol. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Fluoroethanethiol.

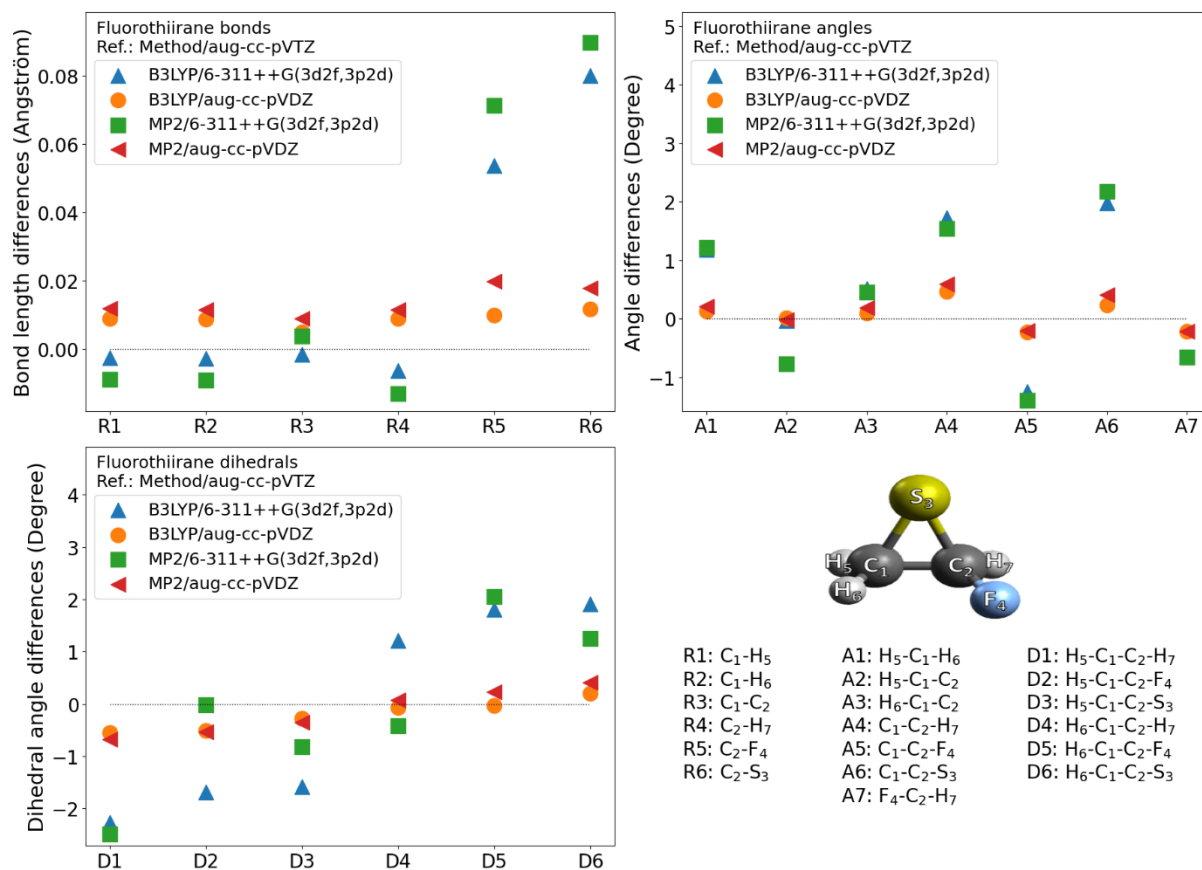


Figure S16. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Fluorothiirane. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Fluorothiirane. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Fluorothiirane.

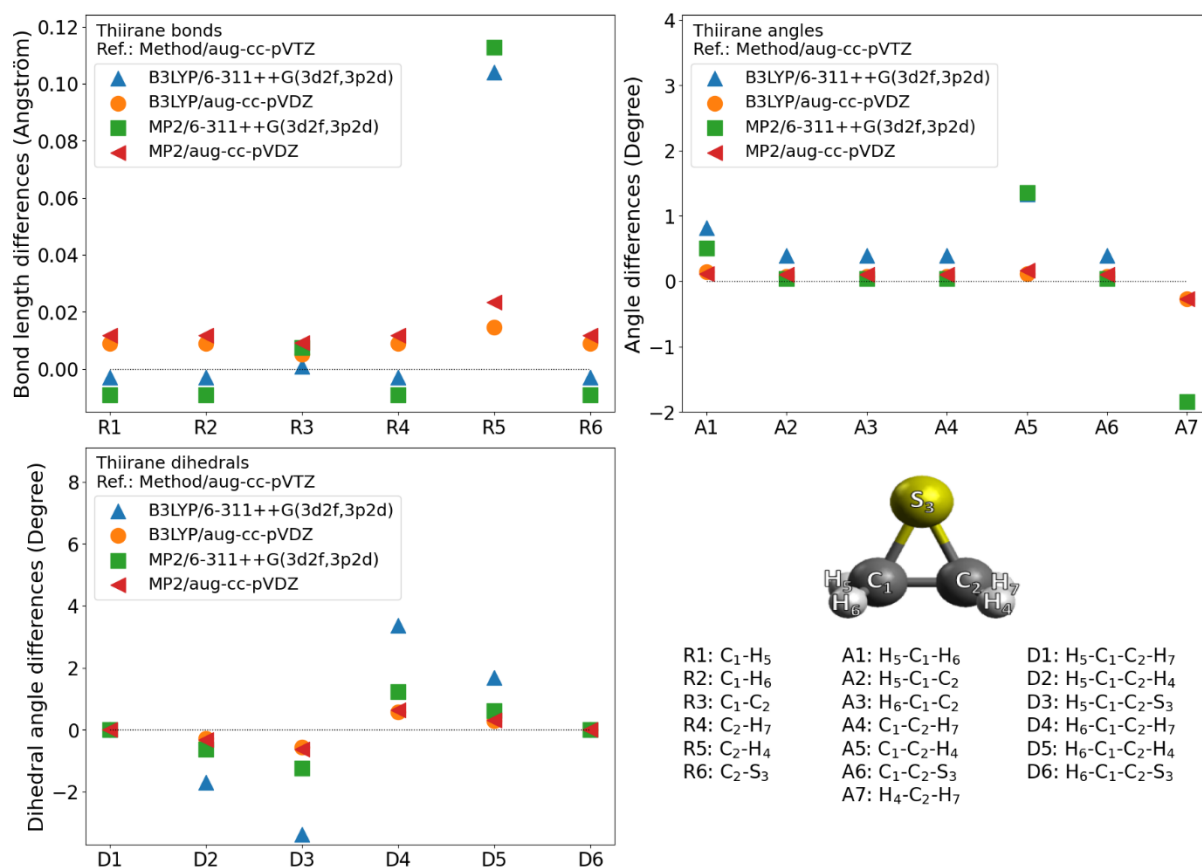


Figure S17. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Thiirane. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Thiirane. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Thiirane.

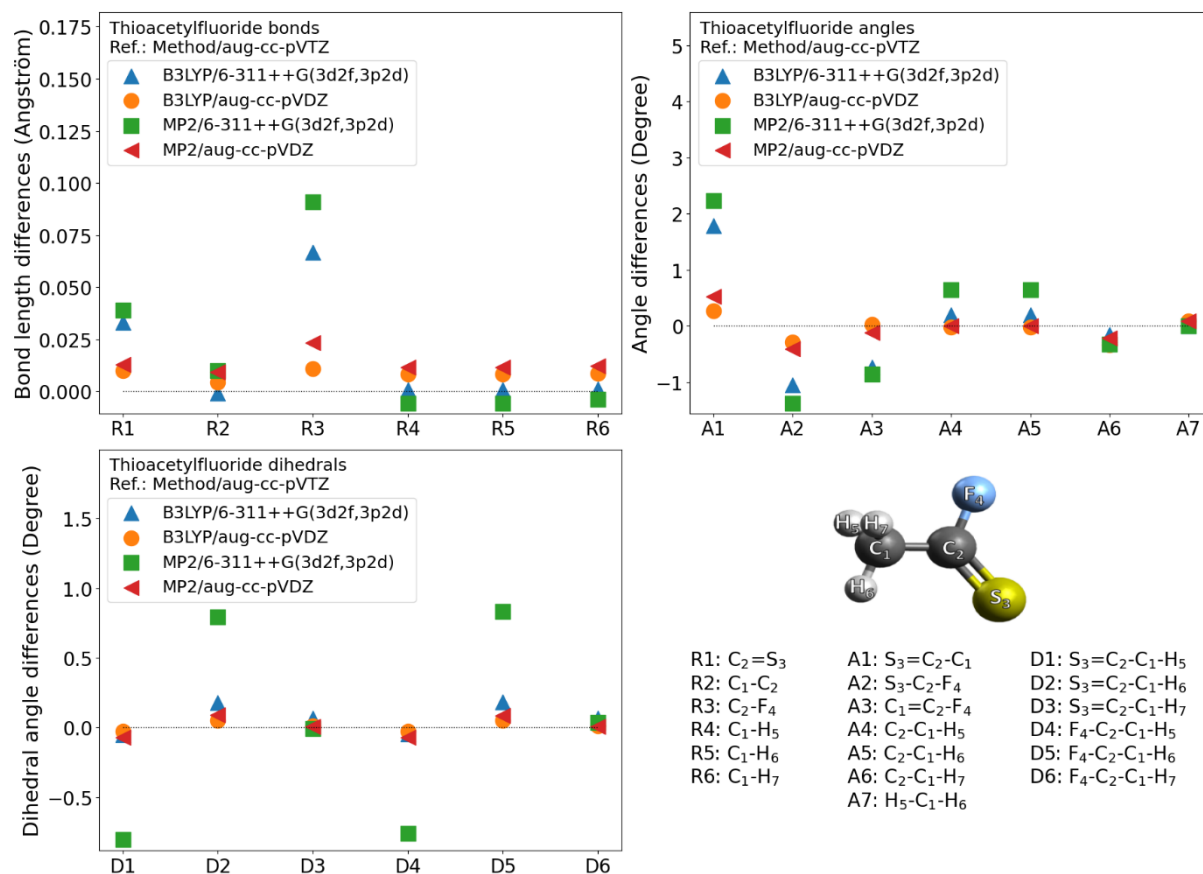


Figure S18. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Thioacetylfluoride. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Thioacetylfluoride. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Thioacetylfluoride.

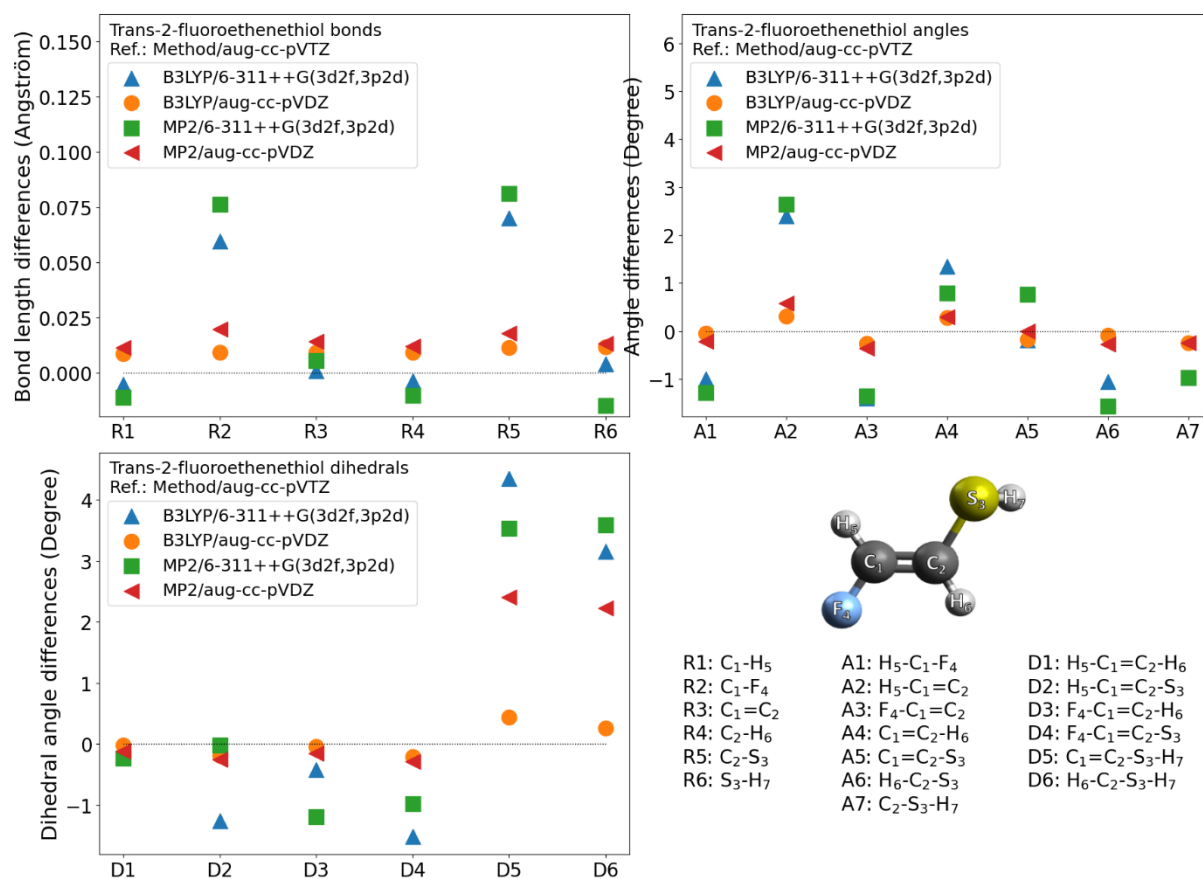


Figure S19. Top left: bond length differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Trans-2-fluoroethenethiol. Top right: angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Trans-2-fluoroethenethiol. Bottom left: dihedral angle differences between (B3LYP or MP2)/6-311++G(3d2f,3p2d) and (B3LYP or MP2)/aug-cc-pVDZ with (B3LYP or MP2)/aug-cc-pVTZ level of theory in the case of Trans-2-fluoroethenethiol.

Boltzmann distribution

In Figure 19, the Boltzmann relative distribution has been computed as function of temperature over range going from 100 K to 100000 K corresponding to an energy range of 0.83 kJ/mol to 831.43 kJ/mol. One can observe that if the thioacetylfluoride is dominating the distribution at low energy, it changes rapidly over ~10 kJ/mol. Over 100 kJ/mol, the relative ratio are between 10 and 20% for every compounds.

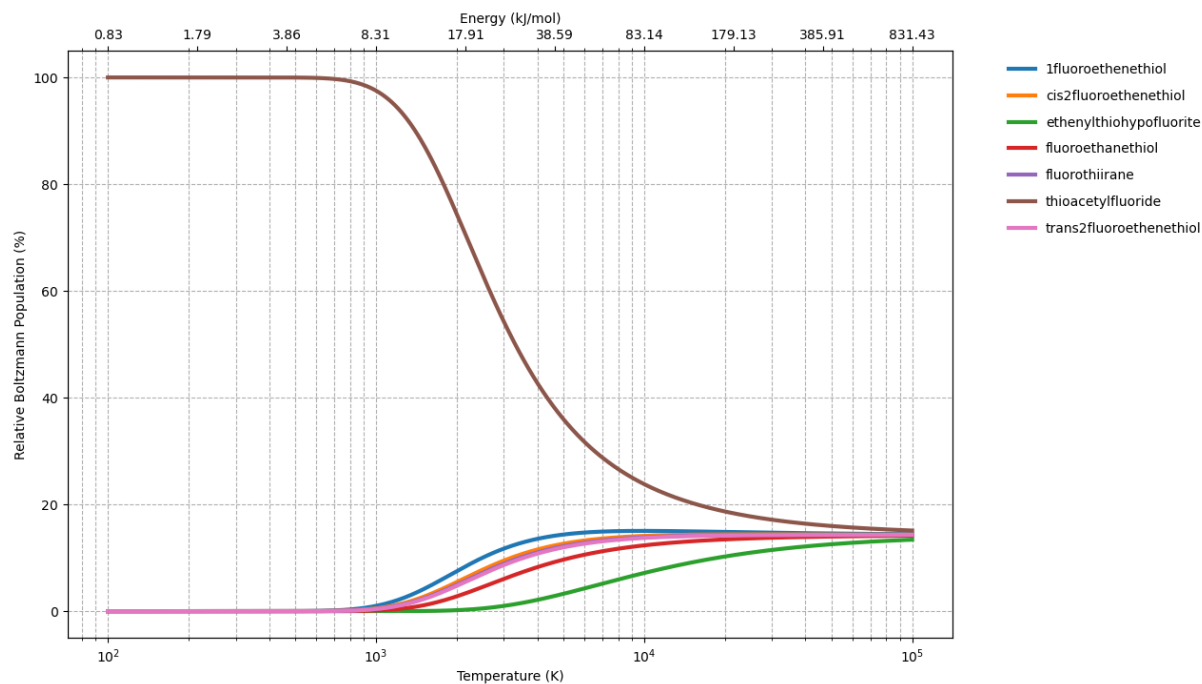


Figure S20. Evolution of the Boltzmann relative distribution of the products of the reaction Thiirane + F₂ as a function of temperature. The corresponding energy (in kJ/mol) is on the upper axis.

Optimized Geometry

Below are listed the optimized geometry at MP2/aug-cc-pVTZ level

- 1-fluoroethenethiol

S	-1.2903230000	0.1550120000	-0.0612490000
F	0.9229400000	-1.2377070000	-0.0338840000
C	0.4597470000	0.0269450000	0.0184800000
C	1.3031290000	1.0555640000	0.0363200000
H	2.3653660000	0.8839030000	-0.0441530000
H	-1.5199020000	-0.7760040000	0.8743530000
H	0.9159780000	2.0562270000	0.1259480000

- Cis-2-fluoroethenethiol

S	1.3314620000	-0.3214670000	-0.0000320000
F	-1.6198550000	-0.7690670000	0.0000290000
C	0.0379090000	0.8684220000	-0.0000070000
C	-1.2470380000	0.5244760000	-0.0000050000
H	2.3204460000	0.5756190000	0.0004330000
H	0.2858930000	1.9178990000	-0.0000610000
H	-2.0762730000	1.2141630000	-0.0000400000

- Ethenylthiohypofluorite

S	-0.5337120000	0.5661310000	0.1372040000
F	-1.6437190000	-0.5757750000	-0.2651470000
C	0.8759000000	-0.4387150000	0.2792570000
C	2.0392450000	-0.0349620000	-0.2485800000
H	0.7978590000	-1.3127200000	0.9142000000
H	2.0859010000	0.8333150000	-0.8911940000
H	2.9582280000	-0.5546400000	-0.0160130000

- F₂

F	0.0000000000	0.0000000000	-0.7006890000
F	0.0000000000	0.0000000000	0.7006890000

- Fluoroethanethiol

S	1.6845210000	-0.0495730000	0.0582620000
F	-2.1847620000	0.2122980000	0.1430590000
C	-1.0176770000	-0.4958070000	-0.1135040000
C	0.1547140000	0.4353290000	-0.1306920000
H	-0.0953760000	1.4798970000	-0.3134030000
H	-0.8954170000	-1.2623410000	0.6497370000
H	-1.1209150000	-0.9722060000	-1.0908920000

- Fluorothiirane

S	-1.0661570000	-0.4645940000	-0.0562860000
F	1.6384290000	-0.3797650000	-0.2368910000
C	0.5672880000	0.0738320000	0.4733420000

C	-0.2175590000	1.1617430000	-0.1241010000
H	0.7625730000	0.0429570000	1.5360490000
H	0.0772970000	1.4667550000	-1.1184400000
H	-0.6255860000	1.9282350000	0.5195320000

- HF

F	0.0000000000	0.0000000000	0.0921840000
H	0.0000000000	0.0000000000	-0.8296520000

- Thiirane

S	0.8653050000	0.0000030000	0.0000000000
C	-0.7984210000	0.7399470000	0.0000000000
C	-0.7984120000	-0.7399530000	0.0000000000
H	-1.0659820000	1.2470000000	-0.9159090000
H	-1.0659820000	1.2470000000	0.9159090000
H	-1.0659610000	-1.2470070000	-0.9159120000
H	-1.0659610000	-1.2470070000	0.9159120000

- Thioacetylfluoride

S	1.3406900000	-0.1673870000	0.0000000000
F	-0.7760870000	1.2963740000	-0.0000030000
C	-1.3460140000	-0.9554910000	-0.0000080000
C	-0.2507030000	0.0510860000	0.0000080000
H	-0.9418960000	-1.9609920000	-0.0009100000
H	-1.9725570000	-0.8002830000	-0.8789820000
H	-1.9714930000	-0.8014640000	0.8799280000

- Trans-2-fluoroethenethiol

S	1.6321570000	-0.1192600000	-0.0758520000
F	-2.3055670000	0.0516070000	-0.0164700000
C	-0.0191370000	0.5004620000	-0.0136190000
C	-1.0302490000	-0.3611590000	0.0608640000
H	2.0720290000	0.4808380000	1.0377390000
H	-0.2066070000	1.5580070000	-0.1355370000
H	-0.9335200000	-1.4309640000	0.1761890000

Gaussian inputs

- 1-fluoroethenethiol

```
%chk=1fluoroethenethiol.MP2.aug-cc-pVTZ.chk  
%mem=1GW  
%Nproc=4  
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

1fluoroethenethiol

```
0 1  
C  
H      1      B1  
C      1      B2  2      A1  
S      3      B3  1      A2  2      D1  0  
H      4      B4  3      A3  1      D2  0  
H      1      B5  3      A4  4      D3  0  
F      3      B6  1      A5  4      D4  0  
  
B1      1.07000000  
B2      1.35520000  
B3      1.78000000  
B4      1.31000000  
B5      1.07000000  
B6      1.35000000  
A1      119.88652694  
A2      119.88652694  
A3      109.50000006  
A4      120.22694612  
A5      120.22694612  
D1      0.00000000  
D2      -168.73540252  
D3      -180.00000000  
D4      -180.00000000
```

- Cis-2-fluoroethenethiol

```
%chk=cis2fluoroethenethiol.MP2.aug-cc-pVTZ.chk  
%mem=1GW  
%Nproc=4  
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

Cis-2-fluoroethenethiol

```
0 1  
C  
H      1      B1  
F      1      B2  2      A1  
C      1      B3  2      A2  3      D1  0  
H      4      B4  1      A3  2      D2  0  
S      4      B5  1      A4  2      D3  0  
H      6      B6  4      A5  1      D4  0
```

```

B1      1.07000000
B2      1.35000000
B3      1.35520000
B4      1.07000000
B5      1.78000000
B6      1.31000000
A1      119.88652694
A2      119.88652694
A3      120.22694612
A4      119.88652694
A5      109.50000006
D1      -180.00000000
D2      -35.53013159
D3      144.46986841
D4      -168.73540252

```

- Ethenylhypofluorite

```

%chk=ethenylthiohypofluorite.MP2.aug-cc-pVTZ.chk
%mem=1GW
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ

```

Ethenylthiohypofluorite

```

0 1
C
H      1      B1
H      1      B2  2      A1
C      1      B3  3      A2  2      D1  0
H      4      B4  1      A3  3      D2  0
S      4      B5  1      A4  3      D3  0
F      6      B6  4      A5  1      D4  0

```

```

B1      1.07000000
B2      1.07000000
B3      1.35520000
B4      1.07000000
B5      1.78000000
B6      1.59000000
A1      119.88652694
A2      119.88652694
A3      119.88652694
A4      120.22694612
A5      109.50000006
D1      -180.00000000
D2      180.00000000
D3      -0.00000000
D4      180.00000000

```

- Fluoroethanethiol

```

%chk=fluoroethanethiol.MP2.aug-cc-pVTZ.chk
%mem=1GW

```



```
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

Fluoroethanethiol

```
0 1
C
S      1      B1
C      1      B2  2      A1
H      3      B3  1      A2  2      D1  0
H      3      B4  1      A3  2      D2  0
F      3      B5  1      A4  2      D3  0
H      1      B6  3      A5  2      D4  0
```

```
B1      1.56640000
B2      1.54000000
B3      1.07000000
B4      1.07000000
B5      1.35000000
B6      1.07000000
A1      119.88652694
A2      109.47120255
A3      109.47120255
A4      109.47123134
A5      119.88652694
D1      -59.99999637
D2      60.00001842
D3      -180.00000000
D4      -180.00000000
```

- Fluorothiirane

```
%chk=fluorothiirane.MP2.aug-cc-pVTZ.chk
%mem=1GW
%nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

Fluorothiirane

```
0 1
C
H      1      B1
H      1      B2  2      A1
C      1      B3  2      A2  3      D1  0
H      4      B4  1      A3  2      D2  0
F      4      B5  1      A4  2      D3  0
S      4      B6  1      A5  2      D4  0
```

```
B1      1.07000000
B2      1.07000000
B3      1.77423324
B4      1.07000000
B5      1.35000000
B6      2.01324228
```

A1	109.47123134
A2	105.91884412
A3	118.29531290
A4	118.29533251
A5	70.47120005
D1	113.76158415
D2	9.80441709
D3	-126.22905142
D4	121.78770000

- Thiirane

```
%chk=thiirane.MP2.aug-cc-pVTZ.chk
%mem=1GW
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

Thiirane

0 1

C

H	1	B1					
H	1	B2	2	A1			
C	1	B3	2	A2	3	D1	0
H	4	B4	1	A3	2	D2	0
S	4	B5	1	A4	2	D3	0
H	4	B6	1	A5	6	D4	0

B1	1.07000000
B2	1.07000000
B3	1.77423324
B4	1.07000000
B5	2.01324228
B6	1.07000000
A1	109.47123134
A2	105.91884412
A3	118.29531290
A4	70.47120005
A5	118.29533251
D1	113.76158415
D2	9.80441709
D3	121.78770000
D4	111.98324858

- Thioacetylfluoride

```
%chk=thioacetylfluoride.MP2.aug-cc-pVTZ.chk
%mem=1GW
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

Thioacetylfluoride

0 1

```

S
C      1      B1
C      2      B2  1      A1
H      3      B3  2      A2  1      D1  0
H      3      B4  2      A3  1      D2  0
H      3      B5  2      A4  1      D3  0
F      2      B6  1      A5  3      D4  0

```

```

B1      1.56640000
B2      1.54000000
B3      1.07000000
B4      1.07000000
B5      1.07000000
B6      1.35000000
A1      119.88652694
A2      109.47120255
A3      109.47120255
A4      109.47123134
A5      120.22694612
D1       60.00007749
D2     -180.00000000
D3     -59.99991511
D4     -180.00000000

```

- Trans-2-fluoroethenethiol

```

%chk=trans2fluoroethenethiol.MP2.aug-cc-pVTZ.chk
%mem=1GW
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ

```

Trans-2-fluoroethenethiol

```

0 1
C
H      1      B1
F      1      B2  2      A1
C      1      B3  2      A2  3      D1  0
H      4      B4  1      A3  2      D2  0
S      4      B5  1      A4  2      D3  0
H      6      B6  4      A5  1      D4  0

```

```

B1      1.07000000
B2      1.35000000
B3      1.35520000
B4      1.07000000
B5      1.78000000
B6      1.31000000
A1      119.88652694
A2      119.88652694
A3      120.22694612
A4      119.88652694
A5      109.50000006
D1     -180.00000000

```

```
D2      -180.00000000
D3       0.00000000
D4     -168.73540252
```

- F2

```
%chk=F2.MP2.aug-cc-pVTZ.chk
%mem=1GW
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

F2

0 1

F

F 1 B1

B1 1.07000000

- HF

```
%chk=HF.MP2.aug-cc-pVTZ.chk
%mem=1GW
%Nproc=4
# opt=calcall freq=noraman MP2/aug-cc-pVTZ
```

HF

0 1

F

H 1 B1

B1 1.07000000

Molpro input

```
memory, 400, m; ! in mWords per processor
file, 1, molecule.int, new;
file, 2, molecule.wfu, new;

gprint, basis;

geomtyp=xyz;
geometry={
include, molecule.xyz;
}

spin=0
charge=0

$l_basis = [aug-cc-pVTZ, aug-cc-pVQZ]

! CCSD(T) calculation with VTZ, VQZ basis sets
do k=1,#i_basis
  basis={
    default=$l_basis(k);
  }

  {hf;}
  {ccsd(t)};

  eref_x(k) = energr;
  ecor_x(k) = energy-energr;

enddo;

! Extrapolation with avtz, avqz basis sets with 2 points
! For HF energy: A. Karton and J. M. L. Martin, Theor. Chem. Acc. 115, 330 (2006)
! For corr. energy by LH3:

extrapolate, basis=avtz:avqz, eref=eref_x, ecorr=ecor_x, method_r=km, npc=2;
ecbs = energy(3);
```