Supplementary Material for:

A kinetic and thermochemical database for organic sulfur and oxygen compounds

Contents:

A separate text file contains the NASA-format thermochemistry polynomials for all the molecules.

1. Calculation of rate parameters for Reactions 21 and 37

Rate parameters were calculated for the two reactions with submerged transition states using the method described in the main article, and the component rate coefficients are presented in the following tables. k_1 is estimated for the high-pressure limit, k_2 is calculated using transition state theory (with the CCSD(T)-F12 energies), K_1 is calculated using thermochemical parameters calculated using CBS-QB3, and k_{-1} is calculated using thermodynamic consistency. k_{eff} provides the effective rate constant calculated at each temperature, while k_{fit} shows the rate constant obtained using the best-fit modified Arrhenius parameters. The ratio of the fitted rate constants to the rate constants calculated at each temperature show that low fitting error was obtained for temperatures between 400 and 2000 K, but significantly greater error was obtained at 300 K. Thus, the specific k_{eff}(300 K) should be used at this temperature.

Rate parameters for Reaction 21 (Hydrogen Abstraction)

T	k_1	k_{-1}	K_1	k_2	k_{eff}	k_{fit}	k_{fit}/k_{eff}
300	1.00E+13	1.27E+11	1.27E-02	1.89E+10	1.30E+12	5.58E+12	4.30
400	1.00E+13	1.69E+10	1.69E-03	9.28E+10	8.46E+12	6.81E+12	0.81
500	1.00E+13	5.36E+09	5.36E-04	2.42E+11	9.78E+12	7.68E+12	0.79
600	1.00E+13	2.58E+09	2.58E-04	4.62E+11	9.94E+12	8.34E+12	0.84
800	1.00E+13	1.11E+09	1.11E-04	1.05E+12	9.99E+12	9.25E+12	0.93
1000	1.00E+13	7.12E+08	7.12E-05	1.76E+12	1.00E+13	9.86E+12	0.99
1500	1.00E+13	4.41E+08	4.41E-05	3.60E+12	1.00E+13	1.08E+13	1.08
2000	1.00E+13	3.80E+08	3.80E-05	5.26E+12	1.00E+13	1.13E+13	1.13

Rate parameters for Reaction 37 (Radical Addition to Double Bond)

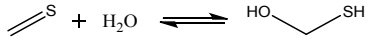
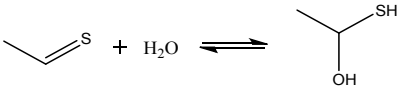
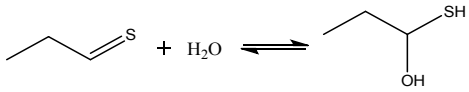
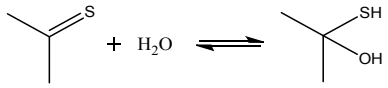
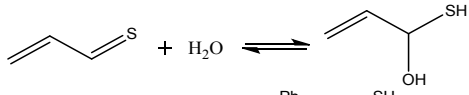
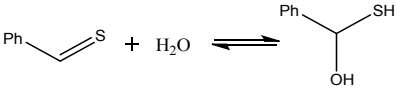
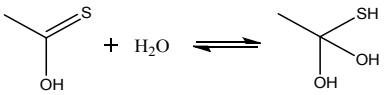
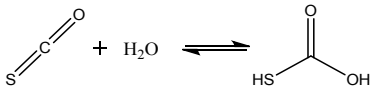
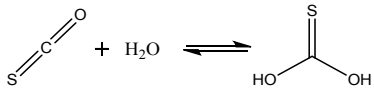
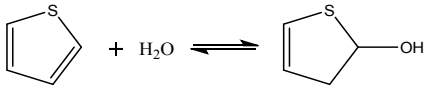
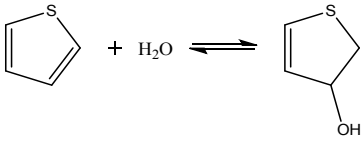
T	k_1	k_{-1}	K_1	k_2	k_{eff}	k_{fit}	k_{fit}/k_{eff}
300	1.00E+13	5.10E+11	5.10E-02	2.82E+11	3.56E+12	6.23E+12	1.75
400	1.00E+13	7.20E+10	7.20E-03	3.96E+11	8.46E+12	7.36E+12	0.87
500	1.00E+13	2.33E+10	2.33E-03	4.93E+11	9.55E+12	8.13E+12	0.85
600	1.00E+13	1.14E+10	1.14E-03	5.77E+11	9.81E+12	8.69E+12	0.89
800	1.00E+13	4.91E+09	4.91E-04	7.19E+11	9.93E+12	9.44E+12	0.95
1000	1.00E+13	3.14E+09	3.14E-04	8.34E+11	9.96E+12	9.93E+12	1.00
1500	1.00E+13	1.96E+09	1.96E-04	1.04E+12	9.98E+12	1.06E+13	1.06
2000	1.00E+13	1.71E+09	1.71E-04	1.18E+12	9.99E+12	1.10E+13	1.10

2. Rate parameters calculated using CBS-QB3

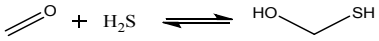
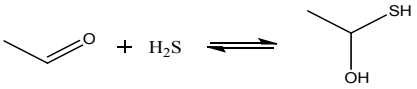
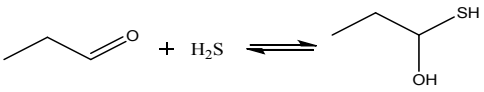
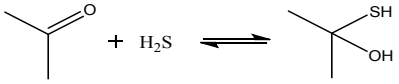
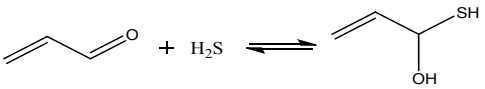
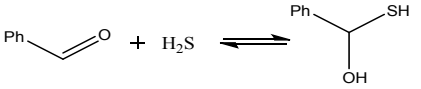
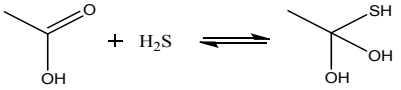
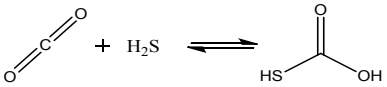
All rate parameters in the Supplementary Materials were calculated using CBS-QB3.

Units: A [cm^3/(mol*s) for bimolecular reactions, s^{-1} for unimolecular reactions], *n* (unitless), E_a (kJ/mol).

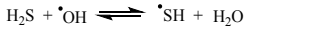
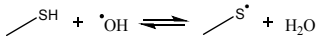
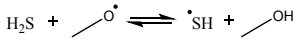
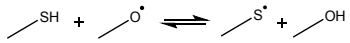
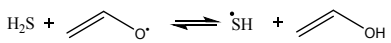
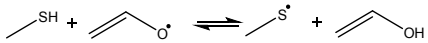
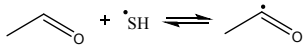
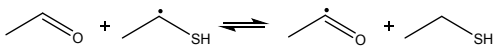
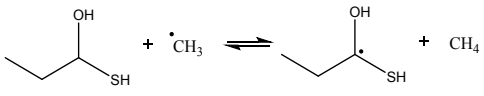
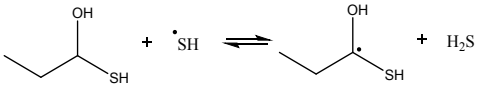
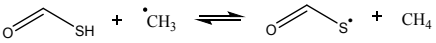
H_2O Addition

Reaction		Forward Rate Parameters			Reverse Rate Parameters		
	T	***log 10A***	***n***	***E_a***	***log 10A***	***n***	***E_a***
1. 	300-2000	-0.63	3.56	106.8	8.72	1.07	167.4
2. 	300-2000	-2.44	3.96	106.3	8.56	1.12	161.3
3. 	300-2000	-2.59	3.95	104.3	8.93	1.03	158.0
4. 	300-2000	-4.31	4.55	103.9	8.31	1.20	158.5
5. 	300-2000	-1.24	3.75	126.7	0.99	1.33	160.4
6. 	300-2000	-1.78	3.90	123.1	7.75	1.44	158.5
7. 	400-2000	-2.53	3.93	143.5	4.79	2.02	151.9
8. 	500-2000	0.20	3.50	172.9	11.87	0.33	171.2
9. 	500-2000	-0.66	3.70	209.9	11.91	0.38	182.9
10. 	600-2000	-2.8	4.32	250.1	7.58	1.79	220.4
11. 	500-2000	-1.6	4.14	250.8	8.60	1.63	216.5

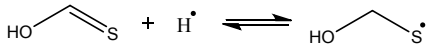
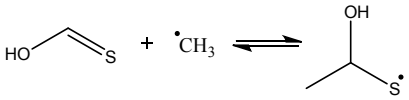
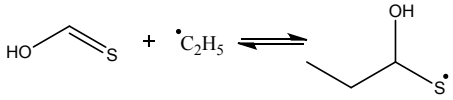
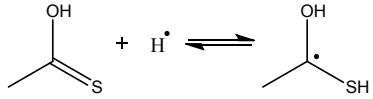
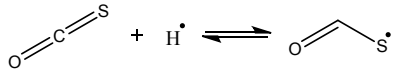
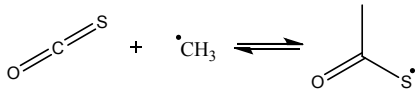
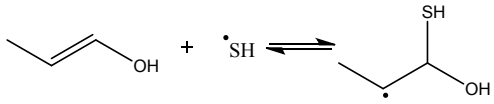
H_2S Addition

Reaction		Forward Rate Parameters			Reverse Rate Parameters		
	T	***log $_{10}$A***	***n***	***E_a***	***log $_{10}$A***	***n***	***E_a***
12. 	300-2000	1.09	3.27	159.6	10.5	0.82	210.4
13. 	300-2000	1.78	2.93	155.3	12.9	0.13	191.4
14. 	300-2000	1.49	2.96	153.6	13.4	0.01	189.5
15. 	300-2000	0.22	3.45	159.0	13.0	0.16	187.7
16. 	300-2000	2.58	2.72	151.9	12.5	0.20	177.7
17. 	300-2000	2.09	2.83	145.1	11.6	0.45	169.9
18. 	300-2000	-0.69	3.60	161.3	7.04	1.65	124.7
19. 	500-2000	0.71	3.52	190.2	11.44	0.59	154.8

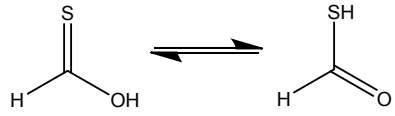
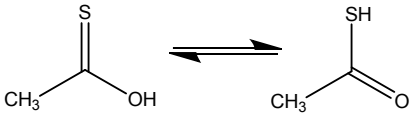
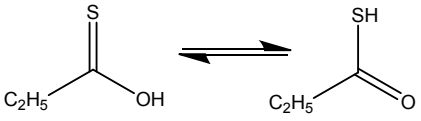
Hydrogen Abstraction

Reaction		Forward Rate Parameters			Reverse Rate Parameters		
	T	***log $_{10}$A***	***n***	***E_a***	***log $_{10}$A***	***n***	***E_a***
20. 	300-2000	7.76	1.72	-1.4	7.04	2.02	112.01
21. 	300-2000	5.3	2.40	-7.6	2.22	3.56	126.20
22. 	300-2000	4.15	2.49	10.6	2.82	2.97	65.62
23. 	300-2000	6.12	2.09	11.7	2.41	3.43	87.10
24. 	500-2000	1.70	3.34	67.2	2.52	3.21	37.62
25. 	500-2000	1.69	3.27	66.2	-0.03	4.05	56.67
26. 	300-2000	4.44	2.80	-2.41	3.00	2.97	5.63
27. 	500-2000	0.34	3.60	29.9	0.19	3.76	47.89
28. 	400-2000	1.14	3.41	13.7	0.40	3.78	72.53
29. 	300-2000	5.79	2.35	-3.0	4.35	2.48	-2.17
30. 	300-2000	0.13	3.51	-5.0	-2.33	4.58	56.23

Radical Addition to Double Bonds

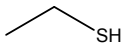
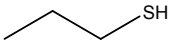
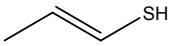
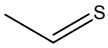
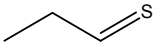
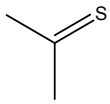
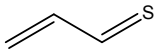
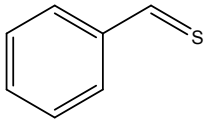
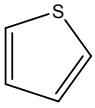
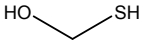
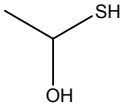
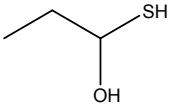
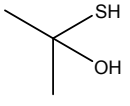
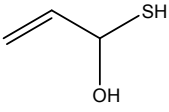
	Reaction		Forward Rate Parameters			Reverse Rate Parameters		
		T	***log 10A***	***n***	***Ea***	***log 10A***	***n***	***Ea***
31.		300-2000	8.45	1.63	10.8	7.84	1.83	141.0
32.		300-2000	4.36	2.35	22.9	10.98	0.99	124.1
33.		300-2000	3.08	2.58	14.3	12.35	0.55	113.7
34.		300-2000	9.30	1.21	-0.6	10.86	0.46	100.8
35.		300-2000	9.92	1.23	33.5	9.02	1.33	71.9
36.		300-2000	6.91	1.68	51.2	11.86	0.59	80.1
37.		300-2000	13.08	0.00	1.7	12.61	0.14	23.7

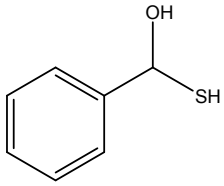
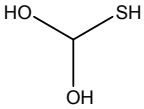
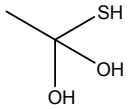
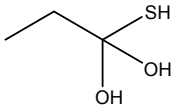
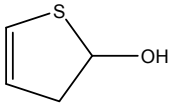
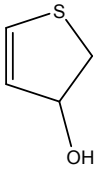
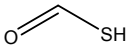
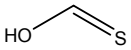
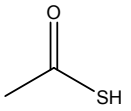
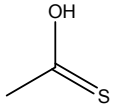
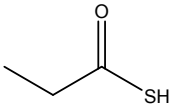
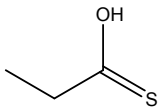
Tautomerization

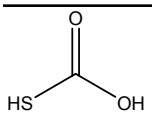
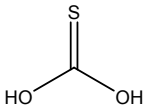
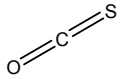
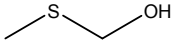
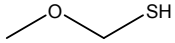
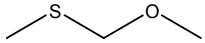
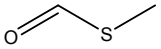
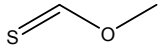
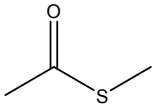
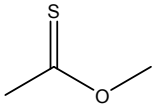
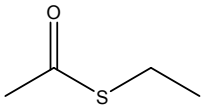
	Reaction		Forward Rate Parameters			Reverse Rate Parameters		
		T	***log 10A***	***n***	***Ea***	***log 10A***	***n***	***Ea***
38.		300-2000	1.18	3.42	91.0	0.81	3.34	99.8
39.		300-2000	1.49	3.35	85.9	1.34	3.17	97.9
40.		300-2000	1.49	3.35	86.1	1.57	3.13	96.6

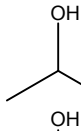
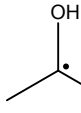
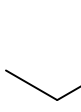
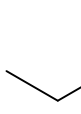
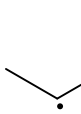
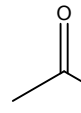
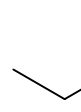
3. Thermochemical Properties Tables

Thermochemical parameters were calculated using CBS-QB3. Enthalpies are presented in units of kJ*mol^{-1}, while the remaining parameters are presented in units of J*mol^{-1}*K^{-1}.

			Cp								
	ΔH_{f}(298 K)	S(298 K)	300 K	400 K	500 K	600 K	800 K	1000 K	1500 K	2000 K	2400 K
H_2S	-26.31	205.59	34.19	35.45	37.03	38.76	42.22	45.30	50.63	53.44	54.72
	-26.82	255.54	50.43	58.06	65.60	72.59	84.40	93.46	107.74	115.37	119.08
	-52.91	302.57	73.81	87.41	100.10	111.56	130.53	144.87	167.19	178.92	184.56
	-74.88	340.89	97.48	116.26	134.07	150.19	176.69	196.47	226.81	242.58	250.12
	44.25	325.41	87.04	102.61	116.87	129.62	150.54	166.20	190.28	202.76	208.69
	111.00	230.69	38.45	43.20	47.86	52.07	58.95	64.02	71.73	75.80	77.80
	64.83	273.70	58.88	69.48	79.40	88.31	102.86	113.70	130.26	138.84	142.93
	41.84	317.85	81.00	97.23	112.57	126.30	148.53	164.86	189.50	202.13	208.14
	19.74	305.35	79.64	95.27	110.34	124.01	146.47	163.15	188.54	201.63	207.86
	157.40	287.09	72.11	88.08	102.09	113.85	131.31	142.74	157.97	165.85	169.76
	185.42	343.03	114.98	147.35	175.41	198.84	233.70	256.85	288.35	303.91	311.15
	111.89	278.57	73.41	95.08	112.97	127.26	147.75	161.27	180.41	190.28	195.18
	-185.89	292.73	77.15	88.08	96.00	101.93	110.54	117.05	129.16	136.75	140.22
	-226.10	322.99	102.87	120.04	132.78	142.58	144.72	168.50	188.49	200.30	205.66
	-247.67	360.90	129.63	150.72	167.18	180.79	202.74	219.85	248.31	263.80	271.01
	-269.89	350.78	129.73	152.91	170.33	184.01	204.94	220.95	248.49	264.14	271.28
	-113.75	345.00	118.96	139.20	153.86	164.90	180.91	192.70	213.02	224.86	230.30

	ΔH_f(298 K)	S(298 K)	*Cp* 300 K	400 K	500 K	600 K	800 K	1000 K	1500 K	2000 K	2400 K
	-86.99	398.69	159.40	196.79	226.36	249.81	284.13	307.88	343.75	362.61	371.37
	-378.54	328.69	88.41	100.15	109.48	117.11	128.78	137.17	150.03	156.88	160.26
	-426.47	361.32	116.25	132.31	145.43	156.49	174.09	187.23	208.03	219.38	225.00
	-450.73	393.78	137.83	160.28	179.23	195.38	220.90	239.60	268.28	283.39	290.73
	-96.92	326.83	105.02	130.86	152.51	170.23	196.44	214.27	240.44	254.37	261.00
	-93.86	325.22	106.93	133.52	155.54	173.28	198.79	215.61	240.42	254.62	261.47
	-132.92	269.68	56.32	63.77	70.05	75.32	83.46	89.20	97.25	100.62	101.79
	-124.29	260.64	49.01	58.00	66.13	73.07	83.52	90.44	99.17	102.45	103.57
	-185.29	312.44	78.23	92.09	103.65	113.31	128.30	139.08	155.07	162.77	166.10
	-175.45	296.90	70.07	84.29	97.43	109.02	127.34	140.25	158.05	165.83	169.01
	-207.91	346.14	105.14	122.52	137.92	151.48	173.46	189.67	213.85	225.74	231.14
	-199.29	338.89	92.67	112.71	131.12	147.26	172.70	190.72	216.47	228.68	234.13

	ΔH_f(298 K)	S(298 K)	*Cp* 300 K	400 K	500 K	600 K	800 K	1000 K	1500 K	2000 K	2400 K
	-379.42	290.84	70.25	82.58	92.47	100.15	110.49	116.41	122.33	123.80	124.15
	-357.65	279.56	71.32	84.88	95.65	103.74	113.62	118.29	122.22	124.48	125.56
	-150.44	231.53	41.04	45.19	48.51	51.08	54.51	56.52	59.09	60.50	61.13
	-199.83	323.88	100.56	119.48	133.64	144.26	159.03	169.37	187.63	199.46	205.17
	-166.71	327.62	98.54	113.83	126.26	136.81	154.00	167.33	189.01	200.54	205.87
	-185.28	353.85	115.21	136.37	155.22	171.78	198.62	218.61	249.58	265.94	273.86
	-144.57	297.81	72.53	85.83	97.67	108.04	124.76	137.06	155.23	163.84	167.52
	-86.24	294.92	66.89	80.46	93.17	104.46	122.53	135.54	154.40	163.43	167.46
	-211.47	335.39	92.91	113.76	132.75	149.06	174.10	191.39	215.64	227.14	232.35
	-156.45	332.77	91.43	109.38	127.03	143.33	170.18	189.71	217.30	229.56	234.62
	-236.37	382.97	117.06	142.80	166.80	187.85	220.80	243.93	276.70	292.26	299.28

	ΔH_f(298 K)	S(298 K)	Cp 300 K	400 K	500 K	600 K	800 K	1000 K	1500 K	2000 K	2400 K
	139.62	192.04	29.03	29.10	29.35	29.75	30.80	31.90	34.08	35.34	35.90
	115.62	238.93	40.17	45.80	51.44	56.69	65.61	72.48	83.40	89.28	92.14
	122.58	305.71	71.22	82.63	93.42	103.13	119.00	130.78	148.78	158.11	162.57
	153.80	306.64	77.50	92.35	105.99	118.07	137.54	151.83	173.38	184.42	189.66
	208.47	324.42	77.01	90.00	103.03	114.98	134.49	148.75	169.94	180.59	185.59
	-38.40	283.93	58.01	67.81	76.28	83.35	93.88	101.01	111.57	117.75	120.89
	-76.45	314.30	83.71	99.46	112.64	123.65	140.65	152.87	171.47	181.32	186.14
	-58.61	333.89	95.52	109.32	120.73	130.31	145.29	156.10	172.29	180.52	184.41
	-99.21	356.87	107.82	128.96	147.34	163.05	187.63	205.29	231.67	245.19	251.67
	-81.89	368.63	118.50	139.98	156.92	170.58	191.23	206.06	229.20	241.99	248.45
	-52.02	369.04	123.28	142.78	158.28	171.07	191.08	205.93	229.48	242.38	248.76
	28.76	268.52	47.04	52.03	56.42	60.16	65.96	70.02	75.83	78.60	79.86
	-31.64	304.74	66.73	77.97	88.00	96.65	110.20	119.90	134.21	141.42	144.82
	-51.99	345.39	92.09	106.93	121.06	133.81	154.59	169.88	192.80	204.41	209.88

4. Computed Geometries of the Saddle Points & Molecules

Z-Matrices for Reaction Transition States

Reaction 1 (H_2O Addition)

0 1
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 5 B5 1 A4 3 D3
H 1 B6 5 A5 3 D4

B1 1.09017221
B2 1.78421227
B3 2.10766562
B4 1.57202431
B5 1.15450839
B6 1.08707034
A1 117.41379967
A2 103.92142842
A3 97.84146984
A4 82.86264147
A5 103.58888573
D1 87.65439124
D2 113.14359777
D3 1.69897839
D4 -120.24280193

Reaction 2 (H_2O Addition)

0 1
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 5 B5 1 A4 3 D3
C 1 B6 5 A5 3 D4
H 7 B7 1 A6 5 D5
H 7 B8 1 A7 5 D6
H 7 B9 1 A8 5 D7

B1 1.09134866
B2 1.79542051
B3 2.12670833
B4 1.59983409
B5 1.15706391
B6 1.50622240
B7 1.09267319
B8 1.09403545
B9 1.09066297
A1 114.67815208
A2 102.02343744
A3 96.48856122
A4 82.05750160
A5 106.38409353
A6 108.34478150
A7 111.63792524
A8 110.34986003
D1 83.74759670
D2 109.03443995
D3 2.27957436
D4 -122.92886315
D5 177.66230166
D6 -62.73455333
D7 59.62031099

Reaction 3 (H_2O Addition)

0 1
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 5 B5 1 A4 3 D3
C 1 B6 5 A5 3 D4
H 7 B7 1 A6 5 D5
H 7 B8 1 A7 5 D6
C 7 B9 1 A8 5 D7
H 10 B10 7 A9 1 D8
H 10 B11 7 A10 1 D9
H 10 B12 7 A11 1 D10

B1 1.09241006
B2 1.79658311
B3 2.12327006
B4 1.59671168
B5 1.15532024
B6 1.51209272
B7 1.09654537
B8 1.09297196
B9 1.53242997
B10 1.09220528
B11 1.09168655
B12 1.09424066
A1 114.59448553
A2 102.07345850
A3 96.55246307
A4 82.19312673
A5 106.23520644
A6 108.90981510
A7 108.35071455
A8 111.33938850
A9 110.26078754
A10 110.54686150
A11 111.54751453
D1 84.00842439
D2 109.35927488
D3 2.33201560
D4 -123.24658056
D5 -59.01941864
D6 58.01521388
D7 179.26799570
D8 179.45862584
D9 -60.67338652
D10 59.72805879

Reaction 4 (H_2O Addition)

0 1
C
C 1 B1
H 2 B2 1 A1

H	2	B3	1	A2	3	D1
H	2	B4	1	A3	4	D2
C	1	B5	2	A4	3	D3
H	6	B6	1	A5	2	D4
H	6	B7	1	A6	2	D5
H	6	B8	1	A7	2	D6
H	1	B9	6	A8	2	D7
O	1	B10	6	A9	2	D8
H	11	B11	1	A10	6	D9
S	1	B12	6	A11	11	D10

B1	1.51645709
B2	1.09174552
B3	1.09202585
B4	1.09556253
B5	1.51344540
B6	1.09436117
B7	1.09250161
B8	1.08917737
B9	1.84815030
B10	1.62342398
B11	0.97085608
B12	1.81232413
A1	111.06292678
A2	108.27815756
A3	111.89594122
A4	114.24038294
A5	111.55925655
A6	108.40918331
A7	110.47764536
A8	117.19857465
A9	104.01180661
A10	108.53901415
A11	116.24452023
D1	117.32750898
D2	118.97844448
D3	174.71921852
D4	-50.29977559
D5	69.46649687
D6	-172.47257991
D7	155.08030502
D8	116.40836204
D9	-138.18293074
D10	103.23612351

Reaction 5 (H_2O Addition)

0 1

C						
H	1	B1				
S	1	B2	2	A1		
H	1	B3	3	A2	2	D1
O	1	B4	3	A3	2	D2
H	5	B5	1	A4	3	D3
C	1	B6	5	A5	3	D4
H	7	B7	1	A6	5	D5
C	7	B8	1	A7	5	D6
H	9	B9	7	A8	1	D7
H	9	B10	7	A9	1	D8

B1	1.09078142
B2	1.79865269
B3	2.14194386
B4	1.60547164
B5	1.16487525
B6	1.48036433
B7	1.08530346
B8	1.33120582
B9	1.08565011
B10	1.08342230
A1	115.05186072
A2	104.16716637
A3	95.68790466
A4	82.26163300
A5	107.28147536
A6	115.52921217
A7	122.83447466
A8	121.73926623
A9	121.47530880
D1	85.21272811
D2	109.37004587
D3	-1.29309548
D4	-122.13382908
D5	61.48411045
D6	-122.48015823
D7	2.54182009
D8	-175.88078465

Reaction 6 (H_2O Addition)

0 1

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	5	B5	4	A4	3	D3
H	1	B6	2	A5	3	D4
H	2	B7	1	A6	6	D5
H	3	B8	2	A7	1	D6
H	5	B9	4	A8	3	D7
H	6	B10	5	A9	4	D8
C	4	B11	3	A10	2	D9
H	12	B12	4	A11	3	D10
S	12	B13	4	A12	3	D11
O	12	B14	4	A13	3	D12
H	15	B15	12	A14	4	D13
H	15	B16	12	A15	4	D14

B1	1.39242070
B2	1.39249311
B3	1.39873197
B4	1.39860331
B5	1.38965698
B6	1.08424430
B7	1.08403460
B8	1.08573194
B9	1.08313936
B10	1.08411689
B11	1.49423944
B12	1.09028348
B13	1.79828556
B14	1.61739360
B15	1.17561394
B16	0.97153264
A1	119.80845608
A2	120.59719482
A3	119.22890460
A4	120.17006798
A5	120.04263380
A6	120.23539897
A7	119.75446152

A8	118.88745778
A9	119.74215418
A10	119.12504538
A11	111.26037646
A12	121.68130130
A13	107.96795048
A14	81.58289588
A15	109.91378487
D1	-0.43102031
D2	-0.13282595
D3	0.71510654
D4	179.97480680
D5	-179.43051088
D6	-179.92397736
D7	-178.24335556
D8	179.93056774
D9	179.83085613
D10	10.79661499
D11	149.65212200
D12	-102.11373971
D13	-127.68003888
D14	122.66994456

Reaction 7 (H_2O Addition)

0 1

C								
C	1	B1						
H	2	B2	1	A1				
H	2	B3	1	A2	3	D1		
H	2	B4	1	A3	3	D2		
O	1	B5	2	A4	5	D3		
H	6	B6	1	A5	2	D4		
S	1	B7	6	A6	2	D5		
H	1	B8	6	A7	2	D6		
O	1	B9	6	A8	2	D7		
H	10	B10	1	A9	6	D8		

B1	1.51060678
B2	1.09208388
B3	1.09623366
B4	1.08756516
B5	1.36698555
B6	0.96713169
B7	1.79537711
B8	2.12601341
B9	1.66613069
B10	1.19989784
A1	108.30095172
A2	111.20327611
A3	110.54145008
A4	114.37433702
A5	109.20373029
A6	114.85054214
A7	81.29559583
A8	106.65854425
A9	78.86291215
D1	120.14102435
D2	-118.75861990
D3	169.93614413
D4	-23.23994867
D5	-142.40633694
D6	121.22054211
D7	114.31226953
D8	119.23164284

Reaction 8 (H_2O Addition)

0 1

O								
C	1	B1						
S	2	B2	1	A1				
H	3	B3	2	A2	1	D1		
O	2	B4	1	A3	3	D2		
H	5	B5	2	A4	1	D3		

B1	1.17191997
B2	1.71475143
B3	1.64450012
B4	1.61682062
B5	0.97144213
A1	143.87237283
A2	66.15992574
A3	119.33921613
A4	111.50060975
D1	174.59101077
D2	179.17272137
D3	-54.37793466

Reaction 8 (H_2O Addition)

0 1

C								
S	1	B1						
O	1	B2	2	A1				
H	3	B3	1	A2	2	D1		
O	1	B4	3	A3	2	D2		
H	5	B5	1	A4	3	D3		

B1	1.60125438
B2	1.25451279
B3	1.25617409
B4	1.64141675
B5	0.96844971
A1	143.91265748
A2	81.08325874
A3	93.42604067
A4	112.09596803
D1	-176.27146736
D2	-179.77554394
D3	-119.72158327

Reaction 9 (H_2O Addition)

0 1

O								
C	1	B1						
S	2	B2	1	A1				
H	3	B3	2	A2	1	D1		
O	2	B4	1	A3	3	D2		
H	5	B5	2	A4	1	D3		

B1	1.16161333
B2	2.31115069
B3	1.34598659
B4	1.24876178
B5	1.21730164
A1	122.77946511
A2	92.32819014
A3	147.41493079
A4	91.42671239
D1	85.96673118

D2 -179.64576783
D3 -179.66288293

Reaction 10 (H_2O Addition)

0 1
C
C 1 B1
C 2 B2 1 A1
C 3 B3 2 A2 1 D1
S 1 B4 2 A3 3 D2
H 1 B5 2 A4 3 D3
H 2 B6 1 A5 5 D4
H 3 B7 2 A6 1 D5
H 4 B8 3 A7 2 D6
O 1 B9 2 A8 3 D7
H 10 B10 1 A9 2 D8
H 10 B11 1 A10 2 D9

B1 1.46181898
B2 1.46015815
B3 1.34477022
B4 1.73790453
B5 1.07906490
B6 1.08604021
B7 1.08314159
B8 1.07908017
B9 1.91246862
B10 0.96938809
B11 1.32286184
A1 109.69957096
A2 114.93080097
A3 111.27816270
A4 125.29914585
A5 119.13761225
A6 122.27509585
A7 129.08823966
A8 89.52387383
A9 111.48081220
A10 63.93677881
D1 1.31313110
D2 2.03997675
D3 154.45150183
D4 -143.37425032
D5 177.79403673
D6 174.36570624
D7 -111.58751100
D8 109.64385961
D9 3.01309568

Reaction 11 (H_2O Addition)

0 1
C
C 1 B1
C 2 B2 1 A1
C 3 B3 2 A2 1 D1
S 1 B4 2 A3 3 D2
H 1 B5 2 A4 3 D3
H 2 B6 1 A5 5 D4
H 3 B7 2 A6 1 D5
H 4 B8 3 A7 2 D6
O 3 B9 2 A8 1 D7
H 10 B10 3 A9 2 D8
H 4 B11 3 A10 2 D9

B1 1.36679654
B2 1.41961460
B3 1.45795706
B4 1.71835951
B5 1.08180541
B6 1.08129894
B7 1.07883597
B8 1.08526562
B9 2.06569549
B10 0.96844066
B11 1.26194395
A1 112.74425826
A2 113.03444774
A3 114.62748153
A4 126.21124849
A5 123.52628789
A6 123.43613671
A7 120.39574359
A8 111.58056836
A9 124.36752276
A10 85.88905227
D1 0.68624824
D2 1.69774083
D3 -176.93490576
D4 -179.56023536
D5 -164.89762285
D6 -136.76051575
D7 93.51777423
D8 4.14413208
D9 107.89007128

Reaction 12 (H_2S Addition)

0 1
C
H 1 B1
H 1 B2 2 A1
S 1 B3 3 A2 2 D1
H 1 B4 4 A3 3 D2
O 1 B5 4 A4 5 D3
H 4 B6 1 A5 6 D4

B1 1.08969160
B2 1.08158277
B3 2.72782771
B4 1.81723435
B5 1.27225209
B6 1.34534178
A1 119.59886546
A2 71.44720185
A3 44.27884888
A4 77.79311639
A5 89.28049073
D1 129.44192593
D2 -115.20049569
D3 -15.17264646
D4 72.87591482

Reaction 13 (H_2S Addition)

0 1
C
H 1 B1
S 2 B2 1 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2

H	3	B5	2	A4	1	D3
C	1	B6	5	A5	3	D4
H	7	B7	1	A6	5	D5
H	7	B8	1	A7	5	D6
H	7	B9	1	A8	5	D7

B1	1.08207438
B2	2.57783332
B3	1.81778015
B4	1.28222502
B5	1.34561337
B6	1.47745109
B7	1.09277643
B8	1.08893567
B9	1.09839600
A1	88.10031074
A2	46.11917006
A3	78.22584260
A4	112.04740588
A5	119.60992962
A6	109.72974081
A7	111.40474012
A8	108.86128785
D1	-113.72635989
D2	-128.53515484
D3	22.12735050
D4	134.38770233
D5	-140.86809741
D6	-18.12246775
D7	102.76938697

Reaction 14 (H_2S Addition)

0 1

C							
H	1	B1					
S	2	B2	1	A1			
H	1	B3	3	A2	2	D1
O	1	B4	3	A3	2	D2
H	3	B5	2	A4	1	D3
C	1	B6	5	A5	3	D4
H	7	B7	1	A6	5	D5
H	7	B8	1	A7	5	D6
C	7	B9	1	A8	5	D7
H	10	B10	7	A9	1	D8
H	10	B11	7	A10	1	D9
H	10	B12	7	A11	1	D10

B1	1.08263566
B2	2.58419939
B3	1.81750188
B4	1.28309019
B5	1.34560587
B6	1.48152946
B7	1.10267814
B8	1.09595158
B9	1.52767534
B10	1.09072160
B11	1.09136697
B12	1.09172499
A1	87.63527427
A2	46.23955852
A3	78.32047736
A4	112.93879552
A5	120.16257597
A6	105.86882580
A7	106.87857733
A8	115.68609744
A9	111.25641026
A10	110.11418597
A11	110.80784736
D1	-113.31573096
D2	-128.09409136
D3	21.36069627
D4	134.07509410
D5	104.74702722
D6	-144.37231026
D7	-18.84596679
D8	58.83587233
D9	179.08327593
D10	-61.16090483

Reaction 15 (H_2S Addition)

0 1

C							
H	1	B1					
H	1	B2	2	A1			
H	1	B3	2	A2	3	D1
C	1	B4	4	A3	3	D2
C	5	B5	1	A4	4	D3
H	6	B6	5	A5	1	D4
H	6	B7	5	A6	1	D5
H	6	B8	5	A7	1	D6
O	5	B9	1	A8	6	D7
H	10	B10	5	A9	1	D8
S	10	B11	5	A10	1	D9
H	12	B12	10	A11	5	D10

B1	1.08871620
B2	1.10282556
B3	1.08650026
B4	1.49386005
B5	1.48943356
B6	1.08862981
B7	1.08999815
B8	1.09920820
B9	1.28993680
B10	1.06142789
B11	2.73250815
B12	1.34604967
A1	107.78989122
A2	110.33004286
A3	111.79951531
A4	119.31437751
A5	110.39692426
A6	111.39720920
A7	108.27586628
A8	121.27146952
A9	102.99695157
A10	78.40316862
A11	121.50766783
D1	118.44193043
D2	116.95719952
D3	174.35609944
D4	-165.02339533
D5	-41.56012878
D6	76.66707489
D7	160.49693221
D8	60.80414988
D9	83.87754436
D10	-78.11837068

Reaction 16 (H_2S Addition)

0 1
C
S 1 B1
H 2 B2 1 A1
H 1 B3 2 A2 3 D1
H 1 B4 2 A3 3 D2
O 1 B5 2 A4 3 D3
C 1 B6 6 A5 2 D4
H 7 B7 1 A6 6 D5
C 7 B8 1 A7 6 D6
H 9 B9 7 A8 1 D7
H 9 B10 7 A9 1 D8

B1 2.80957852
B2 1.34557404
B3 1.08168206
B4 1.82662576
B5 1.29462894
B6 1.43370938
B7 1.08483581
B8 1.34318959
B9 1.08491292
B10 1.08290748
A1 89.02384163
A2 68.64251991
A3 47.01191812
A4 78.04367645
A5 119.18841243
A6 116.80966450
A7 121.41733935
A8 121.40438694
A9 121.54869228
D1 157.19643507
D2 -87.86782341
D3 -73.72861180
D4 -133.62919208
D5 7.90681073
D6 -171.92589798
D7 -1.24184038
D8 179.67861776

Reaction 17 (H_2S Addition)

0 1
C
S 1 B1
H 2 B2 1 A1
H 1 B3 2 A2 3 D1
H 1 B4 2 A3 3 D2
O 1 B5 2 A4 3 D3
C 1 B6 6 A5 2 D4
H 7 B7 1 A6 6 D5
C 7 B8 1 A7 6 D6
H 9 B9 7 A8 1 D7
H 9 B10 7 A9 1 D8

B1 2.80957852
B2 1.34557404
B3 1.08168206
B4 1.82662576
B5 1.29462894
B6 1.43370938
B7 1.08483581
B8 1.34318959
B9 1.08491292
B10 1.08290748
A1 89.02384163
A2 68.64251991
A3 47.01191812
A4 78.04367645
A5 119.18841243
A6 116.80966450
A7 121.41733935
A8 121.40438694
A9 121.54869228
D1 157.19643507
D2 -87.86782341
D3 -73.72861180
D4 -133.62919208
D5 7.90681073
D6 -171.92589798
D7 -1.24184038
D8 179.67861776

Reaction 18 (H_2S Addition)

0 1
C
O 1 B1
H 2 B2 1 A1
O 1 B3 2 A2 3 D1
H 4 B4 1 A3 2 D2
C 1 B5 4 A4 2 D3
H 6 B6 1 A5 4 D4
H 6 B7 1 A6 4 D5
H 6 B8 1 A7 4 D6
S 1 B9 4 A8 2 D7
H 10 B10 1 A9 4 D8

B1 1.31297615
B2 0.97080269
B3 1.29997291
B4 1.06808038
B5 1.48990568
B6 1.08592019
B7 1.08752840
B8 1.09920339
B9 2.69771811
B10 1.34548660
A1 108.01892395
A2 116.86327814
A3 100.00928937
A4 124.14841169
A5 110.55562826
A6 110.86126191
A7 106.82092126
A8 79.38950509
A9 93.92842804
D1 -14.74954915
D2 128.02081375
D3 155.72504653
D4 35.50310735
D5 158.44994891
D6 -83.04422441
D7 -116.26648536
D8 79.79975255

Reaction 19 (H_2S Addition)

0 1
O
C 1 B1
S 2 B2 1 A1
H 3 B3 2 A2 1 D1
O 2 B4 1 A3 3 D2
H 5 B5 2 A4 1 D3

B1 1.16161333
B2 2.31115069
B3 1.34598659
B4 1.24876178
B5 1.21730164
A1 122.77946511
A2 92.32819014
A3 147.41493079
A4 91.42671239
D1 85.96673118
D2 -179.64576783
D3 -179.66288293

Reaction 20 (H Abstraction)

0 2
S
H 1 B1
O 2 B2 1 A1
H 3 B3 2 A2 1 D1
H 1 B4 3 A3 2 D2

B1 1.38468523
B2 1.62057545
B3 0.97256743
B4 1.34351886
A1 127.02134243
A2 105.26482070
A3 83.80557650
D1 62.34538442
D2 -106.99012005

Reaction 21 (H Abstraction)

0 2
S
H 1 B1
O 2 B2 1 A1
H 3 B3 2 A2 1 D1
C 1 B4 3 A3 2 D2
H 5 B5 1 A4 3 D3
H 5 B6 1 A5 3 D4
H 5 B7 1 A6 3 D5

B1 1.37943643
B2 1.63381486
B3 0.97110774
B4 1.82751617
B5 1.08910258
B6 1.08946410
B7 1.08768664
A1 121.02632479
A2 106.63963115
A3 88.19592811
A4 110.67989306
A5 107.30333460
A6 108.45346004
D1 65.33490846
D2 -106.22097855
D3 100.64185973
D4 -139.64326280
D5 -20.84057573

Reaction 22 (H Abstraction)

0 2
S
H 1 B1
H 1 B2 2 A1
O 1 B3 2 A2 3 D1
C 4 B4 1 A3 2 D2
H 5 B5 4 A4 1 D3
H 5 B6 4 A5 1 D4
H 5 B7 4 A6 1 D5

B1 1.34419961
B2 1.45479920
B3 2.74742624
B4 1.39117885
B5 1.09724632
B6 1.09689110
B7 1.10257753
A1 92.49590712
A2 87.84686134
A3 109.15799405
A4 112.28549688
A5 113.55498664
A6 105.12913349
D1 13.01778789
D2 136.12626705
D3 -71.23263401
D4 55.16747303
D5 173.09417135

Reaction 23 (H Abstraction)

0 2
S
H 1 B1
O 2 B2 1 A1
C 1 B3 3 A2 2 D1
H 4 B4 1 A3 3 D2
H 4 B5 1 A4 3 D3
H 4 B6 1 A5 3 D4
C 3 B7 2 A6 1 D5
H 8 B8 3 A7 2 D6
H 8 B9 3 A8 2 D7
H 8 B10 3 A9 2 D8

B1 1.43101528
B2 1.42943649
B3 1.82665054
B4 1.09027225
B5 1.08934430
B6 1.08905715
B7 1.39039535
B8 1.09774314
B9 1.09804405
B10 1.10288802
A1 147.24147867
A2 90.43986584
A3 107.24961938
A4 109.65411538
A5 111.11258757

A6	114.73209711
A7	112.69488768
A8	113.46561240
A9	105.52853797
D1	-110.85287194
D2	-158.84730031
D3	-40.54998379
D4	81.38174328
D5	77.66926435
D6	-84.68870487
D7	41.53949818
D8	158.96508598

Reaction 24 (H Abstraction)

0 2

O							
C	1	B1					
H	2	B2	1	A1			
C	2	B3	1	A2	3	D1	
H	4	B4	2	A3	1	D2	
H	4	B5	2	A4	1	D3	
H	1	B6	2	A5	4	D4	
S	1	B7	2	A6	4	D5	
H	8	B8	1	A7	2	D6	

B1	1.28060775
B2	1.09559864
B3	1.37925396
B4	1.08251751
B5	1.08163638
B6	1.22143397
B7	2.83117292
B8	1.34507960
A1	117.84640957
A2	122.54386553
A3	119.94923259
A4	120.61927724
A5	112.22266191
A6	111.69234761
A7	92.95539430
D1	-179.46547483
D2	-1.06199791
D3	178.08430852
D4	175.02194777
D5	172.66353081
D6	-179.84752636

Reaction 25 (H Abstraction)

0 2

O							
C	1	B1					
H	2	B2	1	A1			
C	2	B3	1	A2	3	D1	
H	4	B4	2	A3	1	D2	
H	4	B5	2	A4	1	D3	
H	1	B6	2	A5	4	D4	
S	1	B7	2	A6	4	D5	
C	8	B8	1	A7	2	D6	
H	9	B9	8	A8	1	D7	
H	9	B10	8	A9	1	D8	
H	9	B11	8	A10	1	D9	

B1	1.28491958
B2	1.09663464
B3	1.37437818
B4	1.08262122
B5	1.08180233
B6	1.26284684
B7	2.81465728
B8	1.82624029
B9	1.09127989
B10	1.08912279
B11	1.09124032
A1	117.82005017
A2	122.94965093
A3	120.00783517
A4	120.65147434
A5	113.04802727
A6	114.53109459
A7	95.39492480
A8	109.68263562
A9	109.16683134
A10	110.26094767
D1	-178.60784817
D2	-2.05041693
D3	175.85509051
D4	165.84180440
D5	159.42702735
D6	176.87518894
D7	37.66252812
D8	157.32635512
D9	-82.24690021

Reaction 26 (H Abstraction)

0 2

C							
H	1	B1					
H	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
C	1	B4	3	A3	4	D2	
O	5	B5	1	A4	3	D3	
H	5	B6	1	A5	6	D4	
S	5	B7	1	A6	6	D5	
H	8	B8	5	A7	1	D6	

B1	1.09285983
B2	1.09177381
B3	1.09286280
B4	1.50423273
B5	1.17923542
B6	1.49504170
B7	3.01734628
B8	1.34472608
A1	110.72431231
A2	110.72368344
A3	110.73083347
A4	129.99429303
A5	110.02014193
A6	109.77322479
A7	90.37034567
D1	-118.94433484
D2	-120.52670408
D3	0.01019044
D4	-180.00000000
D5	-179.99732858
D6	180.00000000

Reaction 27 (H Abstraction)

0 2
C
H 1 B1
O 1 B2 2 A1
C 1 B3 3 A2 2 D1
H 4 B4 1 A3 3 D2
H 4 B5 1 A4 3 D3
H 4 B6 1 A5 3 D4
C 1 B7 3 A6 4 D5
H 8 B8 1 A7 3 D6
C 8 B9 1 A8 3 D7
H 10 B10 8 A9 1 D8
H 10 B11 8 A10 1 D9
H 10 B12 8 A11 1 D10
S 8 B13 1 A12 3 D11
H 14 B14 8 A13 1 D12

B1 1.34171929
B2 1.19385319
B3 1.51057403
B4 1.09362979
B5 1.09210639
B6 1.09421092
B7 2.75270230
B8 1.09111763
B9 1.51095650
B10 1.09401673
B11 1.09600393
B12 1.09408952
B13 1.79452206
B14 1.34617689
A1 119.07340671
A2 126.21592316
A3 109.08571573
A4 110.88150509
A5 109.03270637
A6 115.72880817
A7 105.18404283
A8 101.72964551
A9 111.19055477
A10 111.77846363
A11 110.27580831
A12 109.54340958
A13 97.14726411
D1 -179.84664905
D2 -122.75984401
D3 -0.78827826
D4 120.79788576
D5 -179.91975435
D6 -127.84617836
D7 -8.12062755
D8 59.50970943
D9 -179.98737720
D10 -59.58764149
D11 117.31818985
D12 -66.27100694

Reaction 28 (H Abstraction)

0 2
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 3 B5 1 A4 5 D3
C 1 B6 5 A5 3 D4
H 7 B7 1 A6 5 D5
H 7 B8 1 A7 5 D6
C 7 B9 1 A8 5 D7
H 10 B10 7 A9 1 D8
H 10 B11 7 A10 1 D9
H 10 B12 7 A11 1 D10
C 1 B13 5 A12 7 D11
H 14 B14 1 A13 5 D12
H 14 B15 1 A14 5 D13
H 14 B16 1 A15 5 D14

B1 1.28401690
B2 1.83743859
B3 1.92413156
B4 1.39200497
B5 1.34804105
B6 1.51779464
B7 1.09792751
B8 1.09247091
B9 1.53310162
B10 1.09082838
B11 1.09285789
B12 1.09327468
B13 2.74027251
B14 1.08651785
B15 1.08698310
B16 1.08663810
A1 100.49672243
A2 91.77540660
A3 113.33847887
A4 96.60383564
A5 109.78511408

Reaction 29 (H Abstraction)

0 2
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 3 B5 1 A4 5 D3
C 1 B6 5 A5 3 D4
H 7 B7 1 A6 5 D5
H 7 B8 1 A7 5 D6
C 7 B9 1 A8 5 D7
H 10 B10 7 A9 1 D8
H 10 B11 7 A10 1 D9
H 10 B12 7 A11 1 D10
S 1 B13 5 A12 7 D11
H 14 B14 1 A13 5 D12

B1 1.46664595
B2 1.81756148
B3 1.91431315
B4 1.37037129
B5 1.34774920
B6 1.51255380
B7 1.09954733
B8 1.09211904
B9 1.53195056
B10 1.09079246
B11 1.09228251
B12 1.09253470
B13 2.99108689

B14	1.34461806
A1	100.57953240
A2	90.13791541
A3	115.43903131
A4	95.89326267
A5	112.15417435
A6	107.85654583
A7	107.89153849
A8	113.83341103
A9	111.18423436
A10	109.90874824
A11	110.96690942
A12	104.84859840
A13	89.22988791
D1	100.74273525
D2	114.32517105

Reaction 30 (H Abstraction)

0 2

C							
H	1	B1					
S	1	B2	2	A1			
O	1	B3	3	A2	2	D1	
H	3	B4	1	A3	4	D2	
C	3	B5	1	A4	4	D3	
H	6	B6	3	A5	1	D4	
H	6	B7	3	A6	1	D5	
H	6	B8	3	A7	1	D6	

B1	1.10610232
B2	1.78655887
B3	1.20010636
B4	1.43659437
B5	3.10775670
B6	1.08235535
B7	1.08337107
B8	1.08336976
A1	110.18896318
A2	126.64856393
A3	94.28478093
A4	90.67153687
A5	91.48617080
A6	100.89263206
A7	100.89081839
D1	-180.00000000
D2	0.00000000
D3	0.00000000
D4	0.00693452
D5	119.26389364
D6	-119.24930416

Reaction 31 (R Addition to Multiple Bond)

0 2

C							
H	1	B1					
H	1	B2	2	A1			
O	1	B3	3	A2	2	D1	
H	4	B4	1	A3	3	D2	
S	1	B5	4	A4	5	D3	

B1	2.05616891
B2	1.08745098
B3	1.32944119
B4	0.97164771
B5	1.64411920
A1	80.92840077
A2	110.46443283
A3	107.81533412
A4	125.62349457
D1	100.47043138
D2	177.07429207
D3	5.09247682

Reaction 32 (R Addition to Multiple Bond)

0 2

C							
H	1	B1					
O	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
S	1	B4	3	A3	4	D2	
C	1	B5	3	A4	5	D3	
H	6	B6	1	A5	3	D4	
H	6	B7	1	A6	3	D5	
H	6	B8	1	A7	3	D6	

B1	1.08575744
B2	1.34323684
B3	0.97026639
B4	1.65829303
B5	2.33352562
B6	1.08172270
B7	1.08257750
B8	1.08172037
A1	110.56679198
A2	107.20136517
A3	124.13777696
A4	99.92220580
A5	102.35372855
A6	94.54578138
A7	99.20947367
D1	171.33482287
D2	8.99323752
D3	-110.93215330
D4	-168.89487860
D5	-48.58800636
D6	70.28335675

Reaction 33 (R Addition to Multiple Bond)

0 2

C							
H	1	B1					
S	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
O	1	B4	3	A3	2	D2	
C	1	B5	5	A4	3	D3	
H	6	B6	1	A5	5	D4	
H	6	B7	1	A6	5	D5	
C	6	B8	1	A7	5	D6	
H	9	B9	6	A8	1	D7	
H	9	B10	6	A9	1	D8	
H	9	B11	6	A10	1	D9	

B1	1.08506964
B2	1.66122722
B3	1.87673168
B4	1.34876450
B5	2.31381675
B6	1.08341740

B7	1.08574359
B8	1.48869298
B9	1.09196020
B10	1.10022364
B11	1.09367189
A1	122.64070970
A2	94.23077058
A3	123.58455281
A4	99.97990035
A5	98.83768467
A6	93.23298522
A7	105.56324380
A8	111.85514965
A9	110.34430339
A10	111.35820683
D1	162.25124736
D2	157.88415191
D3	-112.67002903
D4	172.84388360
D5	-70.67873835
D6	49.38602176
D7	67.93941202
D8	-172.67637487
D9	-54.38036989

Reaction 34 (R Addition to Multiple Bond)

0 2							
C							
C	1	B1					
H	2	B2	1	A1			
H	2	B3	1	A2	3	D1	
H	2	B4	1	A3	4	D2	
S	1	B5	2	A4	3	D3	
O	1	B6	2	A5	6	D4	
H	7	B7	1	A6	2	D5	
H	6	B8	1	A7	7	D6	

B1	1.49372289
B2	1.08729115
B3	1.09434835
B4	1.09450227
B5	1.66539738
B6	1.31581309
B7	0.99834934
B8	1.89962646
A1	111.15231564
A2	109.54287857
A3	109.11148925
A4	124.55420476
A5	114.15714215
A6	105.36913802
A7	84.82063081
D1	120.87976765
D2	117.18804933
D3	-5.27084193
D4	179.04807016
D5	-167.88277996
D6	-20.71672733

Reaction 35 (R Addition to Multiple Bond)

0 2							
C							
H	1	B1					
O	1	B2	2	A1			
S	1	B3	3	A2	2	D1	

B1	1.78565321
B2	1.16069312
B3	1.59664649
A1	105.13580154
A2	166.07040528
D1	180.00000000

Reaction 36 (R Addition to Multiple Bond)

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

B1	1.17158053
B2	1.61828392
B3	2.11871837
B4	1.08124638
B5	1.08345031
B6	1.08345031
A1	155.45769884
A2	104.39190869
A3	112.53821962
A4	94.77580593
A5	94.77580593
D1	180.00000000
D2	180.00000000
D3	58.60273649
D4	-58.60273649

Reaction 37 (R Addition to Multiple Bond)

0 2							
C							
H	1	B1					
S	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
O	1	B4	3	A3	2	D2	
H	3	B5	1	A4	5	D3	
C	1	B6	5	A5	3	D4	
H	7	B7	1	A6	5	D5	
C	7	B8	1	A7	5	D6	
H	9	B9	7	A8	1	D7	
H	9	B10	7	A9	1	D8	
H	9	B11	7	A10	1	D9	

B1	1.08737825
B2	2.32711178
B3	1.90259796
B4	1.36468128
B5	1.34423770
B6	1.38917352
B7	1.08578691
B8	1.48898565
B9	1.09654452
B10	1.09588957
B11	1.09194416
A1	90.84821526
A2	86.13139032
A3	104.53407822

A4	89.52893117
A5	117.24339310
A6	116.85291456
A7	123.74474050
A8	110.74728370
A9	111.11958320
A10	111.97287393
D1	95.49214913
D2	117.77567876
D3	-55.41169060
D4	-111.61248856
D5	17.78903281
D6	-167.09299106
D7	125.40734339
D8	-116.10147223
D9	4.50221047

Reaction 38 (Tautomerization)

0 1

C						
H	1	B1				
S	1	B2	2	A1		
O	1	B3	3	A2	2	D1
H	4	B4	1	A3	3	D2

B1	1.09134728
B2	1.69169644
B3	1.25902131
B4	1.36911194
A1	126.21572947
A2	112.29692829
A3	79.53015109
D1	180.00000000
D2	0.00000000

Reaction 39 (Tautomerization)

0 1

C						
S	1	B1				
O	1	B2	2	A1		
H	3	B3	1	A2	2	D1
C	1	B4	3	A3	2	D2
H	5	B5	1	A4	3	D3
H	5	B6	1	A5	3	D4
H	5	B7	1	A6	3	D5

B1	1.71565296
B2	1.26511572
B3	1.35394941
B4	1.49376307
B5	1.09292322
B6	1.09188644
B7	1.08917340
A1	109.91449838
A2	80.51887430
A3	122.18087363
A4	109.54518382
A5	110.14976965
A6	110.00428002
D1	0.03502534
D2	-179.67609045
D3	116.49499242
D4	-125.73087918
D5	-4.16341740

Reaction 40 (Tautomerization)

0 1

C						
S	1	B1				
O	1	B2	2	A1		
H	3	B3	1	A2	2	D1
C	1	B4	3	A3	2	D2
H	5	B5	1	A4	3	D3
H	5	B6	1	A5	3	D4
C	5	B7	1	A6	3	D5
H	8	B8	5	A7	1	D6
H	8	B9	5	A8	1	D7
H	8	B10	5	A9	1	D8

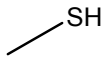
B1	1.71654565
B2	1.26621316
B3	1.35604563
B4	1.49820162
B5	1.09757901
B6	1.09331079
B7	1.53020946
B8	1.09204080
B9	1.09191253
B10	1.09206599
A1	109.86049245
A2	80.39569257
A3	121.63102006
A4	105.80789959
A5	106.98615181
A6	115.17566972
A7	110.19470349
A8	111.14744209
A9	111.11783259
D1	-0.21602671
D2	178.44187920
D3	-87.70774888
D4	25.35274533
D5	150.40376100
D6	178.83805632
D7	-61.31091815
D8	58.90915053

Z-Matrices for Molecules

H_2S

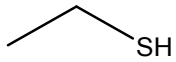
0 1
S
H 1 B1
H 1 B2 2 A1

B1 1.34327993
B2 1.34327993
A1 92.58329996



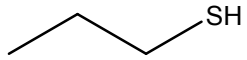
0 1
S
H 1 B1
C 1 B2 2 A1
H 3 B3 1 A2 2 D1
H 3 B4 1 A3 2 D2
H 3 B5 1 A4 2 D3

B1 1.34383796
B2 1.83186600
B3 1.09011110
B4 1.08923069
B5 1.08923069
A1 97.09044649
A2 106.02458786
A3 111.27496891
A4 111.27496891
D1 180.00000000
D2 -61.86427348
D3 61.86427348



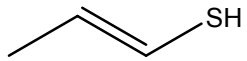
0 1
S
C 1 B1
H 2 B2 1 A1
H 2 B3 1 A2 3 D1
H 1 B4 2 A3 4 D2
C 2 B5 1 A4 5 D3
H 6 B6 2 A5 1 D4
H 6 B7 2 A6 1 D5
H 6 B8 2 A7 1 D6

B1 1.84053942
B2 1.09238710
B3 1.09119687
B4 1.34468713
B5 1.52495257
B6 1.09312266
B7 1.09511375
B8 1.09182844
A1 103.76609343
A2 108.65066099
A3 96.83197082
A4 114.35965187
A5 111.21618781
A6 110.30998782
A7 111.06606383
D1 -113.79907940
D2 62.42213671
D3 -62.92877011
D4 63.33941833
D5 -177.11626126
D6 -56.84849601



0 1
C
H 1 B1
H 1 B2 2 A1
H 1 B3 2 A2 3 D1
C 1 B4 2 A3 4 D2
H 5 B5 1 A4 2 D3
H 5 B6 1 A5 2 D4
C 5 B7 1 A6 2 D5
H 8 B8 5 A7 1 D6
H 8 B9 5 A8 1 D7
S 8 B10 5 A9 1 D8
H 11 B11 8 A10 5 D9

B1 1.09296552
B2 1.09427295
B3 1.09423755
B4 1.53302284
B5 1.09555313
B6 1.09395255
B7 1.52840858
B8 1.09215111
B9 1.09345327
B10 1.83917085
B11 1.34460303
A1 107.66141600
A2 107.65336841
A3 110.95296286
A4 109.62637827
A5 110.19348596
A6 112.29767774
A7 111.28472530
A8 110.55368506
A9 114.64658137
A10 96.87039863
D1 115.84020434
D2 121.99793697
D3 57.88209488
D4 -58.80671228
D5 179.43674741
D6 -58.70398120
D7 60.20350086
D8 177.27783367
D9 63.42757476



0 1
S
H 1 B1
C 1 B2 2 A1
H 3 B3 1 A2 2 D1
C 3 B4 1 A3 2 D2
H 5 B5 3 A4 1 D3
C 5 B6 3 A5 1 D4
H 7 B7 5 A6 3 D5
H 7 B8 5 A7 3 D6

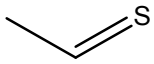
H	7	B9	5	A8	3	D7	

B1	1.34532355
B2	1.78052170
B3	1.08571181
B4	1.33181721
B5	1.08762779
B6	1.50011270
B7	1.09539567
B8	1.09580977
B9	1.09237416
A1	97.31310735
A2	115.85277913
A3	122.48313340
A4	118.86048255
A5	124.35969445
A6	110.89890200
A7	110.98590451
A8	111.74837446
D1	-46.86082688
D2	138.77175358
D3	-6.10052339
D4	173.34810986
D5	123.63308977
D6	-117.94027294
D7	2.68220294

0 1
C

H	1	B1					
H	1	B2	2	A1			
S	1	B3	3	A2	2	D1	

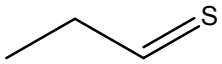
B1	1.08986346
B2	1.08985705
B3	1.61084700
A1	115.92565035
A2	122.03997793
D1	180.00000000



0 1
C

H	1	B1					
C	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
S	3	B4	1	A3	2	D2	
H	1	B5	3	A4	5	D3	
H	1	B6	3	A5	5	D4	

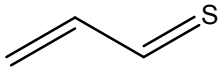
B1	1.08911236
B2	1.49291678
B3	1.09300816
B4	1.61980609
B5	1.09733033
B6	1.09697723
A1	111.78326121
A2	114.81232591
A3	126.45725204
A4	109.77445206
A5	109.77061696
D1	-179.94981833
D2	0.08504453
D3	-121.81265346
D4	121.94294055



0 1
C

C	1	B1					
H	2	B2	1	A1			
S	2	B3	1	A2	3	D1	
H	1	B4	2	A3	4	D2	
H	1	B5	2	A4	4	D3	
C	1	B6	2	A5	4	D4	
H	7	B7	1	A6	2	D5	
H	7	B8	1	A7	2	D6	
H	7	B9	1	A8	2	D7	

B1	1.49928079
B2	1.09327780
B3	1.62101959
B4	1.10069884
B5	1.10021014
B6	1.52446846
B7	1.09248638
B8	1.09173182
B9	1.09173185
A1	113.68135958
A2	127.79107438
A3	106.54145479
A4	106.58648058
A5	117.20947132
A6	110.14116314
A7	111.21517133
A8	111.20612761
D1	-179.99577006
D2	-124.75872528
D3	124.70098749
D4	-0.03955432
D5	-179.97522250
D6	-59.74443602
D7	59.81639596

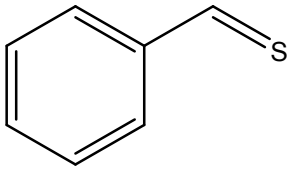


0 1
C

H	1	B1					
H	1	B2	2	A1			
C	1	B3	3	A2	2	D1	
H	4	B4	1	A3	3	D2	
C	4	B5	1	A4	3	D3	
H	6	B6	4	A5	1	D4	
S	6	B7	4	A6	1	D5	

B1	1.08537379
B2	1.08343568
B3	1.34113138
B4	1.08544944
B5	1.44806876
B6	1.09276072
B7	1.63104353
A1	116.94777260
A2	121.70641804

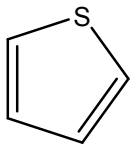
A3	121.00766131
A4	122.16993040
A5	115.20326215
A6	125.48088108
D1	180.00000000
D2	0.00000000
D3	180.00000000
D4	0.00000000
D5	180.00000000



0 1

C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	5	B5	4	A4	3	D3
H	1	B6	2	A5	3	D4
H	2	B7	1	A6	6	D5
H	4	B8	3	A7	2	D6
H	5	B9	4	A8	3	D7
H	6	B10	5	A9	4	D8
C	3	B11	2	A10	1	D9
H	12	B12	3	A11	2	D10
S	12	B13	3	A12	2	D11

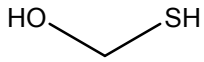
B1	1.38583731
B2	1.40631088
B3	1.40609500
B4	1.38987996
B5	1.39345706
B6	1.08398609
B7	1.08322962
B8	1.08512018
B9	1.08378357
B10	1.08423243
B11	1.45923514
B12	1.09226383
B13	1.63252372
A1	120.31139208
A2	118.85050477
A3	120.73741607
A4	119.74311405
A5	119.88992438
A6	120.99897969
A7	119.21083836
A8	120.07200812
A9	119.96407636
A10	122.56927572
A11	113.69391049
A12	128.27241311
D1	-0.00000000
D2	0.00435527
D3	-0.00380186
D4	-179.99658450



0 1

C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1	D1
S	4	B4	3	A3	2	D2
H	1	B5	2	A4	3	D3
H	2	B6	1	A5	5	D4
H	3	B7	2	A6	1	D5
H	4	B8	3	A7	2	D6

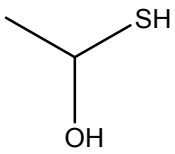
B1	1.36629669
B2	1.42594200
B3	1.36629669
B4	1.72748369
B5	1.07892407
B6	1.08214933
B7	1.08214933
B8	1.07892407
A1	112.67431284
A2	112.67431284
A3	111.46777715
A4	128.49773050
A5	123.34875370
A6	123.97693347
A7	128.49773050
D1	0.00000000
D2	0.00000000
D3	180.00000000
D4	180.00000000
D5	180.00000000
D6	180.00000000



0 1

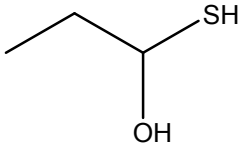
C					
H	1	B1			
H	1	B2	2	A1	
S	1	B3	2	A2	3	D1
H	1	B4	4	A3	3	D2
O	1	B5	4	A4	3	D3
H	4	B6	1	A5	6	D4

B1	1.08805014
B2	1.09631959
B3	1.84497563
B4	1.92992799
B5	1.40086701
B6	1.34441019
A1	108.97259782
A2	109.40309483
A3	96.91328376
A4	114.50396765
A5	96.10911750
D1	-112.84085378
D2	-100.66556114
D3	-123.90770400
D4	62.65185119



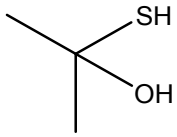
0 1
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 3 B5 1 A4 5 D3
C 1 B6 5 A5 3 D4
H 7 B7 1 A6 5 D5
H 7 B8 1 A7 5 D6
H 7 B9 1 A8 5 D7

B1 1.08942056
B2 1.86212814
B3 1.93258637
B4 1.40618355
B5 1.34374699
B6 1.52450124
B7 1.09213032
B8 1.09216321
B9 1.09430327
A1 107.43710284
A2 95.69966608
A3 112.16537584
A4 95.43657376
A5 112.90485694
A6 111.56130222
A7 108.84778614
A8 110.84308365
D1 139.38757587
D2 115.43728334
D3 56.61660460
D4 -122.50257855
D5 -174.28312724
D6 -54.12186971
D7 64.87864161



0 1
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
H 3 B5 1 A4 5 D3
C 1 B6 5 A5 3 D4
H 7 B7 1 A6 5 D5
H 7 B8 1 A7 5 D6
C 7 B9 1 A8 5 D7
H 10 B10 7 A9 1 D8
H 10 B11 7 A10 1 D9
H 10 B12 7 A11 1 D10

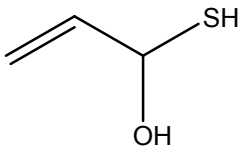
B1 1.09048552
B2 1.86078422
B3 1.93273142
B4 1.40770086
B5 1.34378990
B6 1.53113914
B7 1.09694377
B8 1.09434082
B9 1.53133853
B10 1.09139945
B11 1.09258576
B12 1.09395990
A1 107.60419848
A2 94.96540335
A3 111.97160606
A4 95.39442757
A5 113.24310404
A6 108.55913773
A7 108.92222458
A8 112.26110141
A9 110.80571403
A10 110.75959819
A11 111.12375186
D1 138.92696503
D2 115.38946402
D3 56.37650528
D4 -122.54880092
D5 63.22114369
D6 178.96904156
D7 -58.65623844
D8 56.43656289
D9 176.81078747
D10 -63.38460230



0 1
C
C 1 B1
H 2 B2 1 A1
H 2 B3 1 A2 3 D1
H 2 B4 1 A3 4 D2
C 1 B5 2 A4 3 D3
H 6 B6 1 A5 2 D4
H 6 B7 1 A6 2 D5
H 6 B8 1 A7 2 D6
O 1 B9 6 A8 2 D7
H 10 B10 1 A9 6 D8
S 1 B11 10 A10 6 D9
H 12 B12 1 A11 10 D10

B1 1.53155226
B2 1.09213292
B3 1.09325617
B4 1.09262086
B5 1.52413017
B6 1.09114207
B7 1.09006910
B8 1.09393745
B9 1.41363530
B10 0.96410453
B11 1.88012147
B12 1.34385195
A1 111.66641592

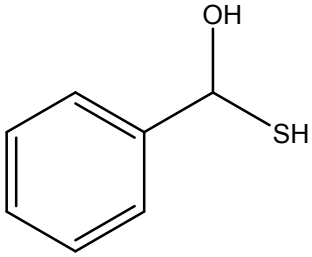
A2	110.92539111
A3	108.69601286
A4	112.21955855
A5	110.38629665
A6	110.99918963
A7	109.09823233
A8	106.06456084
A9	107.85672850
A10	110.27459465
A11	95.37272693
D1	120.93715318
D2	118.97780146



0 1

C					
C	1	B1			
H	1	B2	2	A1	
C	2	B3	1	A2	3	D1
H	4	B4	2	A3	1	D2
S	4	B5	2	A4	1	D3
H	6	B6	4	A5	2	D4
O	4	B7	2	A6	1	D5
H	8	B8	4	A7	2	D6
H	1	B9	2	A8	4	D7
H	2	B10	1	A9	4	D8

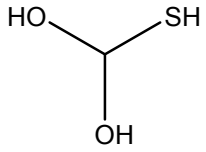
B1	1.32874062
B2	1.08257034
B3	1.49802600
B4	1.09908645
B5	1.86827249
B6	1.34470065
B7	1.40218310
B8	0.96269212
B9	1.08354032
B10	1.08519199
A1	121.18039583
A2	124.22705167
A3	109.62845066
A4	110.97205581
A5	95.49487208
A6	110.23340839
A7	107.84054077
A8	120.94524817
A9	121.15497285
D1	-0.51648923
D2	128.37483887
D3	-120.21786673
D4	55.82968456



0 1

C					
C	1	B1			
C	2	B2	1	A1	
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	1	B5	2	A4	3	D3
H	1	B6	6	A5	5	D4
H	2	B7	1	A6	6	D5
H	4	B8	3	A7	2	D6
H	5	B9	4	A8	3	D7
H	6	B10	1	A9	2	D8
C	3	B11	2	A10	1	D9
H	12	B12	3	A11	2	D10
S	12	B13	3	A12	2	D11
H	14	B14	12	A13	3	D12
O	12	B15	3	A14	2	D13
H	16	B16	12	A15	3	D14

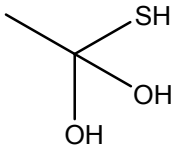
B1	1.39399594
B2	1.39607107
B3	1.39818637
B4	1.39030253
B5	1.39194203
B6	1.08437641
B7	1.08184769
B8	1.08511940
B9	1.08420219
B10	1.08415375
B11	1.51035911
B12	1.09699029
B13	1.86888724
B14	1.34448819
B15	1.40568942
B16	0.96297390
A1	120.16622158
A2	119.27166693
A3	120.47648243
A4	120.35772174
A5	120.05967823
A6	120.62856761
A7	119.67029049
A8	119.77928758
A9	120.23801717
A10	120.79933238
A11	109.65327719
A12	112.51388146
A13	95.76510392
A14	109.59381567



0 1

O					
H	1	B1			
C	1	B2	2	A1	
H	3	B3	1	A2	2	D1
O	3	B4	1	A3	2	D2
H	5	B5	3	A4	1	D3
S	3	B6	1	A5	5	D4
H	7	B7	3	A6	1	D5

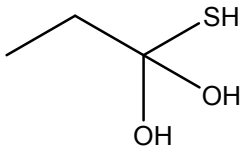
B1	0.96450733
B2	1.40087093
B3	1.09209024
B4	1.39127132
B5	0.96695303
B6	1.84944195
B7	1.34349025
A1	107.18581139
A2	112.43232807
A3	112.92332347
A4	107.16603098
A5	102.98249434
A6	94.45879714
D1	60.00611100
D2	-59.32426671
D3	-61.62227888
D4	-122.76729069
D5	177.78436734



0 1

O							
H	1	B1					
C	1	B2	2	A1			
O	3	B3	1	A2	2	D1	
H	4	B4	3	A3	1	D2	
S	3	B5	1	A4	4	D3	
H	6	B6	3	A5	1	D4	
C	3	B7	1	A6	4	D5	
H	8	B8	3	A7	1	D6	
H	8	B9	3	A8	1	D7	
H	8	B10	3	A9	1	D8	

B1	0.96573042
B2	1.39751830
B3	1.40993358
B4	0.96519364
B5	1.86693523
B6	1.34321863
B7	1.52076055
B8	1.08875039
B9	1.09515860
B10	1.09045662
A1	106.99907985
A2	111.56261190
A3	107.05318157
A4	111.77193134
A5	94.71337707
A6	107.13464078
A7	109.96890141
A8	108.97026857
A9	110.98415161
D1	58.53252613
D2	63.83689487
D3	-112.41827970
D4	-56.36913147
D5	123.35833608
D6	-178.24767173
D7	-58.22874155
D8	60.52428833



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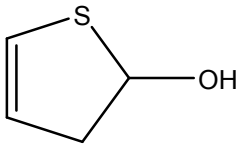
O							
H	1	B1					
C	1	B2	2	A1			
O	3	B3	1	A2	2	D1	
H	4	B4	3	A3	1	D2	
S	3	B5	1	A4	4	D3	
H	6	B6	3	A5	1	D4	
C	3	B7	1	A6	4	D5	
H	8	B8	3	A7	1	D6	
H	8	B9	3	A8	1	D7	
C	8	B10	3	A9	1	D8	
H	11	B11	8	A10	3	D9	
H	11	B12	8	A11	3	D10	
H	11	B13	8	A12	3	D11	

B1	0.96569020
B2	1.39907526
B3	1.40973471
B4	0.96639610
B5	1.87029931
B6	1.34223842
B7	1.52974256
B8	1.09244030
B9	1.09855839
B10	1.52800330
B11	1.09267474
B12	1.09105084
B13	1.09212785
A1	107.12842382
A2	111.72716095
A3	106.86728257
A4	107.99118708
A5	95.42083569
A6	107.41074524
A7	107.36558127
A8	106.17277748
A9	115.35692161
A10	110.26358311
A11	110.83837669
A12	110.94107916



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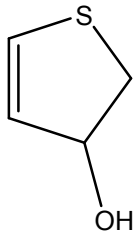
C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	
S	4	B4	3	A3	2	D2	
H	1	B5	2	A4	3	D3	
H	2	B6	1	A5	5	D4	
H	3	B7	2	A6	1	D5	
H	4	B8	3	A7	2	D6	
O	1	B9	2	A8	3	D7	
H	10	B10	1	A9	2	D8	

H	2	B11	1	A10	10	D9	

B1	1.54347599
B2	1.50576422
B3	1.33360103
B4	1.77188183
B5	1.08792001
B6	1.09803283
B7	1.08305518
B8	1.08186800
B9	1.40399859
B10	0.96471838
B11	1.09394445
A1	108.06543259
A2	114.27698576
A3	115.12934632
A4	112.48108506
A5	109.54055737
A6	122.30808844
A7	126.56373789
A8	113.74790597
A9	107.91549141
A10	108.63191291
D1	-20.33596716
D2	2.60079367
D3	144.08074930
D4	-92.41139184
D5	162.24762651
D6	-177.27675365
D7	-95.43821054
D8	63.87867223
D9	28.32066992



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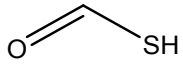
C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	
S	1	B4	2	A3	3	D2	
H	1	B5	2	A4	3	D3	
H	2	B6	1	A5	5	D4	
H	3	B7	2	A6	1	D5	
H	4	B8	3	A7	2	D6	
O	3	B9	2	A8	1	D7	
H	10	B10	3	A9	2	D8	
H	4	B11	3	A10	2	D9	

B1	1.33573441
B2	1.50986926
B3	1.54449580
B4	1.76674467
B5	1.08233700
B6	1.08271631
B7	1.09232878
B8	1.09113458
B9	1.42960265
B10	0.96434332
B11	1.08892949
A1	114.52152719
A2	106.19787183
A3	115.71993957
A4	126.37717583
A5	123.78830655
A6	112.84731665
A7	110.72914650
A8	111.19361008
A9	107.19666734
A10	111.11785060
D1	-20.47763593
D2	5.65313224
D3	-173.57737747
D4	178.10814419
D5	-140.20511218
D6	-91.66780120
D7	102.96726958
D8	-46.15265744
D9	146.12034924



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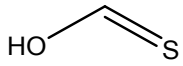
C							
H	1	B1					
S	1	B2	2	A1			
O	1	B3	3	A2	2	D1	
H	3	B4	1	A3	4	D2	

B1	1.10576453
B2	1.79752942
B3	1.19542243
B4	1.34572282
A1	110.08306245
A2	125.69689117
A3	94.50518134
D1	180.00000000
D2	0.00000000



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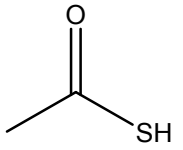
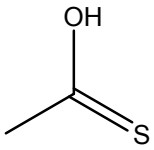
C							
H	1	B1					
S	1	B2	2	A1			
O	1	B3	3	A2	2	D1	
H	4	B4	1	A3	3	D2	

B1	1.08921775
B2	1.62596302
B3	1.32949740
B4	0.97198391
A1	123.57937810
A2	126.29957375
A3	107.80762964
D1	179.90186628
D2	0.02606869



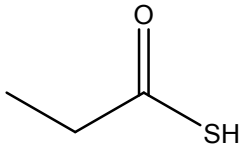
0 1
C
O 1 B1
C 1 B2 2 A1
H 3 B3 1 A2 2 D1
H 3 B4 1 A3 2 D2
S 1 B5 2 A4 3 D3
H 6 B6 1 A5 2 D4
H 3 B7 1 A6 2 D5

B1 1.19774937
B2 1.51283321
B3 1.09401684
B4 1.09140301
B5 1.82512781
B6 1.34345532
B7 1.08963736
A1 124.80862729
A2 108.79436158
A3 111.71651508
A4 122.29708676
A5 93.85479583
A6 108.89599266
D1 98.99780296
D2 -141.86451609
D3 178.68488821
D4 -2.10671347
D5 -19.62516375



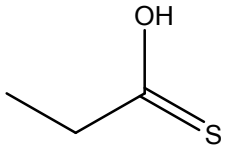
0 1
C
C 1 B1
H 2 B2 1 A1
H 2 B3 1 A2 3 D1
H 1 B4 2 A3 3 D2
S 1 B5 2 A4 3 D3
O 1 B6 2 A5 6 D4
H 2 B7 1 A6 7 D5

B1 1.49848588
B2 1.09420368
B3 1.09430070
B4 1.87292773
B5 1.63969578
B6 1.33885324
B7 1.08597920
A1 109.36107464
A2 109.33581458
A3 140.58749223
A4 126.27908003
A5 110.95040972
A6 111.10217807
D1 116.99247334
D2 -58.36976210
D3 121.65231491
D4 179.98152751
D5 -179.90117543



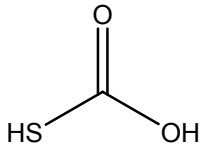
0 1
C
O 1 B1
C 1 B2 2 A1
H 3 B3 1 A2 2 D1
H 3 B4 1 A3 2 D2
S 1 B5 2 A4 3 D3
H 6 B6 1 A5 2 D4
C 3 B7 1 A6 2 D5
H 8 B8 3 A7 1 D6
H 8 B9 3 A8 1 D7
H 8 B10 3 A9 1 D8

B1 1.19806571
B2 1.51965578
B3 1.09575341
B4 1.09575383
B5 1.82812255
B6 1.34321366
B7 1.52713179
B8 1.09130839
B9 1.09216916
B10 1.09130972
A1 125.13150417
A2 107.56973028
A3 107.56822271
A4 122.05276796
A5 93.69649727
A6 112.93415055
A7 111.04721305
A8 110.22878732
A9 111.04721775
D1 123.26628431
D2 -123.24413935
D3 -180.00000000
D4 0.00000000
D5 0.01019880
D6 59.80544331
D7 -180.00000000
D8 -59.80501915



0 1
C
C 1 B1
H 2 B2 1 A1
H 2 B3 1 A2 3 D1
H 1 B4 2 A3 4 D2
C 2 B5 1 A4 5 D3
H 6 B6 2 A5 1 D4
H 6 B7 2 A6 1 D5
H 6 B8 2 A7 1 D6
S 1 B9 2 A8 6 D7
O 1 B10 2 A9 6 D8

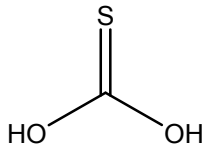
B1	1.50664712
B2	1.09691463
B3	1.09689703
B4	1.87303470
B5	1.52442758
B6	1.09121667
B7	1.09271721
B8	1.09122324
B9	1.63968447
B10	1.34020558
A1	106.34154490
A2	106.34784405
A3	139.79820298
A4	116.39631885
A5	111.27663597
A6	109.79355355
A7	111.27618508
A8	127.46022351
A9	110.14944931
D1	111.61512689
D2	55.72585386
D3	179.92451106
D4	59.97451879
D5	179.98574847
D6	-60.00474805
D7	-0.09332807
D8	179.91491469



0 1

O							
C	1	B1					
S	2	B2	1	A1			
H	3	B3	2	A2	1	D1	
O	2	B4	1	A3	3	D2	
H	5	B5	2	A4	1	D3	

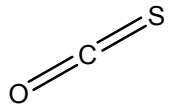
B1	1.19656630
B2	1.79337358
B3	1.34209392
B4	1.34825050
B5	0.96924408
A1	126.42044251
A2	93.01886327
A3	125.20386441
A4	106.74967415
D1	0.05803270
D2	-179.98546304
D3	0.08285471



0 1

C							
S	1	B1					
O	1	B2	2	A1			
H	3	B3	1	A2	2	D1	
O	1	B4	3	A3	2	D2	
H	5	B5	1	A4	3	D3	

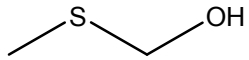
B1	1.56640000
B2	1.43000000
B3	0.96000000
B4	1.43000000
B5	0.96000000
A1	120.00000000
A2	109.47122063
A3	120.00000000
A4	109.47122063
D1	0.56000000
D2	180.00000000
D3	-179.44000000



0 1

C					
O	1	B1			
S	1	B2	2	A1	

B1	1.15621300
B2	1.56794300
A1	180.00000000

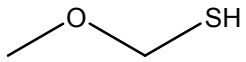


0 1

C							
H	1	B1					
H	1	B2	2	A1			
S	1	B3	2	A2	3	D1	
H	1	B4	4	A3	3	D2	
O	1	B5	4	A4	3	D3	
C	4	B6	1	A5	6	D4	
H	7	B7	4	A6	1	D5	
H	7	B8	4	A7	1	D6	
H	7	B9	4	A8	1	D7	

B1	1.09019552
B2	1.09629413
B3	1.83035144
B4	1.93168186
B5	1.40858001
B6	1.82499384
B7	1.08985360
B8	1.08923157
B9	1.09105195
A1	108.91901707
A2	109.67157730
A3	96.98528466
A4	114.22392100
A5	99.18395258
A6	107.36867120
A7	109.32373450
A8	110.98399140
D1	-114.03398203
D2	-100.37297661
D3	-123.96817685
D4	62.49198961
D5	-167.63680813

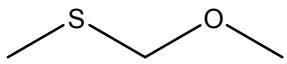
D6	-48.93696672
D7	72.91393937



0 1

C							
H	1	B1					
H	1	B2	2	A1			
S	1	B3	2	A2	3	D1	
O	1	B4	4	A3	3	D2	
H	4	B5	1	A4	5	D3	
C	5	B6	1	A5	4	D4	
H	7	B7	5	A6	1	D5	
H	7	B8	5	A7	1	D6	
H	7	B9	5	A8	1	D7	

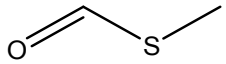
B1	1.08774372
B2	1.09759398
B3	1.85534041
B4	1.39330442
B5	1.34398871
B6	1.42137194
B7	1.08926687
B8	1.09501663
B9	1.09872843
A1	109.46746109
A2	108.43313524
A3	115.57258072
A4	95.81165326
A5	114.64308608
A6	106.61740023
A7	111.39271738
A8	111.01537392
D1	-112.93337943
D2	-123.55173124
D3	66.78540649
D4	71.51810455
D5	177.41615541
D6	-63.24265781
D7	58.56919967



0 1

C							
H	1	B1					
H	1	B2	2	A1			
S	1	B3	2	A2	3	D1	
O	1	B4	4	A3	3	D2	
C	5	B5	1	A4	4	D3	
H	6	B6	5	A5	1	D4	
H	6	B7	5	A6	1	D5	
H	6	B8	5	A7	1	D6	
C	4	B9	1	A8	5	D7	
H	10	B10	4	A9	1	D8	
H	10	B11	4	A10	1	D9	
H	10	B12	4	A11	1	D10	

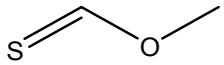
B1	1.09022801
B2	1.09773747
B3	1.83901543
B4	1.40124850
B5	1.42125781
B6	1.08957697
B7	1.09503508
B8	1.09876344
B9	1.82458119
B10	1.09006077
B11	1.08949383
B12	1.09140364
A1	109.37545296
A2	108.66909396
A3	115.26993663
A4	114.38585677
A5	106.65262676
A6	111.50815327
A7	110.95293700
A8	98.79027362
A9	107.24368185
A10	109.69875912
A11	111.07084475
D1	-114.14612563
D2	-123.79678195
D3	73.01386436
D4	177.97934830
D5	-62.47963997
D6	59.21382130
D7	64.03259766
D8	-170.38779319
D9	-51.72850243
D10	70.31510725



0 1

C							
H	1	B1					
C	2	B2	1	A1			
H	3	B3	2	A2	1	D1	
H	3	B4	2	A3	1	D2	
H	3	B5	2	A4	1	D3	
S	1	B6	3	A5	2	D4	
O	1	B7	7	A6	3	D5	

B1	1.10928694
B2	2.66752497
B3	1.08972766
B4	1.08951574
B5	1.08968978
B6	1.78533915
B7	1.19741282
A1	83.99787113
A2	168.11037863
A3	79.99077754
A4	74.29827860
A5	40.24512809
A6	123.26151235
D1	-18.73754102
D2	120.09219308
D3	-124.95246937
D4	-179.51168128
D5	179.63622268

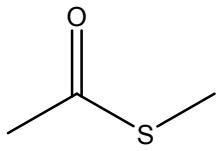


0 1

C							
H	1	B1					
S	1	B2	2	A1			

O	1	B3	3	A2	2	D1	
C	4	B4	1	A3	3	D2	
H	5	B5	4	A4	1	D3	
H	5	B6	4	A5	1	D4	
H	5	B7	4	A6	1	D5	

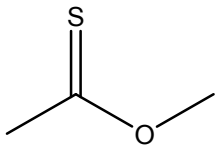
B1	1.09486124
B2	1.62211975
B3	1.32986509
B4	1.44065085
B5	1.08714756
B6	1.09271254
B7	1.09271380
A1	121.98021138
A2	123.92793528
A3	116.79357461
A4	105.79494792
A5	110.60733405
A6	110.61301234
D1	179.98458530
D2	179.98329872
D3	179.89769878
D4	-61.34272497
D5	61.13490359



0 1
C

C	1	B1					
H	2	B2	1	A1			
H	2	B3	1	A2	3	D1	
H	2	B4	1	A3	4	D2	
C	1	B5	2	A4	5	D3	
H	6	B6	1	A5	2	D4	
H	6	B7	1	A6	2	D5	
H	6	B8	1	A7	2	D6	
O	1	B9	6	A8	2	D7	
S	1	B10	10	A9	6	D8	

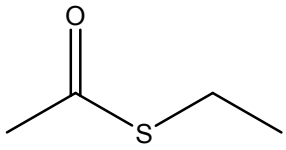
B1	2.75329822
B2	1.08967236
B3	1.08859798
B4	1.08844245
B5	1.51414320
B6	1.09309183
B7	1.09042630
B8	1.09213694
B9	1.20454376
B10	1.79766390
A1	146.86172626
A2	89.22986975
A3	86.27886696
A4	154.47907170
A5	108.45391604
A6	112.81944986
A7	108.65359060
A8	123.80933511
A9	122.42115933
D1	127.76306338
D2	109.76691321
D3	-128.97656032
D4	-113.88031869
D5	7.26130094
D6	129.19552908
D7	178.25716425
D8	179.59082265



0 1
C

S	1	B1					
O	1	B2	2	A1			
C	3	B3	1	A2	2	D1	
H	4	B4	3	A3	1	D2	
H	4	B5	3	A4	1	D3	
H	4	B6	3	A5	1	D4	
C	1	B7	3	A6	4	D5	
H	8	B8	1	A7	3	D6	
H	8	B9	1	A8	3	D7	
H	8	B10	1	A9	3	D8	

B1	1.64248402
B2	1.33419965
B3	1.43750535
B4	1.08790395
B5	1.09093864
B6	1.09093811
B7	1.50365228
B8	1.09411877
B9	1.09412267
B10	1.08626253
A1	125.30852503
A2	119.65391701
A3	104.98663321
A4	110.31165211
A5	110.31163101
A6	109.62485553
A7	109.50995654
A8	109.50913332
A9	110.81107565
D1	0.00000000
D2	179.99619657
D3	-60.34009553
D4	60.33223174
D5	-180.00000000
D6	-58.64127751
D7	58.63185440
D8	179.99440243



0 1
C

H	1	B1					
H	1	B2	2	A1			
H	1	B3	2	A2	3	D1	
C	1	B4	2	A3	4	D2	
H	5	B5	1	A4	2	D3	

H	5	B6	1	A5	2	D4	
S	5	B7	1	A6	2	D5	
C	8	B8	5	A7	1	D6	
O	9	B9	8	A8	5	D7	
C	9	B10	8	A9	5	D8	
H	11	B11	9	A10	8	D9	
H	11	B12	9	A11	8	D10	
H	11	B13	9	A12	8	D11	

B1	1.09089522
B2	1.09224963
B3	1.09461446
B4	1.52563704
B5	1.09172195
B6	1.09048584
B7	1.83226268
B8	1.79984659
B9	1.20507184
B10	1.51414242
B11	1.09357624
B12	1.09037606
B13	1.09168131
A1	108.59397833
A2	108.02269372
A3	110.55578824
A4	111.83022151
A5	111.23531962
A6	113.63925323
A7	99.88432959
A8	122.92527716
A9	113.52319123
A10	108.32216926
A11	112.75605582
A12	108.74781639
D1	117.13455537
D2	120.31258919
D3	-179.34406889
D4	-57.69901315
D5	61.95733941
D6	-83.50223357
D7	-1.80796286
D8	177.61896077
D9	-108.90015306
D10	11.76959408
D11	134.09866230

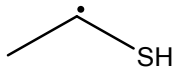
Z-Matrices for Radicals

0 2
S
H 1 B1

B1 1.34805900

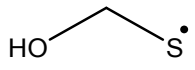
0 2
S
C 1 B1
H 2 B2 1 A1
H 2 B3 1 A2 3 D1
H 2 B4 1 A3 4 D2

B1 1.80509576
B2 1.09426097
B3 1.09426071
B4 1.08936108
A1 108.46557032
A2 108.46546693
A3 112.72803708
D1 115.62679808
D2 122.18654500



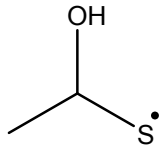
0 2
S
C 1 B1
H 2 B2 1 A1
H 2 B3 1 A2 3 D1
C 2 B4 1 A3 4 D2
H 5 B5 2 A4 1 D3
H 5 B6 2 A5 1 D4
H 5 B7 2 A6 1 D5

B1 1.81255108
B2 1.09664263
B3 1.09673222
B4 1.52576377
B5 1.09500828
B6 1.09200972
B7 1.09200626
A1 105.99738868
A2 105.92913178
A3 115.64533741
A4 110.46961552
A5 110.99351663
A6 110.99466025
D1 111.39208323
D2 124.26821945
D3 -179.90021959
D4 -59.84034334
D5 60.04987358



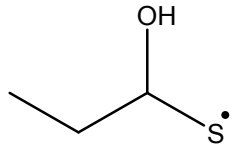
0 2
C
H 1 B1
H 1 B2 2 A1
S 1 B3 2 A2 3 D1
H 1 B4 4 A3 3 D2
O 1 B5 4 A4 3 D3

B1 1.09311270
B2 1.10418734
B3 1.80432166
B4 1.93234767
B5 1.40152428
A1 107.00923608
A2 108.65389903
A3 95.89079776
A4 116.85169040
D1 -111.51684524
D2 -104.96425419
D3 -124.91212420



0 2
C
H 1 B1
S 1 B2 2 A1
H 1 B3 3 A2 2 D1
O 1 B4 3 A3 2 D2
C 1 B5 5 A4 3 D3
H 6 B6 1 A5 5 D4
H 6 B7 1 A6 5 D5
H 6 B8 1 A7 5 D6

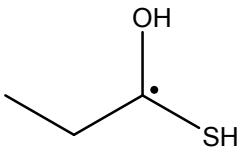
B1 1.10516701
B2 1.82033617
B3 1.93948424
B4 1.40907052
B5 1.52674909
B6 1.08976380
B7 1.09242484
B8 1.09139813
A1 101.58746116
A2 92.09751648
A3 114.41452446
A4 107.42670124
A5 111.02676659
A6 108.65277919
A7 110.13086487
D1 102.00462725
D2 119.74884160
D3 -126.36444999
D4 -174.35188631
D5 -53.94871313
D6 64.46054301



0 2
O

H	1	B1					
C	1	B2	2	A1			
S	3	B3	1	A2	2	D1	
C	3	B4	1	A3	4	D2	
H	5	B5	3	A4	1	D3	
H	5	B6	3	A5	1	D4	
C	5	B7	3	A6	1	D5	
H	8	B8	5	A7	3	D6	
H	8	B9	5	A8	3	D7	
H	8	B10	5	A9	3	D8	
H	3	B11	1	A10	5	D9	

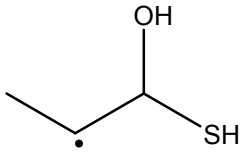
B1	0.96287373
B2	1.41030467
B3	1.81965474
B4	1.53363169
B5	1.09255081
B6	1.09509612
B7	1.52994027
B8	1.09245987
B9	1.09101777
B10	1.09425772
B11	1.10622942
A1	108.17732204
A2	114.30372077
A3	107.94996462
A4	108.31165155
A5	106.40379253
A6	113.74442064
A7	110.60354207
A8	110.60075796
A9	111.17425984
A10	110.83139841
D1	-35.44395080
D2	-128.37936412
D3	-172.09316979
D4	-56.81572264
D5	64.22507928
D6	-175.35633369
D7	-55.32572106
D8	65.03202322
D9	-118.56273288



0 2

C							
S	1	B1					
H	1	B2	2	A1			
O	1	B3	2	A2	3	D1	
H	2	B4	1	A3	4	D2	
C	1	B5	4	A4	2	D3	
H	6	B6	1	A5	4	D4	
H	6	B7	1	A6	4	D5	
C	6	B8	1	A7	4	D6	
H	9	B9	6	A8	1	D7	
H	9	B10	6	A9	1	D8	
H	9	B11	6	A10	1	D9	

B1	1.75965920
B2	1.90549204
B3	1.36854001
B4	1.36335363
B5	1.49506567
B6	1.09589433
B7	1.09212416
B8	1.54320152
B9	1.09213059
B10	1.09314338
B11	1.09338828
A1	90.82784207
A2	118.27894753
A3	101.06512633
A4	113.81308483
A5	107.77239152
A6	108.72197502
A7	113.74015213
A8	110.57572707
A9	110.56979349
A10	111.10904662
D1	-8.93359654
D2	74.21533050
D3	157.78531283
D4	48.08335058
D5	164.23880239
D6	-73.01006545
D7	57.80350341
D8	177.72340540
D9	-62.54702647

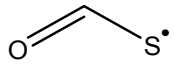


0 2

C							
H	1	B1					
S	1	B2	2	A1			
H	1	B3	3	A2	2	D1	
O	1	B4	3	A3	2	D2	
H	3	B5	1	A4	5	D3	
C	1	B6	5	A5	3	D4	
H	7	B7	1	A6	5	D5	
C	7	B8	1	A7	5	D6	
H	9	B9	7	A8	1	D7	
H	9	B10	7	A9	1	D8	
H	9	B11	7	A10	1	D9	

B1	1.09651509
B2	1.92971600
B3	1.92786065
B4	1.40080777
B5	1.34405244
B6	1.46779444
B7	1.08381588
B8	1.48866792
B9	1.09089885
B10	1.10242750
B11	1.09343151
A1	99.79478914
A2	89.95268401
A3	110.59661434
A4	95.13598490
A5	111.00814141
A6	116.17757267
A7	122.85609902

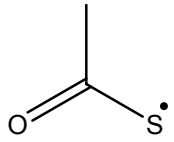
A8	111.22952465
A9	111.92710770
A10	110.86619833
D1	98.80189333
D2	118.73945357
D3	-65.23718839
D4	-123.74529842
D5	-162.83679645
D6	30.47561147
D7	-33.20694160
D8	86.76406766
D9	-154.68969690



0 2

C							
H	1	B1					
O	1	B2	2	A1			
S	1	B3	3	A2	2	D1	

B1	1.10305555
B2	1.20344910
B3	1.77015761
A1	124.75942846
A2	119.12039378
D1	180.00000000



0 2

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

B1	1.76710483
B2	1.21182675
B3	1.50171056
B4	1.09300517
B5	1.09300810
B6	1.09082047
A1	114.19303286
A2	125.24702100
A3	109.80874420
A4	109.80654648
A5	109.53195883
D1	179.99678040
D2	120.78258115
D3	-120.75664928
D4	0.01171873