The Antioxidant Activity of Polysulfides: It's Radical!

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Supporting Information

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Synthetic Procedures

Di-octylsulfide was obtained from commercial suppliers and used as received. tBuS(O)SBu (**6**),[1] tBuS(O)SStBu (**7**),[2] $C_{12}H_{25}SSC_{12}H_{25}$,[3] $C_{12}H_{25}SOSC_{12}H_{25}$,[3] cumyl-SSH[4] and *tert*-dodecyl-SSH[4] were prepared as previously reported.

Di-*tert*-butyltrisulfide[5] **(3).** *tert*-Butylthiol (3.00 g, 33.3 mmol) and Et_3N (3.34 g, 33.3 mmol) were added dropwise as a solution in dry ether (40 mL) to a solution of freshly distilled SCl_2 (1.71 g, 16.6 mmol) in dry ether (40 mL) cooled to -78°C in a dry ice/acetone bath. After the addition is complete, the solution was stirred at -78°C for an additional 30 minutes, after which it was diluted with ether (100 mL) and washed with water, Na_2CO_3 (sat.) and brine. The organic layer was dried over $MgSO_4$, filtered and concentrated in vacuo. The crude oil was purified by column chromatography using 5% EtOAc in Hexanes to obtain the product as a beige oil (3.1 g, 88%). ^{1}H NMR (400 MHz; $CDCl_3$): δ 1.37 (s, 18H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 49.1, 30.0. HRMS (EI, [M+]): m/z calcd for $C_8H_{18}S_3$ 210.0571, found 210.0581.

Di-*tert*-butyltetrasulfide[5] **(4).** A solution of S_2Cl_2 (2.21 mL, 27.7 mmol) in dry ether (70 mL) is cooled to -78°C in a dry ice/acetone bath. A solution of tert-butylthiol (6.25 mL, 55.4 mmol) and Et_3N (7.68 mL, 55.4 mmol) in dry ether (70 mL) is added dropwise over 1 hour. After the addition is complete, the solution is stirred at -78°C for an additional 30 minutes after which is warmed to room temperature and quenched with water. The organic layer was separated and washed with water, Na_2CO_3 (sat.) and brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The crude yellow oil was purified by column chromatography using hexanes as the eluent to yield the product as a yellow oil (5.20 g, 78%). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 1.40 (s, 18H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 49.3, 30.4. HRMS (EI, [M+]): m/z calcd for $C_8H_{18}S_4$ 242.0291, found 242.0298.

Di-*tert*-butylsulfoxide[6] **(5)**. To a solution of di-*tert*-butylsulfide (1.25 g, 8.55 mmol) in dry DCM (20 mL) at 0°C was added m-CPBA (2.00 g, 9.95 mmol) dropwise as a solution in DCM (10 mL). The resulting white suspension was stirred at 0°C for 2 hours after which Na_2CO_3 (0.50 g) was added and the organic layer was washed with water and brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The crude white solid was purified by column chromatography using 10% EtOAc in Hexanes to yield the product as a white solid (1.10 g, 79%). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 1.33 (s, 18H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 57.3, 25.7. HRMS (EI, [M+]): m/z calcd for $C_8H_{18}S$ 162.1078, found 162.1090.

Di-*tert*-butyltetrasulfide-1-oxide[7] **(8).** To a solution of di-*tert*-butyltetrasulfide (0.500 g, 2.10 mmol) in dry DCM (8.0 mL) at 0°C was added m-CPBA (0.470 g, 2.10 mmol) dropwise as a solution in DCM (2.0 mL). The resulting white suspension was stirred at 0°C for 1 hour after which Na_2CO_3 (0.20 g) was added and the organic layer was washed with water and brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The crude oil was purified by column chromatography

using 10% EtOAc in Hexanes to yield the product as a white solid (0.340 g, 63%). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 1.41 (s, 9H), 1.39 (s, 9H). ^{13}C NMR (76 MHz; $CDCl_3$): δ 60.8, 50.0, 30.0, 24.1 HRMS (ESI, [M + Na^+]): m/z calcd for $C_8H_{18}OS_4Na$ 281.0138, found 281.0130.

Di-isopropyltetrasulfide[8] **(9).** Synthesized following the same procedure as **4** starting from 2-propanethiol and obtained as a yellow oil (1.85 g, 70%). ^{1}H NMR (400 MHz; $CDCl_3$): δ 3.31 (7, *J* = 6.8 Hz, 2H), 1.39 (d, *J* = 6.8 Hz, 12H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 42.3, 22.8. HRMS (EI, [M+]): m/z calcd for $C_6H_{14}S_4$ 213.9978, found 213.9968.

Di-*tert*-dodecyltrisulfide (12): 2,2'-thiobis(isoindoline-1,3-dione)[9] (0.200 g, 0.620 mmol) was dissolved in DCM (4.0 mL) and purged with N_2 in a 25 mL RBF. *t*-Dodecylthiol[4] (0.250 g, 1.23 mmol) and Et_3N (170 µL, 1.23 mmol) were added dropwise as a solution in DCM (2.2 mL) and the solution was stirred at room temperature for 2 hours. Upon completion of the reaction as determined by thin layer chromatography, the solution was diluted with DCM (30 mL) and the organic layer was washed with Na_2CO_3 (sat.), water and brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The crude oil was purified by column chromatography using hexanes as the eluent to yield the product as a colourless oil (0.205 g, 74%). ^{1}H NMR (400 MHz; $CDCl_3$): δ 1.60-1.56 (m, 4H), 1.36-1.27 (m, 40H), 0.88 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 52.4, 41.5, 32.1, 30.1, 29.8, 29.8, 29.5, 27.9, 24.8, 22.9, 14.3. HRMS (EI, [M+]): m/z calcd for $C_{24}H_{50}S_3$ 434.3075, found 434.3049.

Di-2-octyltetrasulfide (13). Synthesized following the same procedure as **4** starting from 2-octanethiol[10] and obtained as a yellow oil (0.359 g, 74%). ^{1}H NMR (600 MHz; $CDCl_3$): δ 3.11 (qd, *J* = 6.8, 3.0 Hz, 2H), 1.74 (ddt, *J* = 13.7, 8.8, 6.8 Hz, 2H), 1.58-1.52 (m, 2H), 1.43-1.38 (m, 10H), 1.32-1.29 (m, 12H), 0.89 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR (151 MHz; $CDCl_3$): δ 47.6, 36.3, 31.9, 29.2, 27.1, 22.8, 21.0, 14.2.

Di-octylsulfoxide (14): To a solution of di-octylsulfide (1.00 g, 3.87 mmol) in dry DCM (15 mL) at 0 °C was added m-CPBA (0.908 g, 4.06 mmol) dropwise as a solution in DCM (5 mL). The resulting white suspension was stirred at 0 °C for 2 hours after which Na_2CO_3 (0.50 g) was added and the organic layer was washed with water, brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The crude white solid was purified by column chromatography using 10% EtOAc in hexanes to obtain the product as a white solid (0.950 g, 90%). ^{1}H NMR (400 MHz; $CDCl_3$): δ 2.72-2.57 (m, 4H), 1.79-1.71 (m, 4H), 1.49-1.39 (m, 4H), 1.33-1.27 (m, 16H), 0.87 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (101 MHz; $CDCl_3$): δ 52.6, 31.9, 29.3, 29.2, 29.0, 22.7, 14.2. HRMS (ESI, [M+Na^+]): m/z calcd for $C_{16}H_{34}OSNa$ 297.2228, found 297.2246.

Di-*tert*-dodecyltrisulfide-1-oxide (16): To a solution of di-*tert*-dodecyltrisulfide (0.200 g, 0.460 mmol) in dry DCM (1.5 mL) at 0 °C was added m-CPBA (0.110 g,

0.480 mmol) dropwise as a solution in DCM (0.8 mL). The resulting white suspension was stirred at 0 °C for 2 hours after which Na_2CO_3 (0.10 g) was added and the organic layer was washed with water, brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The crude white solid was purified by column chromatography using 10% EtOAc in hexanes to yield the product as a white solid (0.127 g, 61%). ^{1}H NMR (600 MHz; $CDCl_3$): δ 1.80 (m, 1H), 1.65-1.59 (m, 3H), 1.39-1.33 (m, 15H), 1.28 (m, 25H), 0.88 (t, *J* = 7.0 Hz, 6H). ^{13}C NMR (151 MHz; $CDCl_3$): δ 64.2, 52.4, 41.5, 37.1, 32.1, 32.0, 30.2, 30.1, 29.7, 29.7, 29.6, 29.5, 29.4, 27.9, 27.7, 24.9, 23.9, 22.8, 22.8, 21.5, 21.3, 14.3, 14.3. HRMS (ESI, [M+Na$^+$]): m/z calcd for $C_{24}H_{50}OS_3Na$ 473.2922, found 473.2929.

Inhibited Co-Autoxidation of 1-Hexadecene at 100 °C

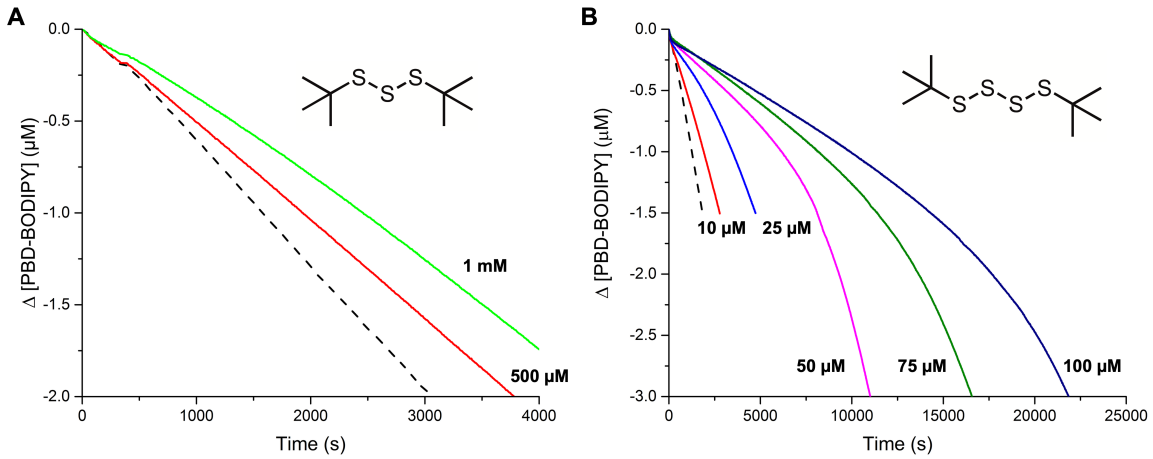


Figure S1. Co-autoxidations of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumylperoxide (1 mM) in chlorobenzene at 100 °C (dashed black trace) and inhibited by organosulfur **3** (A) and **4** (B). Reaction progress was monitored by absorbance at 587 nm (ε = 119 166 M^{-1} cm^{-1}).

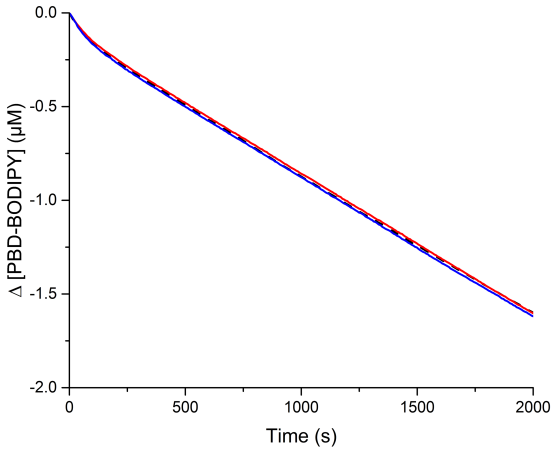


Figure S2. Co-autoxidations of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumylperoxide (1 mM) in chlorobenzene at 100 °C (dashed black trace) and inhibited by 50 μM (red) and 100 μM (blue) of sulfur. Reaction progress was monitored by absorbance at 587 nm (ε = 119 166 M^{-1} cm^{-1}).

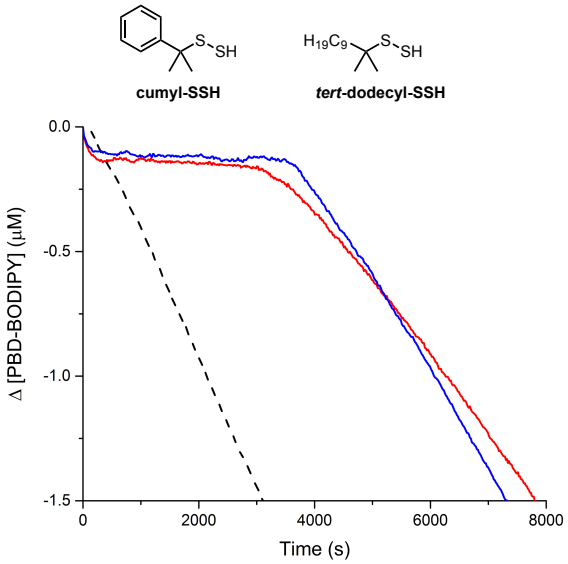


Figure S3. Co-autoxidations of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumylperoxide (1 mM) in chlorobenzene at 100 °C (dashed black trace) and inhibited by 50 μM of cumyl-SSH (red) and *tert*-dodecyl-SSH (blue). Reaction progress was monitored by absorbance at 587 nm (ε = 119 166 M^{-1} cm^{-1}).

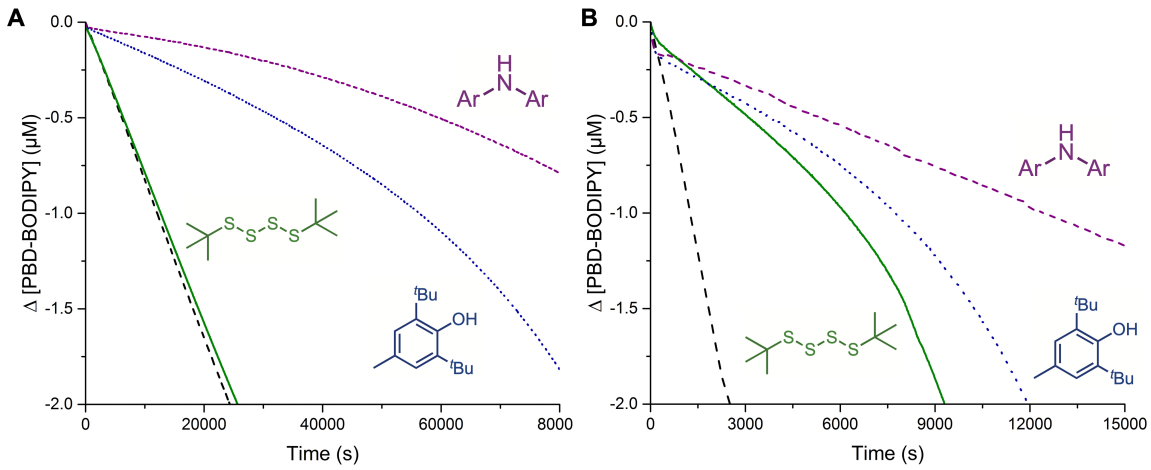


Figure S4. Co-autoxidation of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated with AIBN (6 mM) in chlorobenzene at 37 °C (dashed black trace) and inhibited by 50 μM of 50 μM of **4** (green), BHT (blue) and ^{t}Bu-DPA (purple) (A). Reaction progress was monitored by absorbance at 588 nm (ε = 148 700 M^{-1} cm^{-1}). Co-autoxidation of 1-hexadecene (2.8 M) and PBD-BODIPY (10 μM) initiated by dicumylperoxide (1 mM) in chlorobenzene at 100 °C (dashed black trace) and inhibited by 50 μM of **4** (green), BHT (blue) and ^{t}*Bu*-DPA (purple). Reaction progress was monitored by absorbance at 587 nm (ε = 119 166 M^{-1} cm^{-1}) (B).

Variation of R_i in 1-Hexadecene Autoxidation at 100 °C

Table S1. Inhibition rate constants and stoichiometries obtained from thermally-initiated (0.5-2 mM dicumylperoxide) co-autoxidation of 1-hexadecene and PBD-BODIPY in chlorobenzene at 100 °C in the presence of 50 μM of organosulfur.

[DCP] (mM)	**0.5**		**1**		**2**	
Substrate	k_{inh} (10^6 M^{-1} s^{-1})	*n*	k_{inh} (10^6 M^{-1} s^{-1})	*n*	k_{inh} (10^6 M^{-1} s^{-1})	*n*
4	(0.15 ± 0.02)	1.2 ± 0.2	(0.23 ± 0.04)	1.4 ± 0.3	(1.7 ± 0.2)	1.1 ± 0.1
5	(2.1 ± 0.5)	0.3 ± 0.1	(1.4 ± 0.2)	0.4 ± 0.1	(2.4 ± 0.2)	0.5 ± 0.1
6	(3.5 ± 0.9)	1.0 ± 0.1	(1.5 ± 0.5)	1.0 ± 0.1	(1.4 ± 0.5)	0.5 ± 0.1

Tetralin Hydroperoxide Decomposition by Polysulfides

Tetralin hydroperoxide (1 mM) was loaded in a screw cap vial containing either ^{t}BuSSS^{t}Bu or ^{t}BuSSSS^{t}Bu (0.2 mM) in PhCl and heated at 100 °C under air. Aliquots (100 µL) were taken every 15 minutes and diluted to 500 µL in an autosampler vial containing 350 µL of hexanes and 50 µL of a benzyl alcohol stock solution (2 mM). The samples (10 µL injections) were separated using a Waters Acquity UPLC (1.5% 2-propanol in hexanes, 1.2 mL min^{-1}; Sunfire Silica column (5 µm, 4.6 mm × 250 mm)) and analyzed by UV absorbance at 215 nm.

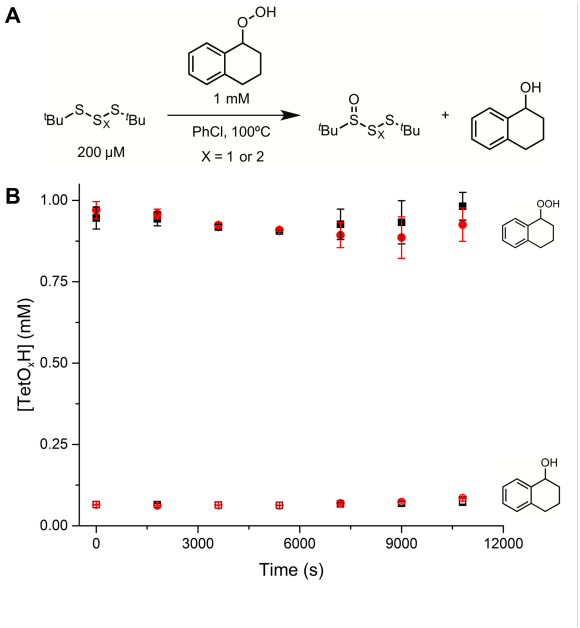


Figure S5. Tetralin hydroperoxide (full) decomposition to tetralin alcohol (empty) by **3** (square, black) or **4** (circle, red) in PhCl at 100 °C.

Inhibited *n*-Hexadecane Autoxidation

Acid Formation

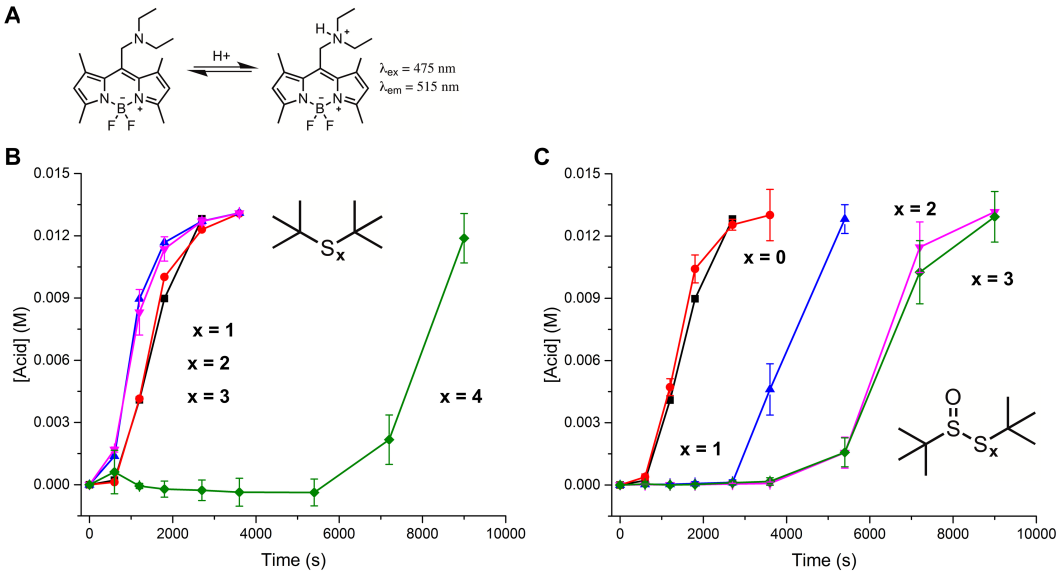
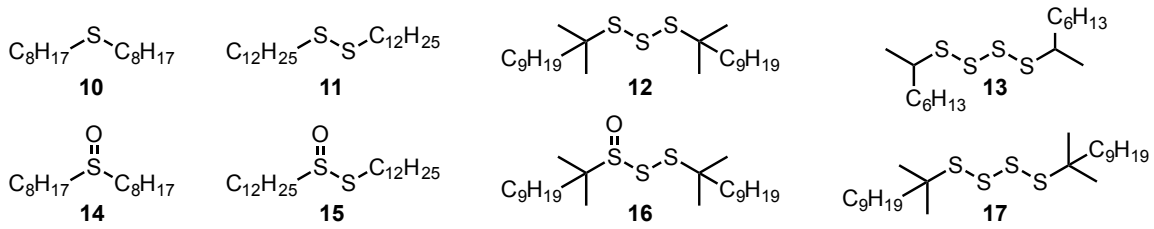


Figure S6. BODIPY probe (A) allows the quantification of acids formed during n-hexadecane autoxidation at 160 °C inhibited by polysulfides (B) and their corresponding 1-oxides (C).

Long Chain Analogues

Since the autoxidation of *n*-hexadecane was conducted at 160 °C, one should consider the boiling points of compounds **1-8** to exclude that the absence of activity of some compounds may be due to their volatility at 160 °C. Therefore, we performed inhibited n-hexadecane autoxidation at 160 °C inhibited by long chain (poly)sulfides **10-17** (Figure S6) and found that their inhibition, or lack of, corresponded well to their shorter chain analogues.



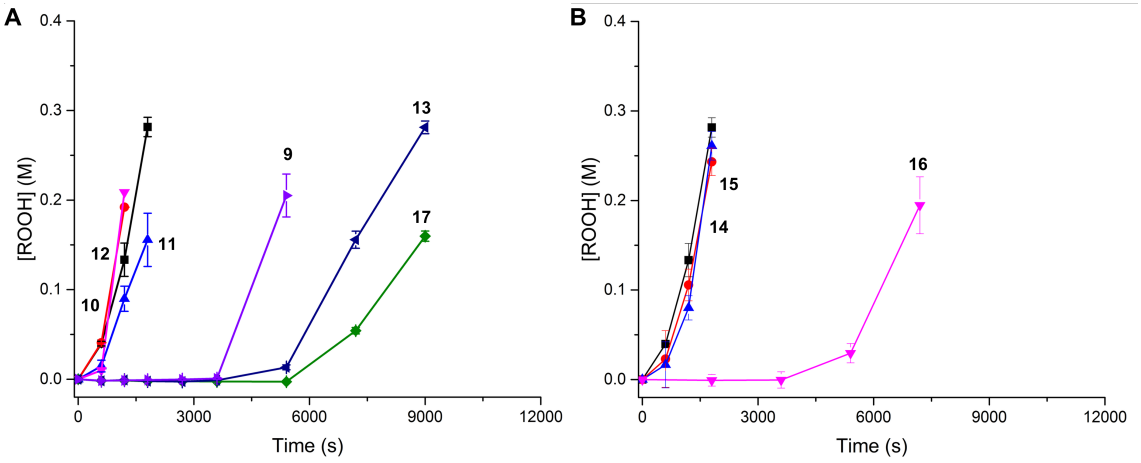
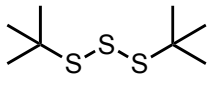


Figure S7. Hydroperoxide production over the course of a *n*-hexadecane autoxidation at 160 °C (black square) inhibited by 500 μM polysulfides (A) and their corresponding oxides (B).

The synthesis of long chain analogues also highlights the effect of the side chain substituent on the RTA activity of tetrasulfides. The *tert*-butyl group is not necessary for the activity of those compounds as both **9** and **13** are potent RTA at 160 °C. (Figure S6A).

NMR Spectra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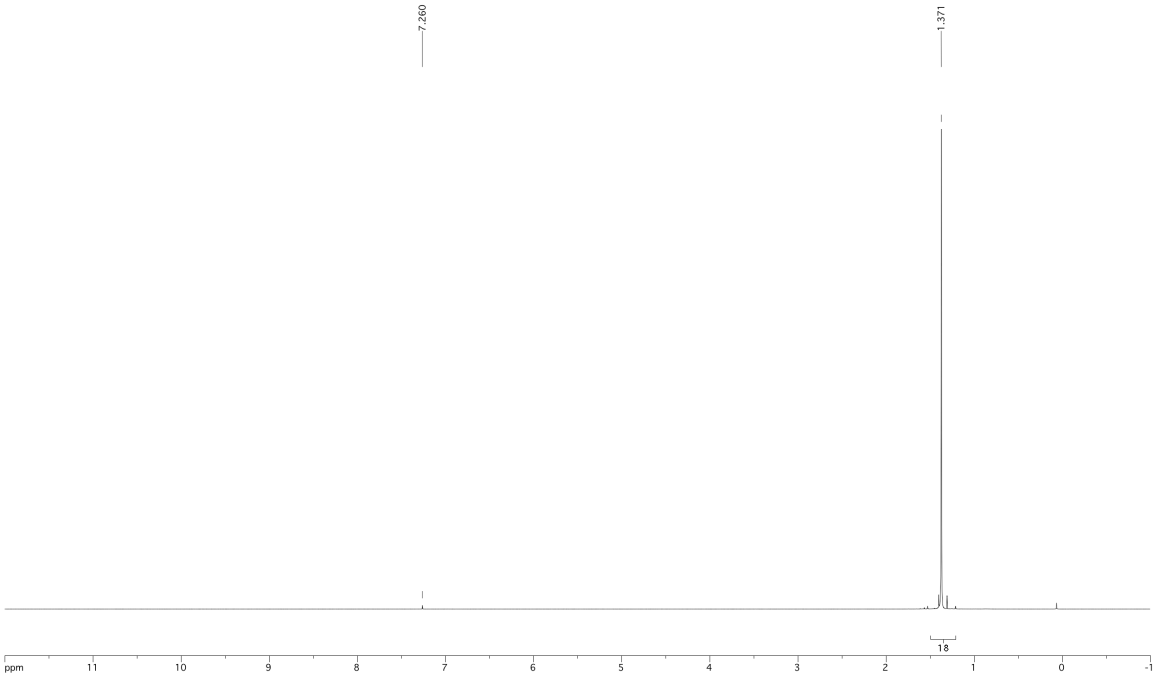

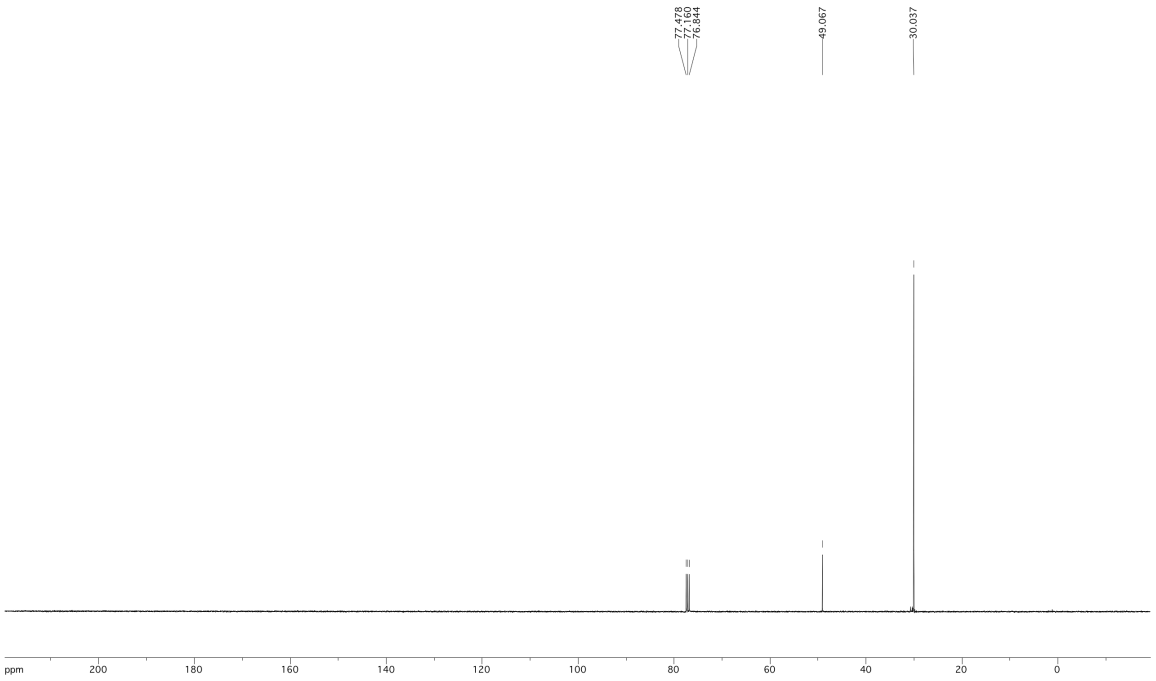

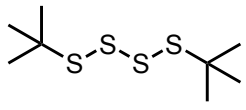

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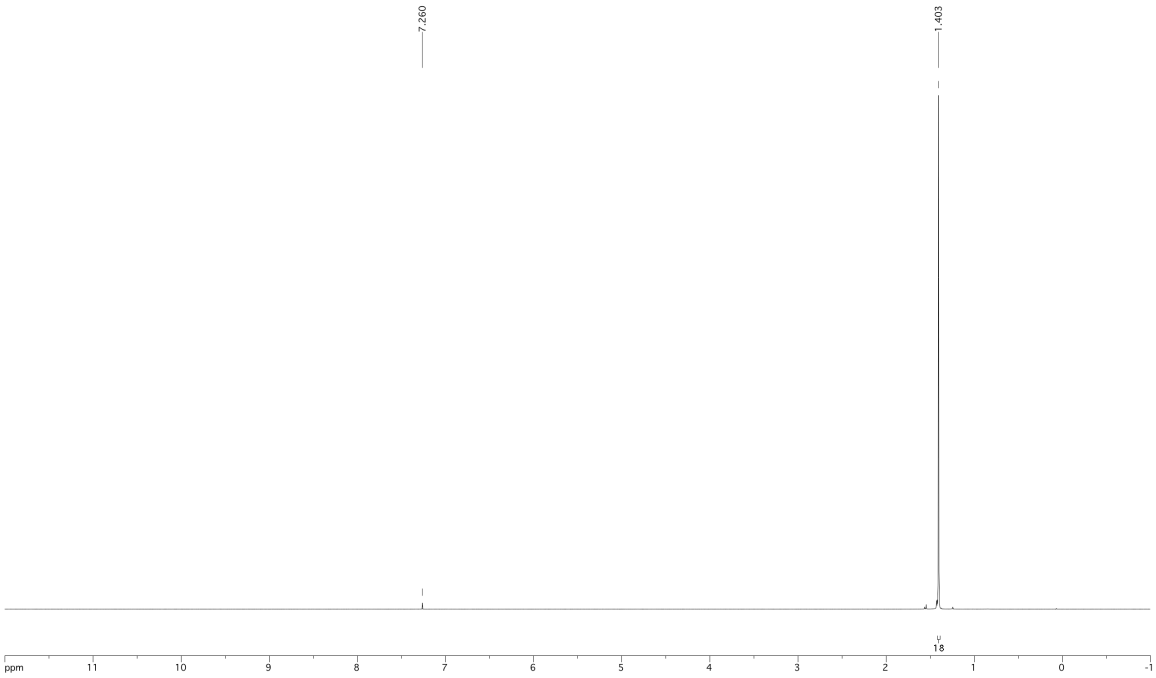
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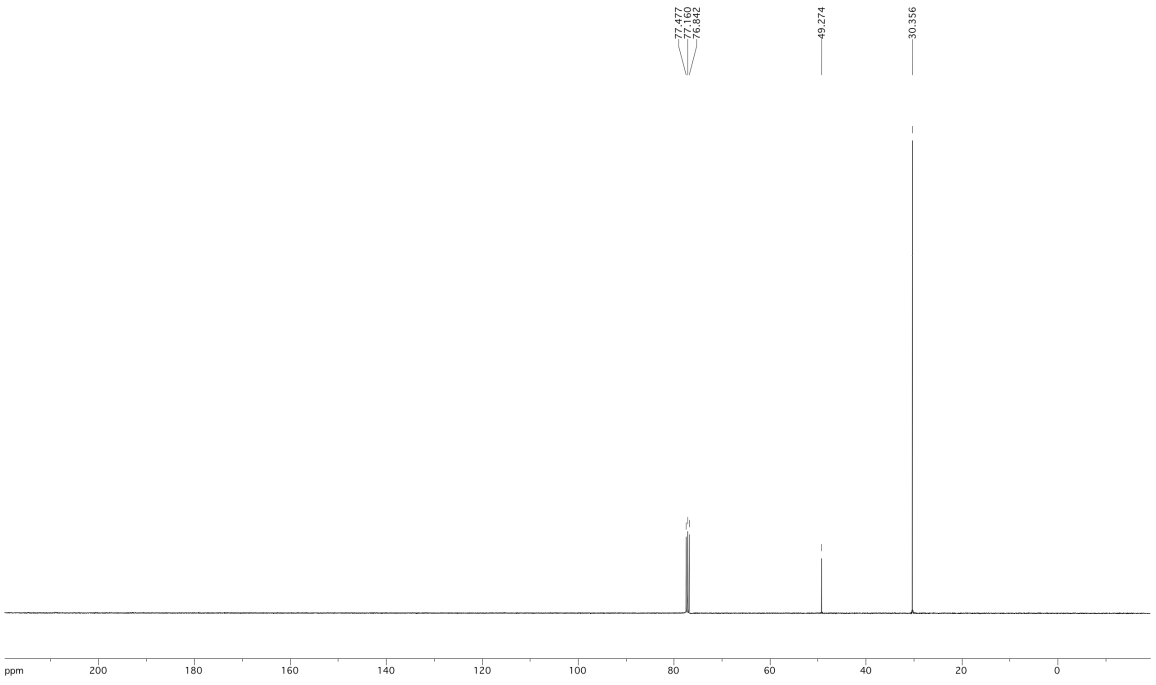
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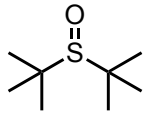

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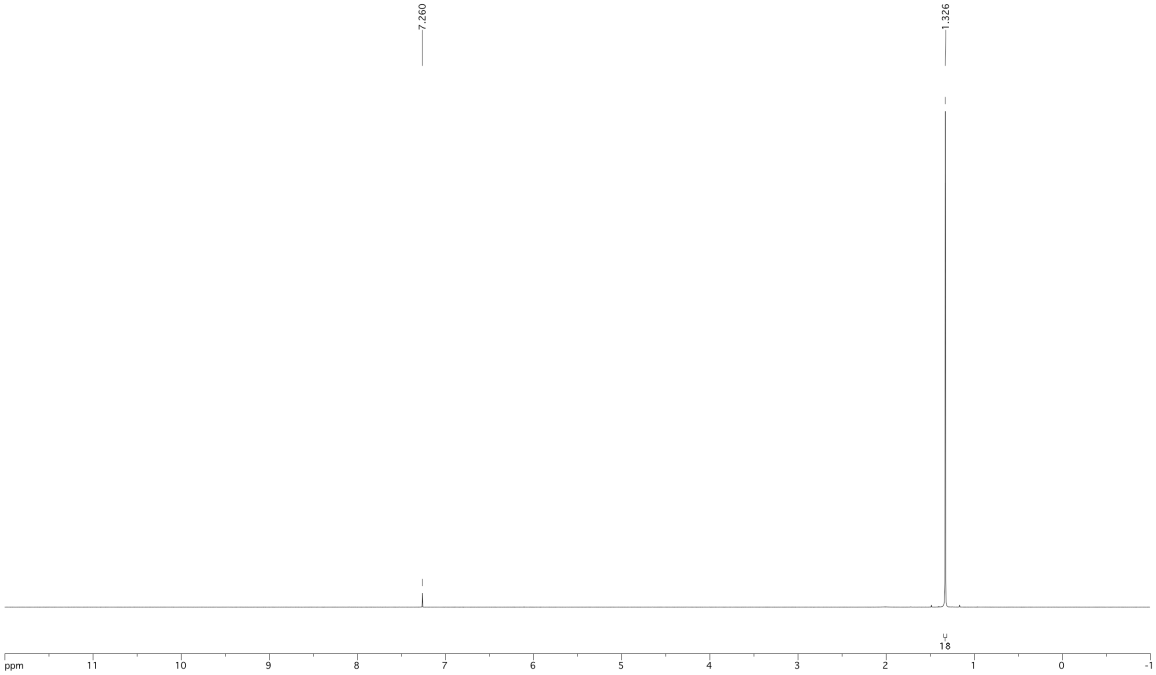
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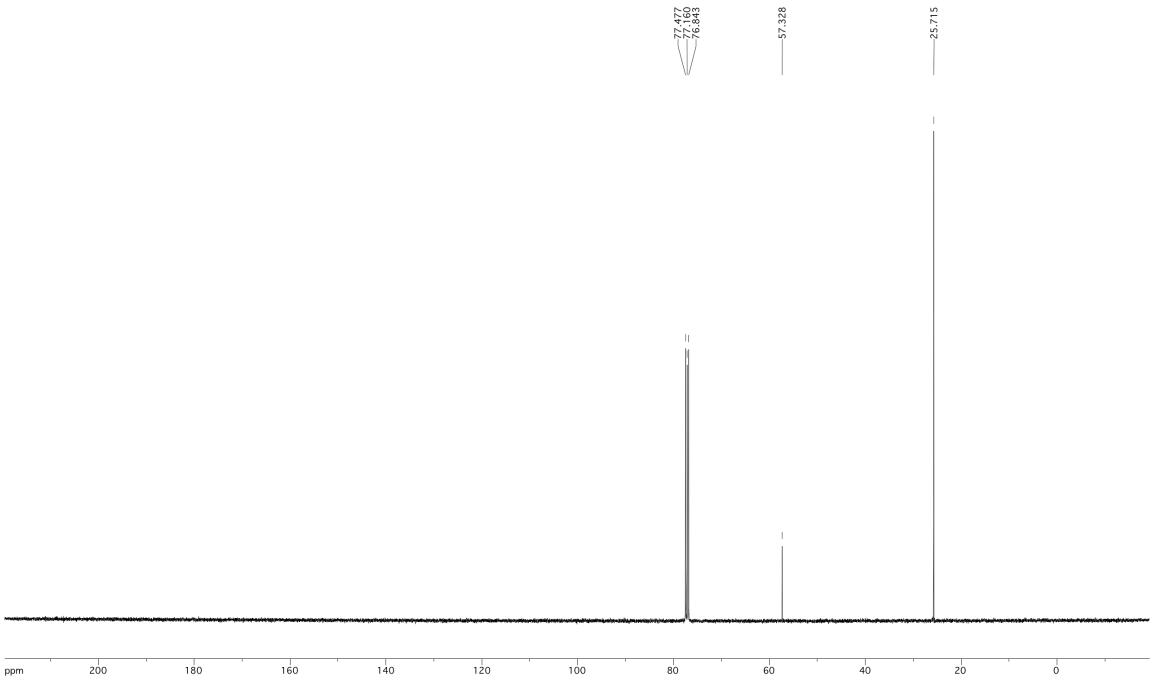
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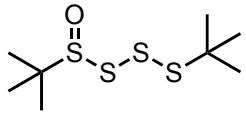

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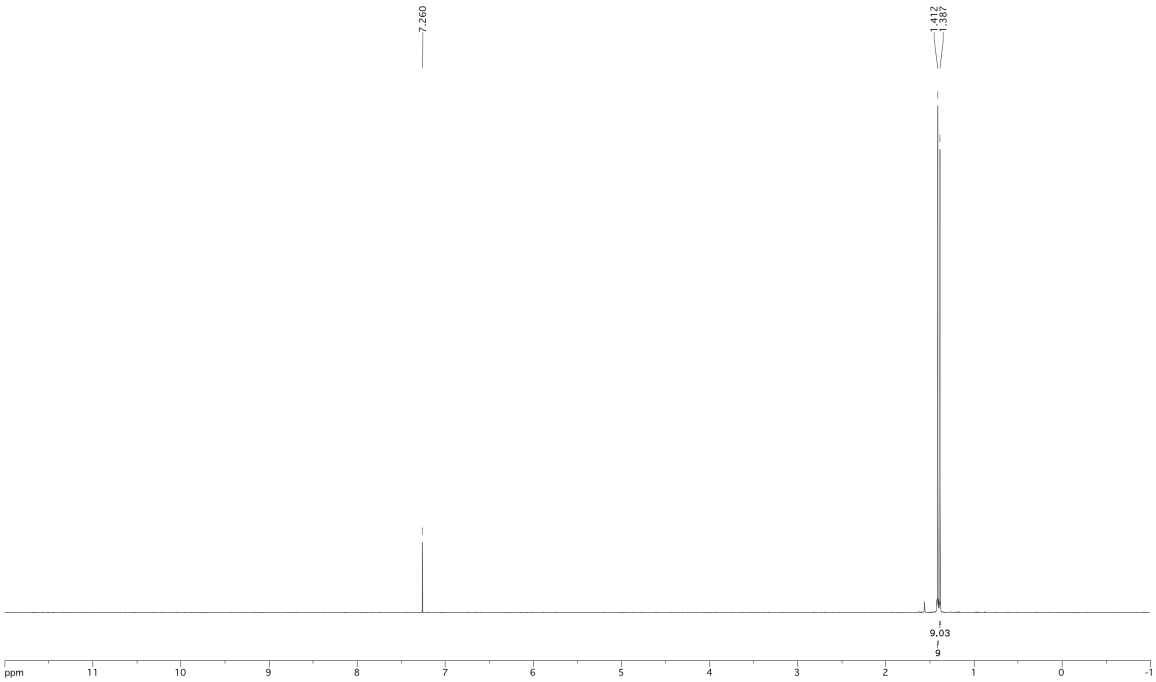
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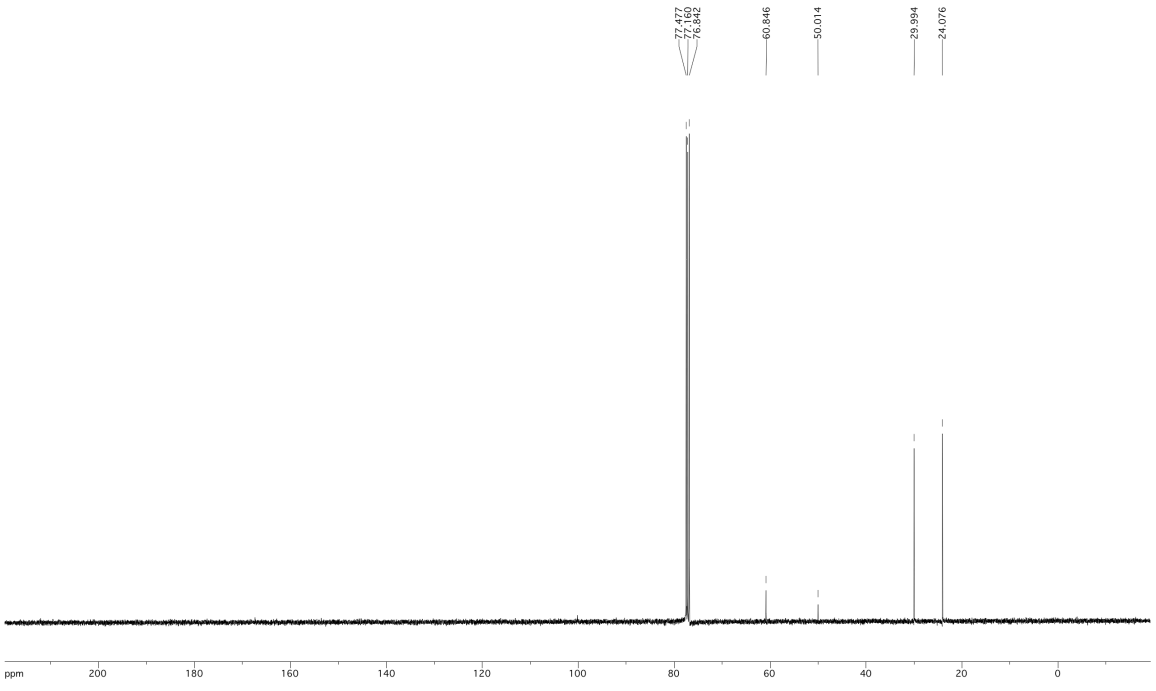
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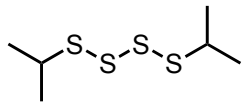

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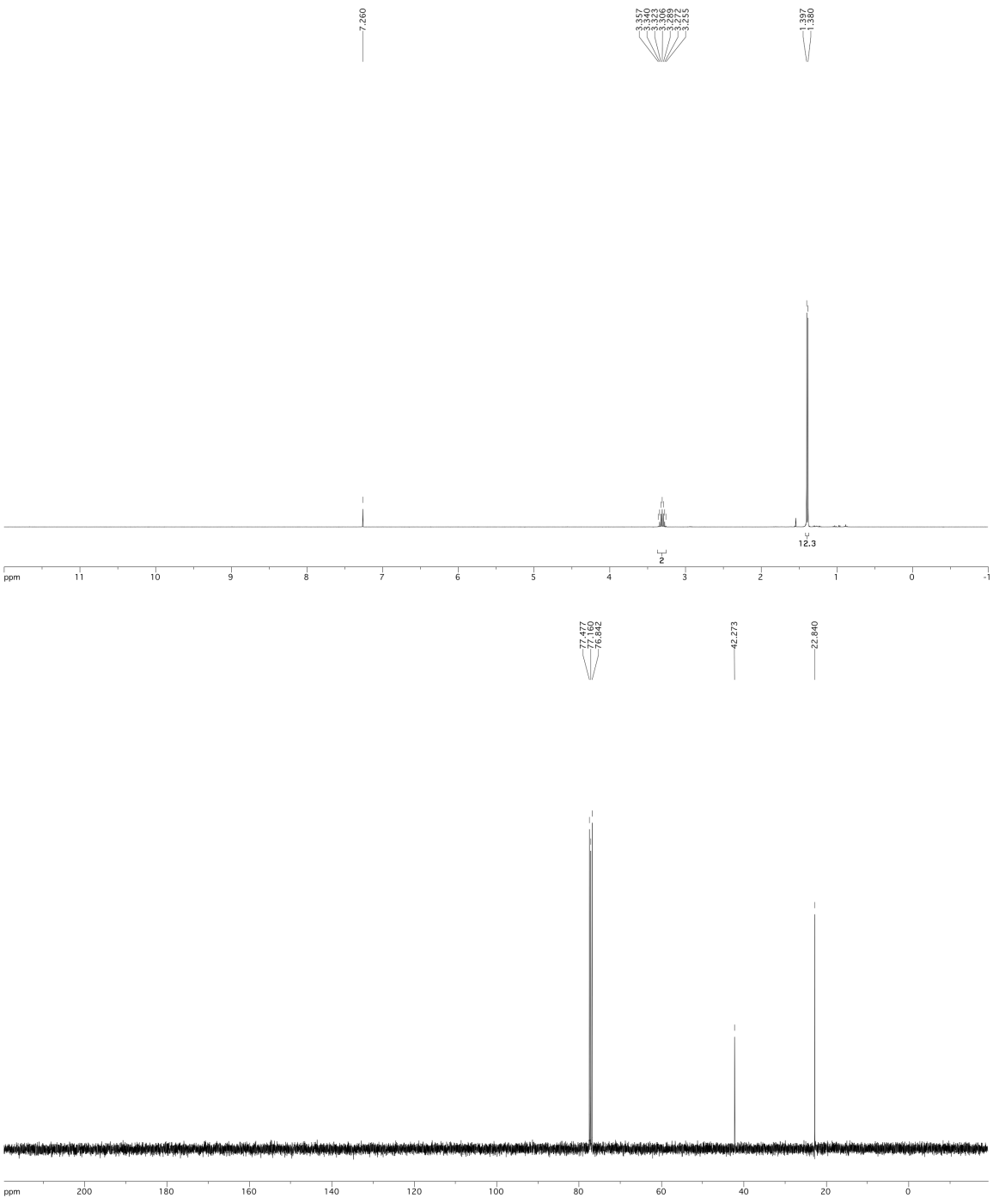
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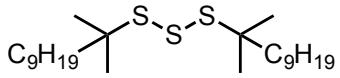
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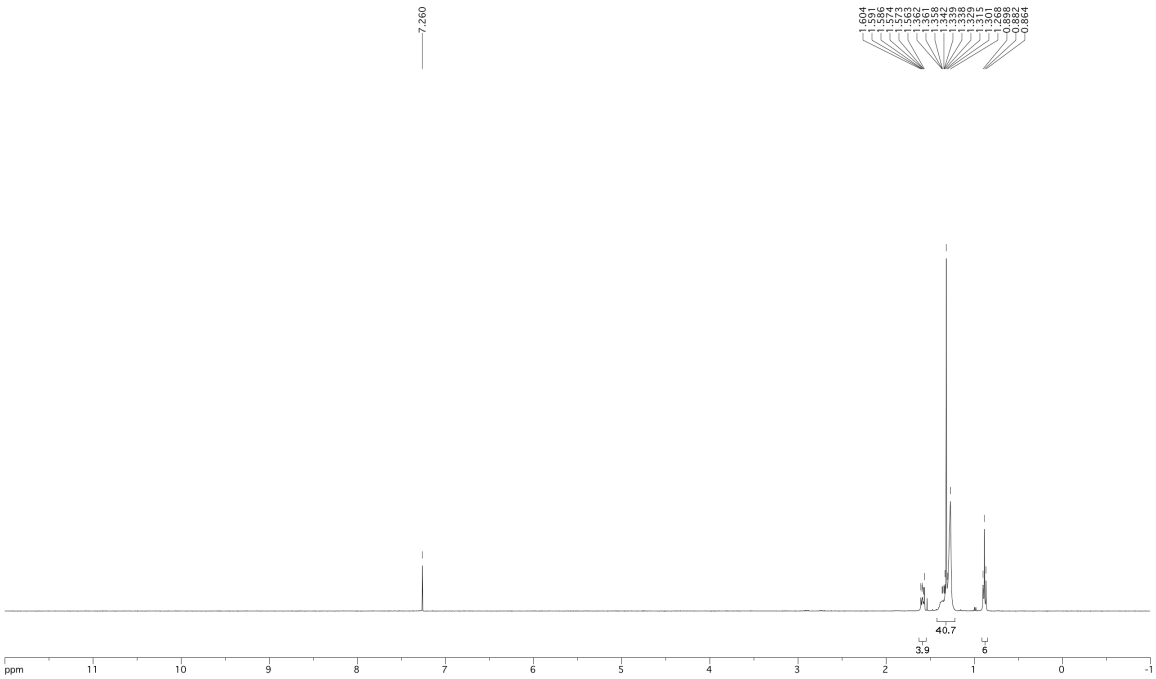
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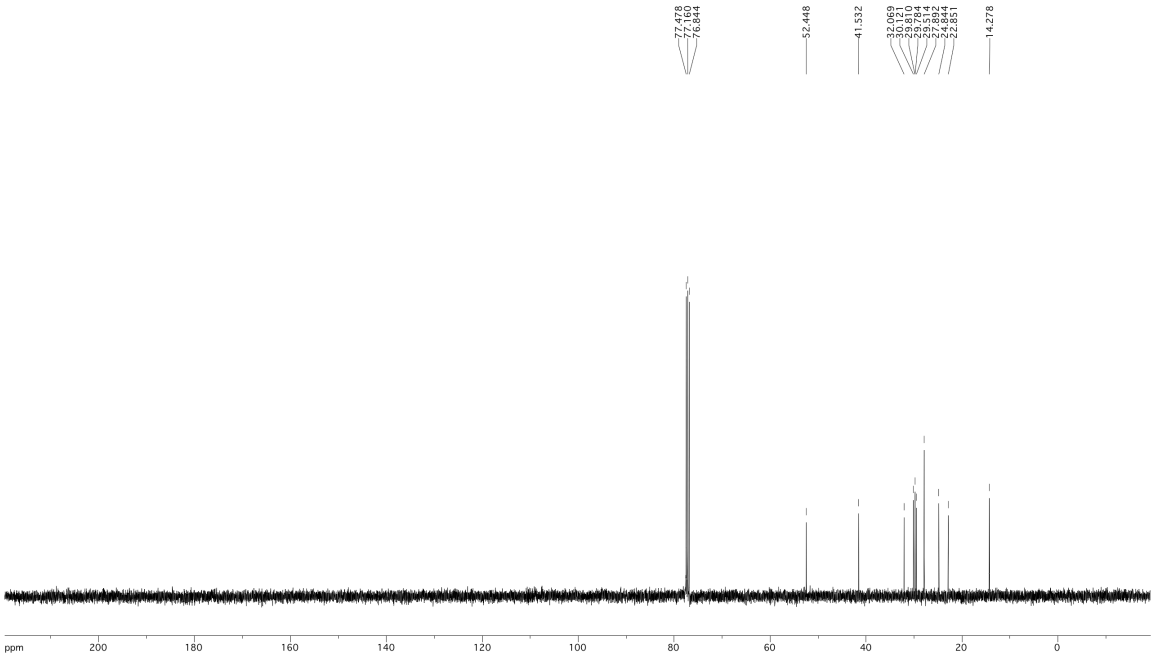
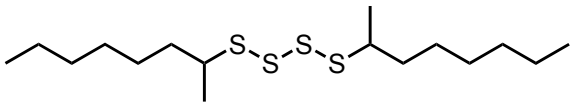
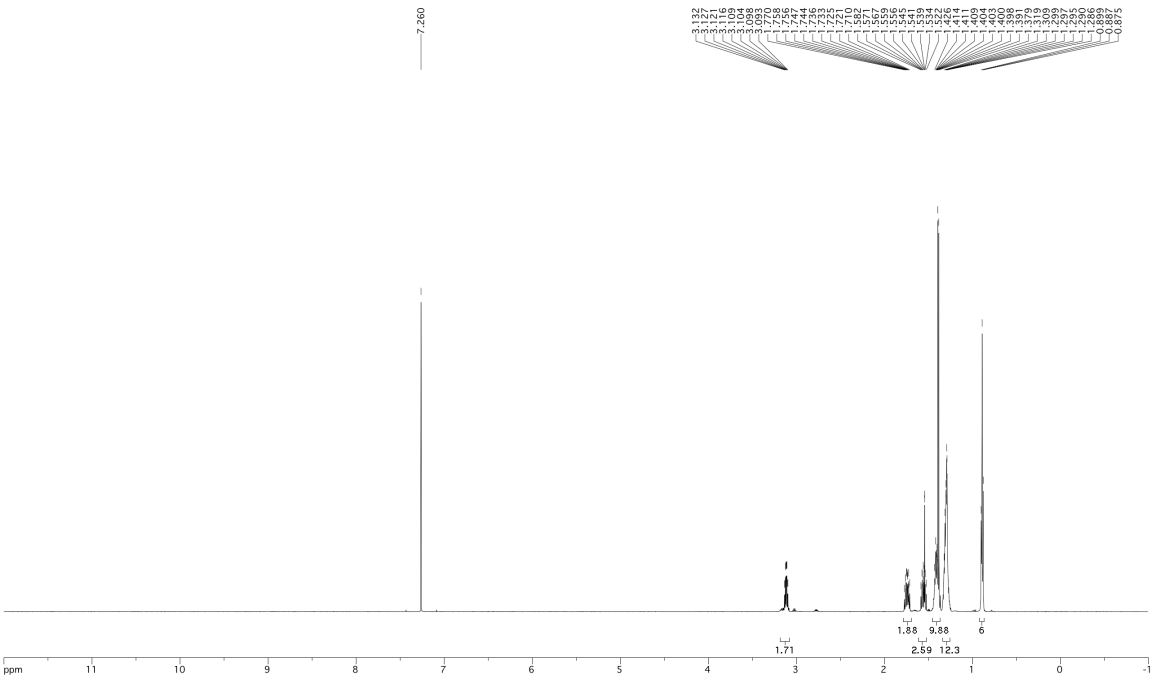
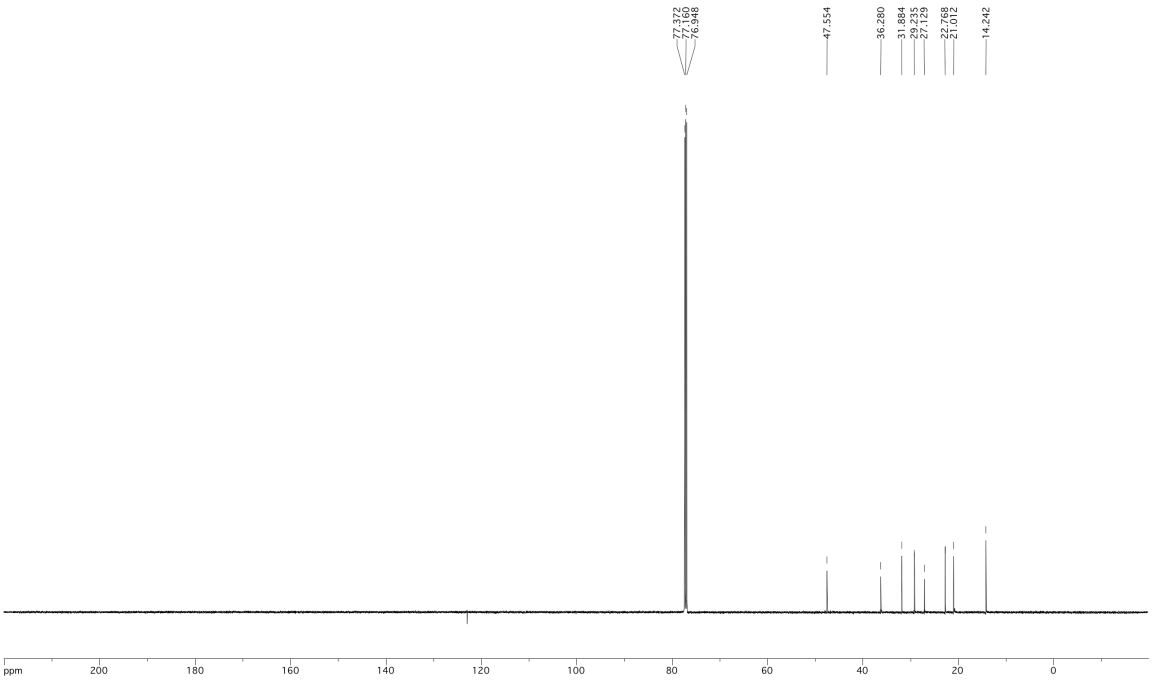
6
ppm
11
10
9
8
7
6
5
4
3
2
1
0
-1

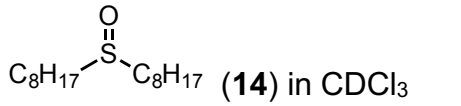

77.478
77.160
76.844
52.448
41.532
32.069
30.121
30.010
29.784
29.592
29.312
24.844
22.851
14.278
ppm
200
180
160
140
120
100
80
60
40
20
0



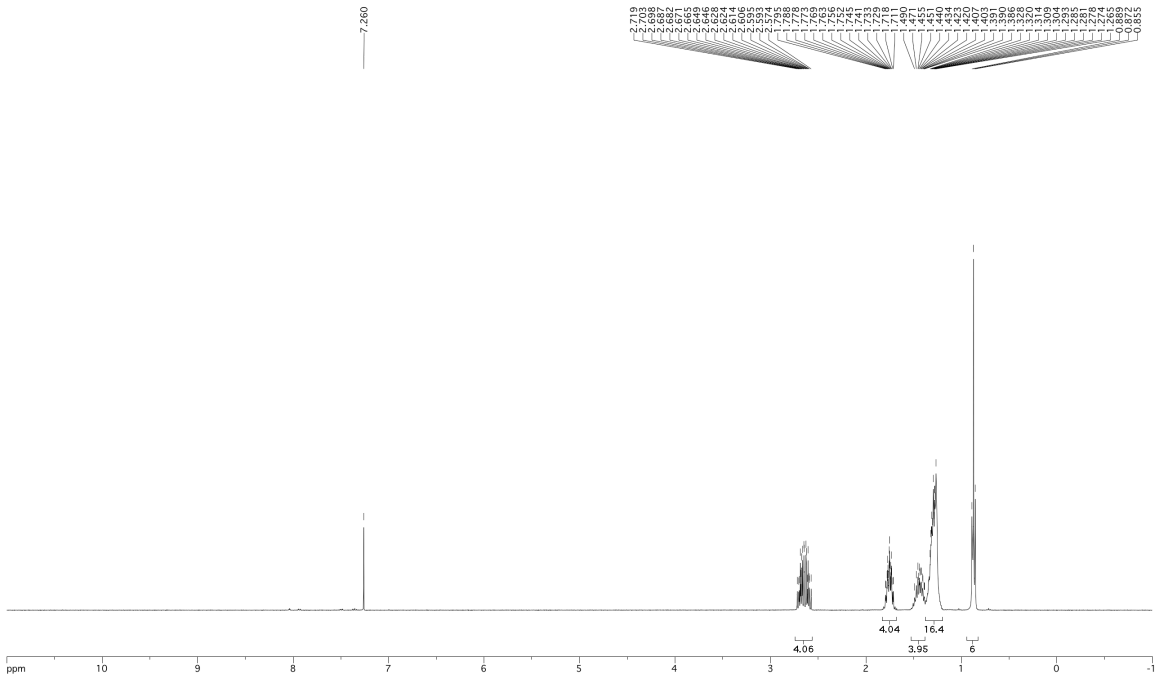
(**13**) in $CDCl_3$

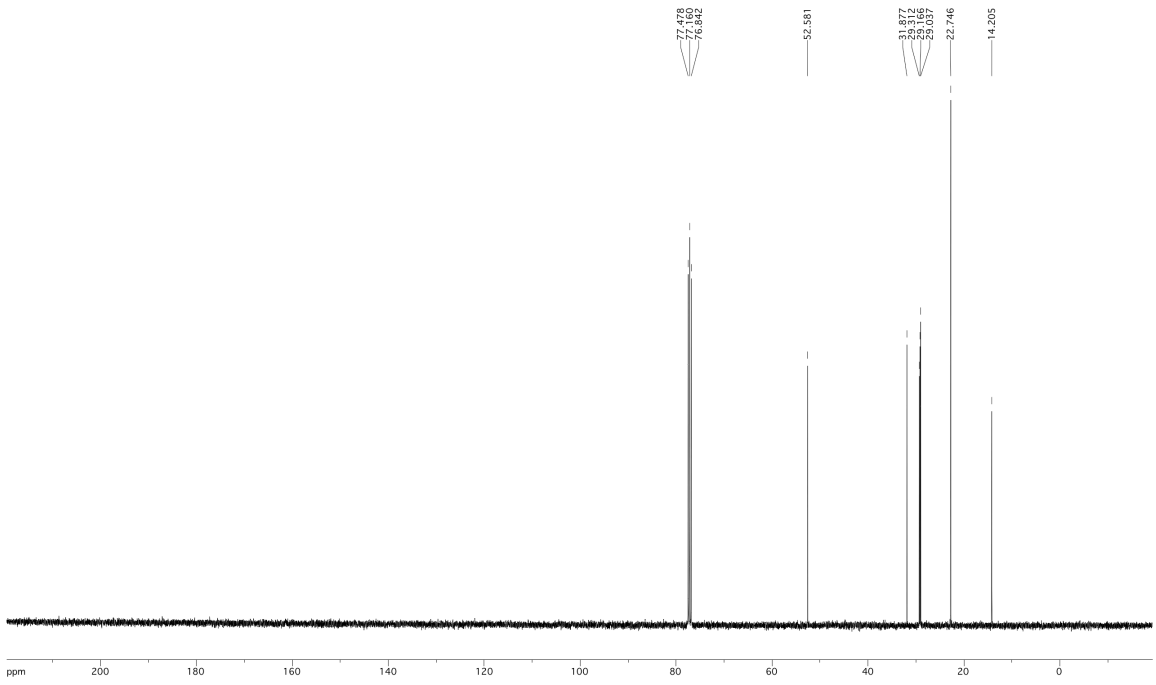

7.260
1.71
1.88
9.88
2.59
12.3
6
ppm

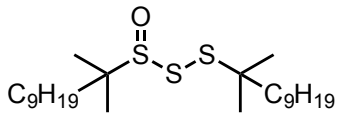

77.372
77.160
76.948
47.554
36.280
31.884
29.235
27.129
22.768
21.012
14.242
ppm

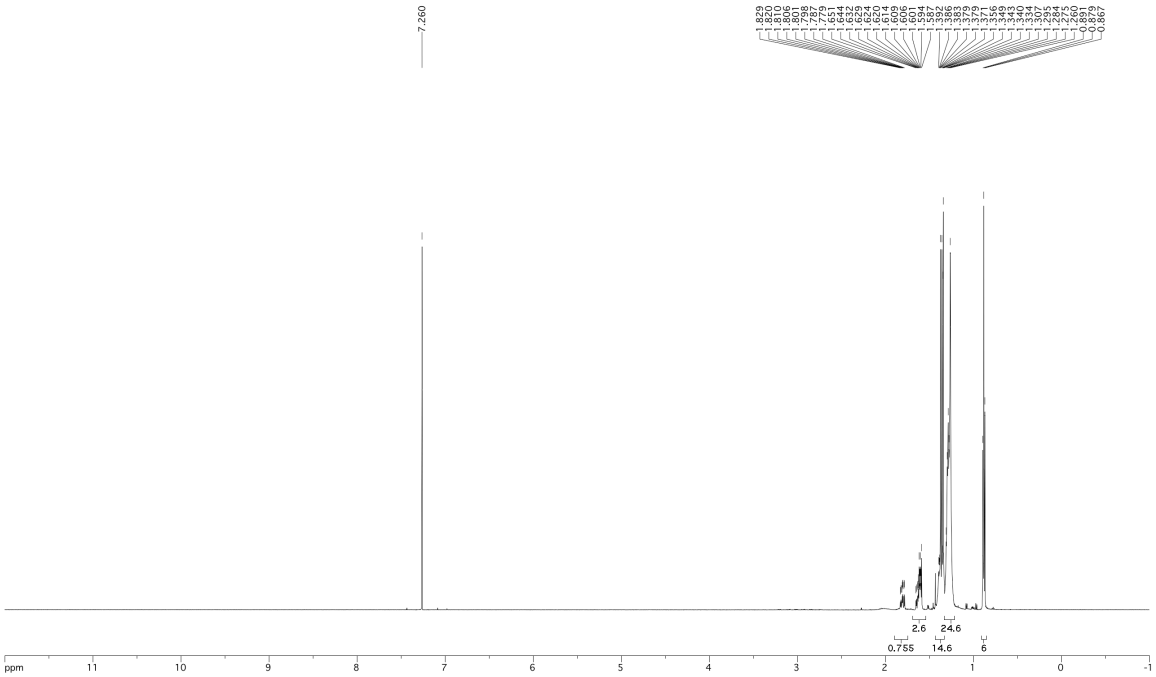

O
S
C8H17
C8H17

(**14**) in $CDCl_3$


7.260
4.04
16.4
4.06
3.95
6
ppm


77.478
77.160
76.842
52.581
31.877
29.312
29.166
29.037
22.746
14.205
ppm


O
S
S
S
C9H19
C9H19
(**16**) in $CDCl_3$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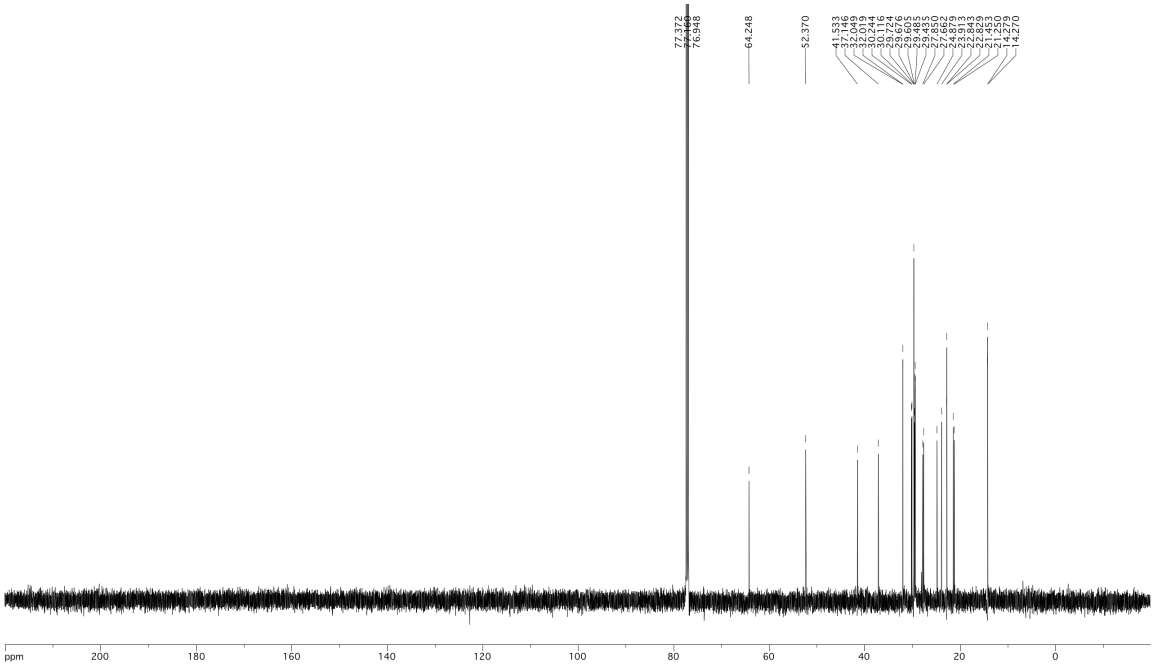
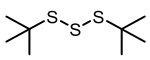
2.6
24.6
0.755
14.6
6
ppm


77.372
77.160
76.948
64.248
52.370
ppm

Computational Data

Optimized Gaussian Structures and CBS-QB3 Energies

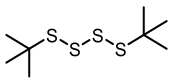
di-*tert*-butyl trisulfide



CBS-QB3 Enthalpy= -1508.258015 CBS-QB3 Free Energy= -1508.319037

```
0 1
 C                -2.80780600   -0.23892000   -0.12150900
 S                 0.00000000    1.24320000   -0.00000900
 S                 1.35350700    0.04231300   -1.04334900
 C                 2.80780600   -0.23891700    0.12151100
 S                -1.35351000    0.04233500    1.04335000
 C                -3.77593700   -1.07008600    0.73527200
 H                -4.07788500   -0.53202500    1.63742900
 H                -4.67806200   -1.28487800    0.15362100
 H                -3.33240600   -2.02355600    1.03292800
 C                -3.44054300    1.09891700   -0.51234800
 H                -2.73495900    1.72396200   -1.06354000
 H                -4.30822400    0.92266500   -1.15768300
 H                -3.77406700    1.65111600    0.36886900
 C                -2.36439300   -1.02521400   -1.35719200
 H                -1.65191300   -0.45602500   -1.95695900
 H                -1.89679400   -1.97220000   -1.08049000
 H                -3.23508400   -1.24015100   -1.98674600
 C                 2.36439800   -1.02518400    1.35721400
 H                 1.65192200   -0.45597900    1.95697200
 H                 1.89679400   -1.97217400    1.08053400
 H                 3.23509200   -1.24011000    1.98676800
 C                 3.77593400   -1.07010300   -0.73525400
 H                 4.07787700   -0.53206400   -1.63742600
 H                 4.67806300   -1.28487900   -0.15360300
 H                 3.33240300   -2.02358100   -1.03288400
 C                 3.44054600    1.09892800    0.51231900
 H                 4.30822900    0.92269100    1.15765500
 H                 3.77406800    1.65110700   -0.36891100
 H                 2.73496400    1.72398600    1.06349900
```

di-*tert*-butyl tetrasulfide



CBS-QB3 Enthalpy= -1906.015841 CBS-QB3 Free Energy= -1906.082022

```
0 1
 S                 0.60321700    0.87864700   -0.63223500
 C                 3.53286800   -0.14933700    0.04122000
 S                -0.60321700   -0.87865100   -0.63220700
 S                 2.04907300    0.69855600    0.83795900
 S                -2.04906200   -0.69852100    0.83799100
 C                -3.53287200    0.14933200    0.04123200
 C                 4.55804700   -0.17986500    1.18606300
 H                 4.19354800   -0.76060000    2.03705800
 H                 5.48142300   -0.64727200    0.82979800
 H                 4.80358400    0.82691200    1.53348100
```

C	3.17038400	-1.56855100	-0.40120500
H	2.42311700	-1.55933300	-1.19688200
H	4.06383700	-2.07048600	-0.78882700
H	2.77669300	-2.15772400	0.42925600
C	4.05186700	0.68399500	-1.13275100
H	4.32853900	1.69067000	-0.81221900
H	4.93751100	0.20387200	-1.56324400
H	3.30038100	0.76816800	-1.92056100
C	-3.17041700	1.56855400	-0.40119000
H	-2.77676400	2.15774200	0.42927900
H	-2.42312900	1.55935400	-1.19684800
H	-4.06387400	2.07046300	-0.78883800
C	-4.55806500	0.17983400	1.18606100
H	-5.48145400	0.64720200	0.82978000
H	-4.80356700	-0.82694800	1.53348900
H	-4.19359900	0.76059300	2.03705500
C	-4.05183300	-0.68401600	-1.13274400
H	-4.32847700	-1.69069900	-0.81221500
H	-4.93748800	-0.20392000	-1.56324500
H	-3.30033700	-0.76816500	-1.92054700

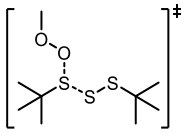
MeOO•

CBS-QB3 Enthalpy= -189.954731 CBS-QB3 Free Energy= -189.985244

0 2

C	1.09605800	-0.18318200	0.00000000
H	1.87467600	0.57860400	0.00000800
H	1.14883700	-0.80072600	0.89698200
H	1.14884100	-0.80070700	-0.89699400
O	-0.15733600	0.54388500	0.00000000
O	-1.18625200	-0.27864500	0.00000000

Trisulfide substitution on S1 by MeOO• TS



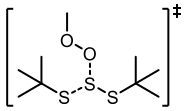
TS freq.: -304.51 cm^{-1}
CBS-QB3 Enthalpy= -1698.196157 CBS-QB3 Free Energy= -1698.270551

0 2

S	-1.14224400	0.08977900	-0.18910400
O	-2.50695400	1.40000400	-0.59635700
O	-2.55514500	2.37524800	0.43565900
C	-1.93379800	3.56012900	-0.04728100
H	-2.40149000	3.89075400	-0.97841800
H	-2.09090900	4.30237600	0.73839800
H	-0.86094300	3.40378000	-0.20154200
S	0.74431000	-1.10799600	-0.97147600
C	-2.40670300	-1.28023000	0.21211400
S	2.12593600	-1.03881900	0.53461900
C	3.31925600	0.36046500	0.11009200
C	4.00107000	0.07596500	-1.22996200
H	3.27199000	0.03397300	-2.04169800
H	4.71450900	0.87544400	-1.45773000
H	4.54414400	-0.87136300	-1.20530800
C	2.57168200	1.69518300	0.08201400

H	2.07705000	1.89454600	1.03501900
H	3.27921700	2.50756800	-0.11700600
H	1.81730800	1.70570500	-0.70740600
C	4.33151100	0.31983700	1.26458800
H	5.08610400	1.09762400	1.11133200
H	3.84993700	0.50341100	2.22835600
H	4.84723200	-0.64259200	1.31364400
C	-3.15570800	-1.63885300	-1.07484100
H	-2.48025700	-2.06174700	-1.82191200
H	-3.92743500	-2.38467100	-0.85433500
H	-3.64104500	-0.75907900	-1.49986800
C	-1.68156800	-2.49702200	0.79631900
H	-1.08396100	-2.22909600	1.67051400
H	-2.43947100	-3.22040600	1.11547600
H	-1.03168300	-2.98289000	0.07049400
C	-3.35877200	-0.70076500	1.26936800
H	-4.08820000	-1.47376600	1.53420300
H	-2.81929300	-0.41692100	2.17532300
H	-3.89586800	0.16966300	0.89895000

Trisulfide substitution on S2 by MeOO• TS



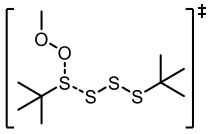
TS freq.: -226.16 cm^{-1}
CBS-QB3 Enthalpy= -1698.188069 CBS-QB3 Free Energy= -1698.262263

0 2

C	2.93479400	-0.82813600	0.23430700
S	-0.20030300	0.54138700	-0.64290800
S	-1.24964400	-0.42076700	0.85317200
C	-2.84371800	-1.01285600	0.03082200
S	1.72571900	-0.87826300	-1.18625900
O	-0.88397800	2.25304300	-0.57944900
O	-0.48997100	2.98606300	0.57849600
C	0.51436900	3.91226100	0.17953700
H	0.14773700	4.56669900	-0.61569400
H	0.72401100	4.49610800	1.07846700
H	1.42175100	3.39380900	-0.14705300
C	-3.66847000	0.18476100	-0.44613800
H	-3.14301400	0.75102600	-1.21663800
H	-4.61456300	-0.17020400	-0.86971700
H	-3.89120400	0.86569000	0.37755500
C	-3.55617300	-1.74699700	1.17789000
H	-4.51588000	-2.12866800	0.81560800
H	-2.97111700	-2.59647500	1.53907900
H	-3.75715000	-1.07961200	2.01973400
C	-2.52377600	-1.97117700	-1.11723600
H	-1.93072200	-2.82101200	-0.77359600
H	-3.45735500	-2.35119600	-1.54624400
H	-1.97094700	-1.46760700	-1.91237700
C	3.28279800	0.62532300	0.58231600
H	2.40567900	1.16420000	0.94594600
H	4.04251300	0.64223100	1.37188100
H	3.67830900	1.15468700	-0.28714200
C	4.18308600	-1.55655800	-0.29955200
H	4.94827800	-1.57864000	0.48442700
H	3.95713800	-2.58881700	-0.57766800
H	4.59966600	-1.04760000	-1.17124500

C	2.37487500	-1.56420300	1.45742200
H	3.12799300	-1.58723700	2.25351700
H	1.48514400	-1.06952000	1.84952200
H	2.10626500	-2.59292700	1.20897300

Tetrasulfide substitution on S1 by MeOO• TS

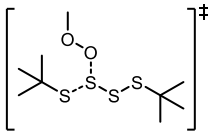


TS freq.: -286.39 cm^{-1}
CBS-QB3 Enthalpy= -2095.952850 CBS-QB3 Free Energy= -2096.031532

0 2

S	2.13326000	0.01740200	-0.91220900
O	3.84296500	-0.61198200	-0.37603200
O	3.90687400	-1.10083300	0.95331300
C	3.72250600	-2.51279300	0.91717400
H	4.45281100	-2.98031600	0.25226500
H	3.88084100	-2.84297300	1.94588700
H	2.70482300	-2.75976000	0.59734300
S	-0.08160400	-0.43920500	-1.63862400
C	2.02247700	1.57324400	0.18543700
S	-1.15824200	-1.48403600	-0.21999500
S	-2.21086600	-0.17526000	1.02314900
C	-3.87886100	0.11824000	0.18994000
C	1.00578400	2.53159500	-0.44641900
H	1.01896100	3.46514500	0.12629800
H	1.26185200	2.76671700	-1.48204500
H	-0.00727300	2.13301700	-0.42012400
C	1.60804300	1.18192900	1.60768100
H	2.32149600	0.48418300	2.04503500
H	1.57491300	2.08214400	2.23168900
H	0.61576200	0.72909300	1.62306900
C	3.41608700	2.21823300	0.17092800
H	3.36304400	3.15106400	0.74214800
H	4.16836400	1.57680100	0.62519900
H	3.73510800	2.45903800	-0.84545300
C	-4.61799200	-1.20916400	0.00552900
H	-5.60445200	-1.02269500	-0.43281200
H	-4.07439400	-1.87620400	-0.66659000
H	-4.75715300	-1.72072900	0.96019000
C	-4.60869900	1.01293600	1.20441700
H	-4.08264000	1.95816900	1.35993600
H	-5.60919800	1.24314600	0.82475600
H	-4.72186800	0.51588500	2.17105300
C	-3.69779300	0.84466700	-1.14438400
H	-3.16386500	1.78840000	-1.01596600
H	-3.14565500	0.23452700	-1.86131300
H	-4.68029300	1.06213200	-1.57775400

Tetrasulfide substitution on S2 by MeOO• TS



TS freq.: -377.04 cm^{-1}
CBS-QB3 Enthalpy= -2095.954803 CBS-QB3 Free Energy= -2096.035520

```
0 2
 S                -0.74719900    0.54104600   -0.56049900
 S                -1.77306700   -0.38045800    0.94068100
 C                -3.24806300   -1.23889100    0.13205600
 S                 1.06428700   -1.04797000   -1.13721600
 O                -1.73511800    2.32939100   -0.72557000
 O                -1.61879300    3.12509800    0.39763900
 C                -0.53881700    4.04039200    0.21573900
 H                -0.67929000    4.61874200   -0.70051100
 H                -0.56463500    4.69281400    1.09003000
 H                 0.41098000    3.49751300    0.17833900
 S                 2.29355100   -1.32279800    0.43687000
 C                 3.77739900   -0.17403200    0.20809700
 C                -2.77204800   -2.24968000   -0.91140300
 H                -3.63649700   -2.77570900   -1.33114900
 H                -2.25121000   -1.75408500   -1.73274200
 H                -2.09700200   -2.98839100   -0.47468200
 C                -4.18018200   -0.19238300   -0.48310000
 H                -5.05222100   -0.69079900   -0.92115600
 H                -4.52878200    0.51810000    0.26911000
 H                -3.67801300    0.37350200   -1.26924500
 C                -3.92089500   -1.94716400    1.31799400
 H                -4.81824800   -2.46521000    0.96538400
 H                -3.25979100   -2.68955800    1.77219700
 H                -4.22677700   -1.23644200    2.09019400
 C                 4.49930600   -0.51116500   -1.09781500
 H                 3.84700500   -0.35601700   -1.95947500
 H                 5.37326900    0.13897900   -1.21289700
 H                 4.84117600   -1.54857500   -1.10677600
 C                 3.30751000    1.28183100    0.22713000
 H                 2.78678600    1.52012700    1.15722500
 H                 4.17303500    1.94708300    0.13608200
 H                 2.63380000    1.48722000   -0.60708100
 C                 4.65724400   -0.48914300    1.42643500
 H                 4.96936600   -1.53661400    1.43740400
 H                 5.55946300    0.12926900    1.39078200
 H                 4.13897500   -0.27356900    2.36425500
```

tert-BuS•

CBS-QB3 Enthalpy= -555.194016 CBS-QB3 Free Energy= -555.232306

```
0 2
 S                 1.53335100    0.06144400    0.00000000
 C                -0.30965200   -0.03414700    0.00000000
 C                -0.79610900   -0.75720800    1.26526200
 H                -1.89126700   -0.79698700    1.27529200
 H                -0.42313300   -1.78359600    1.30213000
 H                -0.45905900   -0.24183400    2.16634500
 C                -0.79610900   -0.75720800   -1.26526200
 H                -1.89126700   -0.79698700   -1.27529200
```

H	-0.45905900	-0.24183400	-2.16634500
H	-0.42313300	-1.78359600	-1.30213000
C	-0.79610900	1.43020300	0.00000000
H	-1.89171300	1.43746400	0.00000000
H	-0.45355900	1.96720700	0.88726100
H	-0.45355900	1.96720700	-0.88726100

tert-BuSS•

CBS-QB3 Enthalpy= -952.978966 CBS-QB3 Free Energy= -953.021731
CBS-QB3 Enthalpy= -952.974910 CBS-QB3 Free Energy= -953.032948 (100 °C)

0 2

S	-0.59123600	-0.93896400	-0.00001200
S	-2.16182400	0.27303400	-0.00000500
C	0.98123900	0.11913500	0.00000500
C	1.00917300	0.97909500	1.26472500
H	1.92559900	1.57833900	1.27895300
H	0.15705500	1.66086000	1.29413200
H	0.99020500	0.36369400	2.16730400
C	1.00919000	0.97910700	-1.26470700
H	1.92561700	1.57834900	-1.27891900
H	0.99023100	0.36371400	-2.16729200
H	0.15707300	1.66087300	-1.29411700
C	2.11286300	-0.91716600	0.00000800
H	3.07759400	-0.40069800	0.00001400
H	2.07538900	-1.55564300	0.88645200
H	2.07539800	-1.55563800	-0.88644000

tert-BuSSS•

CBS-QB3 Enthalpy= -1350.731516 CBS-QB3 Free Energy= -1350.779629
CBS-QB3 Enthalpy= -1350.726819 CBS-QB3 Free Energy= -1350.792265 (100 °C)

0 2

S	2.69014800	0.66681700	-0.19041800
S	1.44892400	-0.73675800	0.46600600
S	-0.26948100	-0.86771900	-0.76167900
C	-1.56021000	0.22433700	0.08022200
C	-1.83752500	-0.27180000	1.50166300
H	-0.95449400	-0.18113800	2.13785100
H	-2.63356300	0.33185500	1.95089800
H	-2.15647700	-1.31588300	1.50196500
C	-2.79480600	0.02985100	-0.81451900
H	-3.11281600	-1.01513800	-0.84068500
H	-3.62193900	0.62441900	-0.41372600
H	-2.60678400	0.36224000	-1.83818500
C	-1.10959200	1.68662200	0.07359100
H	-0.21735300	1.83656800	0.68397900
H	-0.89118700	2.03136700	-0.93876300
H	-1.90604000	2.31421900	0.48838800

tert-BuSOOMe

CBS-QB3 Enthalpy= -745.232102 CBS-QB3 Free Energy= -745.280837

0 1

C	3.19670600	0.05987900	-0.35995100
H	3.76190100	-0.37470900	0.47019200
H	2.96987900	-0.70634200	-1.11040900

H	3.78159100	0.85745800	-0.82634300
S	0.05661700	-1.02036400	-0.18391200
O	1.20703700	-0.34230800	0.80437100
O	2.02147500	0.70247600	0.09577100
C	-1.37175100	0.16120500	-0.03647000
C	-2.50817100	-0.56103200	-0.77760900
H	-3.40454000	0.06608700	-0.75996700
H	-2.25417600	-0.74624500	-1.82526200
H	-2.75665200	-1.51557000	-0.30642900
C	-1.71104200	0.36420600	1.44341000
H	-0.85180400	0.76354400	1.98487400
H	-2.53872600	1.07474800	1.54162700
H	-2.00531200	-0.57634000	1.91433200
C	-1.03418300	1.49407400	-0.71645600
H	-0.79156000	1.34854100	-1.77135900
H	-1.89416200	2.16994400	-0.64970000
H	-0.17976600	1.97337200	-0.23763700

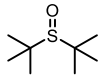
tert-BuSSOOMe

CBS-QB3 Enthalpy= -1142.992969 CBS-QB3 Free Energy= -1143.046147

0 1

C	3.96134000	0.21395400	-0.09090800
H	4.31565100	0.58197000	0.87649000
H	3.92617500	-0.88129800	-0.09450200
H	4.63029800	0.55547100	-0.88485800
S	0.89831300	-0.99299500	0.29396200
S	-0.61230400	-0.47166500	-0.98044000
C	-2.00480300	0.21669400	0.09436500
O	1.76111200	0.41250900	0.64869600
O	2.70374500	0.77580400	-0.42810000
C	-1.53621200	1.50111800	0.78390300
H	-2.36068300	1.92600000	1.36715400
H	-0.70283800	1.30892100	1.46153600
H	-1.21016700	2.24559100	0.05465200
C	-2.46070600	-0.83175200	1.11041700
H	-3.28900300	-0.43158400	1.70504700
H	-2.80384100	-1.74258800	0.61474900
H	-1.65360500	-1.09525400	1.79687700
C	-3.11535100	0.51337800	-0.92458800
H	-3.44227700	-0.39321400	-1.44028500
H	-3.98058500	0.93448900	-0.40307200
H	-2.78973200	1.23919200	-1.67404700

Di-*tert*-butyl sulfoxide



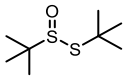
CBS-QB3 Enthalpy= -787.851085 CBS-QB3 Free Energy= -787.904169

0 1

C	1.55508200	1.74699300	-0.28084700
C	1.57353200	0.25194300	0.03060000
S	-0.00474500	-0.64507600	-0.60247100
C	2.65531600	-0.45002200	-0.81104200
C	1.78721900	-0.05481000	1.51166100
O	0.01342500	-1.96576600	0.12736100
C	-1.57336200	0.24762400	0.02941800

C	-1.55320200	0.44907400	1.54257400
C	-1.77924100	1.54669500	-0.75388300
C	-2.66812900	-0.76571700	-0.34982400
H	2.56124600	2.15492400	-0.13544100
H	0.88290900	2.29867400	0.37771600
H	1.27169900	1.94545400	-1.31854200
H	2.64284900	-1.52863700	-0.64265500
H	3.64038800	-0.06897800	-0.52421600
H	2.51631600	-0.26528800	-1.87943100
H	2.83819100	0.10759000	1.77155300
H	1.18089200	0.58000100	2.15807800
H	1.53846300	-1.09911700	1.71301700
H	-2.56077600	0.69479900	1.89483400
H	-1.23665000	-0.46907500	2.04230200
H	-0.89149200	1.26346300	1.84246000
H	-2.79750000	1.91156100	-0.58323200
H	-1.66581100	1.38502300	-1.82981300
H	-1.09352500	2.33710800	-0.45102600
H	-2.50183400	-1.72285200	0.14482100
H	-3.64098300	-0.36991200	-0.04223000
H	-2.69913800	-0.93808300	-1.42948100

Di-*tert*-butyl thiosulfinate

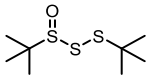


CBS-QB3 Enthalpy= -1185.618570 CBS-QB3 Free Energy= -1185.677755
CBS-QB3 Enthalpy= -1185.610832 CBS-QB3 Free Energy= -1185.693518 (100 °C)

0 1

C	2.16335900	-1.68279000	0.74844500
C	2.24589400	-0.33544600	0.03087000
S	0.66025400	0.66385500	0.38915300
C	3.33912800	0.54939000	0.65097900
C	2.44053000	-0.45315700	-1.47991600
O	0.80672300	1.93916800	-0.36926500
S	-0.73392900	-0.66523600	-0.62335500
C	-2.37214600	-0.06775400	0.08747100
C	-3.40450200	-0.99524300	-0.57343000
C	-2.40185500	-0.24090500	1.60979700
C	-2.62978600	1.38904300	-0.31764500
H	3.14046600	-2.17489800	0.70259100
H	1.42594200	-2.34502600	0.29489300
H	1.90737600	-1.55823400	1.80490900
H	3.35458700	1.53744100	0.18884400
H	4.31293000	0.07649700	0.49274500
H	3.19577400	0.67247800	1.72840200
H	3.46055200	-0.78769700	-1.69451000
H	1.74865800	-1.16970500	-1.92630900
H	2.28980600	0.51860400	-1.95542500
H	-4.40695400	-0.71558000	-0.23338700
H	-3.38115900	-0.90792200	-1.66225900
H	-3.23560600	-2.04106500	-0.30572700
H	-3.38722200	0.04832000	1.99129600
H	-1.65773800	0.38688900	2.10307600
H	-2.21601900	-1.27931500	1.89198100
H	-2.60034500	1.50420400	-1.40276500
H	-3.62013700	1.69580000	0.03728700
H	-1.88961900	2.06913400	0.10628200

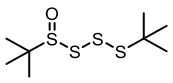
Di-*tert*-butyl trisulfide-1-oxide



CBS-QB3 Enthalpy= -1583.377038 CBS-QB3 Free Energy= -1583.441316
CBS-QB3 Enthalpy= -1583.368655 CBS-QB3 Free Energy= -1583.458435 (100 °C)

```
0 1
 C                -2.24053800    1.97497500   -0.10003900
 C                -2.70290400    0.52079100    0.00636000
 S                -1.25085900   -0.54867700    0.62474300
 C                -3.74382600    0.35801800    1.12559200
 C                -3.22999900   -0.05340400   -1.30847400
 O                -1.75890500   -1.94464300    0.63398700
 S                 0.08619800   -0.25172900   -1.14821700
 C                 2.87009900    0.35494200    0.23878800
 H                -3.10944700    2.61831400   -0.27286900
 H                -1.54046500    2.12725700   -0.92243100
 H                -1.76301400    2.31293300    0.82471500
 H                -4.02711600   -0.68827400    1.24920500
 H                -4.63936400    0.93173600    0.86796000
 H                -3.36933800    0.73090100    2.08334900
 H                -4.20479200    0.38786600   -1.53939300
 H                -2.56002600    0.15484000   -2.14525000
 H                -3.35311400   -1.13538200   -1.22475900
 S                 1.84072000   -1.07091900   -0.44084000
 C                 3.15567600    1.37484100   -0.86574600
 H                 2.23233500    1.82770600   -1.23328500
 H                 3.79074300    2.17699000   -0.47412400
 H                 3.66992400    0.91051100   -1.70981000
 C                 4.16253000   -0.34885100    0.68223400
 H                 4.85548500    0.39335900    1.09049900
 H                 3.96947500   -1.09235500    1.45959400
 H                 4.65785300   -0.84534100   -0.15601400
 C                 2.17020500    1.00872900    1.43147800
 H                 1.96317100    0.28198800    2.21947100
 H                 2.80827400    1.79654900    1.84675900
 H                 1.22627000    1.46849000    1.13234600
```

Di-*tert*-butyl tetrasulfide-1-oxide

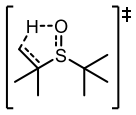


CBS-QB3 Enthalpy= -1981.134025 CBS-QB3 Free Energy= -1981.204070
CBS-QB3 Enthalpy= -1981.125001 CBS-QB3 Free Energy= -1981.222712 (100 °C)

```
0 1
 S                -0.50105700   -0.70903900    0.53741300
 C                -3.55503700   -0.15360100    0.17514300
 S                 0.95477500   -0.95940500   -0.94482900
 S                -1.95512700    0.58643700   -0.55156800
 O                -1.88808000    1.97257500   -0.02147300
 S                 2.30190900    0.61697100   -0.86953200
 C                 3.66057100    0.10173700    0.33180900
 C                -4.64917600    0.72913300   -0.44620900
 H                -4.51857600    1.77469200   -0.16380800
 H                -5.62645300    0.39163900   -0.08801600
 H                -4.65060800    0.66237700   -1.53803800
```

C	-3.53483300	-0.00281400	1.69571300
H	-2.84170100	-0.70470200	2.16525700
H	-4.53298600	-0.19708300	2.10084600
H	-3.24543400	1.01388400	1.97087300
C	-3.68395300	-1.60159800	-0.29751200
H	-3.58368900	-1.67876900	-1.38430600
H	-4.67597000	-1.98057500	-0.03134300
H	-2.93789500	-2.25093300	0.16146500
C	3.09578800	-0.05483400	1.74542400
H	2.38243400	-0.87929100	1.80135600
H	2.59174200	0.85499900	2.07677500
H	3.91194300	-0.27261800	2.44314700
C	4.33486800	-1.18618200	-0.14591900
H	5.14860500	-1.45146300	0.53784700
H	4.75334700	-1.06647000	-1.14749000
H	3.62955300	-2.01966800	-0.16482200
C	4.63544800	1.28824400	0.26248100
H	5.02402700	1.43166000	-0.74893400
H	5.48480800	1.09388400	0.92489500
H	4.16141400	2.21791200	0.58674200

Di-*tert*-butyl sulfoxide fragmentation TS

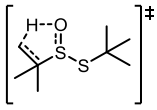


TS freq.: -1037.24 cm^{-1}
CBS-QB3 Enthalpy= -787.806234 CBS-QB3 Free Energy= -787.859836

0 1

C	2.75054400	-0.03904600	-1.18659100
C	2.05723500	0.24841400	0.12057600
S	-0.25330300	-0.61452300	-0.72264900
C	2.11165500	-0.72358400	1.14889700
C	1.85167500	1.70472100	0.43685300
O	-0.00884300	-1.83935200	0.23843100
C	-1.74077700	0.26300000	0.02117100
C	-1.88032700	1.58167700	-0.74622200
C	-2.94991200	-0.65004300	-0.23025300
C	-1.54438100	0.47768600	1.52198100
H	3.81091400	0.23708300	-1.09780300
H	2.32880000	0.53665000	-2.01319900
H	2.70751400	-1.09947700	-1.44225300
H	1.05278700	-1.42394400	0.90197400
H	2.00519100	-0.36191100	2.17038300
H	2.86370900	-1.50497800	1.03404500
H	2.83593700	2.16787400	0.60071200
H	1.37765000	2.24724800	-0.38403100
H	1.27065500	1.85306000	1.34711700
H	-2.80797400	2.08472900	-0.45500500
H	-1.05146200	2.26231200	-0.53906800
H	-1.92410000	1.41245800	-1.82665600
H	-3.85436500	-0.20065600	0.19519700
H	-2.79585600	-1.62526600	0.23567800
H	-3.11412200	-0.80513600	-1.29934200
H	-0.75341700	1.19976700	1.72972300
H	-2.47044800	0.85568000	1.96795100
H	-1.29208500	-0.46525600	2.01103200

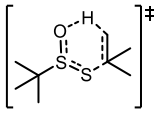
Di-*tert*-butyl thiosulfinate fragmentation TS



TS freq.: -912.46 cm^{-1}
CBS-QB3 Enthalpy= -1185.571215 CBS-QB3 Free Energy= -1185.629957
CBS-QB3 Enthalpy= -1185.563597 CBS-QB3 Free Energy= -1185.645595 (100 °C)

```
0 1
 C                -3.50433200    0.05627700    1.17692300
 C                -2.79757400    0.34494400   -0.11977600
 S                -0.47020300   -0.68959500    0.61439300
 C                -2.89828600   -0.57612900   -1.19033300
 C                -2.44311600    1.78089500   -0.38330000
 O                -0.70964100   -1.75340500   -0.50386100
 S                 0.80011900    0.82470800   -0.11913100
 C                 2.53394400    0.08923300    0.00131100
 C                 3.44423900    1.23294400   -0.47021900
 C                 2.85518400   -0.29349900    1.44815800
 C                 2.64882800   -1.11794200   -0.93584100
 H                -4.53716600    0.42712800    1.10715600
 H                -3.03347200    0.55825500    2.02421000
 H                -3.55414400   -1.01441900    1.38305300
 H                -1.84633000   -1.27775600   -1.05762900
 H                -2.80843700   -0.16173200   -2.19356600
 H                -3.66771200   -1.34256500   -1.09494700
 H                -3.36818600    2.32798000   -0.61688300
 H                -1.98987300    2.26493300    0.48359500
 H                -1.77465100    1.88780800   -1.23860000
 H                 4.48549500    0.89454800   -0.45676300
 H                 3.20426500    1.54088800   -1.49099200
 H                 3.36433400    2.10589600    0.18248300
 H                 3.88021900   -0.67578000    1.50760600
 H                 2.18516700   -1.07501000    1.81151300
 H                 2.77131000    0.56867500    2.11344200
 H                 2.43562000   -0.83366600   -1.96850600
 H                 3.66722300   -1.52071400   -0.89170400
 H                 1.95149100   -1.90938800   -0.65830700
```

Di-*tert*-butyl thiosulfinate fragmentation TS (6-membered ring)

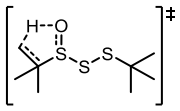


TS freq.: -815.73 cm^{-1}
CBS-QB3 Enthalpy= -1185.548607 CBS-QB3 Free Energy= -1185.608074

```
0 1
 C                -2.97684800   -1.35511700   -0.29533200
 C                -2.36729400   -0.04032200    0.19150800
 S                -0.77215100    0.23825800   -0.80692000
 C                -3.24842000    1.15920600   -0.18064200
 C                -2.04467500   -0.05682100    1.68117200
 O                -0.20680100    1.54786300   -0.16631800
 S                 0.44888000   -1.34014900   -0.28028400
 C                 2.82579800    0.22084200    0.18674200
 C                 3.20887000   -0.84650000    1.15395200
```

C	3.32303600	0.10291300	-1.21684500
C	2.30314200	1.45010400	0.64296100
H	-3.95298700	-1.49850400	0.17954400
H	-2.34204400	-2.20574900	-0.04314900
H	-3.13170000	-1.34939100	-1.37850000
H	-2.76663500	2.09931700	0.09367900
H	-4.20133800	1.09063100	0.35357700
H	-3.46455300	1.18068400	-1.25257200
H	-2.97315700	-0.13961700	2.25564700
H	-1.40260300	-0.90220500	1.93375500
H	-1.53976600	0.86602200	1.97385600
H	4.24465100	-0.63494600	1.46484100
H	2.58386700	-0.83000400	2.04570000
H	3.18883700	-1.84068200	0.70859600
H	4.38131200	0.40723600	-1.21324400
H	2.79015100	0.77173500	-1.89259000
H	3.26343000	-0.91763100	-1.59070900
H	2.31345100	1.60487600	1.72058400
H	2.59151500	2.32417300	0.05661500
H	1.10266500	1.41558700	0.32909000

Di-*tert*-butyl trisulfide-1-oxide fragmentation TS



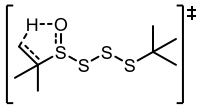
TS freq.: -929.49 cm^{-1}
CBS-QB3 Enthalpy= -1583.327591 CBS-QB3 Free Energy= -1583.391617
CBS-QB3 Enthalpy= -1583.319328 CBS-QB3 Free Energy= -1583.408657 (100 °C)

0 1

C	-3.37448700	0.49517500	0.00242800
C	-2.94449000	1.65862600	-0.84687900
H	-2.24013600	2.31484900	-0.33243600
H	-2.50677000	1.33773000	-1.79312100
H	-3.83443900	2.25978200	-1.08406600
C	-3.76908200	0.81277200	1.41922500
H	-4.73720700	1.33430000	1.40780900
H	-3.89047000	-0.09013400	2.02016300
H	-3.05028600	1.47120600	1.91069300
C	-3.83167600	-0.70010200	-0.60030700
H	-2.85853100	-1.50037600	-0.41142600
H	-4.62950800	-1.22909500	-0.07874200
H	-3.94360400	-0.68457000	-1.68351600
S	-1.06047900	-0.66670100	0.63418500
O	-1.68421100	-1.96595600	0.05294100
S	0.14689800	0.26010300	-0.87531600
C	3.09993900	0.26001200	0.28438800
S	1.97999500	-0.72023800	-0.86965400
C	2.56534300	0.22469200	1.71772500
H	2.44200900	-0.80061700	2.07172400
H	3.26563400	0.73991900	2.38462600
H	1.60057300	0.73029600	1.79353800
C	4.43409000	-0.49667500	0.18229100
H	4.81452400	-0.50390900	-0.84226600
H	5.17848800	-0.00235500	0.81446500
H	4.33643700	-1.53058500	0.52250500
C	3.25117000	1.69848300	-0.21630600
H	2.29205600	2.22065300	-0.21153300

H	3.93678800	2.24871900	0.43760000
H	3.65066300	1.72331900	-1.23235500

Di-*tert*-butyl tetrasulfide-1-oxide fragmentation TS



TS freq.: -918.28 cm^{-1}
CBS-QB3 Enthalpy= -1981.085430 CBS-QB3 Free Energy= -1981.154560
CBS-QB3 Enthalpy= -1981.076527 CBS-QB3 Free Energy= -1981.172959 (100 °C)

0 1

C	3.90209800	0.70641100	-0.12175100
C	3.47481400	1.29780700	-1.43567700
H	3.30498800	0.53850500	-2.20102800
H	2.57913100	1.91285300	-1.33833400
H	4.28288000	1.94976300	-1.79855300
C	4.98637200	-0.33456300	-0.17934500
H	5.93893000	0.16170400	-0.41556100
H	5.11181200	-0.84574900	0.77666200
H	4.80470200	-1.07781500	-0.95786400
C	3.65358200	1.39398500	1.08939000
H	2.70292000	0.72417400	1.60471200
H	4.41255200	1.29294000	1.86540300
H	3.24178100	2.39832900	0.99998400
S	1.93171100	-1.01641600	0.42061600
O	1.80495400	-0.26935100	1.77667200
S	0.48459200	-0.25547200	-0.94055700
S	-1.24635200	-1.43439100	-0.62920200
C	-3.57951200	0.61207800	0.01851400
S	-2.38486000	-0.57208500	0.86873400
C	-2.81493700	1.74763400	-0.66532200
H	-2.19403900	1.37372000	-1.48176400
H	-3.52564600	2.46619000	-1.08850400
H	-2.16983600	2.27465700	0.04043200
C	-4.46144800	-0.14419700	-0.97758800
H	-5.17950100	0.54602800	-1.43400400
H	-3.86476900	-0.58472800	-1.77910000
H	-5.01898400	-0.94359300	-0.48488000
C	-4.41537000	1.14666300	1.19252100
H	-3.79511600	1.67755700	1.91896800
H	-5.16442700	1.84802500	0.81159200
H	-4.94205500	0.34118200	1.71056500

Isobutylene

CBS-QB3 Enthalpy= -156.871528 CBS-QB3 Free Energy= -156.905174

0 1

C	-1.27595500	-0.67829100	0.00000000
H	-1.32650900	-1.33185200	0.87868000
H	-1.32650400	-1.33186300	-0.87867100
H	-2.15878000	-0.03656500	-0.00000600
C	-0.00000200	0.12423600	0.00000000
C	0.00000000	1.45722000	0.00000000

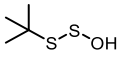
```
 H                -0.92400300    2.02565700   -0.00000200
 H                 0.92400700    2.02565400    0.00000100
 C                 1.27595700   -0.67829100   -0.00000200
 H                 1.32651800   -1.33184200    0.87868600
 H                 1.32649600   -1.33187400   -0.87866200
 H                 2.15877600   -0.03655900   -0.00001600
```

tert-Butyl sulfenic acid

CBS-QB3 Enthalpy= -630.958987 CBS-QB3 Free Energy= -631.000322

```
0 1
 C                 1.70311700   -1.04068600   -0.09297100
 C                 0.65925900    0.08175200    0.00082300
 S                -0.96313000   -0.81679400   -0.01806600
 C                 0.79150600    0.85864700    1.31598500
 C                 0.75607500    1.02495200   -1.20368900
 O                -2.06273100    0.47278100    0.11034800
 H                 2.70742400   -0.60760100   -0.05934900
 H                 1.61011300   -1.60077800   -1.02734100
 H                 1.61380600   -1.74144800    0.74156200
 H                -0.04178800    1.55396700    1.43455200
 H                 1.72415800    1.43350400    1.32525200
 H                 0.79346000    0.18097500    2.17219300
 H                 1.71880700    1.54723900   -1.19935900
 H                 0.66677100    0.47657800   -2.14438000
 H                -0.02879100    1.78460400   -1.16730200
 H                -2.31176800    0.71141300   -0.79045600
```

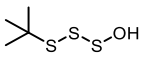
tert-Butylthiosulfoxylic acid



CBS-QB3 Enthalpy= -1028.722819 CBS-QB3 Free Energy= -1028.768600

```
0 1
 S                 1.79704700   -0.40817800    0.44609200
 O                 2.44689000    0.96938700   -0.31403300
 S                 0.11804100   -0.92252100   -0.59462300
 C                -1.28181600    0.16590800    0.06055300
 C                -2.51022300   -0.33107700   -0.71523700
 C                -1.45787500   -0.05114000    1.56399500
 C                -0.98402200    1.63304300   -0.26269500
 H                -3.38710600    0.25253500   -0.41763100
 H                -2.37955400   -0.21263100   -1.79404100
 H                -2.72019000   -1.38322400   -0.50632700
 H                -2.28515400    0.56610500    1.93061000
 H                -0.55793100    0.23492500    2.11195500
 H                -1.68298900   -1.09568200    1.79086400
 H                -0.87008000    1.78541800   -1.33830400
 H                -1.80979300    2.26204500    0.08802800
 H                -0.06695500    1.97015200    0.22320600
 H                 2.94684200    0.65603400   -1.07930600
```

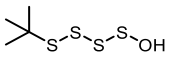
tert-Butyl trisulfide oxyacid



CBS-QB3 Enthalpy= -1426.479081 CBS-QB3 Free Energy= -1426.529338

```
0 1
 S                -2.49427800   -0.00515000   -0.41285000
 O                -2.33218100    1.59844700    0.11515200
 S                -1.05001300   -1.10150800    0.56674200
 C                 1.75417800    0.33436700    0.03292000
 S                 0.71778100   -1.12627200   -0.55347700
 C                 1.12697800    1.65312400   -0.42665800
 H                 0.14441600    1.81548800    0.01887400
 H                 1.77544900    2.48644400   -0.13323200
 H                 1.01174000    1.67713300   -1.51254100
 C                 3.09657200    0.09386000   -0.67804800
 H                 3.78410700    0.90801200   -0.42814100
 H                 3.55646400   -0.84629500   -0.36456400
 H                 2.97952900    0.07768400   -1.76470700
 C                 1.93287500    0.29650400    1.55196400
 H                 2.38530000   -0.64330400    1.87560200
 H                 2.58614800    1.11863500    1.86360400
 H                 0.97881300    0.41537900    2.06915500
 H                -2.78397000    1.66298600    0.96702700
```

tert-Butyl tetrasulfide oxyacid



CBS-QB3 Enthalpy= -1824.237299 CBS-QB3 Free Energy= -1824.293459

```
0 1
 S                 1.65355800   -0.80146400    0.81405100
 S                 0.21602600   -1.25694000   -0.70573700
 S                 3.23141900    0.14407000   -0.08233300
 O                 2.89920900    1.79601400    0.01456000
 S                -0.99179100    0.40098200   -0.97736100
 C                -2.43161400    0.23887300    0.23052300
 C                -3.21005300   -1.04760400   -0.05246700
 H                -2.58717300   -1.93042200    0.10591000
 H                -3.58187100   -1.06818900   -1.07900800
 H                -4.06711200   -1.11590200    0.62613900
 C                -1.92905600    0.28205200    1.67478900
 H                -2.78366400    0.26273100    2.35977600
 H                -1.35102300    1.18714700    1.87101500
 H                -1.30132200   -0.58101900    1.90437600
 C                -3.28154700    1.47799300   -0.09205000
 H                -2.73115400    2.40371600    0.09350400
 H                -4.16920900    1.48059700    0.54801600
 H                -3.61776900    1.47637000   -1.13198400
 H                 2.36285200    2.02260000   -0.75693300
```

2-Methylpropane-2-sulfinothioic acid

CBS-QB3 Enthalpy= -1028.711647 CBS-QB3 Free Energy= -1028.756687

```
0 1
 C                -1.28440400   -1.61674100   -0.55053600
 C                -1.09259700   -0.22811500    0.06437600
 S                 0.57336100    0.40020500   -0.62644800
 C                -2.13251900    0.76790000   -0.45981800
 C                -1.04988900   -0.27361100    1.58647300
 O                 0.63112000    1.89176200    0.17114100
 S                 2.02400500   -0.71448300    0.11252300
 H                -2.27967000   -1.98717400   -0.28677800
 H                -0.54263500   -2.32464300   -0.17859300
 H                -1.21922300   -1.58902000   -1.64216700
 H                -1.94471000    1.77444300   -0.08369700
 H                -3.12683500    0.45673200   -0.12524800
 H                -2.14316000    0.80091200   -1.55256600
 H                -1.98326400   -0.70593400    1.95959200
 H                -0.22235900   -0.89261000    1.93898800
 H                -0.95230400    0.72714300    2.01221300
 H                 1.16379100    1.73788900    0.96895100
```

tert-BuSO•

CBS-QB3 Enthalpy= -630.352256 CBS-QB3 Free Energy= -630.393921
CBS-QB3 Enthalpy= -630.348299 CBS-QB3 Free Energy= -630.404850 (100 °C)

```
0 2
 S                 0.51173100   -1.16329100    0.00000000
 O                -0.78578900   -1.94371900    0.00000000
 C                 0.03808900    0.64692500    0.00000000
 C                -0.78578900    0.91613000    1.26438000
 H                -1.13698900    1.95312400    1.26798400
 H                -1.65600000    0.25765300    1.30066700
 H                -0.19433900    0.75403800    2.16921800
 C                -0.78578900    0.91613000   -1.26438000
 H                -1.13698900    1.95312400   -1.26798400
 H                -0.19433900    0.75403800   -2.16921800
 H                -1.65600000    0.25765300   -1.30066700
 C                 1.36361000    1.41533800    0.00000000
 H                 1.16776500    2.49183800    0.00000000
 H                 1.96238800    1.18689600    0.88633300
 H                 1.96238800    1.18689600   -0.88633300
```

tert-BuSSO•

CBS-QB3 Enthalpy= -1028.109556 CBS-QB3 Free Energy= -1028.155846

```
0 2
 S                 1.95574600   -0.29931200    0.23911600
 O                 2.11610000    1.08630200   -0.31433300
 S                 0.10110000   -1.16204600   -0.30040300
 C                -1.19807900    0.17527000    0.04097100
 C                -2.52414600   -0.59720200   -0.01045400
 C                -0.98321800    0.79837300    1.42207100
 C                -1.13350000    1.23019200   -1.06996900
 H                -3.35123100    0.10893900    0.11634700
```

H	-2.66033100	-1.10049700	-0.97097500
H	-2.58726200	-1.34348500	0.78455500
H	-1.80291000	1.49412800	1.63031700
H	-0.05143200	1.36414500	1.46718600
H	-0.97250500	0.03927000	2.20677500
H	-1.29307200	0.77719800	-2.05078000
H	-1.91832700	1.97723200	-0.90597800
H	-0.16761000	1.73458200	-1.07790900

tert-BuSSSO•

CBS-QB3 Enthalpy= -1425.868035 CBS-QB3 Free Energy= -1425.919234

0 2

S	-2.53246700	0.15753000	-0.30825700
O	-2.33461600	1.55974000	0.18068500
S	-1.04722200	-1.17267700	0.51210000
C	1.72607800	0.31607500	0.06484500
S	0.61320800	-0.98927200	-0.72063600
C	1.07819800	1.69908700	-0.02161300
H	0.14809600	1.74914600	0.54602500
H	1.76519100	2.44814400	0.38718600
H	0.85626200	1.96919400	-1.05647300
C	2.98287600	0.24155400	-0.81836100
H	3.71156800	0.97614100	-0.46232100
H	3.45019500	-0.74522800	-0.77526600
H	2.75734100	0.47456600	-1.86221500
C	2.05178200	-0.06267000	1.51060800
H	2.51780100	-1.04865700	1.56861700
H	2.74606900	0.67183700	1.93227600
H	1.15448300	-0.06664900	2.13249800

tert-BuSSSSO•

CBS-QB3 Enthalpy= -1823.624187 CBS-QB3 Free Energy= -1823.681265

0 2

S	1.64810800	-0.88706400	0.78857700
S	0.27592900	-1.08717000	-0.82043400
S	3.24563500	0.24228900	-0.07787100
O	2.98953400	1.70843100	0.06494900
S	-0.94670900	0.57302800	-0.87541500
C	-2.42790400	0.19360900	0.22928300
C	-3.16793400	-1.04323100	-0.28432600
H	-2.53580500	-1.93246200	-0.23680500
H	-3.49628200	-0.90877900	-1.31708000
H	-4.05137000	-1.22709600	0.33650300
C	-1.98143000	0.01643600	1.68179300
H	-2.86121200	-0.12048000	2.31981800
H	-1.42852800	0.88706500	2.03956300
H	-1.34709200	-0.86417900	1.79992900
C	-3.29063400	1.45576900	0.07052100
H	-2.76760300	2.34835200	0.42229200
H	-4.20270800	1.34326500	0.66474200
H	-3.58567200	1.61404600	-0.96989300

tert-BuS(S)O•

CBS-QB3 Enthalpy= -1028.091699 CBS-QB3 Free Energy= -1028.136968

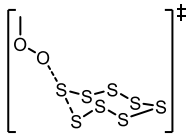
```
0 2
 C                 -1.13812200   -1.63077400   -0.64054400
 C                 -1.09491400   -0.26417300    0.03214200
 S                  0.60559300    0.55096700   -0.39292600
 C                 -2.12770000    0.70278000   -0.55044000
 C                 -1.17583000   -0.33864000    1.55644000
 O                  0.56798200    1.91796200    0.18732100
 S                  2.08218500   -0.67291300    0.06845300
 H                 -2.12303000   -2.07460400   -0.46190300
 H                 -0.38109000   -2.30458300   -0.23988300
 H                 -0.99762400   -1.55439500   -1.72141900
 H                 -2.01874700    1.70215700   -0.12877800
 H                 -3.12870100    0.33238400   -0.30881200
 H                 -2.04774900    0.77145400   -1.63802300
 H                 -2.17493800   -0.68553500    1.83992600
 H                 -0.44278200   -1.03778400    1.96166500
 H                 -1.01425300    0.64317600    2.00463400
```

Sulfur S_8

CBS-QB3 Enthalpy= -3182.059726 CBS-QB3 Free Energy= -3182.110857

```
0 1
 S                  1.60091600   -1.79267800    0.50023900
 S                 -0.13557200   -2.39955800   -0.50025000
 S                 -1.79269200   -1.60093200    0.50020600
 S                  2.39964100   -0.13558800   -0.50019800
 S                  1.79268700    1.60093400    0.50021700
 S                  0.13558100    2.39955800   -0.50025400
 S                 -1.60093200    1.79267700    0.50023500
 S                 -2.39963100    0.13558700   -0.50019500
```

S_8 substitution by MeOO• TS

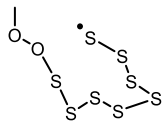


TS freq.: -376.61 cm^{-1}
CBS-QB3 Enthalpy= -3371.994902 CBS-QB3 Free Energy= -3372.059661

```
0 2
 O                 -3.50113700    0.50377400    0.02503700
 O                 -3.46572600   -0.45683900    1.02568300
 C                 -3.43438000    0.19005000    2.30044100
 H                 -2.48394000    0.71721200    2.43052800
 H                 -4.27218900    0.88359700    2.39469200
 H                 -3.51850300   -0.61813000    3.02794500
 S                  0.26764000    2.37486100   -0.92247000
 S                 -1.72503600    0.93833500   -0.67943400
 S                  1.55917000    2.17753400    0.61292400
 S                 -1.25557900   -0.84011000   -1.59823500
```

S	3.03799000	0.72197100	0.14180900
S	-0.51470800	-2.16639000	-0.13516400
S	2.48539300	-1.06641200	1.06271800
S	1.55862000	-2.29594200	-0.36099600

S_8 - MeOO• adduct



CBS-QB3 Enthalpy= -3372.011315 CBS-QB3 Free Energy= -3372.081448

0 2

O	-3.40389600	-1.34163800	-0.33295000
O	-3.93191100	-0.47529900	0.74511800
C	-4.14919900	-1.30284100	1.87838800
H	-3.20771900	-1.69821600	2.27484800
H	-4.84129400	-2.11677500	1.64678200
H	-4.59919000	-0.63174200	2.61401500
S	3.00737400	-2.87941600	-0.46234000
S	-1.74452700	-1.22525800	-0.45202200
S	1.84952100	-1.50113200	0.30346700
S	-1.41053400	0.42966100	-1.62615800
S	3.03728900	0.34221800	0.31905000
S	-1.24631700	2.07940700	-0.28898300
S	1.79549800	1.71399100	1.21491600
S	0.72606200	2.71548400	-0.32688700

*i*PrO•

CBS-QB3 Enthalpy= -193.328687 CBS-QB3 Free Energy= -193.362846

0 2

O	0.22345500	1.37047700	-0.15647700
C	-0.02188400	0.12553300	0.36486800
H	0.02306200	0.16490700	1.46769800
C	-1.35742700	-0.46312700	-0.09993900
H	-1.52841200	-1.44787200	0.34534800
H	-2.18019000	0.19204200	0.19514500
H	-1.37064700	-0.55935600	-1.18857500
C	1.18890600	-0.73972000	-0.09300500
H	2.12343300	-0.30715400	0.26434700
H	1.07315500	-1.74471400	0.31881300
H	1.21439300	-0.79778800	-1.18249900

*i*PrOO•

CBS-QB3 Enthalpy= -268.416420 CBS-QB3 Free Energy= -268.453609

0 2

O	-1.92887500	-0.16110900	-0.11641200
O	-0.77879100	-0.62631000	0.32205300
C	0.37278200	0.02196900	-0.34197000
H	0.15575400	-0.03594400	-1.41139200
C	0.45777100	1.47017500	0.11018200
H	1.26901800	1.97990300	-0.41591100
H	-0.47740600	1.98597000	-0.11139100

```
 H                  0.65001300    1.52875600    1.18473200
 C                  1.57369400   -0.83106200    0.02521100
 H                  1.42920200   -1.86532300   -0.29286400
 H                  2.46921200   -0.44103800   -0.46408200
 H                  1.74004900   -0.81946200    1.10524500
```

*t*BuO•

CBS-QB3 Enthalpy= -232.559991 CBS-QB3 Free Energy= -232.597221

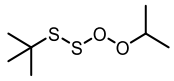
```
0 2
 O                 -0.51504300    1.35749900    0.00000000
 C                 -0.06471700    0.05489400    0.00000000
 C                 -0.51504300   -0.67961200    1.27723900
 H                 -0.18332600   -0.13225500    2.16166200
 H                 -1.60556800   -0.74508500    1.30469300
 H                 -0.11054400   -1.69502700    1.31475700
 C                 -0.51504300   -0.67961200   -1.27723900
 H                 -0.18332600   -0.13225500   -2.16166200
 H                 -0.11054400   -1.69502700   -1.31475700
 H                 -1.60556800   -0.74508500   -1.30469300
 C                  1.48764400    0.22435400    0.00000000
 H                  1.94050400   -0.77022900    0.00000000
 H                  1.81084000    0.76741200   -0.88873800
 H                  1.81084000    0.76741200    0.88873800
```

*i*PrOO*i*Pr

CBS-QB3 Enthalpy= -386.726066 CBS-QB3 Free Energy= -386.775008

```
0 1
 C                  1.67354000    0.03968700    0.30901200
 H                  1.36684400    0.29137400    1.33185100
 O                 -0.55187300   -0.57270700   -0.00113800
 O                  0.54275200    0.23185300   -0.54983300
 C                  2.70170800    1.04990400   -0.18983600
 H                  2.31246000    2.06790500   -0.12576400
 H                  3.60916700    0.98552300    0.41530700
 H                  2.96573800    0.84390500   -1.23024600
 C                  2.17497600   -1.40084200    0.25926200
 H                  3.02738700   -1.53158900    0.93227700
 H                  1.38619300   -2.08968100    0.56256800
 H                  2.48896200   -1.65804700   -0.75619300
 C                 -1.76658900    0.10992900   -0.33618100
 H                 -1.73826300    0.32767800   -1.41079500
 C                 -2.86381500   -0.90933500   -0.04822600
 H                 -2.86686800   -1.18047800    1.01087500
 H                 -3.84006200   -0.48670200   -0.29754700
 H                 -2.71361100   -1.81545400   -0.63782500
 C                 -1.92466300    1.40698500    0.45135000
 H                 -1.07951800    2.06970500    0.26179600
 H                 -2.84097600    1.92587000    0.15523600
 H                 -1.97544100    1.19885400    1.52393800
```

1-*tert*-butyl 4-isopropyl peroxydisulfane



CBS-QB3 Enthalpy= -1221.453830 CBS-QB3 Free Energy= -1221.514707

```
0 1
 C                  3.33214600    0.33717100    0.41361700
 H                  3.21388500    0.61821700    1.46727300
 S                  0.05746200   -1.12954800   -0.35433200
 S                 -1.41829400    0.06995600   -1.11379500
 C                 -2.72391200    0.23355500    0.24136800
 O                  1.04081600   -0.17182700    0.59092800
 O                  2.06933500    0.53164000   -0.23827000
 C                 -2.12674400    0.96346000    1.44771400
 H                 -2.89866400    1.10106200    2.21306600
 H                 -1.30571700    0.39661600    1.88965400
 H                 -1.74223700    1.94564000    1.16500900
 C                 -3.26262200   -1.14424900    0.63028000
 H                 -4.03946000   -1.03368800    1.39461300
 H                 -3.69896300   -1.65715100   -0.22972000
 H                 -2.47369100   -1.77527900    1.04436000
 C                 -3.81660400    1.08097200   -0.42747700
 H                 -4.23465600    0.58023200   -1.30451700
 H                 -4.63094200    1.24836800    0.28451900
 H                 -3.43503700    2.05746600   -0.73636800
 C                  4.25304700    1.33874400   -0.27987000
 H                  3.86404200    2.35330200   -0.18019600
 H                  5.24805100    1.29773500    0.17000000
 H                  4.34407200    1.10324200   -1.34308000
 C                  3.81933800   -1.10394800    0.30619600
 H                  4.78901500   -1.21483700    0.79992800
 H                  3.11716400   -1.78756300    0.78595300
 H                  3.92735200   -1.39261000   -0.74270900
```

Acetone

CBS-QB3 Enthalpy= -192.813154 CBS-QB3 Free Energy= -192.849015

```
0 1
 C                  1.29153900   -0.61333400   -0.00000300
 H                  1.33816400   -1.26332800    0.87955200
 H                  2.14309200    0.06549700   -0.00018800
 H                  1.33800600   -1.26364000   -0.87933500
 C                  0.00000000    0.18642200    0.00000000
 O                 -0.00000100    1.39555300    0.00000000
 C                 -1.29153800   -0.61333500    0.00000400
 H                 -1.33816700   -1.26332200   -0.87955800
 H                 -1.33800000   -1.26364900    0.87933000
 H                 -2.14309200    0.06549600    0.00019800
```

tert-BuSH

CBS-QB3 Enthalpy= -555.832080 CBS-QB3 Free Energy= -555.870425

```
0 1
 C                  0.82250100    1.45704800   -0.00005300
 C                  0.35568100   -0.00608100    0.00000100
 S                 -1.51334800    0.07624600   -0.00000700
 C                  0.84669100   -0.72492200   -1.26267900
 C                  0.84668500   -0.72482700    1.26273700
 H                  1.91619400    1.49255900   -0.00004400
```

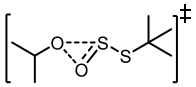
```
 H                  0.46673600    1.98839800    0.88607500
 H                  0.46675200    1.98832700   -0.88623100
 H                  0.50364800   -1.76250300   -1.28854900
 H                  1.94244100   -0.73419300   -1.28592300
 H                  0.48689500   -0.22646600   -2.16465600
 H                  1.94243400   -0.73410000    1.28598700
 H                  0.48688700   -0.22630200    2.16467400
 H                  0.50363800   -1.76240500    1.28868500
 H                 -1.73140500   -1.25055000    0.00006900
```

SO

CBS-QB3 Enthalpy= -472.840210 CBS-QB3 Free Energy= -472.865418

```
0 3
 S                  0.00000000    0.00000000    0.49933000
 O                  0.00000000    0.00000000   -0.99866000
```

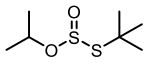
peroxydisulfane concerted TS



TS freq.: -187.72 cm^{-1}
CBS-QB3 Enthalpy= -1221.434095 CBS-QB3 Free Energy= -1221.495690

```
0 1
 C                  3.20046600    0.23160000    0.19830400
 H                  3.73310500   -0.28027400    1.02330000
 S                 -0.13240500   -1.75195100    0.23590000
 S                 -1.58138600   -0.81799400   -0.98082800
 C                 -2.22416000    0.68079400   -0.02021200
 O                  0.34666000   -0.87194000    1.32980000
 O                  1.93605600   -0.28342900    0.04674600
 C                 -1.12643500    1.75009600    0.02336700
 H                 -1.50770400    2.62750800    0.55767000
 H                 -0.23274800    1.38789600    0.52840000
 H                 -0.84359400    2.05907200   -0.98498900
 C                 -2.69217100    0.26969300    1.37856600
 H                 -3.14707600    1.13939300    1.86447500
 H                 -3.44218400   -0.52245900    1.32975900
 H                 -1.86271800   -0.06370200    2.00066600
 C                 -3.41330900    1.14740500   -0.87435100
 H                 -4.20447900    0.39532500   -0.91473900
 H                 -3.82906000    2.05492900   -0.42520100
 H                 -3.10804600    1.38959300   -1.89513600
 C                  3.19421900    1.74326400    0.46957700
 H                  2.61760800    1.95567000    1.37337900
 H                  4.20980100    2.12710100    0.61219700
 H                  2.73075300    2.27564000   -0.36611900
 C                  3.98397500   -0.09841500   -1.10138400
 H                  5.01215100    0.26707400   -1.01977600
 H                  3.99859100   -1.17690100   -1.26497700
 H                  3.49901700    0.37958200   -1.95564100
```

S-(*tert*-butyl) O-isopropyl sulfurothioite

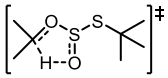


CBS-QB3 Enthalpy= -1221.530465 CBS-QB3 Free Energy= -1221.590435

```
0 1
 C                  3.05102600   -0.11955600    0.23812300
 H                  2.97099000    0.23815900    1.27285500
 S                  0.47678000    0.41120900    0.55620800
 S                 -0.94316000   -0.92474500   -0.40824600
 C                 -2.58513900   -0.08727000   -0.03315600
 O                  0.32794600    1.77496900    0.03481400
 O                  1.69719300   -0.39526600   -0.25280000
 C                 -2.76466800    1.13954100   -0.93743600
 H                 -3.74167200    1.59730100   -0.74418400
 H                 -1.98931600    1.88391500   -0.75692500
 H                 -2.72219100    0.85428500   -1.99074200
 C                 -2.69487900    0.29100300    1.44929900
 H                 -3.70593400    0.65890300    1.65459700
 H                 -2.50618500   -0.56884800    2.09532600
 H                 -2.00004800    1.08993300    1.71722200
```

C	-3.62151100	-1.16847300	-0.38035600
H	-3.52386000	-2.04180100	0.26840500
H	-4.62702500	-0.75477200	-0.25101800
H	-3.52681700	-1.49654600	-1.41864500
C	3.68217500	0.95567700	-0.63684700
H	3.09849000	1.87654200	-0.59999600
H	4.70026200	1.17061700	-0.29952400
H	3.72358300	0.61699900	-1.67502200
C	3.79385000	-1.44642300	0.21467600
H	4.82085600	-1.31026700	0.56419100
H	3.30033600	-2.17820900	0.85678700
H	3.82438300	-1.84424300	-0.80265000

Sulfurothioite fragmentation TS



TS freq.: -985.67 cm^{-1}
CBS-QB3 Enthalpy= -1221.478266 CBS-QB3 Free Energy= -1221.536598

0 1

S	0.32031700	-1.07836300	-0.28796700
C	2.80209300	0.28135600	-0.01601600
O	0.92581700	-0.95411200	1.11190600
S	-0.90687300	0.58043800	-0.67517200
C	-2.56129300	0.12672600	0.11427500
C	-3.46647800	1.30360300	-0.28234800
C	-3.10050100	-1.18399200	-0.46613700
C	-2.41242300	0.04768000	1.63710300
H	2.08223200	-0.27595000	0.86909800
H	-4.46211800	1.15035500	0.14604100
H	-3.08062900	2.25311800	0.09680900
H	-3.57322000	1.38134300	-1.36693900
H	-4.09327900	-1.38666000	-0.05013900
H	-2.45867900	-2.03111100	-0.21435100
H	-3.18868700	-1.13018000	-1.55306900
H	-2.03367500	0.98688400	2.04525300
H	-3.38903100	-0.15574200	2.09015100
H	-1.72768700	-0.74775700	1.93510800
C	2.84075800	1.73491500	0.48019000
H	1.83316200	2.15215800	0.50296500
H	3.27927300	1.80777000	1.47858600
H	3.44481100	2.33746900	-0.20673800
C	4.11920900	-0.50298300	0.06804700
H	3.95161300	-1.54848500	-0.19716400
H	4.83985000	-0.08549700	-0.64337600
H	4.55631300	-0.45455700	1.06838100
O	2.08373900	0.06283900	-1.08704200

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