Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Living polymerizations of propylene sulfide initiated with potassium xanthates characterized with unprecedentedly high propagation rates

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Table S1. Conditions and results of xanthate initiated ROP of PS carried out in non-inert atmosphere.

Entry*	PS/xanthate $[M]_0/[I]_0$	Xanthate	Additive	Reaction time	T, °C	Mn predicted	Mn (GPC)	Mw/Mn
1	35	PMX	PC*	5 h	100	2595	700	1.26
2	50	PMX	-	5 h	80	3708	1600	1.34
3	150	PMX	PC	5 h	80	11123	1360	1.22
4	25	PMX	PC	5 h	80	1853	2700	1.7
5	35	PMX	PC	5 h	100	2595	671	1.45
6	25	PMX	-	5 h	80	1853	1400	1.52
7	25	PMX	PC	5 h	50	1853	670	1.43
8	150	PIBX	-	5 h	60	11123	2130	1.42
9	150	PIBX	PC	5 h	60	11123	700	1.3
10	150	PIBX	-	6 h	30	11123	2600	1.4
11	150	PIBX	PC	6 h	30	11123	550	1.2

* Obtained polymers were found to demonstrate bimodal distribution according to GPC.

** PC = propylene carbonate. Was used to give the ration $[PC]_0/[I]_0 = 1$

Table S2. Conditions and results of xanthate initiated emulsion polymerization of PS.

Entry	PS/PMX[18C6]	Reaction time, h	T, °C	Mn predicted	Mn (GPC)	Mw/Mn
1	10	2	5-20	742	12641	1.49
2	25	2	5-20	1854	8010	1.45
3	50	2	5-20	3708	3200	1.36
4	100	2	5-20	7415	2715	1.1/1.05
5	200	2	5-20	14830	820	1.1

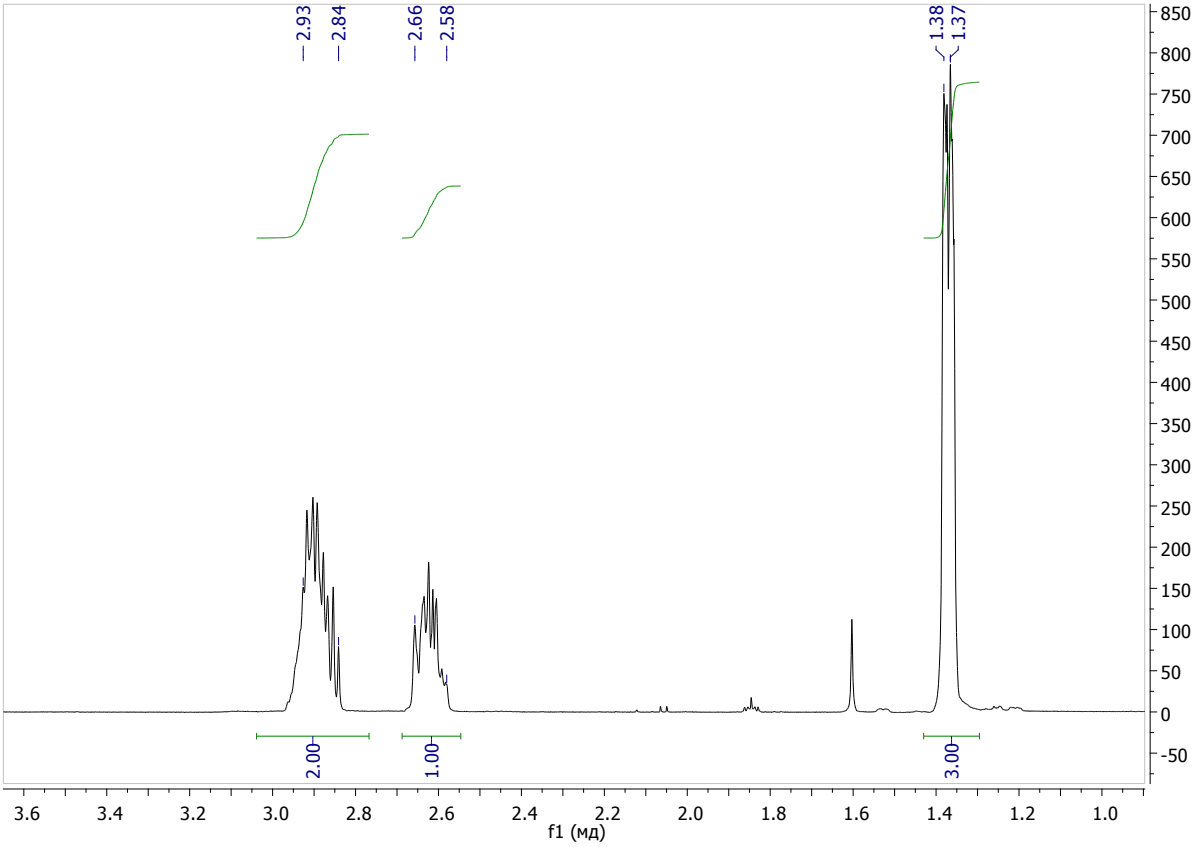


Figure S1. 1H NMR spectra of PPS synthesized in acetone at 0 °C (entry 8, Table S1) recorded in $cdcl_3$ at 25°C.

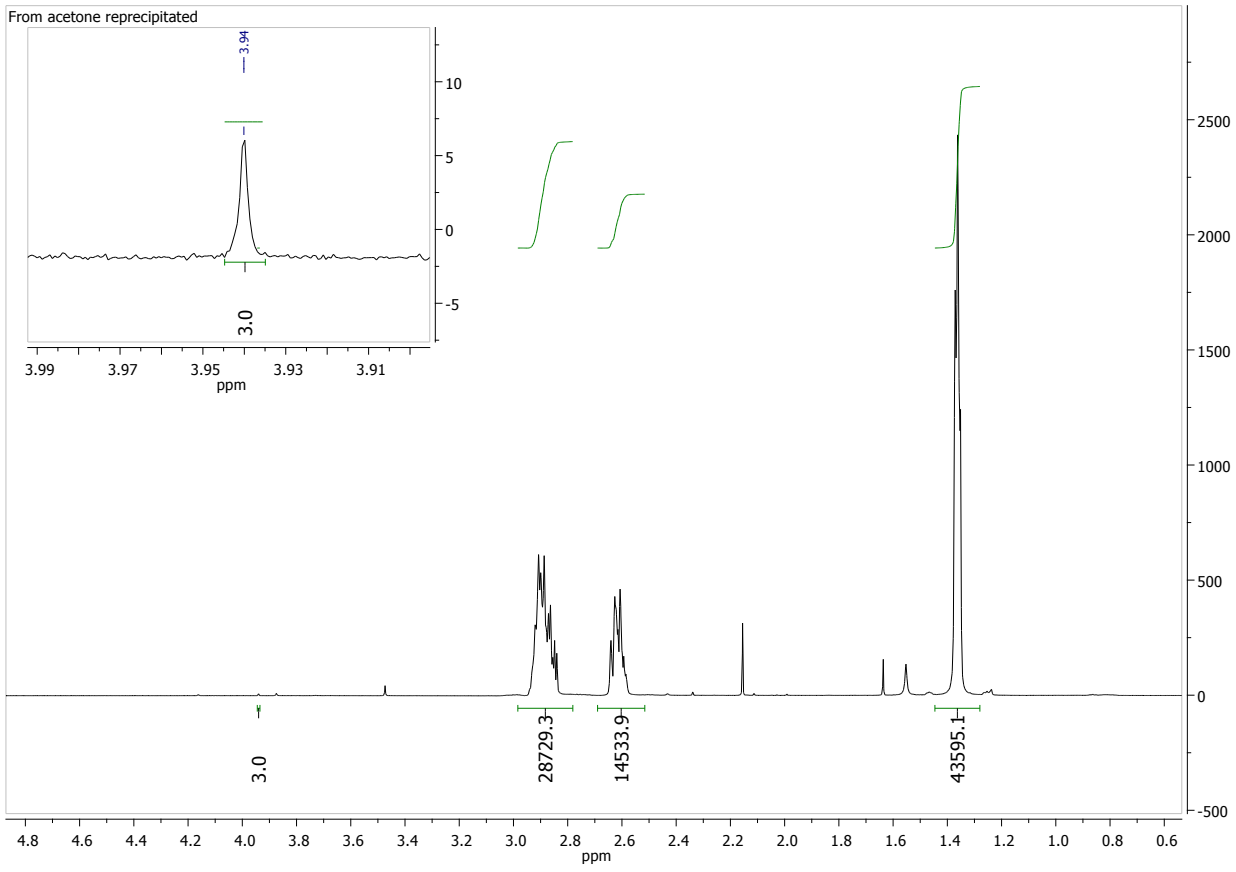


Figure S2. 1H NMR spectra of PPS synthesized in acetone at 0 °C (entry 10, Table 1) recorded in $cdcl_3$ at 25°C.

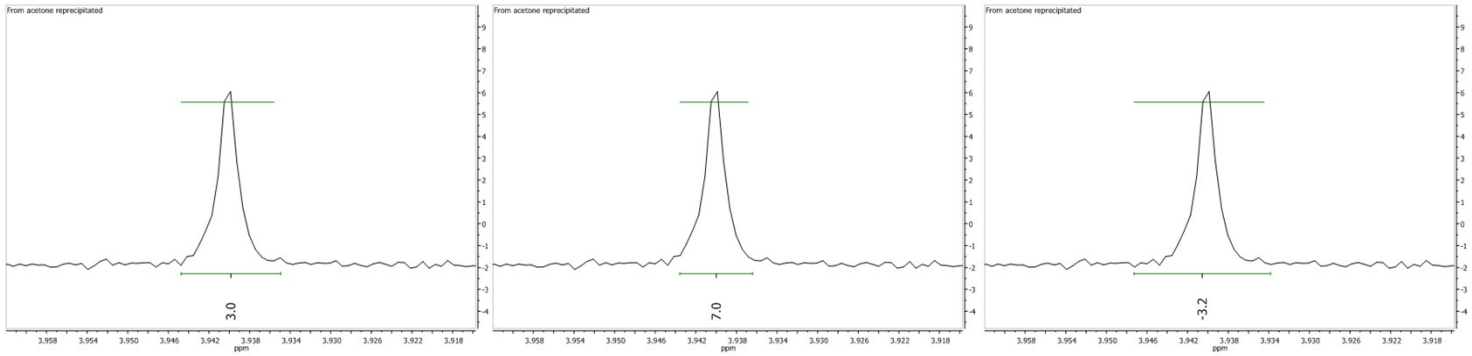


Figure S3. Fragments of 1H NMR in the region of xanthate CH_3 group demonstrating the uncertainties in determination of integral intensities for PPS characterized with high Mn values.

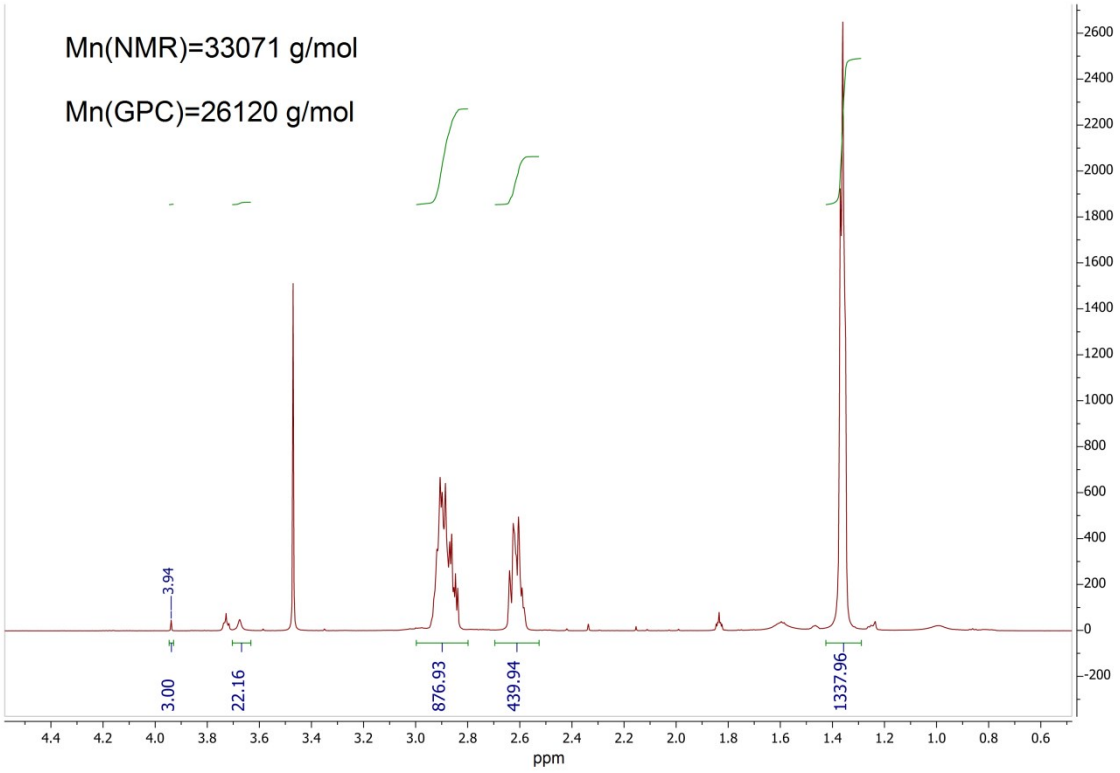


Figure S4. 1H NMR spectra of PPS synthesized in $cdcl_3$ at 0 °C (entry 13, Table 1) recorded in $cdcl_3$ at 25°C. Polymer was purified by double precipitation from CH_2Cl_2 to MeOH and washed with MeOH.

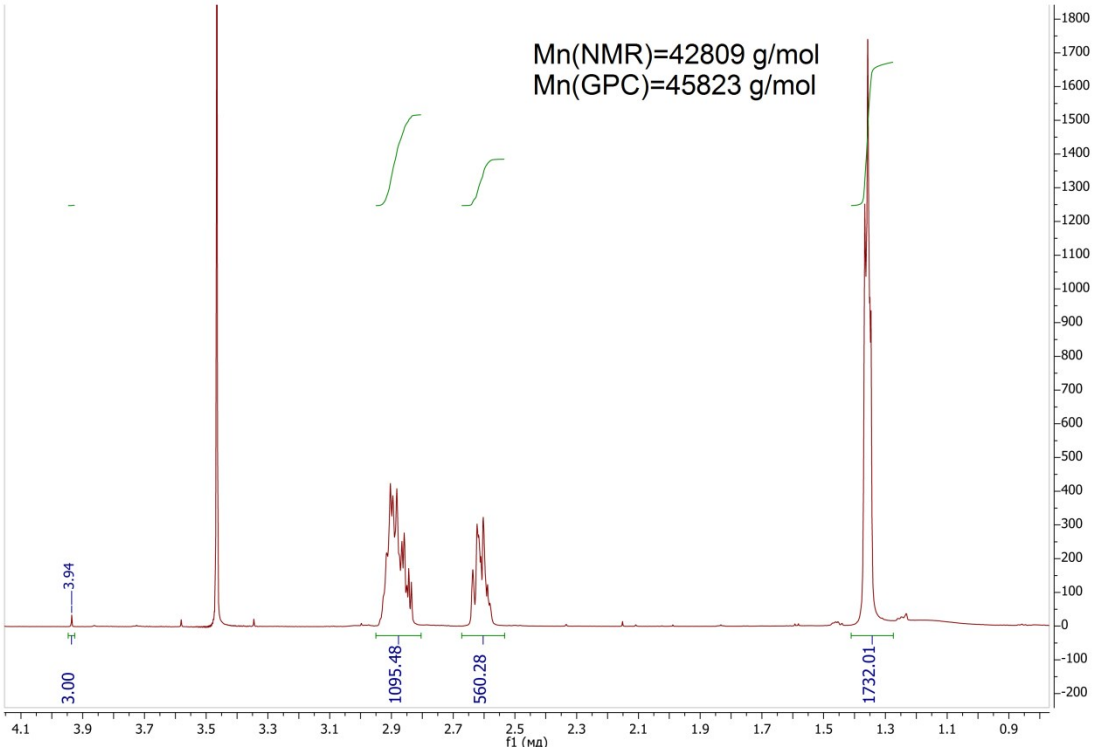


Figure S5. 1H NMR spectra of PPS synthesized in cdcl$_3$ at 0 °C (entry 16, Table 1) recorded in cdcl$_3$ at 25°C. Polymer was purified by double precipitation from CH_2Cl_2 to MeOH and washed with MeOH.

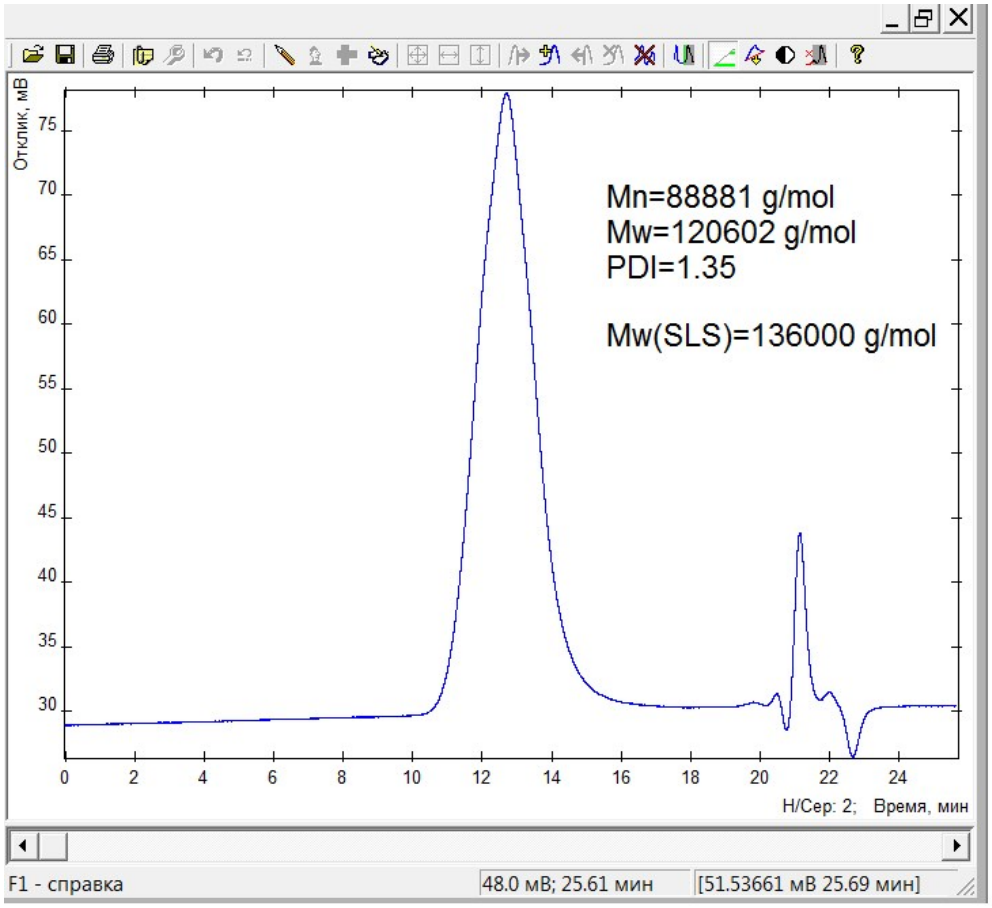


Figure S6. GPC trace recorded for PPS synthesized in acetone at 0 °C (entry 10, Table 1). Mean average molecular weight determined with static light scattering method was given for the comparative purpose.

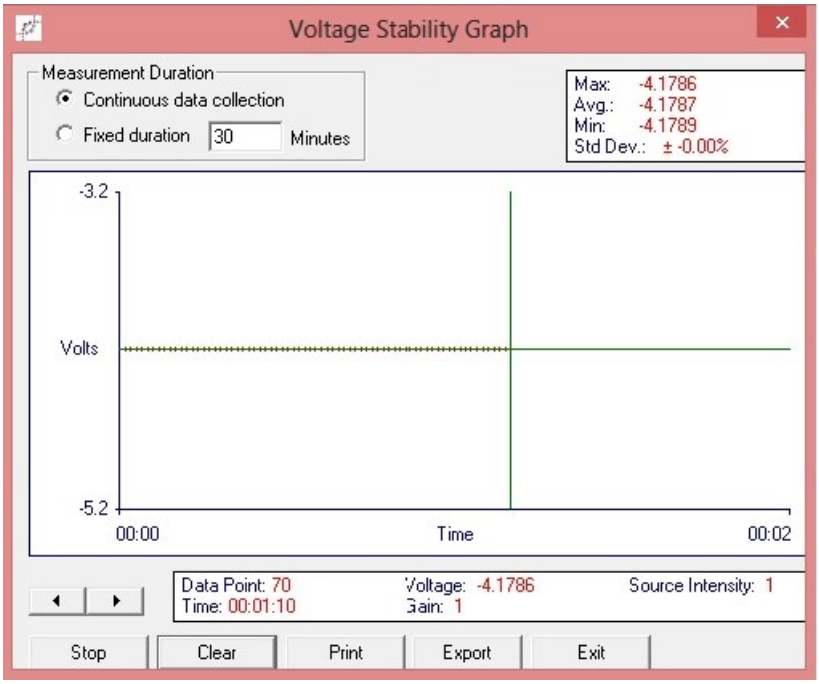


Figure S7. Voltage stability for cuvette filled with toluene determined prior to the dn/dc calculations.

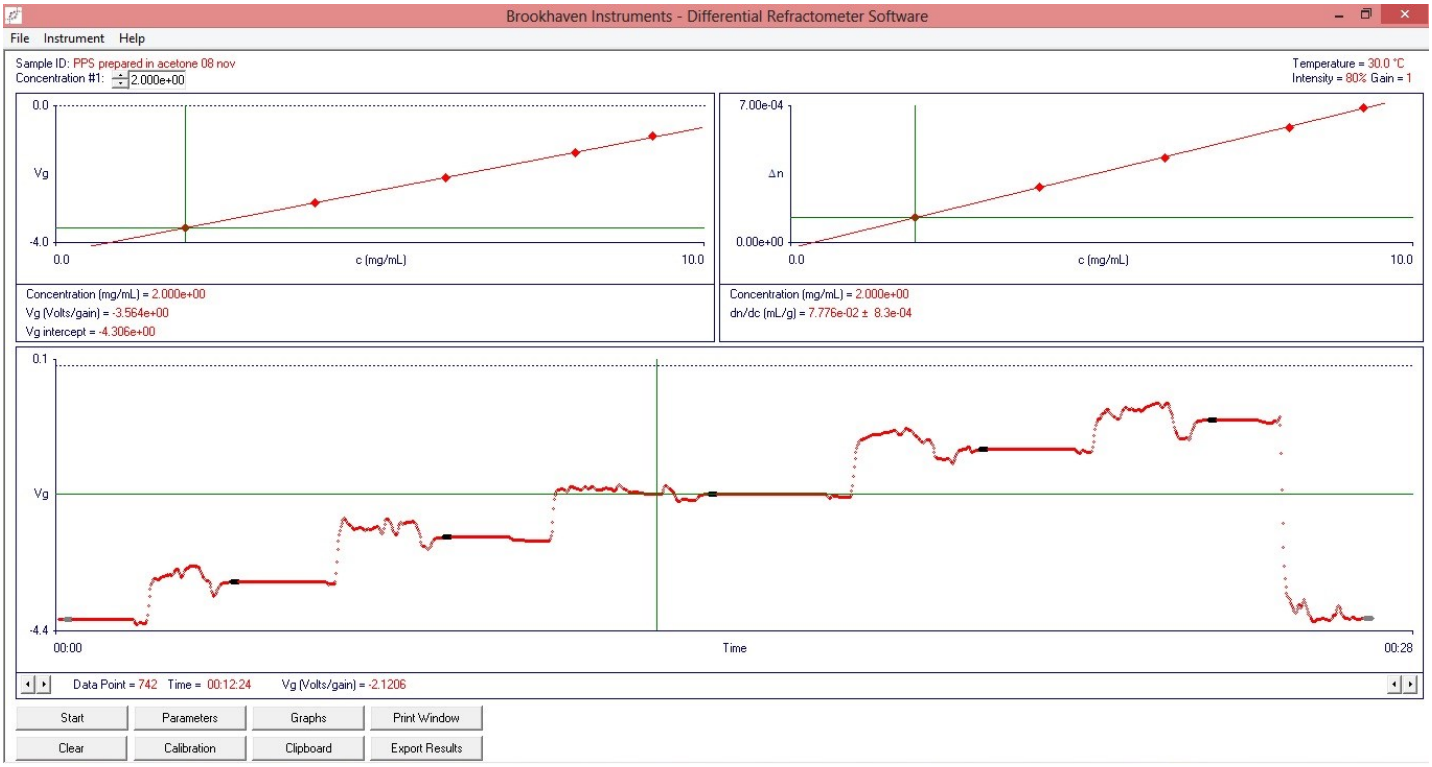


Figure S8. dn/dc (mL/g) calculated based on five PPS-toluene solutions using Brookhaven DNDC apparatus at 30 ^{o}C.

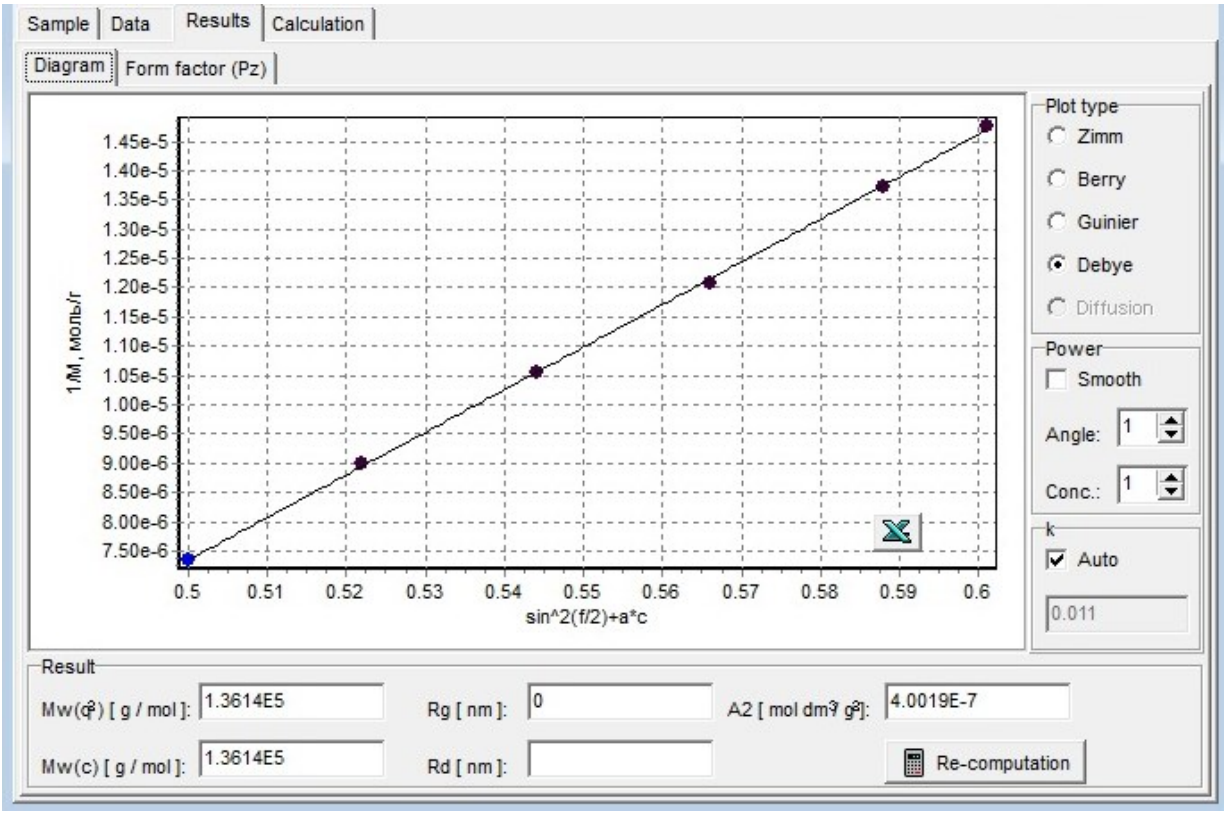


Figure S9. Debye plot for PPS synthesized in acetone at 0 °C (entry 10, Table 1) giving the desired Mw value.

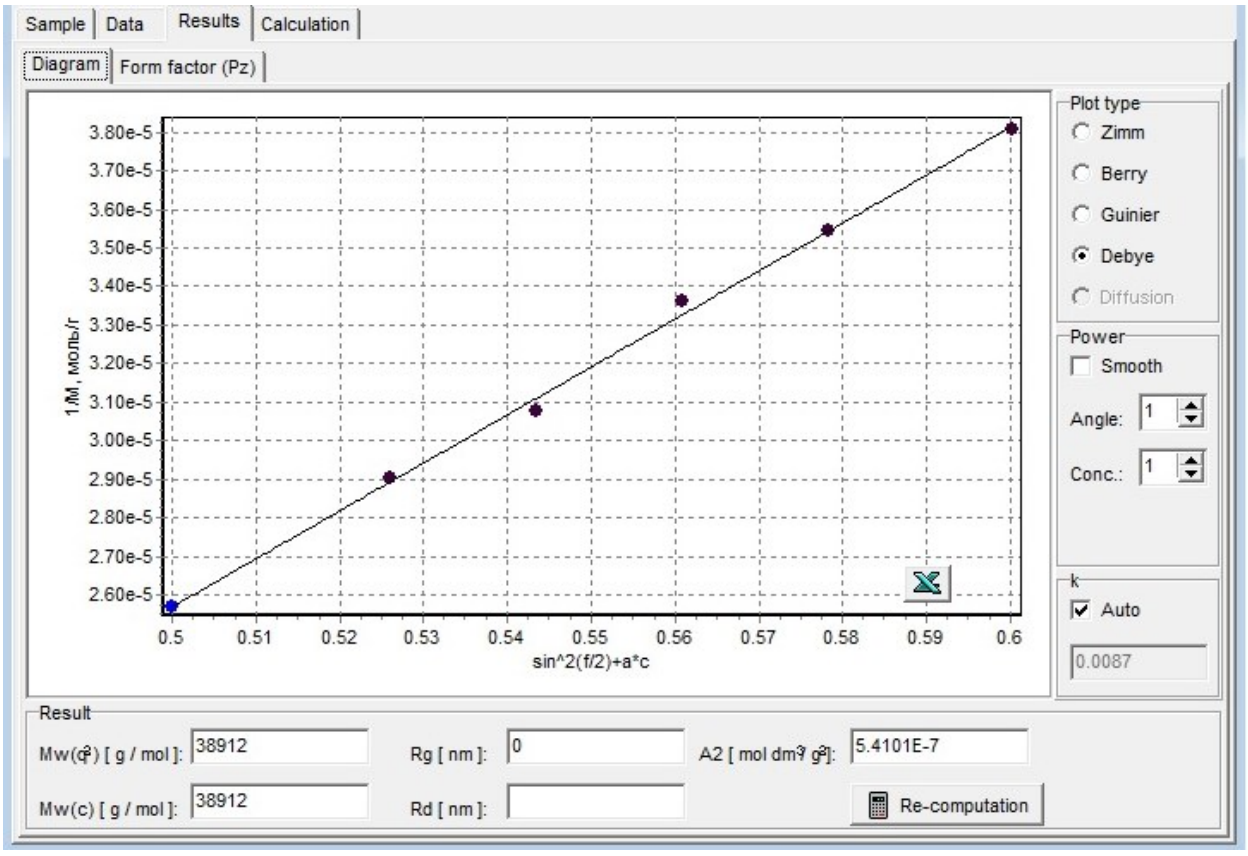


Figure S10. Debye plot for PPS synthesized in $cdcl_3$ at 0 °C (entry 14, Table 1) giving the desired Mw value.

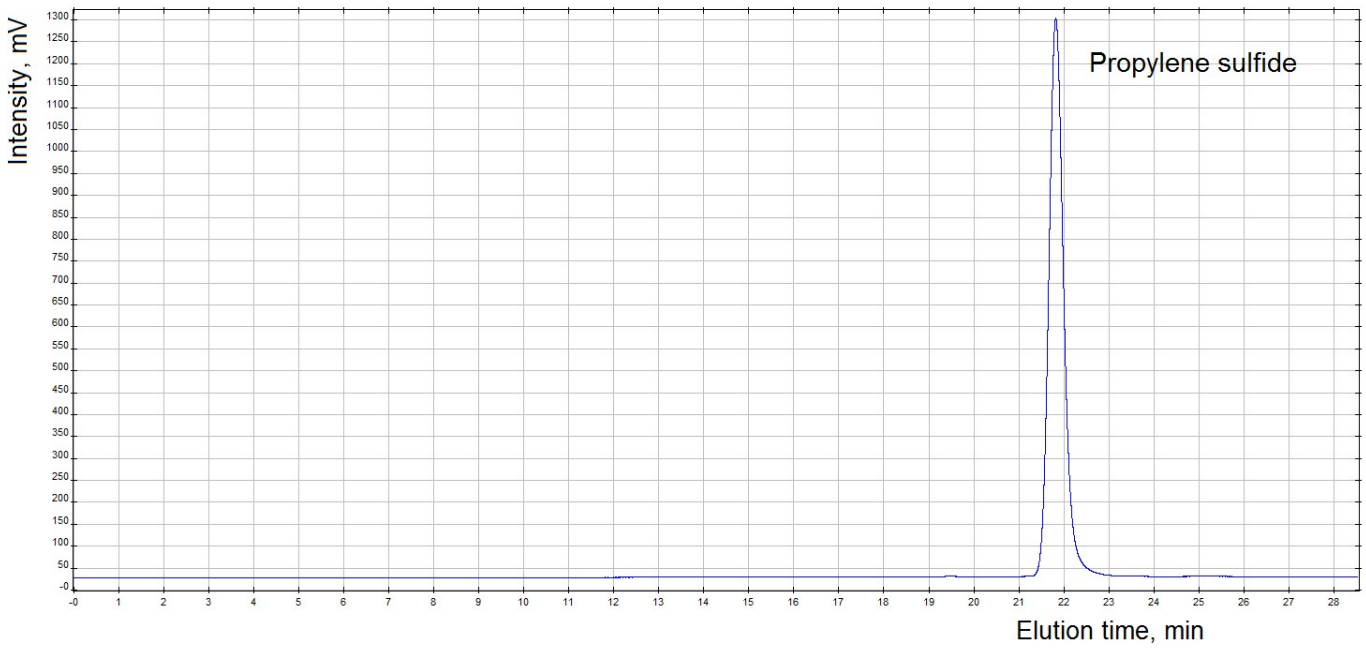


Figure S11. GPC trace recorded for the solution after the completion of test polymerization of PS carried out for 5 h at 80 ^{o}C under N_2 atmosphere without addition of solvent or initiator.

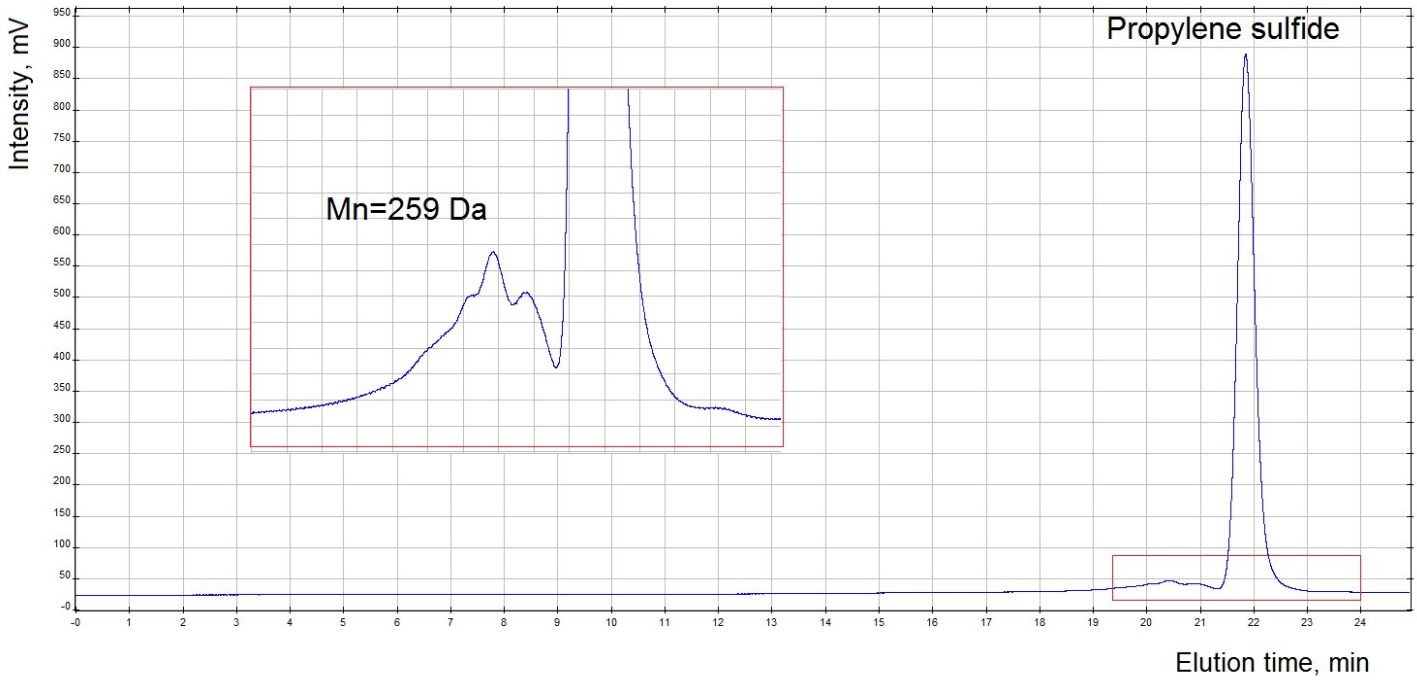


Figure S12. GPC trace recorded for the solution after the completion of test polymerization of PS carried out for 5 h at 120 ^{o}C in stainless still autoclave without addition of solvent or initiator.

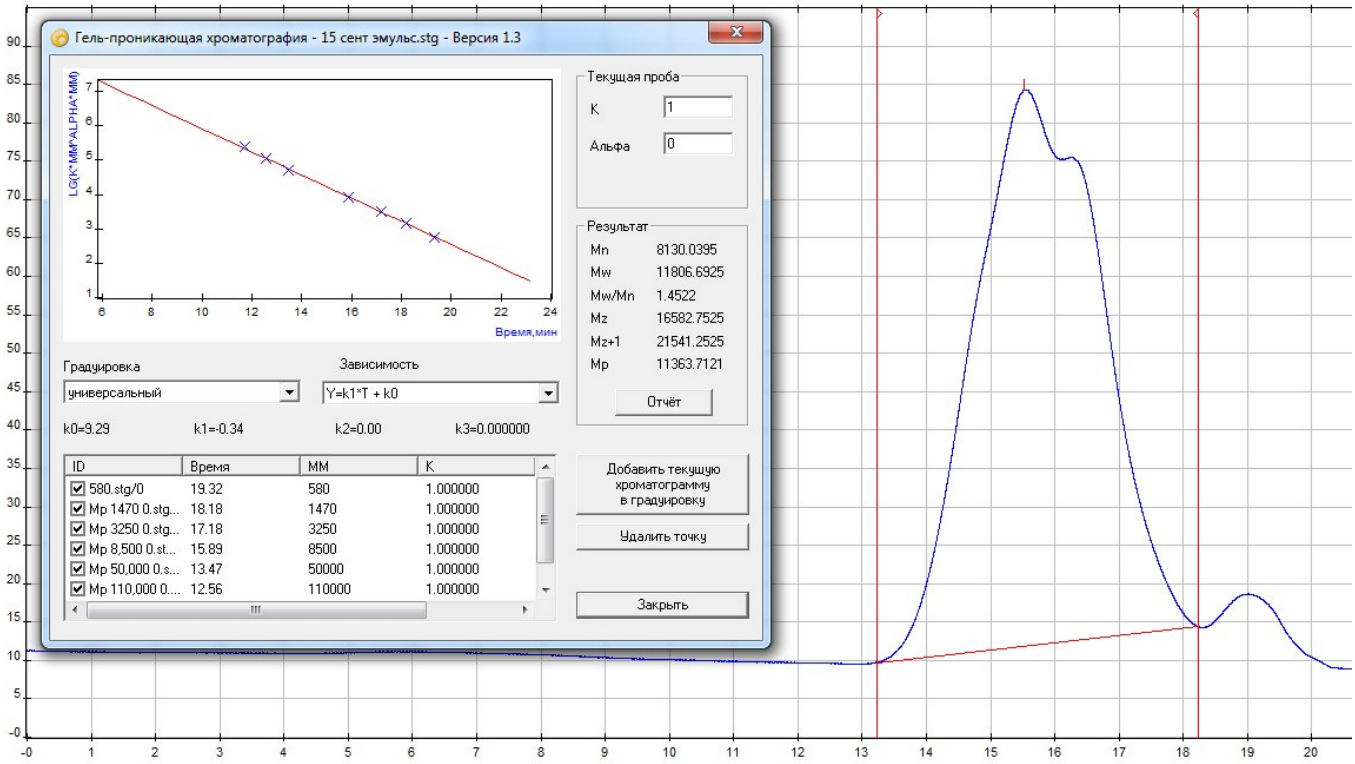


Figure S13. GPC trace recorded for PPS synthesized via emulsion polymerization technique at [monomer]/[initiator] ratio equal to 25 (entry 2, Table S2).

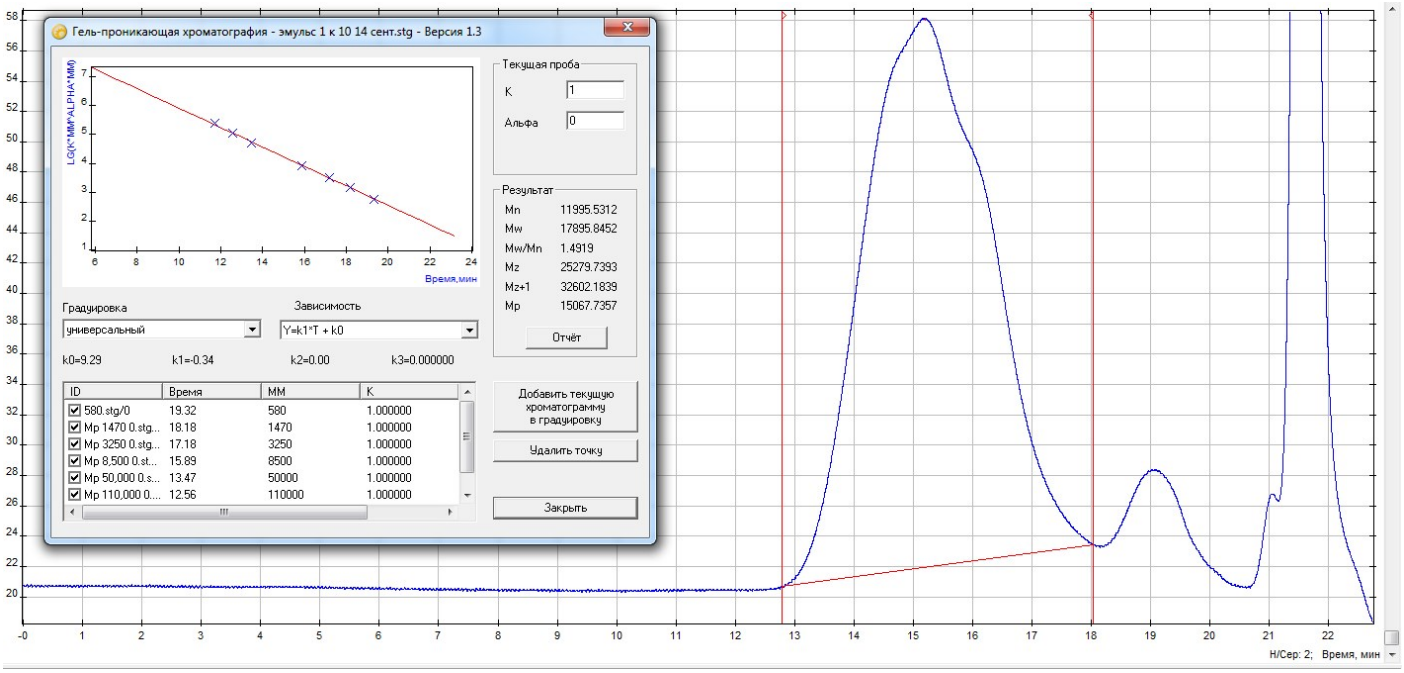
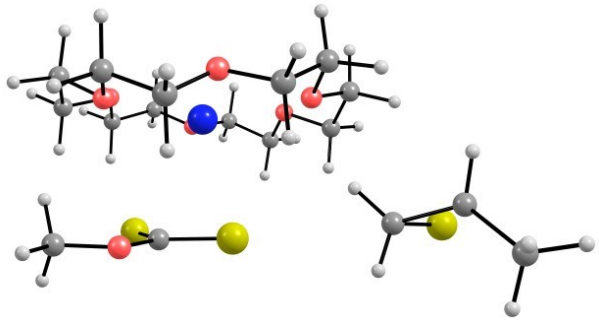


Figure S14. GPC trace recorded for PPS synthesized via emulsion polymerization technique at [monomer]/[initiator] ratio equal to 10 (entry 1, Table S2).

Calculated atomic coordinates, frequencies and energies

Complex **a1** (Figure 5)



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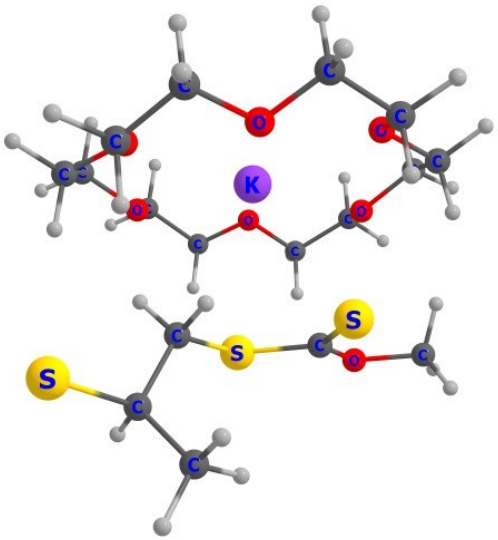
Complex **a3** (Figure 5)



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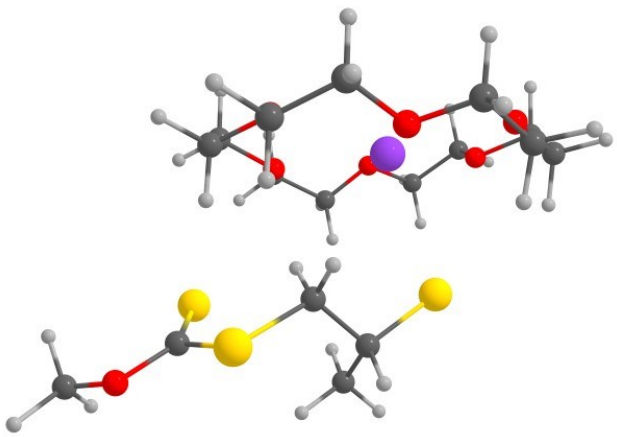

atomic coordinates:
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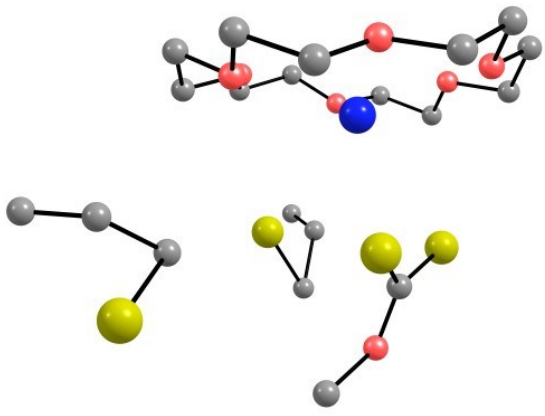
O	-5.354739000	0.584898000	0.665417000
C	-1.380439000	0.609355000	1.240995000
C	-0.912770000	0.072563000	2.595966000
H	-1.364084000	-0.169206000	0.468781000
H	-0.736492000	1.436913000	0.925615000
H	-1.037607000	0.873552000	3.335534000
C	-1.737130000	-1.132012000	3.042795000
H	-1.401398000	-1.471976000	4.025780000
H	-2.806382000	-0.890366000	3.107653000
H	-1.612436000	-1.956732000	2.333100000
S	0.877513000	-0.318624000	2.457651000

Zero-point correction= 0.513413 (Hartree/Particle)
Thermal correction to Energy= 0.547245
Thermal correction to Enthalpy= 0.548189
Thermal correction to Gibbs Free Energy= 0.445751
Sum of electronic and zero-point Energies= -2987.675972
Sum of electronic and thermal Energies= -2987.642139
Sum of electronic and thermal Enthalpies= -2987.641195
Sum of electronic and thermal Free Energies= -2987.743633

Number of imaginary frequencies = 0
Lowest frequency = 20.575

Complex **b1** (Figure 5)



atomic coordinates:

C	-0.68640300	0.10680200	0.05829900
H	-0.78006900	0.13008400	1.15482000
H	0.38265400	0.14070700	-0.19754200
C	-1.29563200	-1.16327400	-0.47453500
H	-0.83928100	-2.02143400	0.04015900
H	-2.37957100	-1.17684300	-0.28830000
C	-1.40916500	-2.47355600	-2.42519300
H	-2.49482100	-2.61279400	-2.33143400
H	-0.89377100	-3.29392400	-1.90449500
C	-1.00849400	-2.47992600	-3.87812600
H	0.06937700	-2.28125600	-3.97588600
H	-1.22150300	-3.46949500	-4.30827600
C	-1.48425000	-1.46066700	-5.94236200
H	-0.42686000	-1.21449600	-6.12176100
H	-1.69325300	-2.44519300	-6.38570300
C	-2.37629100	-0.42903700	-6.58393500
H	-3.42673300	-0.64146200	-6.34332200
H	-2.24194600	-0.45818300	-7.67510700
C	-2.82340900	1.88059700	-6.61532800
H	-2.86194000	1.81168800	-7.71230500
H	-3.84814400	1.79301900	-6.22439500
C	-2.20910600	3.20309600	-6.23250000
H	-1.16917800	3.23553100	-6.58837100
H	-2.76657300	4.02559200	-6.70569000
C	-1.40888800	4.39866500	-4.38244600
H	-0.35528700	4.14471900	-4.57009200
H	-1.64171800	5.32566200	-4.92856500
C	-1.63636900	4.62891900	-2.91069800
H	-1.00144700	5.46271100	-2.57670800
H	-2.68654500	4.89046700	-2.72185500
C	-1.47422300	3.57441100	-0.81222700
H	-1.04968000	4.52475000	-0.45753500
H	-2.54663700	3.55758400	-0.56349600
C	-0.75374500	2.43819400	-0.13461000
H	0.30546300	2.44455300	-0.43098900
H	-0.80580100	2.56806500	0.95750100
C	-5.76243800	-0.08387400	-2.82967600
C	-7.33037100	0.34548800	-1.05394000
H	-6.61779000	0.92829400	-0.46415800

H	-7.35832500	-0.67913700	-0.67774000
H	-8.32122600	0.79708200	-1.01711200
O	-1.35266400	1.21627200	-0.51534900
O	-1.03226200	-1.22927200	-1.86282200
O	-1.74852500	-1.48376100	-4.55413400
O	-2.01498600	0.84753000	-6.08529400
O	-2.24048900	3.34266800	-4.82368200
O	-1.29384200	3.44693800	-2.21071700
K	-2.41872700	0.94710100	-3.22432900
S	-5.44675100	0.17410400	-4.48245100
S	-4.71453100	-0.82989500	-1.72352200
O	-6.96417600	0.36820300	-2.43466700
C	-6.45761300	3.45135200	-3.17597400
C	-5.28978200	3.80989000	-4.00372500
H	-7.09829700	4.25856300	-2.83073100
H	-6.93374900	2.49063900	-3.34832800
H	-4.97478500	3.04215200	-4.70659300
C	-5.06105400	5.23470000	-4.43633800
H	-4.00993700	5.40185100	-4.68617300
H	-5.66086200	5.44750800	-5.32796800
H	-5.35071000	5.93342600	-3.64614400
S	-4.86419600	3.33324000	-2.28918200
C	-4.34498600	1.97520300	0.85289100
C	-3.42394500	1.99137800	2.00659300
H	-4.08573500	1.38175200	-0.02126400
H	-2.54464700	1.35895900	1.90823900
H	-4.91609800	2.88102100	0.65840100
C	-3.23533200	3.25517800	2.80838200
H	-2.88837500	3.03453800	3.82054800
H	-2.49120800	3.89691900	2.32155200
H	-4.17654000	3.80766700	2.87401100
S	-4.93981700	1.00505100	2.27941000

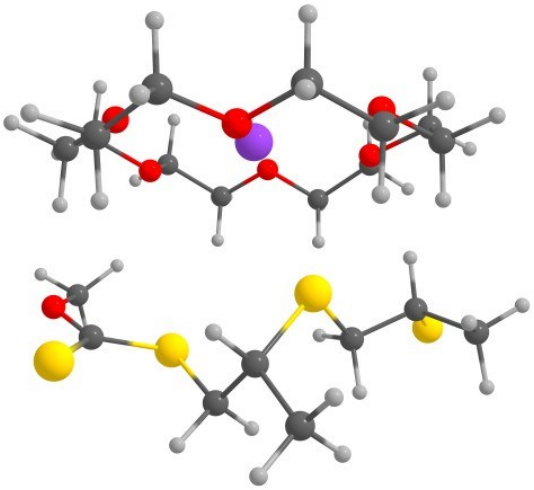
Zero-point correction= 0.596693 (Hartree/Particle)
Thermal correction to Energy= 0.637981
Thermal correction to Enthalpy= 0.638925
Thermal correction to Gibbs Free Energy= 0.517471
Sum of electronic and zero-point Energies= -3503.620115
Sum of electronic and thermal Energies= -3503.578827
Sum of electronic and thermal Enthalpies= -3503.577882

Sum of electronic and thermal Free Energies= -3503.699337

Number of imaginary frequencies = 0

Lowest frequency = 6.2737

Complex **b5** (Figure 5)



atomic coordinates:

KC20H39S4O7

C	-3.005691000	0.054978000	2.575323000
H	-3.949764000	-0.455721000	2.335783000
H	-3.123978000	0.619183000	3.511421000
C	-1.926213000	-0.987591000	2.709202000
H	-2.197395000	-1.693505000	3.506606000
H	-1.834138000	-1.548440000	1.767380000
C	0.337012000	-1.267390000	3.279572000
H	0.454098000	-1.954320000	2.426313000
H	0.099007000	-1.860815000	4.173555000
C	1.617584000	-0.503562000	3.506389000
H	1.459291000	0.280624000	4.260367000
H	2.396804000	-1.186187000	3.877277000
C	3.218067000	0.826841000	2.400163000
H	3.061975000	1.668782000	3.090200000
H	4.023727000	0.193829000	2.801041000
C	3.619355000	1.329900000	1.037210000
H	3.730191000	0.486719000	0.342906000
H	4.586902000	1.846853000	1.111664000
C	2.885816000	2.634643000	-0.768970000

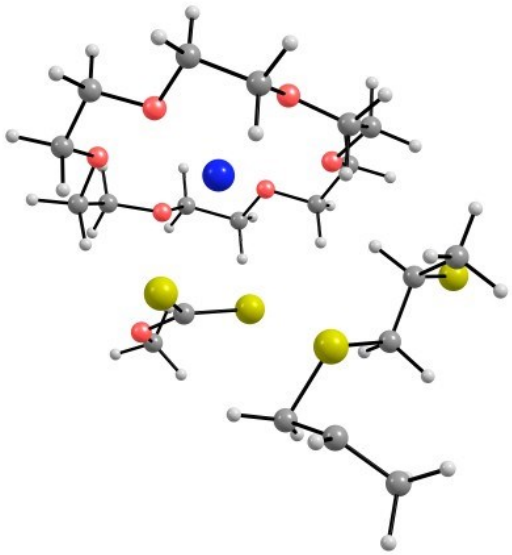
H	3.894563000	3.065729000	-0.841454000
H	2.827288000	1.768985000	-1.445257000
C	1.874625000	3.679415000	-1.163751000
H	1.900251000	4.518086000	-0.452769000
H	2.123327000	4.061809000	-2.163915000
C	-0.412768000	4.007812000	-1.587366000
H	-0.452467000	4.859052000	-0.892165000
H	-0.181002000	4.388227000	-2.592313000
C	-1.743265000	3.301677000	-1.619751000
H	-2.500232000	3.981174000	-2.037440000
H	-1.682711000	2.406335000	-2.256249000
C	-3.367726000	2.292595000	-0.271229000
H	-4.149425000	2.994319000	-0.596640000
H	-3.361260000	1.428251000	-0.950222000
C	-3.659304000	1.826630000	1.133925000
H	-3.703360000	2.673993000	1.832690000
H	-4.635298000	1.320078000	1.135090000
C	3.191269000	-1.835778000	-0.885417000
C	3.672114000	-2.640902000	1.342026000
H	3.484435000	-3.692160000	1.113281000
H	2.796437000	-2.178521000	1.802720000
H	4.538833000	-2.544281000	1.992472000
O	-2.638306000	0.926819000	1.520266000
O	-0.698845000	-0.341761000	3.016776000
O	2.022488000	0.075557000	2.276382000
O	2.625948000	2.222386000	0.562450000
O	0.586190000	3.092023000	-1.173174000
O	-2.099580000	2.926433000	-0.301329000
K	-0.037364000	1.513612000	1.022986000
S	3.710314000	-1.082846000	-2.260610000
S	1.604194000	-2.538212000	-0.610530000
O	4.024252000	-1.927232000	0.144873000
C	0.803632000	-2.383390000	-2.230691000
C	0.162168000	-1.032562000	-2.550878000
H	0.052561000	-3.178978000	-2.225795000
H	1.553752000	-2.627711000	-2.987825000
H	0.937336000	-0.260111000	-2.518974000
C	-0.442669000	-1.085749000	-3.953832000
H	-0.844196000	-0.108562000	-4.230734000
H	0.319310000	-1.370760000	-4.687285000

H	-1.256078000	-1.817274000	-4.004874000
S	-1.057010000	-0.476278000	-1.304678000
C	-2.088539000	-1.975438000	-1.029890000
C	-3.510349000	-1.579774000	-0.610395000
H	-1.613351000	-2.584239000	-0.256398000
H	-3.422513000	-0.735197000	0.081851000
H	-2.130885000	-2.560223000	-1.956546000
C	-4.310407000	-1.118806000	-1.829508000
H	-5.283156000	-0.722860000	-1.523768000
H	-3.776994000	-0.339995000	-2.392178000
H	-4.488083000	-1.967707000	-2.499362000
S	-4.320582000	-2.964427000	0.278949000

Zero-point correction= 0.600559 (Hartree/Particle)
Thermal correction to Energy= 0.639901
Thermal correction to Enthalpy= 0.640845
Thermal correction to Gibbs Free Energy= 0.525857
Sum of electronic and zero-point Energies= -3503.620968
Sum of electronic and thermal Energies= -3503.581626
Sum of electronic and thermal Enthalpies= -3503.580682
Sum of electronic and thermal Free Energies= -3503.695670

Number of imaginary frequencies = 0
Lowest frequency = 19.1009

Complex **c1**/**b3** (Figure 5)



Atomic coordinates:

KC20H39S4O7

C	-0.687984000	0.359350000	-0.015154000
H	-0.816967000	0.688694000	1.024754000
H	0.340081000	-0.002590000	-0.165317000
C	-1.682834000	-0.734854000	-0.296497000
H	-1.510409000	-1.565213000	0.403947000
H	-2.704255000	-0.355806000	-0.148128000
C	-2.372182000	-2.277978000	-1.919403000
H	-3.413723000	-2.005461000	-1.701515000
H	-2.092108000	-3.144253000	-1.301605000
C	-2.230262000	-2.646314000	-3.374226000
H	-1.184060000	-2.892134000	-3.608966000
H	-2.848215000	-3.534070000	-3.578019000
C	-2.684350000	-1.900575000	-5.551205000
H	-1.713738000	-2.322887000	-5.850715000
H	-3.465051000	-2.653389000	-5.738426000
C	-2.975466000	-0.663410000	-6.360962000
H	-3.915057000	-0.198139000	-6.031966000
H	-3.068475000	-0.946569000	-7.419916000
C	-2.023831000	1.370649000	-7.046712000
H	-1.978291000	1.051884000	-8.098523000
H	-2.984971000	1.871536000	-6.864943000
C	-0.889206000	2.321668000	-6.762768000
H	0.077466000	1.805787000	-6.859724000
H	-0.919458000	3.146507000	-7.489293000
C	-0.100093000	3.826330000	-5.128500000
H	0.918805000	3.412554000	-5.148130000
H	-0.157883000	4.649151000	-5.855533000
C	-0.422816000	4.352502000	-3.753153000
H	0.217923000	5.216440000	-3.525716000
H	-1.474091000	4.676119000	-3.720005000
C	-0.578605000	3.704942000	-1.500840000
H	-0.059213000	4.629203000	-1.208107000
H	-1.663311000	3.891191000	-1.467408000
C	-0.210633000	2.598628000	-0.544708000
H	0.868727000	2.394340000	-0.603101000
H	-0.457225000	2.901075000	0.484548000
C	-5.098232000	0.763907000	-3.607810000
C	-5.994077000	-1.462921000	-3.784438000

H	-6.668667000	-1.375298000	-2.930230000
H	-5.062326000	-1.941067000	-3.472295000
H	-6.466557000	-2.023484000	-4.590593000
O	-0.944787000	1.443011000	-0.893943000
O	-1.523352000	-1.182192000	-1.633441000
O	-2.658317000	-1.560694000	-4.177403000
O	-1.900324000	0.246879000	-6.193900000
O	-1.043961000	2.823992000	-5.449329000
O	-0.203603000	3.319737000	-2.811086000
K	-1.804451000	0.997605000	-3.457029000
S	-4.740124000	2.183633000	-4.478728000
S	-4.726320000	0.486433000	-1.977442000
O	-5.714870000	-0.177572000	-4.342868000
C	-6.846316000	3.221290000	-1.613462000
C	-6.868155000	4.588377000	-1.058437000
H	-7.216699000	2.409657000	-0.992450000
H	-6.896293000	3.064467000	-2.688086000
H	-6.867361000	5.397756000	-1.784712000
C	-7.515409000	4.900343000	0.263014000
H	-6.989627000	5.703094000	0.784360000
H	-8.536780000	5.234881000	0.059385000
H	-7.572715000	4.022152000	0.908172000
S	-5.193335000	3.781879000	-1.116554000
C	-4.888254000	3.026543000	0.554223000
C	-3.395595000	3.110396000	0.857421000
H	-5.230032000	1.994023000	0.471397000
H	-2.858134000	2.621773000	0.033740000
H	-5.469850000	3.576770000	1.297515000
C	-2.949388000	4.568247000	0.983463000
H	-1.883271000	4.621056000	1.219678000
H	-3.117948000	5.147784000	0.063815000
H	-3.494772000	5.053353000	1.800653000
S	-3.102338000	2.152274000	2.388336000

Zero-point correction= 0.598987 (Hartree/Particle)
Thermal correction to Energy= 0.639004
Thermal correction to Enthalpy= 0.639949
Thermal correction to Gibbs Free Energy= 0.523857
Sum of electronic and zero-point Energies= -3503.587802
Sum of electronic and thermal Energies= -3503.547785

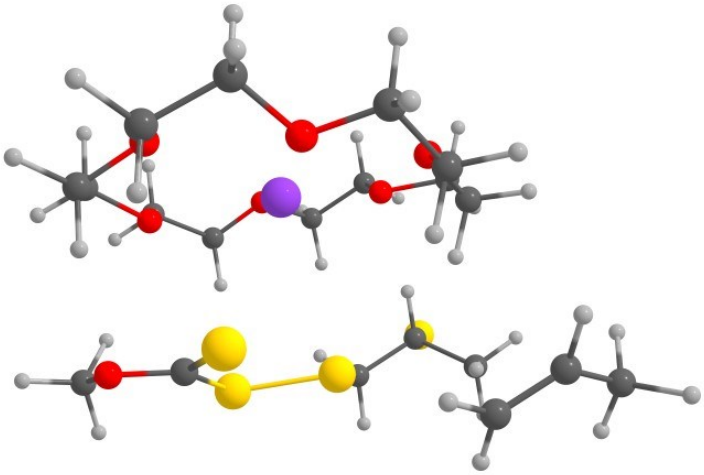
Sum of electronic and thermal Enthalpies= -3503.546840

Sum of electronic and thermal Free Energies= -3503.662932

Number of imaginary frequencies = 0

Lowest frequency = 18.0795

Complex **c3** (Figure 5)



Atomic coordinates:

KC20H39S4O7

C	1.547614000	-1.392644000	-3.050824000
H	2.599818000	-1.693372000	-3.151439000
H	1.130292000	-1.201307000	-4.049125000
C	0.811429000	-2.508282000	-2.352507000
H	0.862187000	-3.421260000	-2.962674000
H	1.296399000	-2.713664000	-1.388477000
C	-1.250050000	-3.099020000	-1.404387000
H	-0.842324000	-3.160205000	-0.384404000
H	-1.153165000	-4.087354000	-1.876108000
C	-2.709092000	-2.724443000	-1.370650000
H	-3.081381000	-2.608189000	-2.398227000
H	-3.282359000	-3.528701000	-0.885404000
C	-4.231163000	-1.067149000	-0.737070000
H	-4.534999000	-1.002273000	-1.791566000
H	-4.890900000	-1.787519000	-0.230282000
C	-4.376128000	0.281549000	-0.081799000
H	-4.060072000	0.242509000	0.968210000
H	-5.436795000	0.570870000	-0.119978000

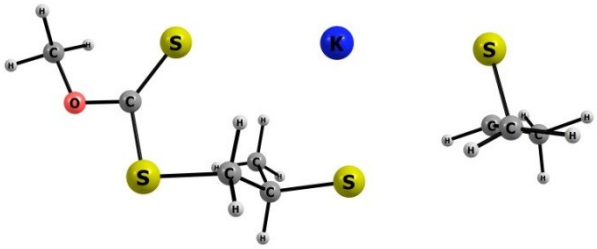
C	-3.794259000	2.538949000	-0.291617000
H	-4.832296000	2.852138000	-0.475008000
H	-3.602271000	2.560577000	0.790235000
C	-2.853146000	3.483750000	-0.994291000
H	-3.007456000	3.449099000	-2.082595000
H	-3.051899000	4.507318000	-0.646143000
C	-0.569756000	4.072840000	-1.079321000
H	-0.668286000	4.286558000	-2.153434000
H	-0.719997000	5.006361000	-0.519097000
C	0.802238000	3.519050000	-0.790214000
H	1.560016000	4.300037000	-0.948982000
H	0.856965000	3.183523000	0.256856000
C	2.299192000	1.825256000	-1.461035000
H	3.101291000	2.568203000	-1.582528000
H	2.360902000	1.409833000	-0.442405000
C	2.463086000	0.724848000	-2.480355000
H	2.388337000	1.128767000	-3.499911000
H	3.451900000	0.257797000	-2.355310000
C	-1.746897000	-0.652571000	2.328044000
C	-3.210595000	-2.559399000	2.507077000
H	-2.641229000	-3.086296000	3.276855000
H	-2.962111000	-2.931515000	1.509334000
H	-4.276507000	-2.661124000	2.697693000
O	1.441855000	-0.226835000	-2.251126000
O	-0.542076000	-2.127390000	-2.151737000
O	-2.883441000	-1.506812000	-0.660768000
O	-3.588884000	1.226873000	-0.786157000
O	-1.525503000	3.107662000	-0.681036000
O	1.032262000	2.428399000	-1.661772000
K	-0.886854000	0.430199000	-1.022135000
S	-1.536330000	0.981145000	2.220248000
S	-0.476839000	-1.857716000	2.184691000
O	-2.952488000	-1.147069000	2.569824000
C	2.616659000	2.494723000	2.617887000
C	3.455675000	3.149762000	1.813573000
H	2.954637000	1.657473000	3.225298000
H	1.566700000	2.764140000	2.694280000
H	3.076570000	3.981277000	1.218303000
C	4.910628000	2.826253000	1.645242000
H	5.125623000	2.537510000	0.609559000

H	5.533232000	3.698451000	1.870307000
H	5.212347000	2.002796000	2.298150000
S	1.179751000	-0.680503000	1.682555000
C	2.274495000	-2.100717000	1.183393000
C	3.321984000	-1.607027000	0.186289000
H	1.642748000	-2.864920000	0.725079000
H	2.775094000	-1.128984000	-0.631996000
H	2.745916000	-2.514253000	2.079005000
C	4.238651000	-0.564008000	0.823540000
H	4.967693000	-0.202925000	0.091900000
H	3.676953000	0.304909000	1.197677000
H	4.790304000	-1.002483000	1.663203000
S	4.230992000	-3.051459000	-0.478743000

Zero-point correction= 0.596418 (Hartree/Particle)
Thermal correction to Energy= 0.637851
Thermal correction to Enthalpy= 0.638795
Thermal correction to Gibbs Free Energy= 0.518935
Sum of electronic and zero-point Energies= -3503.586851
Sum of electronic and thermal Energies= -3503.545419
Sum of electronic and thermal Enthalpies= -3503.544474
Sum of electronic and thermal Free Energies= -3503.664335

Number of imaginary frequencies = 0
Lowest frequency = 20.6276

Prereaction (propagation) thiolate-PS complex (no 18-crown-6)



Atomic coordinates:

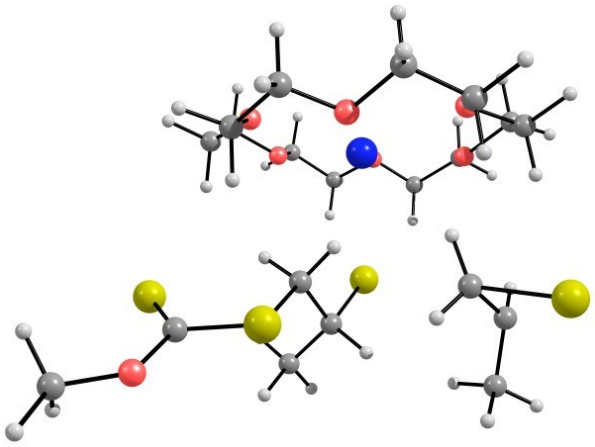
C	3.60221600	0.17919800	-0.17246300
C	5.61038300	1.32316700	0.43244800
H	5.22712800	1.66216400	1.39620100
H	5.48593800	2.10899900	-0.31433900
H	6.65150400	1.01899500	0.51057600
K	-0.96329200	1.56621200	0.08651700

S	3.12003400	-1.41664300	-0.72179700
S	2.66423800	1.52468800	0.05189300
O	4.91256200	0.14037000	0.01780200
C	1.29899500	-1.30323000	-0.85239300
C	0.51193900	-1.84269800	0.34735200
H	1.07158000	-0.25482600	-1.05464300
H	1.04903800	-1.87807500	-1.74666500
H	0.67479900	-2.92642700	0.38422100
C	0.94964700	-1.25978600	1.68970300
H	0.36746100	-1.71750000	2.49298400
H	2.01283000	-1.44401000	1.88749300
H	0.78391600	-0.17852000	1.72929800
S	-1.27225800	-1.54321200	0.01212600
C	-4.37734500	-0.29105100	-1.12611600
C	-4.59041600	-0.24342200	0.33249700
H	-5.25102100	-0.41583900	-1.75979900
H	-3.76138500	-0.61968400	0.92897200
H	-3.45057300	-0.72420800	-1.49196900
C	-5.96995400	-0.43997100	0.90744700
H	-6.16125200	-1.51095600	1.03136600
H	-6.06195200	0.04056300	1.88413100
H	-6.72938500	-0.02383000	0.23994100
S	-4.20697400	1.38822500	-0.42065100

Zero-point correction= 0.223131 (Hartree/Particle)
Thermal correction to Energy= 0.243145
Thermal correction to Enthalpy= 0.244089
Thermal correction to Gibbs Free Energy= 0.168266
Sum of electronic and zero-point Energies= -2581.287395
Sum of electronic and thermal Energies= -2581.267382
Sum of electronic and thermal Enthalpies= -2581.266437
Sum of electronic and thermal Free Energies= -2581.342261

Number of imaginary frequencies = 0
Lowest frequency = 7.7166

Thiolate+18-crown-6 – PS complex (propagation)



Atomic coordinates:

C	-4.50135700	-1.15887600	-1.10562400
H	-5.22645400	-0.57600900	-1.69107900
H	-5.04733700	-1.91900200	-0.52768800
C	-3.52282500	-1.82989200	-2.03624800
H	-4.08011000	-2.39560300	-2.79705500
H	-2.89688800	-1.07738000	-2.53844000
C	-1.81754500	-3.44774700	-2.09610600
H	-1.18971500	-2.75818500	-2.67823300
H	-2.38618500	-4.09035100	-2.78391700
C	-0.94780500	-4.30494800	-1.21071600
H	-1.56921700	-4.92136200	-0.54415300
H	-0.33748000	-4.97148000	-1.83668900
C	0.79082000	-4.14938200	0.38301900
H	0.24466600	-4.68137200	1.17609700
H	1.36275400	-4.88428100	-0.20149600
C	1.74471400	-3.14578700	0.98097400
H	2.26237700	-2.59641100	0.18183300
H	2.49677800	-3.66981200	1.58833500
C	1.83050800	-1.28434700	2.42413300
H	2.66232900	-1.77994100	2.94545900
H	2.25661400	-0.59336400	1.68285700
C	1.00247300	-0.53760000	3.43762200
H	0.56864400	-1.25332500	4.15087000
H	1.64386200	0.16275300	3.99120000
C	-0.94201200	0.72479300	3.72093200
H	-1.41479500	-0.08360500	4.29744300
H	-0.40722000	1.38393900	4.41974100
C	-1.99833800	1.52437900	3.00289900
H	-2.67992100	1.95721400	3.74921000

H	-1.54380200	2.34903400	2.43642500
C	-3.82230000	1.29546600	1.52591000
H	-4.46491300	1.74953500	2.29384300
H	-3.48130600	2.09195100	0.84931600
C	-4.61584400	0.26216200	0.76726400
H	-4.97217300	-0.52345300	1.44977400
H	-5.48895200	0.74958400	0.30985700
C	4.44220400	0.71288100	-0.16815300
C	6.79492100	0.91756200	0.16961400
H	7.05115900	0.59554300	-0.84106000
H	6.85211000	0.06918200	0.85382300
H	7.44152400	1.72841500	0.49712000
O	-3.78846000	-0.30447400	-0.22916000
O	-2.70835600	-2.70784100	-1.27737800
O	-0.11230200	-3.45305900	-0.45045000
O	1.00635000	-2.24650800	1.79150200
O	-0.03713000	0.16966000	2.78169600
O	-2.71026100	0.65970800	2.13584400
K	-1.25056300	-1.12825100	0.50532500
S	3.00125000	1.70369200	0.01974200
S	4.54148600	-0.85902800	-0.65201900
O	5.47247700	1.47157700	0.18561000
C	1.62183100	0.67335500	-0.61177300
C	1.14576000	1.03846800	-2.01911100
H	1.93393300	-0.37525300	-0.56942800
H	0.82741800	0.83534300	0.12260600
H	0.92410800	2.11400800	-2.03230500
C	2.21836200	0.75904200	-3.06904900
H	1.85953800	1.05909800	-4.05701600
H	3.14517700	1.30844600	-2.85700700
H	2.44855500	-0.31086200	-3.09747900
S	-0.40757100	0.11619700	-2.34116600
C	-0.97391400	3.02369200	-0.20645500
C	-1.76705200	3.39312000	-1.38986800
H	0.08609800	3.26576200	-0.20633700
H	-2.60676300	2.73568700	-1.60500100
H	-1.24163500	2.10753200	0.31600800
C	-1.10189400	4.00524900	-2.59482800
H	-0.74245900	3.19763200	-3.24286500
H	-1.80207400	4.62320100	-3.16189100

H	-0.25274700	4.62518300	-2.29248400
S	-2.06876400	4.45455900	0.08098700

Zero-point correction= 0.598669 (Hartree/Particle)

Thermal correction to Energy= 0.639037

Thermal correction to Enthalpy= 0.639981

Thermal correction to Gibbs Free Energy= 0.521414

Sum of electronic and zero-point Energies= -3503.612465

Sum of electronic and thermal Energies= -3503.572097

Sum of electronic and thermal Enthalpies= -3503.571153

Sum of electronic and thermal Free Energies= -3503.689721

Number of imaginary frequencies = 0

Lowest frequency = 12.0871