

Antioxidant Activity of Propyl Gallate in Aqueous and Lipid Media.

A Theoretical Study

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Supporting Information

Cartesian coordinates relative energies of main stationary points and imaginary frequencies of transition states for studied reactions.

Transition states geometries calculated in water.

Neutral PG

TS($\bullet$ OOH)₃(OH)
H= -915.261264
G= -915.327475
if= -2440.7221
O 2

C	0.0118021293	0.0212227552	0.0071391804
C	0.0010227579	0.0497559641	1.4144458769
H	0.9230158064	0.1012251923	1.9746046822
C	-1.1930091722	0.0104954474	2.1014038603
O	-1.1944015474	0.037632351	3.4655480191
H	-2.1022936816	0.0020088944	3.7926677616
C	-2.3937337731	-0.0601357368	1.3903181375
O	-3.5436236716	-0.1134144044	2.0765688525
H	-4.2870764583	-0.1245774805	1.4537471891
C	-2.3852256383	-0.0888763201	-0.0245203836
O	-3.5561988997	-0.1287269133	-0.6461548979
H	-3.8716188624	-1.2001512729	-0.7276707636
C	-1.162253799	-0.0488045154	-0.7120941988
H	-1.1651868219	-0.0748029401	-1.7919393504
C	1.2914303211	0.0561504702	-0.7470780646
O	1.3556492391	0.1062313026	-1.9590358536
O	2.3605389688	0.0192105374	0.0375939257
C	3.654787979	0.0379411748	-0.6245749282
H	3.7313405136	0.9632461685	-1.1936797954
H	3.6998479302	-0.8101807337	-1.3060666769
C	4.7146173967	-0.0494522755	0.4472819013
H	4.600927357	0.7914560456	1.1327970838
H	4.5704505054	-0.9680188127	1.017545431
C	6.1027985706	-0.0312339197	-0.1853781791
H	6.2622648089	0.8898444167	-0.7476953288
H	6.8760352885	-0.098705333	0.5786501982
H	6.2293881489	-0.8716492096	-0.8694018118
O	-3.9343788719	-2.4625082207	-0.5898027293
O	-2.782223523	-2.7320244277	0.071133293
H	-3.0284959126	-2.7988869907	1.0091942521

TS($\bullet$ OOCH₃)₃(OH)
H= -954.537339
G= -954.607474
if= -2617.0141
O 2

C	0.0222803459	0.0226454927	-0.0171053526
C	0.0253495064	-0.0457113431	1.3890712918
H	0.9534021896	-0.0946391047	1.9391391526
C	-1.1632252773	-0.0552731516	2.0868671828
O	-1.1500591637	-0.1285744788	3.4498947613
H	-2.0549006536	-0.1543076975	3.7862626341
C	-2.3716393537	0.0026948925	1.3896948939
O	-3.5150625252	-0.01598782	2.0868547435
H	-4.2634697681	0.0092822911	1.4692091292
C	-2.3801890933	0.0634895372	-0.0248021983
O	-3.5557622402	0.1059274113	-0.6293609168
H	-3.7628074038	-0.9464923168	-1.0260480321

C	-1.1597986437	0.0787344111	-0.7232683659
H	-1.173077267	0.1212301629	-1.8026622616
C	1.2957134724	0.0212818736	-0.7820692492
O	1.3518452697	0.0627502815	-1.9947213253
O	2.3694796957	-0.0343023539	-0.0048900685
C	3.6594267709	-0.0635198356	-0.6747715128
H	3.7530439403	0.8414348738	-1.2730179545
H	3.6818197264	-0.9336860553	-1.329122669
C	4.7222206611	-0.1413388084	0.3949711635
H	4.6342260594	0.7259475787	1.0507356829
H	4.5557899307	-1.0347638263	0.9983218092
C	6.1075923113	-0.184287694	-0.242361756
H	6.2899913289	0.711646496	-0.8374853838
H	6.8820049903	-0.2460230284	0.5210484858
H	6.2084098552	-1.0516664791	-0.8963748871
O	-3.7415463848	-2.1783966884	-1.1987539771
O	-2.7101932387	-2.5490191812	-0.4039822117
C	-3.2108362667	-3.1362068769	0.8078172431
H	-2.3368149725	-3.2979121209	1.4326984772
H	-3.9130251035	-2.4499393525	1.2771641923
H	-3.6964476979	-4.0787280889	0.5622052799

TS($\bullet$ OOCHCH₂)₃(OH)
H= -992.623781
G= -992.693727
if= -2238.08
O 2

C	-0.2620978649	0.1012960313	0.0546890987
C	-0.2815598007	0.1105634015	1.4564763761
H	0.6345301748	0.0752561378	2.0274076998
C	-1.4922765777	0.1995372784	2.1382959388
O	-1.4835115233	0.229534727	3.5003636079
H	-2.3909306688	0.2650026447	3.830348202
C	-2.6809302634	0.2048226781	1.4301287657
O	-3.8473765175	0.2093641236	2.1135463649
H	-4.5769720909	0.1655406244	1.4764005988
C	-2.667810282	0.1226448711	0.0216018243
O	-3.8252634811	-0.0587260957	-0.5969789264
H	-3.8822123416	-1.2142983954	-0.7755565171
C	-1.440944215	0.1220004755	-0.6651746272
H	-1.4455310826	0.0716418255	-1.7442524864
C	1.0138628082	-0.0070290503	-0.6938645505
O	1.0865604437	0.0390147631	-1.9058105215
O	2.0697806265	-0.1728368811	0.0925504186
C	3.358007728	-0.2999022709	-0.5696806222
H	3.5391856213	0.6122291617	-1.1365490663
H	3.3065639917	-1.1460772859	-1.2529185456
C	4.4013208358	-0.5094493018	0.5010482773
H	4.3963809808	0.3450331255	1.1789895861
H	4.1443042791	-1.397634194	1.0799357072
C	5.7782227071	-0.6743891798	-0.1345540374
H	6.0537742168	0.2141357907	-0.7043127373
H	6.5381761513	-0.8365704884	0.6287265991
H	5.7928381466	-1.5286368919	-0.8129873392
O	-3.6954679599	-2.4336415958	-0.7887025814
O	-2.3382482764	-2.520230967	-0.6449617817
C	-1.9461122443	-2.8736712159	0.6096284849

C -0.6372060452 -2.9744985025 0.855957904
H -2.7534815418 -3.025926973 1.3120426053
H -0.310941894 -3.2635840454 1.8435789949
H 0.0943010298 -2.808081807 0.0771828095

TS($\bullet$ OOH)_{4(OH)}
H= -915.264958
G= -915.330834
if= -2038.7051
O 2

C -0.3262623042 0.5352423588 -0.3076233345
C -0.0080563495 -0.8223081058 -0.3392291127
H -0.7625716447 -1.5841680619 -0.219322372
C 1.3126075157 -1.1881617669 -0.5170855866
O 1.6625979496 -2.4908473334 -0.5313158587
H 2.6148082276 -2.562974154 -0.6910658664
C 2.3143376221 -0.202974078 -0.6735243339
O 3.5768794327 -0.5554988094 -0.8810609894
H 4.0623105359 -0.7027474852 0.0967047918
C 1.9545568258 1.1639255029 -0.6373339556
O 2.9174171825 2.1003571961 -0.778350516
H 3.7647179138 1.6599482473 -0.939780486
C 0.6372508425 1.5336160885 -0.4536576282
H 0.3654544674 2.5781285797 -0.4260620372
C -1.7373347764 0.9759524894 -0.1097995244
O -2.0596577696 2.1367423117 0.0379834454
O -2.6023092568 -0.027197271 -0.1160147038
C -4.002785931 0.3194064495 0.0685086327
H -4.296016952 0.984198843 -0.7426650655
H -4.100541804 0.8424585545 1.0184665755
C -4.7915963198 -0.9678987341 0.0569234038
H -4.6295996613 -1.4794268922 -0.8927576811
H -4.4233628983 -1.616177127 0.8533726148
C -6.2761435757 -0.6782033141 0.2554364587
H -6.6620156628 -0.048813378 -0.547758422
H -6.8501507741 -1.6037234996 0.2647324855
H -6.4486776892 -0.1638298371 1.201914838
O 4.2592055491 -0.7505735133 1.3847628295
O 3.0327032106 -0.4400829439 1.85403198
H 3.0446802241 0.5186883433 2.0211333584

TS($\bullet$ OOCH₃)_{4(OH)}
H= -954.541459
G= -954.610255
if= -2249.64
O 2

C -0.0389120679 0.1341572469 -0.0316968237
C -0.050927615 0.0504142364 1.3588372082
H 0.8613907046 -0.0002955844 1.9325951641
C -1.2704217657 0.0190723551 2.0106116857
O -1.3167065337 -0.0846556795 3.3531100941
H -2.2384629533 -0.0723073385 3.6486887188
C -2.480106408 0.0678281682 1.2756822092
O -3.6514174373 0.0506578801 1.8910189801
H -3.8550883686 -1.009272746 2.2084589475
C -2.4255702043 0.1612560796 -0.1358175087
O -3.5830041095 0.2037757538 -0.8298184196
H -4.3226338032 0.1836330664 -0.2043085245
C -1.2123569648 0.1928243557 -0.7882850374

H -1.1764743057 0.2582364539 -1.8654221562
C 1.2518297778 0.1549434957 -0.7781925267
O 1.3215952267 0.1462204422 -1.9900359648
O 2.3130758925 0.1798426508 0.0142098403
C 3.6134373607 0.1739880574 -0.637748336
H 3.6792522998 1.0576002801 -1.2707932126
H 3.6786736303 -0.7204707656 -1.2552721226
C 4.66260978 0.1825187902 0.4477120583
H 4.52261906 1.0655860194 1.0725320873
H 4.5301199712 -0.6982756227 1.0776275845
C 6.0581584763 0.1869824027 -0.1685153824
H 6.207620467 1.0735268661 -0.7865115401
H 6.8212526086 0.1838832772 0.6085610526
H 6.2101825695 -0.6928289308 -0.7953705935
O -3.7565642379 -2.2751106491 2.3348459696
O -2.5901345184 -2.4997928288 1.6947435331
C -2.8312196689 -3.0673267741 0.3940267145
H -3.5565625004 -2.4534704891 -0.1359938449
H -3.2031303694 -4.0814653944 0.5260253804
H -1.8655719926 -3.0659330748 -0.1036552344

TS($\bullet$ OOCHCH₂)_{4(OH)}
H= -992.626937
G= -992.697911
if= -2174.94
O 2

C -0.2192376812 0.2979554113 -0.0140709209
C -0.2247793783 0.1666128439 1.3705322736
H 0.6906405809 0.1035693578 1.9382365705
C -1.4446514015 0.0907490718 2.0208602258
O -1.490951861 -0.067436423 3.3583507542
H -2.4158113156 -0.1285608256 3.6401000739
C -2.6536799688 0.1262956965 1.2856023218
O -3.8150852058 -0.069777549 1.8930614297
H -3.918654733 -1.197365218 2.0107110412
C -2.6080068622 0.3046719369 -0.1140546883
O -3.7717466884 0.3237038356 -0.8097268523
H -4.5064296234 0.2409108733 -0.1844141473
C -1.4006745036 0.3923762453 -0.7640143548
H -1.3646170049 0.4975301934 -1.8382732104
C 1.0660136623 0.3432621374 -0.7670335823
O 1.1334709662 0.5798690806 -1.9556921891
O 2.1248179619 0.0913050411 -0.0113197094
C 3.417536784 0.1268953978 -0.6771722852
H 3.557711663 1.1259951538 -1.0872510269
H 3.4004825515 -0.5981614575 -1.4893946285
C 4.4702213371 -0.2076372942 0.3516538336
H 4.4005007319 0.5019812997 1.1771913173
H 4.2789850104 -1.2048659711 0.7501353633
C 5.8568277882 -0.1469725467 -0.2814720214
H 6.0618724181 0.8511023527 -0.6711423582
H 6.6260132512 -0.3887267811 0.4507263047
H 5.9396999036 -0.8558983008 -1.1065477083
O -3.7279759083 -2.4526545377 1.9530587573
O -2.402246827 -2.5049166329 1.6541128824
C -2.1520687129 -2.8970131344 0.3654910555
H -3.0378166223 -3.0546795792 -0.2332370155
C -0.8842324625 -3.0282086656 -0.0164640704
H -0.6718231353 -3.3357137899 -1.029168072

H	-0.0696727144	-2.850108222	0.6715156366
Deprotonated PG TS(•OOCH ₃) H= -954.092290 G= -954.161098 if= -2846.0190 -1 2			
C	0.4897941685	-0.3956900798	-0.4378469209
C	0.235153729	0.9943997333	-0.4218916636
H	1.0353033819	1.7006171134	-0.2577707966
C	-1.0435033899	1.4358510514	-0.6241911924
O	-1.3621478897	2.7570962736	-0.6268641038
H	-2.3154023832	2.778616412	-0.8161851271
C	-2.1397428651	0.5397969241	-0.8832728048
O	-3.2923685259	1.0138755678	-1.108014237
C	-1.8451302299	-0.8619091011	-0.8284420788
O	-2.8601513374	-1.7298595225	-0.9906370606
H	-3.5749614113	-1.4715465191	-0.3111840413
C	-0.5437753877	-1.3057344671	-0.6255505699
H	-0.3432987293	-2.3675332061	-0.603785805
C	1.8504022939	-0.927259196	-0.2383655842
O	2.1406623091	-2.1066201392	-0.2552178783
O	2.7628842039	0.0310868394	-0.0295996627
C	4.1220290173	-0.4104779131	0.1753264121
H	4.4434754395	-0.9695419734	-0.7029802319
H	4.147153067	-1.0742641827	1.0390398584
C	4.9740557963	0.8191583431	0.3944391619
H	4.8865987805	1.4715116722	-0.4755042438
H	4.5918829456	1.3668375375	1.2569729472
C	6.4329217917	0.4290694295	0.6190189802
H	6.829645792	-0.1081092185	-0.2434227822
H	7.0487648154	1.3127400525	0.7782135831
H	6.5335618978	-0.2145481269	1.4938882752
O	-4.1982454057	-1.0118235614	1.0237423525
O	-3.0732508635	-0.539775434	1.604053317
C	-3.2798166435	0.8066187474	2.0315420441
H	-3.5688427423	1.4046282624	1.1673569415
H	-4.0614045885	0.8194854456	2.7894884419
H	-2.3307157439	1.13696233	2.4458205848

Transition states geometries calculated in
pentylethanoate.

TS(•OOH) _{3(OH)} H= -915.254570 G= -915.321301 if= -2094.9204 0 2			
C	-0.011312721	-0.0203395284	0.0721147054
C	0.0004903822	0.0574754808	1.4749566435
H	0.9343878918	0.11746529	2.0144592534
C	-1.1868329962	0.0690199536	2.1840553244
O	-1.1719272633	0.1498357428	3.5366379242
H	-2.0771990921	0.1923739521	3.8659056599
C	-2.3918238003	-0.0065993131	1.4914129111

O	-3.5367440335	0.0024886019	2.1944303737
H	-4.2778699765	0.0249258876	1.5697535647
C	-2.4120136511	-0.085191191	0.0809750994
O	-3.5990557289	-0.1205883246	-0.4959871625
H	-3.8179250109	-1.1774522393	-0.8153901299
C	-1.1985577049	-0.0907721122	-0.627594291
H	-1.2093483967	-0.1524415198	-1.7060956297
C	1.2572513527	-0.0252696304	-0.7088228147
O	1.3019425099	-0.036194961	-1.9145129161
O	2.3372636293	-0.016858333	0.0705446176
C	3.6161370681	-0.0064257496	-0.609319638
H	3.6737620756	0.8945753062	-1.2197378841
H	3.6677992534	-0.8761991797	-1.2632975062
C	4.6981835426	-0.0357767731	0.4447695733
H	4.5807161352	0.8259584969	1.1036884457
H	4.581588873	-0.9351418294	1.0515192004
C	6.0758138811	-0.0155608983	-0.2110797413
H	6.2131731509	0.88931396	-0.8053112953
H	6.8637970828	-0.0464460219	0.5407320403
H	6.2071202277	-0.8748260166	-0.8709402525
O	-3.8510231079	-2.4327251046	-0.8489527953
O	-2.6437917597	-2.7607988121	-0.3242206199
H	-2.8378047252	-3.0835539206	0.5708540221

TS(•OOCH ₃) _{3(OH)} H= -954.534507 G= -954.604125 if= -2346.02 0 2			
C	0.0150468889	0.0075832666	0.0070798084
C	0.0175125238	-0.0270902972	1.4126614501
H	0.94767237	-0.0594072449	1.9605150935
C	-1.1751319707	-0.0130932708	2.1117954191
O	-1.1727567167	-0.0482401195	3.4672573519
H	-2.0786412909	0.0132887627	3.7913182001
C	-2.3736095993	0.0338764847	1.4058522564
O	-3.5274528865	0.0434603829	2.0940098059
H	-4.2520479287	0.1521465765	1.4577941801
C	-2.3870255278	0.0627208489	-0.0078168854
O	-3.5661272969	0.109010797	-0.590297182
H	-3.7773936742	-0.9506349112	-1.0183217665
C	-1.1656081415	0.0546994378	-0.7046014957
H	-1.1655966981	0.0741990277	-1.7847352752
C	1.2883801123	-0.0027286973	-0.7659520587
O	1.3410396517	0.0459625336	-1.970503911
O	2.364024685	-0.0705771501	0.0171341455
C	3.6446229952	-0.0752974776	-0.6592472517
H	3.7331870495	0.8458470142	-1.2348322908
H	3.6700868956	-0.9207191628	-1.3461886739
C	4.7227547493	-0.1796592	0.3939088195
H	4.6301921327	0.6589143978	1.0859497196
H	4.5779742128	-1.0979542748	0.965029749
C	6.1014193065	-0.1745667873	-0.260117346
H	6.2642576152	0.7472202853	-0.8209927694
H	6.8872185258	-0.2539483064	0.4903886386
H	6.2102596811	-1.0123771352	-0.9509650054
O	-3.7980300022	-2.1593249715	-1.1698653385
O	-2.723364835	-2.5509864184	-0.4483073507
C	-3.1567883017	-3.20713474	0.7501005327

H -2.2488068638 -3.4220513303 1.3079321604
H -3.8185228133 -2.55048986 1.3138148174
H -3.6750038479 -4.1263594606 0.481360453

TS($\bullet$ OOCHCH₂)₃(OH)

H= -992.621978

G= -992.692527

if= -2152.65

0 2

C -0.2019179817 -0.0229413574 0.0863698474
C -0.2076438168 0.0253400557 1.4875840147
H 0.7149127824 -0.0345918757 2.0456739955
C -1.4055540475 0.1750032436 2.178783088
O -1.3968342026 0.2288792897 3.5320228982
H -2.3022426323 0.3179792237 3.852792377
C -2.5942910345 0.2293614232 1.4724392776
O -3.7507378095 0.3174416476 2.158658339
H -4.4768165694 0.3335780882 1.5171634437
C -2.602952094 0.1330658337 0.0637730064
O -3.7783831596 0.0672772629 -0.525897776
H -3.9391120622 -1.0505717398 -0.8118514315
C -1.3823108258 0.0401693932 -0.6294629587
H -1.3843396134 -0.0198571477 -1.7078724986
C 1.066529344 -0.1762645277 -0.6767111732
O 1.1196836225 -0.2491436569 -1.8803938112
O 2.1383963412 -0.2265432539 0.1134694541
C 3.4178602541 -0.360050968 -0.5524353214
H 3.5189439609 0.4515335621 -1.2719430208
H 3.4296073 -1.308044987 -1.0901923547
C 4.4954535987 -0.3041010888 0.5051281831
H 4.4247283988 0.646863328 1.0355683782
H 4.329077722 -1.1017887977 1.2308410586
C 5.8730004843 -0.4512337106 -0.1344636169
H 6.0540874686 0.3428047321 -0.8607792761
H 6.657386946 -0.400284991 0.6200212007
H 5.964845806 -1.408032795 -0.651099765
O -3.8811281231 -2.2759631746 -0.8688172803
O -2.5476813855 -2.5042434795 -0.7236640327
C -2.2234560011 -2.9787723788 0.5140797001
C -0.9500642347 -3.2526243414 0.7848339358
H -3.0640918704 -3.0851178133 1.1859799903
H -0.6910684516 -3.635541958 1.7602716094
H -0.1749530435 -3.1211505226 0.0427260429

TS($\bullet$ OOH)₄(OH)

H= -915.258685

G= -915.325253

if= -1633.5324

0 2

C -0.3180207067 0.5404859904 -0.3861171372
C -0.004266671 -0.815794024 -0.4590821023
H -0.770258664 -1.5736619545 -0.4043605689
C 1.3215567587 -1.1832661999 -0.6022635143
O 1.6686954753 -2.4766981479 -0.6751132873
H 2.6200725255 -2.5362122222 -0.8372306236
C 2.3293906641 -0.1950521292 -0.6611179034
O 3.6027955761 -0.5413714415 -0.8083151771
H 4.0499176636 -0.6693253823 0.186172875
C 1.9740167082 1.1721917015 -0.6148607119

O 2.9463470362 2.0982060902 -0.6938412561
H 3.7789940781 1.6532867652 -0.9040665467
C 0.6519122643 1.5407497639 -0.4678471492
H 0.3722002607 2.5826432198 -0.423145861
C -1.7351271911 0.9877815699 -0.2185254035
O -2.0663002038 2.1468392895 -0.1720146949
O -2.585383843 -0.0291174925 -0.1215809124
C -3.981810057 0.3192181029 0.0482476093
H -4.2912895448 0.9248093816 -0.8030428905
H -4.07927895 0.9149100365 0.9555902244
C -4.7662884877 -0.9687697033 0.1366260644
H -4.6117035775 -1.5444489966 -0.7773567967
H -4.3843826118 -1.5614536447 0.9693800445
C -6.251231571 -0.6776832434 0.3333767668
H -6.6509737194 -0.0944594981 -0.4979000558
H -6.8198530416 -1.6048342136 0.3967559242
H -6.4217251375 -0.1153613255 1.2529521062
O 4.2118829338 -0.6527986727 1.4837471211
O 2.9333733047 -0.552831891 1.9025911016
H 2.8191828584 0.3750769315 2.1719066953

TS($\bullet$ OOCH₃)₄(OH)

H= -954.539584

G= -954.609045

if= -2042.84

0 2

C -0.0306199158 0.1141608486 -0.0109808793
C -0.0356520376 0.0502476844 1.3816245692
H 0.8832714944 0.010745858 1.945714926
C -1.2517353781 0.0344978802 2.0406371931
O -1.3031633716 -0.0352640011 3.3785980682
H -2.2268546709 0.0191855149 3.6593572936
C -2.4610675374 0.0752186838 1.3073676905
O -3.6296881217 0.0694330245 1.9257874681
H -3.8839040501 -1.0080596024 2.1753701561
C -2.4161421794 0.1634113834 -0.1033757183
O -3.5784078819 0.2113147934 -0.7784462498
H -4.2976117153 0.2815719287 -0.1345697123
C -1.2059635353 0.1752283075 -0.7636464393
H -1.1647401781 0.233655678 -1.8409098516
C 1.2561769699 0.1291833897 -0.7710425991
O 1.317755674 0.1450263857 -1.9759946452
O 2.322141575 0.1246543936 0.0234604073
C 3.6118421587 0.1523018386 -0.6364943746
H 3.6525511642 1.0341509353 -1.2751948749
H 3.6985702326 -0.7366303062 -1.2609398548
C 4.6730166388 0.1897997747 0.4382087107
H 4.5170314976 1.0723914968 1.0606197734
H 4.5654193095 -0.6883385895 1.0768751952
C 6.0655483002 0.2222803324 -0.1849880915
H 6.1922280919 1.1026574313 -0.8173630086
H 6.8324171873 0.2517185951 0.5883180911
H 6.2414709728 -0.6624792058 -0.7990868964
O -3.8690610515 -2.2639046263 2.2191381784
O -2.6728779373 -2.5192806445 1.6534095442
C -2.8516839347 -3.1265873133 0.3631210129
H -3.5085255598 -2.5088347431 -0.2466290714
H -3.2786984744 -4.1181588262 0.5026725929
H -1.8564917357 -3.1895563001 -0.0687686035

TS($\bullet$ OOCHCH₂)₄(OH)

H= -992.625753

G= -992.696780

if= -1940.97

0 2

C	-0.2054106896	0.268887146	-0.0079327059
C	-0.1970064136	0.132077559	1.378009826
H	0.726567377	0.0648755015	1.9316673935
C	-1.409466802	0.0675179229	2.0426630595
O	-1.4527046098	-0.0787896299	3.3748418116
H	-2.3793416408	-0.0874500111	3.6527111164
C	-2.6221234002	0.1131848045	1.317815652
O	-3.7798621316	-0.0592095393	1.9374853605
H	-3.9574708396	-1.1821346188	1.9751374786
C	-2.5942861024	0.3085360105	-0.0800250817
O	-3.7637912544	0.3596062527	-0.7467668044
H	-4.480552897	0.3391833332	-0.0974219311
C	-1.3917941298	0.3797189573	-0.7446091945
H	-1.3587104997	0.4968462257	-1.8174628658
C	1.0733541073	0.3052120348	-0.7794833284
O	1.1284677135	0.4938686977	-1.9699781955
O	2.1407835839	0.0992694292	-0.0131367395
C	3.4248531484	0.1231904032	-0.6838978779
H	3.5490790151	1.0982107131	-1.1543358617
H	3.4228217393	-0.6422690905	-1.4594705966
C	4.4894872134	-0.1355104236	0.3563279804
H	4.4185106002	0.6248686676	1.1354660507
H	4.3059903802	-1.105051108	0.8221518468
C	5.8745300631	-0.10885011	-0.2828929192
H	6.0771370712	0.8622794238	-0.7375194667
H	6.6473158023	-0.2984744357	0.4613398779
H	5.9627399694	-0.869721448	-1.0601910599
O	-3.8486797102	-2.4343672069	1.8121756934
O	-2.5146885332	-2.5453757264	1.5940251414
C	-2.2097797407	-2.9095126942	0.3129481879
H	-3.0659334834	-2.9978622107	-0.3415358974
C	-0.9341023956	-3.1083459909	-0.0043744488
H	-0.6821824976	-3.3942821702	-1.0143391356
H	-0.1491213771	-3.0040376253	0.7314993602