

## Supplemental Material

### Ab Initio Rate Coefficients for Reactions of 2,5-dimethylhexyl Isomers with O<sub>2</sub>: Temperature -and Pressure-Dependent Branching Ratios

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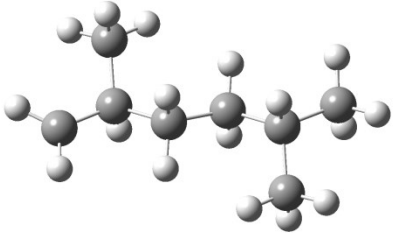
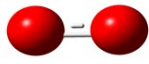
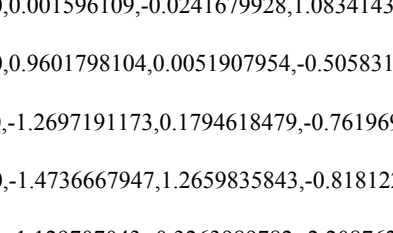
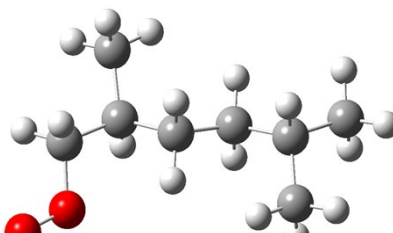
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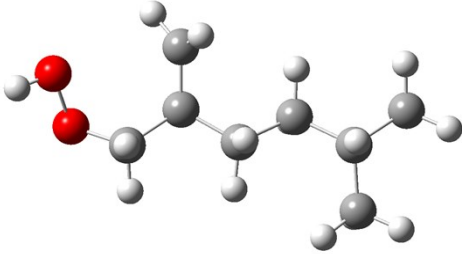
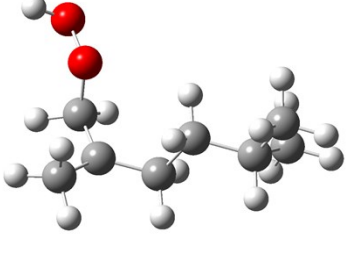
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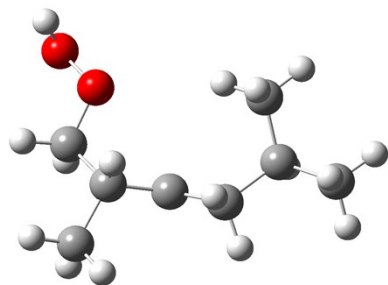
2,5-Dimethylhexyl-1-yl Radical	O <sub>2</sub>
	 O,0,0.,0.,0. O,0,0.,0.,1.205752
2,5-Dimethylhexyl-1-peroxy Radical (ROO-1)	2,5-Dimethylhexyl-1-peroxy Radical (ROO-1)
 C,0,0.0012735919,-0.0104899153,-0.0006515133 H,0,0.001596109,-0.0241679928,1.0834143153 H,0,0.9601798104,0.0051907954,-0.5058312232 C,0,-1.2697191173,0.1794618479,-0.7619695988 H,0,-1.4736667947,1.2659835843,-0.818122901 C,0,-1.129707043,-0.3263989782,-2.2087622655 H,0,-2.0095778405,-0.0891049294,-2.8106402205 H,0,-0.2645243404,0.1321909936,-2.6957251366 H,0,-0.9867793445,-1.4114574313,-2.2254864896 C,0,-2.4652646962,-0.4533570458,-0.0113010991 H,0,-2.4132975173,-0.1291723987,1.0332810847 H,0,-2.3354555032,-1.5433315606,-0.0009162592 C,0,-3.8436199988,-0.1051845752,-0.5865815719 H,0,-3.9676104431,0.9869035878,-0.5976407971 H,0,-3.8924764662,-0.426911041,-1.632492856 C,0,-5.0380950669,-0.7330046756,0.15965783 H,0,-4.8687476065,-1.8179033346,0.2007106253 C,0,-6.3408785547,-0.4931290122,-0.6165349464 H,0,-6.2799820099,-0.8939988553,-1.6326015784 H,0,-7.1923466649,-0.9674969183,-0.1198317912 H,0,-6.5572892172,0.5781158693,-0.6938160055	 C,0,0.0223940199,-0.0023034801,-0.3499525505 H,0,0.2325274086,0.3999683222,0.6446987276 H,0,0.9487103562,-0.0393780421,-0.9281502607 C,0,-0.680730952,-1.3535019004,-0.2969644604 C,0,0.3226276646,-2.4168191547,0.175328543 H,0,-0.130971242,-3.4090630419,0.1947567794 H,0,1.1920252733,-2.4662370461,-0.4862786224 C,0,-1.9461822347,-1.2849272178,0.5815535151 H,0,-1.6401424425,-1.1787197028,1.6315097323 C,0,-2.8794372651,-2.4940004029,0.4387984943 H,0,-3.210106158,-2.5716871357,-0.6060003329 H,0,-2.3240677556,-3.4140619129,0.6519524089 C,0,-4.1217802917,-2.4648421807,1.3511435858 H,0,-3.7700576702,-2.342280612,2.3849546119 C,0,-4.877053231,-3.7989015236,1.2695464484

C,0,-5.1719862435,-0.2223437859,1.6014363024	H,0,-4.2324774821,-4.6407085923,1.5395165918
H,0,-4.2926594991,-0.4551658936,2.2064325145	H,0,-5.7390987656,-3.8080665962,1.9427275872
H,0,-5.3111053,0.8645477012,1.6166318297	H,0,-5.2481919951,-3.9754112013,0.2540207578
H,0,-6.0377454224,-0.6736273248,2.094783406	C,0,-5.0628113328,-1.2946362209,1.0308730856
	H,0,-4.576112696,-0.3246956556,1.1558348238
	H,0,-5.4219428575,-1.3575370193,-0.002462817
	H,0,-5.9381896601,-1.3090941923,1.686501529
	H,0,-0.9849627308,-1.5960523051,-1.3232859554
	H,0,0.6814066979,-2.19539097,1.1859559549
	H,0,-2.49227969,-0.3738331739,0.3244170233
	O,0,-0.8588121219,0.9494797292,-1.0239066613
	O,0,-0.3603972998,2.1682155554,-1.0161201038

QOOH-1 <sub>p</sub>	QOOH-2 <sub>p</sub>
	
C,0,0.1040047914,0.1368396805,0.0099711403	C,0,-0.0658916413,0.0283836883,0.0128107786
H,0,0.0048480794,0.1519635852,1.101189692	H,0,-0.1441437461,0.0836393732,1.1035377267
C,0,1.592470336,0.152785943,-0.4214700028	H,0,0.9943824417,0.0377582525,-0.2713972426
C,0,2.3236191067,1.3494451668,0.0875526184	C,0,-0.7755509949,-1.1591172437,-0.538648066
H,0,2.2388104141,2.3052101925,-0.4111505283	C,0,-0.475697902,-1.5919132823,-1.9382134932
H,0,-1.3138873892,2.5757310765,0.5210331067	H,0,-1.0639374841,-1.0249749706,-2.676368485
C,0,2.2535648524,-1.1714756169,0.020501156	H,0,0.5768207068,-1.4316406725,-2.1918945139
H,0,2.3121637134,-1.1900772095,1.1173753255	C,0,-1.9835924793,1.6947251764,0.1672021949
C,0,3.6554843326,-1.3782695164,-0.5659042672	H,0,-2.0777386828,-2.7708317859,-0.0304296908
H,0,3.5850389401,-1.4183655621,-1.6615759581	C,0,-3.3062633309,-1.0050346988,-0.2601727884

H,0,4.2636353162,-0.4965727645,-0.3348825006  
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 C,0,3.6937916799,-3.9368453988,-0.4741570408  
 H,0,2.6833667869,-4.0080176439,-0.0642250749  
 H,0,3.6188478119,-4.0121727113,-1.5648597775  
 H,0,4.2527961625,-4.8079528864,-0.1201675542  
 H,0,1.5746092262,0.1860646429,-1.5191334929  
 H,0,2.7605714532,1.3354975216,1.0809563246  
 H,0,1.6040308224,-2.0050532375,-0.2680058843  
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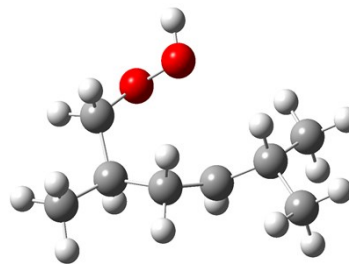
**QOOH-3<sub>p</sub>**



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 C,0,-0.7792114473,-1.2614406669,-0.5276558638  
 C,0,0.1148719902,-2.4833078504,-0.1944522048

H,0,-3.2308362008,0.0681442239,-0.0529334598  
 H,0,-3.4097074124,-1.1010876918,-1.3468869667  
 C,0,-4.5720170995,-1.5753521931,0.407519372  
 H,0,-4.582934057,-2.6600834756,0.2307964686  
 C,0,-5.8299982017,-0.983120906,-0.2437845548  
 H,0,-5.8559668644,-1.1853521386,-1.3185598523  
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 H,0,-5.8643824168,0.1033557444,-0.10884008  
 C,0,-4.593069199,-1.3436512673,1.9253115561  
 H,0,-3.7482565338,-1.8202776435,2.4284776442  
 H,0,-4.5577631193,-0.2728080812,2.1537881439  
 H,0,-5.5079982695,-1.7476780492,2.3684523682  
 H,0,-0.7112269721,-2.6499157802,-2.0918247937  
 H,0,-1.8515869691,-1.5785812253,1.2478181338  
 O,0,-0.7004912332,1.2017068799,-0.5533294048  
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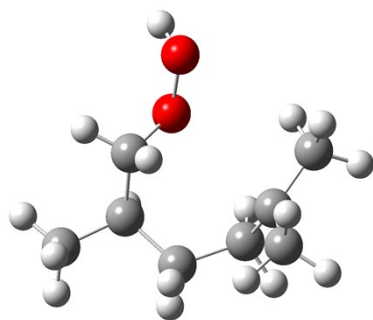
**QOOH-4<sub>p</sub>**



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 H,0,0.8583801009,0.0836008855,-0.7155208534  
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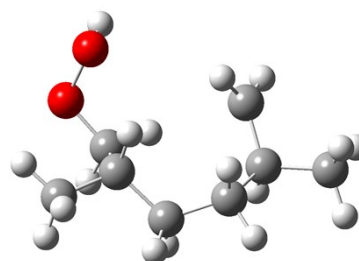
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C,0,-2.1590559608,-1.3987511865,0.0366534749  
H,0,-2.3278634996,-1.0557842653,1.0551053671  
C,0,-3.2785195417,-2.0892333666,-0.6677989772  
H,0,-2.9823680618,-2.3301242627,-1.6975625707  
H,0,-3.4940248452,-3.0556837655,-0.1820876095  
C,0,-4.6020394933,-1.28176603,-0.7041115975  
H,0,-4.849500885,-1.0204020958,0.3334343435  
C,0,-5.7462982288,-2.1358837123,-1.2630745854  
H,0,-5.8912095936,-3.0473950552,-0.6752490161  
H,0,-6.6897590881,-1.5822451189,-1.2604285545  
H,0,-5.5417082757,-2.4346288125,-2.2972084072  
C,0,-4.4402784154,0.0220471341,-1.4956005417  
H,0,-3.6233388008,0.6294237567,-1.0990293267  
H,0,-4.2191858143,-0.190857771,-2.548003618  
H,0,-5.3576659224,0.6174300445,-1.4644238658  
H,0,0.2557023247,-2.5792450774,0.8860569335  
O,0,-0.8370296619,1.1185215424,-0.5273451374  
O,0,-0.2232470072,2.3188030499,0.0170598731  
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**QOOH-5<sub>p</sub>**



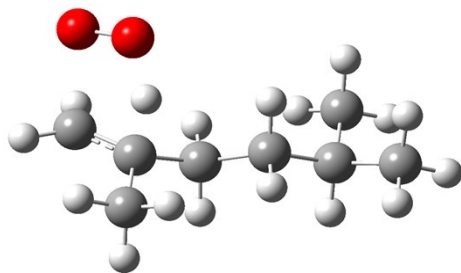
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C,0,-3.1007569101,-2.4719044107,-0.5745978503  
H,0,-3.0635223067,-2.6167397728,-1.6518884304  
C,0,-4.1674270297,-3.1815026447,0.1998491665  
H,0,-3.7840897717,-3.3473807988,1.2159308589  
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H,0,-5.2463774007,-5.0814646962,0.1668202342  
H,0,-4.862206814,-4.4437885931,-1.4367119782  
C,0,-5.4533105483,-2.3283331529,0.3295260083  
H,0,-5.2455902292,-1.3621599826,0.7976559237  
H,0,-5.8915293597,-2.1366834179,-0.6551471569  
H,0,-6.2035644815,-2.8432817183,0.9390965657  
H,0,-0.8852068164,-1.4626511087,-1.6669661911  
H,0,0.331366544,-2.3496277297,0.9953382883  
H,0,-2.6813720425,-0.4277154125,-0.1172955064  
H,0,-0.7430402564,0.8281013113,-0.7203539915  
O,0,-0.2316615666,-3.784101994,-0.3725510782  
O,0,-1.0810303316,-4.2614774307,0.7104985618  
H,0,-0.5392819241,-4.9979412891,1.0260831156

**QOOH-6<sub>p</sub>**



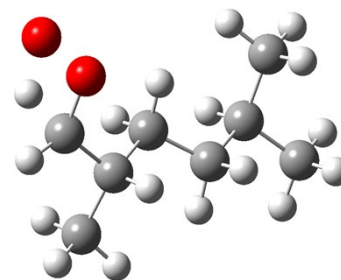
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C,0,1.3319885955,0.1113887933,2.2530026145	C,0,1.4980322036,-0.0064414982,2.0371852732
C,0,2.0491413016,1.4258179109,2.4039476474	C,0,2.1990352275,1.3170778386,2.4050011893
C,0,1.0067177855,1.0111627296,-0.7406208389	C,0,1.5069307828,3.042253103,0.6611051982
H,0,1.1134001083,-0.2849911723,3.2611945894	C,0,2.6301788737,2.2595891115,1.261289147
H,0,-0.5473598827,1.0704062541,1.7221936176	H,0,0.5121647123,1.0077471603,-0.3126651195
H,0,-0.6422551962,-0.670011506,1.8407600249	H,0,-0.4502850542,0.9360103818,2.0247542952
H,0,0.4575335849,-0.9876753479,-0.2918454769	H,0,2.0946652504,-0.5330574778,1.2790809568
H,0,0.9940813977,1.9861666813,-0.2419666662	H,0,1.568691228,1.878162548,3.1072824519
H,0,0.7304163163,1.1481911413,-1.7939184968	H,0,0.2138142549,-0.7457478453,-0.4268841621
H,0,1.9981309562,-0.6170933917,1.7824073975	H,0,1.5445502709,-0.6405889402,2.9287789271
C,0,-1.339913342,0.1255435448,-0.6646671577	H,0,3.1025318047,1.0503544504,2.9647609167
H,0,-1.3322091602,-0.0961475505,-1.7353434826	H,0,3.0905123724,1.6451896248,0.4713228177
H,0,-2.0306432845,-0.5707084592,-0.1819923538	O,0,-1.4429812377,0.3397085908,-0.3957888019
H,0,-1.7443099394,1.1349558007,-0.5339172663	O,0,-1.9164295385,1.6394985191,0.0567828077
C,0,1.3987217917,2.5138996655,3.201595438	C,0,-0.7582478238,-1.1872230781,2.0671444474
H,0,1.5833808124,2.3828647076,4.2834597468	H,0,-0.7978972161,-1.2259442686,3.1592516795
H,0,1.7950454908,3.4999053278,2.9378856728	H,0,-1.7816262768,-1.1747376637,1.6874298396
H,0,0.3128762461,2.5431413801,3.0740341844	H,0,-0.27890967,-2.1087388852,1.7171959137
C,0,3.5379238248,1.4568559951,2.2682313466	H,0,0.5665748265,3.1794009961,1.1802815752
H,0,3.9111746381,2.4794106926,2.1540860214	H,0,1.67079784,3.6151988325,-0.2453953501
H,0,4.0359502384,1.0381614061,3.1619829081	C,0,3.7394255532,3.2249454248,1.7558732839
H,0,3.8716440729,0.8757237864,1.4062775165	H,0,4.0596783275,3.8987288744,0.9571048626
O,0,2.3221411124,0.4587181192,-0.6765789065	H,0,3.3759829987,3.8380063793,2.5858067079
O,0,3.2309843282,1.447060984,-1.2354224615	H,0,4.614460412,2.6647998151,2.1004745484
H,0,3.5317103413,0.9759889298,-2.0247324824	H,0,-1.8936844918,2.1300526134,-0.7763847302

**TS1<sub>p</sub>**



C,0,0.0577483602,-0.3335458557,0.0606543234  
 H,0,0.0674680112,-0.4330743846,1.1389597358  
 H,0,1.0109323353,-0.4622703052,-0.4370403111  
 C,0,-1.1354560574,-0.2363303227,-0.6534761142  
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 H,0,-1.8689544871,-0.0179074821,-2.7029002132  
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 C,0,-2.4470218535,-0.5443204846,0.0878090706  
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 H,0,-3.4740033122,1.3324940997,-0.244165619  
 H,0,-3.7957229724,0.1142267709,-1.4649360705  
 C,0,-4.9902986982,-0.1070440475,0.3091733753  
 H,0,-5.125121982,-1.1933741941,0.2112350951  
 C,0,-6.1729039458,0.5749419347,-0.3930347836  
 H,0,-6.2212367986,0.3001097781,-1.4508685514  
 H,0,-7.1236405092,0.2948147802,0.0696365012

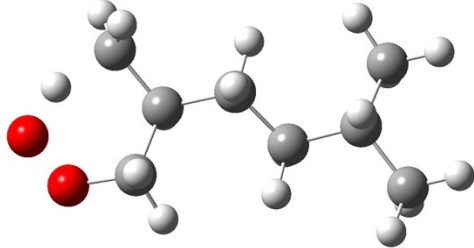
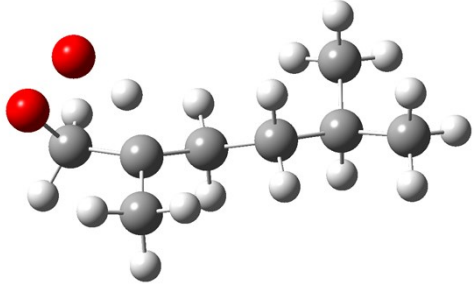
**TS2<sub>p</sub>**



C,0,-0.004736781,-0.0004079856,-0.0007576163  
 H,0,-0.0025066056,0.0017057134,1.3341383689  
 H,0,1.0580420486,-0.0006749508,-0.2627351874  
 C,0,-0.8887683695,-1.0651056602,-0.60917803  
 C,0,-0.1352417794,-2.4014501409,-0.654794381  
 H,0,-0.7142134943,-3.1639294794,-1.1778104618  
 H,0,0.8222793615,-2.3029679549,-1.1742512013  
 C,0,-2.2558297955,-1.1468518768,0.0997667778  
 H,0,-2.1140125682,-1.6089353572,1.0853588539  
 C,0,-3.3207385986,-1.9217271401,-0.685714102  
 H,0,-3.483891175,-1.4301695948,-1.6548264746  
 H,0,-2.9528514441,-2.9287101759,-0.9127152436  
 C,0,-4.6766861388,-2.0611959152,0.0342417601  
 H,0,-4.4839433307,-2.5182385323,1.0147489309  
 C,0,-5.6026836158,-3.0042740358,-0.7466399851  
 H,0,-5.146379773,-3.989113534,-0.8844152229  
 H,0,-6.5541099969,-3.1459071457,-0.2260588133

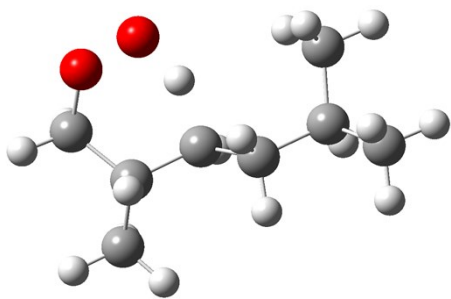


H,0,-6.0851339097,1.665405836,-0.3361768318	H,0,-5.8258453497,-2.5985997003,-1.7395631624
C,0,-4.9836862777,0.2345404458,1.806366534	C,0,-5.3614677337,-0.7075778777,0.2713835886
H,0,-4.1979804196,-0.297212745,2.3483034926	H,0,-4.7578681679,-0.0410763113,0.8913175005
H,0,-4.8271926699,1.3082320548,1.9581497242	H,0,-5.5529359739,-0.1979985297,-0.6796681231
H,0,-5.9379822153,-0.030151212,2.2706565384	H,0,-6.3236060543,-0.8417830934,0.7740695597
H,0,-1.2959643257,-1.6383801598,-2.3062202846	H,0,-1.0714476097,-0.7332301345,-1.6447526543
H,0,-2.2849267156,-0.3713029712,1.1556738148	H,0,0.0661880269,-2.7680390326,0.3566046689
H,0,-1.0902725425,1.0822740005,-0.6480459858	H,0,-2.5977039008,-0.1261562002,0.2813806036
O,0,-0.5756123603,2.257436443,-0.3664852554	O,0,-0.5345560967,1.2782371866,0.1078794513
O,0,0.4473626128,1.8383074645,0.2548986413	O,0,-0.4355646176,1.1771303421,1.6027855455

TSQ1 <sub>p</sub>	TSQ2 <sub>p</sub>
	
C,0,0.0120283551,0.0885880422,-0.0642390613	C,0,0.0021267021,-0.0008993111,-0.003502176
C,0,0.0461224738,0.0873802484,1.4465645589	H,0,-0.000013169,0.0045935955,1.0925260717
C,0,1.5125297258,-0.0418628477,1.9431219908	H,0,1.0298621406,-0.0046624513,-0.3808163438
H,0,1.5942807379,0.1545938216,3.0134770958	C,0,-0.8777817532,-1.151082895,-0.5328580421
H,0,-0.3169931696,1.0560009517,1.8063647746	C,0,-0.6937338874,-1.4371281317,-2.0048317156
H,0,0.0041935979,-0.8884751212,-0.5472328476	H,0,-1.5292523918,-1.9993021827,-2.4261749393
H,0,-0.6229834556,0.8259995923,-0.5496757894	H,0,-0.5885102087,-0.504991705,-2.5638777865
H,0,1.9181284663,-1.034142618,1.7129319447	C,0,-1.0848637849,-2.3196312674,0.4046194883
O,0,2.4346802978,0.6263521111,-0.0385844828	H,0,-0.1457207091,-2.8963434231,0.4578951083

O,0,2.3115272726,0.9588669438,1.330266453  
H,0,1.3290042644,0.499081544,-0.3260641122  
C,0,-0.8516737818,-1.0287164849,2.0373401952  
H,0,-1.8374256629,-0.9409046322,1.5722254973  
H,0,-0.4530636365,-2.0032559525,1.7277172832  
C,0,-0.9962090852,-0.9931285623,3.5652971729  
H,0,-0.0167550486,-1.1560860406,4.0281661089  
H,0,-1.3194427934,0.0090601422,3.8780961661  
C,0,-1.9768437994,-2.0351259488,4.1422032993  
H,0,-1.6953259822,-3.0164318345,3.7362076549  
C,0,-1.8441933592,-2.1057886048,5.6700720936  
H,0,-2.5122307912,-2.8627759912,6.0905443874  
H,0,-0.8228368503,-2.3558701192,5.9716218548  
H,0,-2.1017911123,-1.1449868523,6.1289980429  
C,0,-3.4333443686,-1.7570673795,3.7433414566  
H,0,-3.7560731698,-0.7782904483,4.1152976757  
H,0,-3.5780161122,-1.7673257612,2.6604800678  
H,0,-4.1032099316,-2.5097211725,4.168631042

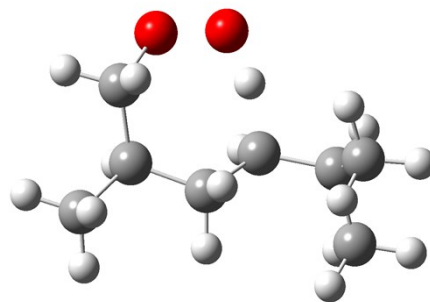
**TSQ3<sub>p</sub>**



C,0,-0.0195976501,0.0132563459,-0.0194874833  
H,0,-0.0034957788,0.0207410356,1.0766185893  
H,0,1.0034061139,0.032530475,-0.4040276675  
C,0,-0.7957008071,-1.2136437142,-0.5581738423

C,0,-2.2259538094,-3.2752661051,0.022382457  
H,0,-3.1593405489,-2.7043077926,-0.0674099108  
H,0,-2.0270362939,-3.697050656,-0.9681684416  
C,0,-2.4446270493,-4.4407732608,1.0074839761  
H,0,-1.4794921793,-4.9492429493,1.1401003641  
C,0,-3.4316654927,-5.4580341321,0.417769263  
H,0,-3.079569988,-5.8469668285,-0.5421302872  
H,0,-3.5735898795,-6.3077341984,1.0915618931  
H,0,-4.4124567444,-4.9992299994,0.2522402891  
C,0,-2.9242797879,-3.9669189938,2.3871604287  
H,0,-2.2087788498,-3.2965875884,2.8692490569  
H,0,-3.8778574742,-3.4340797787,2.3033247828  
H,0,-3.077789114,-4.8169017294,3.0579507177  
H,0,0.2171031182,-2.0322195078,-2.1667943979  
H,0,-1.2494528994,-1.9242164597,1.4118744773  
O,0,-0.6137445698,1.181816771,-0.5117371554  
O,0,-1.9894248683,0.9557265085,-0.2351839085  
H,0,-1.8992773957,-0.2712419801,-0.4283527792

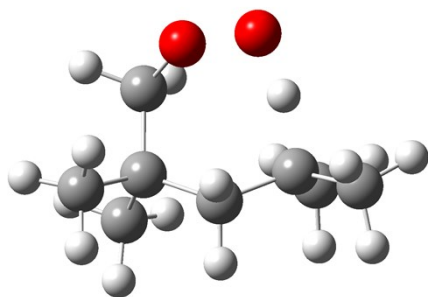
**TSQ4<sub>p</sub>**



C,0,-0.0029060642,0.0033325962,-0.0036794071  
H,0,-0.0001388047,0.0034682502,1.0899367485  
H,0,1.0371869429,0.00620176,-0.3398593922  
C,0,-0.7564083811,-1.2113162459,-0.5647906458

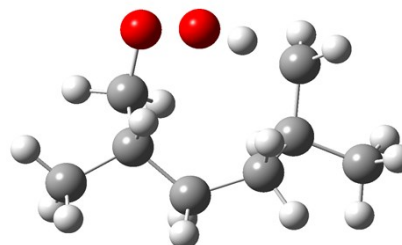
C,0,-0.1854964731,-2.5126550235,-0.0002785389	C,0,-2.1852944476,-1.2170122038,0.0009186982
H,0,-0.6965732195,-3.389607725,-0.4044625849	H,0,-2.1475903975,-1.1839323146,1.0941049216
H,0,0.874164644,-2.5936132068,-0.2605767467	C,0,-0.6900200216,-1.2189717804,-2.1098597641
C,0,-2.2782947221,-1.0885730566,-0.2502566868	H,0,-1.2328796677,-0.3463727381,-2.4908498708
H,0,-2.5455765799,-1.4235208731,0.7569880714	C,0,-1.2135633517,-2.4831895466,-2.7609075667
C,0,-3.2629064936,-1.4881117128,-1.3244697877	H,0,-0.7967529393,-3.3951913349,-2.3227614129
H,0,-3.0818177804,-0.8869628618,-2.2259052979	C,0,-1.3613677238,-2.5631863505,-4.2725385911
H,0,-3.0471784969,-2.5286342682,-1.6194496594	H,0,-1.8950161847,-3.4980130365,-4.4845108222
C,0,-4.7497274713,-1.3925296532,-0.9341193204	C,0,0.0188427316,-2.6681783063,-4.9589158077
H,0,-4.8926532285,-2.002498043,-0.0314676646	H,0,0.5950122583,-3.5125895088,-4.571008391
C,0,-5.6315132665,-1.9837769966,-2.0425327556	H,0,-0.1026099169,-2.8103790866,-6.0368245807
H,0,-5.3637032182,-3.0225757223,-2.2576998615	H,0,0.6068922595,-1.7582427819,-4.8073988256
H,0,-6.6875083271,-1.9623651299,-1.7593802355	C,0,-2.1869899004,-1.412027927,-4.8675496101
H,0,-5.5261051145,-1.41245268,-2.9711801191	H,0,-3.1501734704,-1.3100981249,-4.3611139315
C,0,-5.1756746767,0.0452770672,-0.6070138158	H,0,-1.6613649532,-0.4560108591,-4.7877981905
H,0,-4.6199111636,0.4589340662,0.2374634903	H,0,-2.3803047853,-1.5906596109,-5.9286724713
H,0,-5.0104762348,0.7060787977,-1.4644808105	H,0,-0.2668046756,-2.1223863155,-0.1976136694
H,0,-6.2390110759,0.0853822426,-0.3543488001	H,0,-2.7611964417,-0.3567965596,-0.3596089963
H,0,-0.2701611473,-2.5477461598,1.0899316619	H,0,0.3602241114,-1.0723890378,-2.4046822039
O,0,-0.6229426399,1.2065463142,-0.4977071469	H,0,-0.4614991192,0.9405701755,-0.3362557223
H,0,-0.6704476196,-1.2030518373,-1.6468167431	O,0,-2.9207297199,-2.4128554145,-0.27229393
H,0,-2.3301252241,0.2691582466,-0.0596277389	O,0,-3.4215963218,-2.3595120407,-1.5915794373
O,0,-1.8716549028,1.3313702822,0.1555400888	H,0,-2.4725441546,-2.5544573471,-2.2455128156

TSQ5<sub>p</sub>



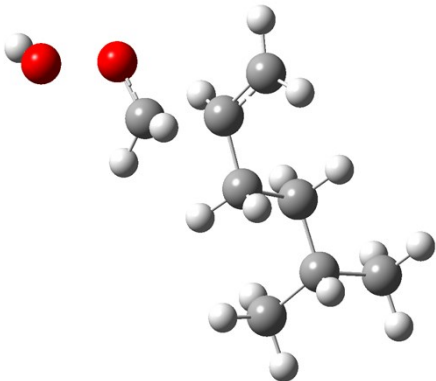
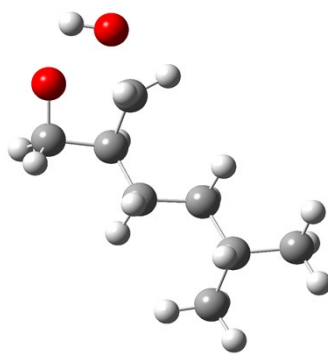
C,0,0.0069532587,-0.0009109025,-0.0022502597  
 C,0,0.0051049532,0.002195956,1.5232003101  
 C,0,1.3430372288,-0.0014904243,2.3326680284  
 C,0,2.4079733313,-0.9336179745,1.7035050963  
 H,0,-0.5575937904,-0.8827259316,1.8340135788  
 H,0,-0.5872045349,0.8646286544,1.8694423976  
 H,0,3.1134692174,-1.2642568744,2.472710157  
 H,0,2.9725108813,-0.444812827,0.9057887539  
 O,0,1.8357486681,-2.1326603007,1.1639894906  
 O,0,1.5984377442,-1.9389102158,-0.2139338989  
 H,0,0.7789643437,-1.0801393603,-0.2418116375  
 C,0,0.7105400322,1.1275182096,-0.7285885081  
 H,0,0.640622569,0.9957439432,-1.811423675  
 H,0,0.2461917043,2.0935692328,-0.4831899782  
 H,0,1.7683398721,1.1983769598,-0.4723011264  
 C,0,-1.3408054194,-0.3664674596,-0.5940764242  
 H,0,-1.2782860139,-0.5035758874,-1.6767757286  
 H,0,-1.7387107306,-1.2843678879,-0.15478897  
 H,0,-2.0730879691,0.4332743646,-0.4074451171  
 C,0,1.002330349,-0.5306003222,3.7411847924  
 H,0,1.8705505676,-0.4646961074,4.4039443775  
 H,0,0.1914812272,0.0482625308,4.1939508219

TSQ6<sub>p</sub>



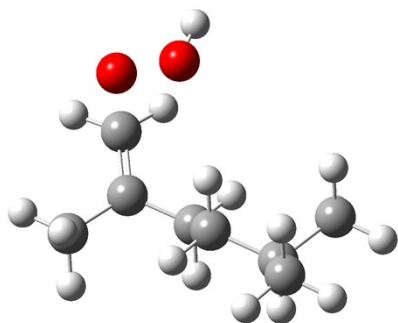
C,0,0.0288092964,0.0183820529,-0.0103538798  
 C,0,0.0111493941,0.0069399367,1.5326853201  
 C,0,1.4190390521,-0.0185874759,2.1694103156  
 C,0,2.3323631194,1.2197969953,2.0231559706  
 C,0,2.5538875585,2.4321465192,-0.2405302196  
 C,0,3.1187545405,1.3754427599,0.6851248559  
 H,0,1.0402713754,-0.1485331746,-0.4006818937  
 H,0,-0.4815781935,0.933021819,1.8403195822  
 H,0,1.9587322239,-0.9058407112,1.8091450736  
 H,0,1.7507955683,2.1264805895,2.2183812208  
 H,0,-0.6173271454,-0.7594804602,-0.4258480051  
 H,0,1.2762458331,-0.1825901523,3.2435116022  
 H,0,3.0677730719,1.1569614171,2.8316395106  
 H,0,3.1016579414,0.4129295278,0.162144106  
 O,0,-0.4957726686,1.2089328899,-0.6181561822  
 O,0,0.0313221488,2.3524296864,0.0160683805  
 H,0,1.1371652198,2.3704935729,-0.217091475  
 C,0,-0.8210195743,-1.1783308266,2.0483994788  
 H,0,-0.8915825999,-1.1671783426,3.1394943503  
 H,0,-1.8376431556,-1.1463690985,1.6468448878  
 H,0,-0.3754979074,-2.1358243938,1.7559688444  
 H,0,2.6451458137,3.4593563175,0.1184123876  
 H,0,2.7810804892,2.3312124041,-1.3013839687

H,0,0.6879514922,-1.5766467719,3.6956676332	C,0,4.6038267984,1.7056686242,0.9638390916
C,0,1.9492919576,1.4071917225,2.4748795624	H,0,5.1710188583,1.8166218734,0.0357591496
H,0,1.2544559737,2.0728235807,2.9956719102	H,0,4.6939146337,2.6391425443,1.5280573703
H,0,2.8722997748,1.3724204819,3.0629410817	H,0,5.0683485046,0.9085296702,1.5524314589
H,0,2.1895688289,1.8616907286,1.5123318369	

TS3 <sub>p</sub>	TS4 <sub>p</sub>
	
C,0,0.0072239714,0.0128857708,0.0265456907	C,0,-0.1623077995,0.0920461206,0.1924365396
C,0,-0.0121243521,0.0021906758,1.9571576874	H,0,-0.3381790264,-0.4931182571,1.1087356441
C,0,1.3304228164,-0.00696216,2.3574483904	C,0,1.2798831626,-0.0320945245,-0.2960851178
H,0,1.9165225165,-0.9171408971,2.3374243852	C,0,1.782449804,1.2501855594,0.3388955913
C,0,-0.8661899118,1.216360076,2.3099872808	H,0,2.6148689066,1.7622514115,-0.1195749051
H,0,-0.3259637285,2.1307610219,2.0369103797	H,0,0.1723095695,2.9699620431,-0.658879996
C,0,-1.2177408205,1.2595716936,3.8077685001	C,0,2.0605000197,-1.3021115168,0.0679822515
H,0,-1.7458637373,0.3368361522,4.0828130747	H,0,2.0628968038,-1.4233800966,1.1587324539
H,0,-0.2860727599,1.2593894036,4.3840267146	C,0,3.5031590035,-1.3119506428,-0.4563371329
C,0,-2.0690082271,2.4705940995,4.2365462281	H,0,3.4926320681,-1.2171392802,-1.5502850482
H,0,-1.5557399973,3.3776395455,3.8884876606	H,0,4.0275284828,-0.4248188913,-0.0809770497
C,0,-2.1561434752,2.5415555968,5.7677655827	C,0,4.3271903344,-2.5558264699,-0.0696047767
H,0,-1.162725752,2.6026618735,6.2214734484	H,0,4.2797255562,-2.6576585154,1.0234150442

H,0,-2.7269937416,3.4165189549,6.0912996293  
H,0,-2.6530181339,1.6530797564,6.1723160964  
C,0,-3.4740971812,2.454730105,3.6173572992  
H,0,-3.4476039939,2.4813080178,2.5253570949  
H,0,-4.0199962371,1.553583541,3.9178475654  
H,0,-4.0551442409,3.3194574436,3.9500432907  
H,0,-0.5352176947,-0.9474663621,2.047422557  
H,0,1.8578274363,0.9210721148,2.5536487849  
H,0,-1.7842247651,1.2030790417,1.7183619947  
H,0,0.7253275761,0.8129250865,-0.1870449159  
H,0,-1.0373755985,0.3125443068,-0.127591599  
O,0,0.3300165293,-1.2008878074,-0.3021225799  
O,0,0.2459969247,-1.2847944833,-2.0861554597  
H,0,-0.2716568917,-2.102074392,-2.0460214852

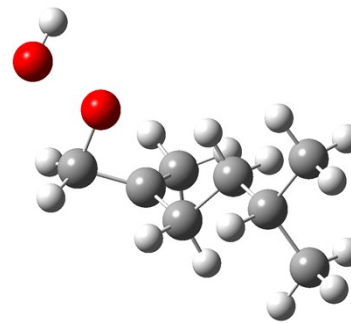
**TS5<sub>p</sub>**



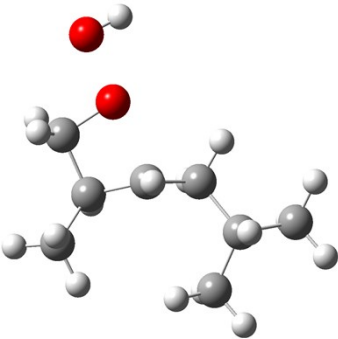
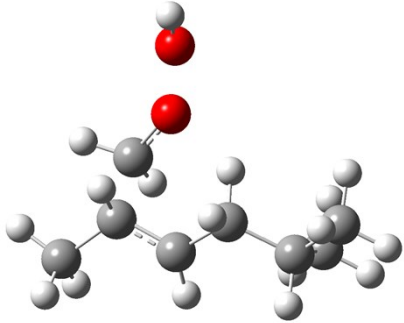
C,0,0.1494255661,-0.1447961923,-0.1467149874  
H,0,0.2173641327,-0.1715134085,0.935128522  
H,0,1.0935298293,-0.2146007364,-0.6750264863  
C,0,-1.0091670493,-0.5827259593,-0.763076217  
C,0,-1.0577255465,-0.7595867084,-2.2520496239  
H,0,-1.5685473029,0.0859898665,-2.7289061222  
H,0,-0.0575351048,-0.8220105434,-2.6848817821

C,0,5.7998661299,-2.3644010539,-0.4580023659  
H,0,6.2245021639,-1.4727875584,0.0125220071  
H,0,6.4042828249,-3.2235520621,-0.1535908573  
H,0,5.90643835,-2.2515601555,-1.5423366198  
C,0,3.770009908,-3.84588789,-0.6883549584  
H,0,2.7458918623,-4.0512548415,-0.3675906019  
H,0,3.7730700789,-3.7847302375,-1.7823508616  
H,0,4.3800506252,-4.7078758793,-0.4039989483  
H,0,1.2988056505,0.1190390009,-1.3784549664  
H,0,1.8035798046,1.2952251807,1.4218581506  
H,0,1.5083852725,-2.1575692739,-0.3350832802  
O,0,-0.1608682356,1.4778877974,0.5090118337  
H,0,-0.9234709603,-0.170549741,-0.5503170577  
O,0,1.1100864012,2.8594026952,-0.8748896457

**TS6<sub>p</sub>**

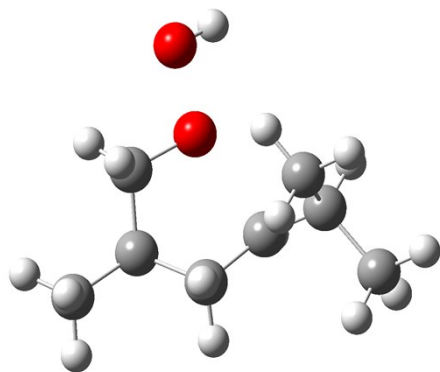


C,0,-0.0978450786,0.0880296933,-0.0265310582  
H,0,0.4456471152,-0.2110923228,0.8825628306  
H,0,0.6282294314,0.4960170244,-0.7304679835  
C,0,-0.8084514682,-1.0920521152,-0.5977122058  
C,0,-0.2720362728,-1.7472761535,-1.8129529374  
H,0,-0.5590120477,-2.796600193,-1.9435324305  
H,0,0.8034421706,-1.6169641092,-1.9793675274  
C,0,-2.0870975257,-1.5686490657,0.0146863859

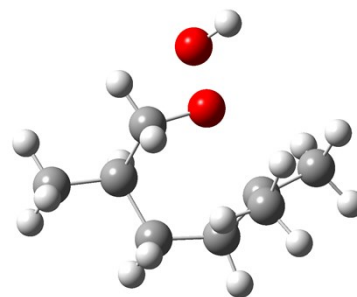
C,0,-2.291574496,-0.7289829192,0.0099345466	H,0,-2.3365069494,-2.5560947913,-0.3852850489
H,0,-2.7315271808,-1.7129864725,-0.2084540715	C,0,-3.2925909912,-0.6248240849,-0.2044076198
C,0,-3.34248552,0.3563479702,-0.3207691306	H,0,-3.0843491627,0.3543062453,0.2439289822
H,0,-2.9064338575,1.3402748322,-0.1207363254	H,0,-3.3878040517,-0.4647080159,-1.2812987197
H,0,-3.56152621,0.3193530305,-1.3933040785	C,0,-4.6238536149,-1.1587043448,0.3554024238
C,0,-4.6681781857,0.2129917344,0.451151281	H,0,-4.7827252564,-2.1602326716,-0.0672082029
H,0,-5.0370958114,-0.8114892817,0.3003540502	C,0,-5.7857270483,-0.2683814528,-0.1077133356
C,0,-5.7194910436,1.1770516233,-0.1170354883	H,0,-5.8287248438,-0.2072382745,-1.1985880969
H,0,-5.8920517251,0.9971478809,-1.1822362915	H,0,-6.7454881325,-0.6559316915,0.2459598314
H,0,-6.6771871177,1.0690945547,0.4006925069	H,0,-5.676373283,0.7504546485,0.2798739391
H,0,-5.3953340634,2.2171366033,-0.0036990273	C,0,-4.6175657964,-1.2861233376,1.8853785325
C,0,-4.497584844,0.437465728,1.9607105072	H,0,-3.8496719769,-1.9777737604,2.241683863
H,0,-3.8188192024,-0.2894237444,2.4137426178	H,0,-4.4362940677,-0.3129281858,2.3555523228
H,0,-4.0971966149,1.4375455975,2.1586561185	H,0,-5.5807851362,-1.6544413351,2.2498256217
H,0,-5.4576170103,0.3535706157,2.4784253928	H,0,-0.7868714663,0.8848797346,0.2664661103
H,0,-1.6152895255,-1.6618825387,-2.5271937176	O,0,-1.0582515921,-0.8576369627,-2.5488548238
H,0,-2.0687239151,-0.7111102264,1.0793948399	O,0,-0.7380877038,-1.1797868385,-4.2549416037
O,0,0.147249946,1.766779685,-0.3069987282	H,0,-0.7432977015,-0.2390865545,-4.4802074622
O,0,-0.6867286221,2.3440909186,0.65981348	H,0,-1.9157148831,-1.6919742417,1.093336752
H,0,-0.1070586099,2.4245941871,1.4319211627	
<b>TS7<sub>p</sub></b>	<b>TS8<sub>p</sub></b>
	
C,0,0.0038346189,0.0015385867,0.0602557734	C,0,-0.0129407278,-0.0208030986,0.0260731035

H,0,0.0233119884,-0.0499626161,1.1527862532	H,0,-0.0333914274,-0.0236134051,1.126049254
H,0,1.0397417032,0.0181639277,-0.2916706296	H,0,1.0201165714,-0.0019604442,-0.3495561599
C,0,-0.7481753576,-1.1952763173,-0.5296386276	C,0,-0.4200048375,-1.6817807783,-0.4333435844
C,0,-0.1543984602,-2.5605954509,-0.1603160367	C,0,0.747516075,-2.549683596,0.0284723488
H,0,0.4048367474,-2.532217568,0.7830783874	H,0,0.6161249357,-3.5790066292,-0.3142854874
H,0,0.465382178,-3.0261751434,-0.9302215215	H,0,1.6960643704,-2.1835665705,-0.3692556454
C,0,-2.1534043487,-1.4106600722,-0.0076284511	C,0,-1.6952792272,-1.9561416705,0.1377978273
H,0,-2.3007385645,-1.2662934369,1.0603255771	H,0,-1.7305792222,-2.4314436102,1.1161709505
C,0,-3.3812929525,-1.480630181,-0.8508142714	C,0,-2.9257338174,-1.3633114878,-0.4265846908
H,0,-3.1057972135,-1.6264863167,-1.901744341	H,0,-2.6769770975,-0.2970606117,-0.6226144016
H,0,-3.9417391622,-2.3753750703,-0.5492452944	H,0,-3.1081124764,-1.7806348734,-1.4285569427
C,0,-4.3384788772,-0.2645270944,-0.7344040221	C,0,-4.1971751156,-1.4712356656,0.4339569465
H,0,-4.5741935315,-0.1343227749,0.3298653213	H,0,-4.3400589144,-2.5291435479,0.6929098995
C,0,-5.649909038,-0.5517126719,-1.4772084496	C,0,-5.42422771,-1.0126559829,-0.3644804076
H,0,-6.1397436277,-1.4499322032,-1.0907752276	H,0,-5.5558234525,-1.6077665576,-1.2730822598
H,0,-6.349950959,0.2825091128,-1.3758337087	H,0,-6.3374942226,-1.1028047213,0.2300020734
H,0,-5.4678703159,-0.7041821535,-2.5465187692	H,0,-5.323320952,0.0359902116,-0.6631497148
C,0,-3.6943744541,1.0319359425,-1.2413917818	C,0,-4.0633386248,-0.6706903097,1.7372712447
H,0,-2.7905754693,1.2821445228,-0.6799288797	H,0,-3.2141796337,-1.0061559651,2.3393267344
H,0,-3.4190967009,0.9433209017,-2.2981258699	H,0,-3.9144318894,0.3924779429,1.5238911875
H,0,-4.3856579426,1.8743732174,-1.1487460661	H,0,-4.9623264405,-0.7705993687,2.3518184733
H,0,-0.4608036592,0.9480387956,-0.2276688437	H,0,0.8208246487,-2.565716788,1.1193275766
O,0,-1.3761829308,-3.2945343124,0.0130945546	O,0,-0.8397154704,0.804001235,-0.5736866996
O,0,-0.7756460506,-4.8615093883,0.2639851624	O,0,-0.1602694531,2.5202964016,-0.2251769423
H,0,-1.5771323121,-5.2979700863,-0.0536563788	H,0,-0.329494683,2.7517827177,-1.1499745354
H,0,-0.7895402323,-1.1006287285,-1.6192698202	H,0,-0.447242111,-1.556074203,-1.5168065208

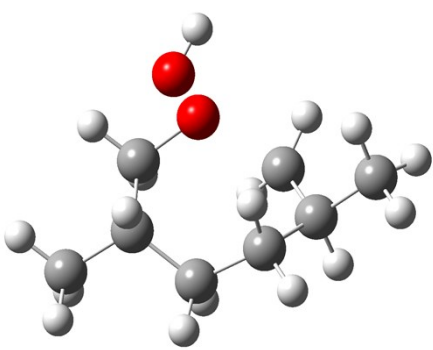


**TS9<sub>p</sub>**

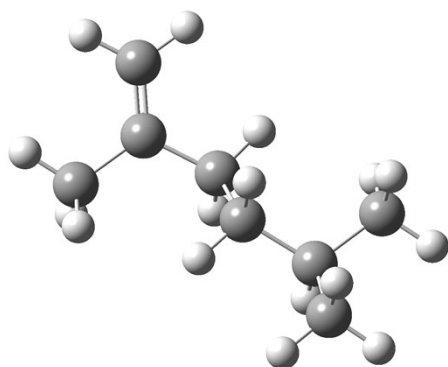
C,0,0.0040826959,-0.0018268172,-0.0086876675  
 H,0,-0.0014362141,0.0070563962,1.0848883552  
 H,0,1.0473510786,-0.0116503703,-0.3353463502  
 C,0,-0.7522796017,-1.2141374086,-0.558672343  
 C,0,-2.1980853305,-1.2490894249,-0.0528579164  
 H,0,-2.2270469754,-1.4425876522,1.0234894856  
 C,0,-0.7885754946,-1.2637031794,-2.0990376381  
 H,0,-1.2124900725,-0.3301014429,-2.4830111252  
 C,0,-1.5911442284,-2.4433973409,-2.5360256367  
 H,0,-1.1960777186,-3.414114742,-2.2482427736  
 C,0,-2.5804707552,-2.4442296034,-3.6661160501  
 H,0,-3.1683933767,-3.364939526,-3.56553299  
 C,0,-1.8456209093,-2.5232080016,-5.0270335731  
 H,0,-1.1762106882,-3.3865586646,-5.0726217749  
 H,0,-2.5666503333,-2.610901873,-5.8456543965  
 H,0,-1.2484036622,-1.6230218011,-5.2019671181  
 C,0,-3.5647356247,-1.264283309,-3.638194665  
 H,0,-4.0910491636,-1.2308006721,-2.6834328858  
 H,0,-3.0556339646,-0.3074896571,-3.788896237  
 H,0,-4.3003947507,-1.3690015228,-4.440808512  
 H,0,-0.2577911262,-2.1280081484,-0.2070582992

**TS10<sub>p</sub>**

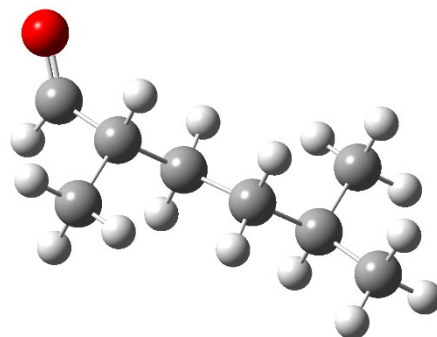
C,0,0.0033171498,0.0033577425,-0.0029551402  
 C,0,0.0040413878,0.0091849739,1.5350980059  
 C,0,1.3996513793,0.0077928362,2.1876025898  
 C,0,2.2589420018,1.216669298,1.9422214454  
 C,0,0.7687090514,1.1962525766,-0.5823359373  
 H,0,1.2652266473,-0.1095801123,3.2778885051  
 H,0,-0.5747311629,0.8724422572,1.8878231621  
 H,0,-0.5360168472,-0.8752825852,1.8905383489  
 H,0,0.5242275108,-0.898067358,-0.3488775605  
 H,0,0.3910361712,2.1403129383,-0.1659646784  
 H,0,0.6537911714,1.2450376362,-1.6665346984  
 H,0,1.9445366992,-0.8820636273,1.8559429777  
 C,0,-1.4310144248,-0.0192615241,-0.5472130263  
 H,0,-1.4405149627,-0.087301285,-1.6387305982  
 H,0,-1.9891406284,-0.8735334582,-0.1543320141  
 H,0,-1.9763847835,0.8883842727,-0.2650302561  
 C,0,1.7552474174,2.572839354,2.3255365054  
 H,0,1.9325315309,2.7598816665,3.3983962785  
 H,0,2.2823821951,3.3587263709,1.7770067332  
 H,0,0.6835819557,2.6965148619,2.1573315576  
 C,0,3.7400216366,1.0146920359,1.9636966453

H,0,-2.6954085561,-0.2886241664,-0.2475372214	H,0,4.2710957947,1.9026266105,1.6104292108
H,0,0.2422241163,-1.3249640196,-2.480236802	H,0,4.0957174806,0.8062362364,2.985780753
H,0,-0.446648772,0.9339926308,-0.3538340889	H,0,4.025561131,0.1685160294,1.3344893298
O,0,-2.8904840173,-2.2919390997,-0.7288618971	O,0,2.1686097059,1.1378495904,-0.3029934195
O,0,-4.3424994999,-2.2749652602,0.0650625923	O,0,2.8257938823,0.5303102762,-1.6808367144
H,0,-4.595316897,-3.1672485632,-0.2071020244	H,0,3.5650845352,1.1522420978,-1.705073198
<p><b>TS11<sub>p</sub></b></p> 	
C,0,-0.0283617579,-0.0271856885,0.0045956176	
C,0,-0.0028139071,-0.0037090203,1.5341437109	
C,0,1.4178894293,-0.0431111302,2.1350641447	
C,0,2.3126339345,1.1727597663,1.8065784874	
C,0,2.7894739303,0.3401629679,-0.567694677	
C,0,3.3451998334,0.989526754,0.6612337023	
H,0,0.3935907543,-0.9628405255,-0.3786131297	
H,0,-0.4648094962,0.9416130952,1.8413409896	
H,0,1.9164582539,-0.9774834101,1.8430732768	
H,0,1.6775719726,2.0262747624,1.5565579764	
H,0,-1.0545908727,0.0483969707,-0.3634399236	
H,0,1.302334095,-0.1046017281,3.2224013146	
H,0,2.8812837158,1.4525631749,2.7000088372	
H,0,4.1226233296,0.3103966078,1.0518423346	
O,0,0.7242668706,1.0292094509,-0.6049272085	

C,0,-0.8615322369,-1.1576923612,2.0707123868	
H,0,-0.9208029363,-1.1285727125,3.1619001634	
H,0,-1.8826530254,-1.1115461131,1.6808938701	
H,0,-0.4410867315,-2.1295952986,1.788551022	
O,0,-0.3016193035,2.313870046,-0.4616369554	
H,0,-0.0565775519,2.7073729323,-1.3096977778	
C,0,4.0089872393,2.3348661896,0.3355347256	
H,0,4.4261933083,2.7978000484,1.2340979707	
H,0,4.8193644428,2.2153170089,-0.3891072243	
H,0,3.2732786012,3.0259213793,-0.0868264892	
H,0,3.0059208365,0.7595366486,-1.5421586918	
H,0,2.5670415646,-0.7197609767,-0.5534162006	

**P1<sub>p</sub>,P5<sub>p</sub>**

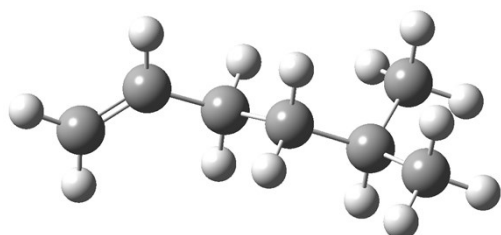
C,0,-0.0027958934,0.024225489,-0.0028720642  
 H,0,-0.0030778765,0.0391994671,1.0821666776  
 H,0,0.9663002182,0.029333958,-0.4909500136  
 C,0,-1.1391928714,-0.0010252715,-0.7007313872  
 C,0,-1.1428015401,-0.040668895,-2.2089169708  
 H,0,-1.6717649175,0.8186949595,-2.6340172697  
 H,0,-0.1286398268,-0.0448703163,-2.6124324041  
 C,0,-2.4899975441,0.0012093669,-0.0163112915  
 H,0,-3.1061637424,-0.8056297187,-0.4368717025  
 C,0,-3.256203424,1.3311448727,-0.1621353401  
 H,0,-2.6724537265,2.1308277207,0.3114080405  
 H,0,-3.3267587574,1.5917990776,-1.2238870997  
 C,0,-4.6800490716,1.3259029796,0.4268692048  
 H,0,-5.2273729457,0.4937931311,-0.0375593141  
 C,0,-5.4124164414,2.6262502064,0.0668116656  
 H,0,-5.4544243017,2.7743488734,-1.0163222395  
 H,0,-6.439177328,2.6208984362,0.4441949961  
 H,0,-4.9036756589,3.4934499096,0.5018478125  
 C,0,-4.6898857805,1.1067551941,1.9466509131  
 H,0,-4.2475263512,0.1484456616,2.2288498919

**P2<sub>p</sub>**

C,0,-0.0003747008,0.0203488431,-0.0191432125  
 H,0,0.0366437125,-0.3963256413,1.0160317801  
 C,0,1.3411910679,0.0599279268,-0.7236360909  
 C,0,2.3361707896,0.8711228392,0.123537006  
 H,0,3.3037473641,0.9539474536,-0.3743243191  
 H,0,1.9677493844,1.8853430478,0.2986707179  
 C,0,1.8007682818,-1.3946583107,-0.9849330348  
 H,0,1.9698561275,-1.8978492398,-0.023596113  
 C,0,3.0653184302,-1.5072856039,-1.8471564638  
 H,0,2.8953697348,-0.9983302481,-2.8053975279  
 H,0,3.8871008726,-0.9737529296,-1.3582454432  
 C,0,3.5305463111,-2.9511098565,-2.1241793547  
 H,0,3.6326941291,-3.4584525174,-1.1549293151  
 C,0,4.9105859982,-2.9465640857,-2.7968757774  
 H,0,5.6525725737,-2.4262000284,-2.1841107386  
 H,0,5.2714409832,-3.9650122919,-2.966616551  
 H,0,4.869056236,-2.4435974626,-3.769135265  
 C,0,2.5239863275,-3.7445121352,-2.9699158715  
 H,0,1.5500212105,-3.8321590576,-2.4827865932  
 H,0,2.3700097304,-3.2623982766,-3.9417245692

H,0,-4.1279670463,1.8978871268,2.4557572623  
H,0,-5.7118597115,1.1234827301,2.3363870958  
H,0,-1.6590345432,-0.9373746443,-2.5712817809  
H,0,-2.3499028312,-0.2291132712,1.0427434078

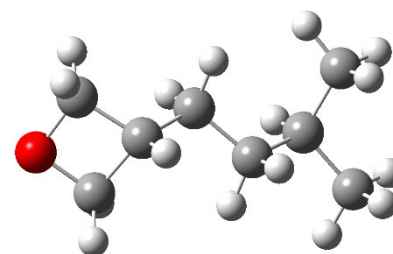
**P3<sub>p</sub>**



C,0,-0.0003913609,0.3732149832,-0.119118718  
H,0,-0.0375100139,0.8509224174,0.8557267979  
C,0,1.1228038067,-0.1609664497,-0.5897521062  
C,0,2.4474750371,-0.17109175,0.1201297244  
H,0,2.33451527,0.2758514022,1.1143353286  
C,0,3.5446070118,0.5765361867,-0.6609836816  
H,0,3.6631968542,0.1175064297,-1.6518640054  
H,0,3.2000884584,1.6014286742,-0.8397082471  
C,0,4.9188423908,0.6280340375,0.0335146701  
H,0,4.7664118566,1.0444757774,1.0388645781  
C,0,5.8656078875,1.5703647809,-0.7231688192  
H,0,5.4467961492,2.5777351304,-0.8023164833  
H,0,6.8335361799,1.6480629083,-0.2194231608  
H,0,6.049489124,1.2053543156,-1.7395986034  
C,0,5.5539922562,-0.7609653076,0.1899182494

H,0,2.8877428278,-4.7587173265,-3.1576827701  
H,0,1.1715041089,0.5600627051,-1.6824299108  
H,0,2.500685888,0.3983424578,1.0975374059  
H,0,0.978701455,-1.9270160416,-1.4735748667  
O,0,-1.0455955303,0.384771755,-0.4937164546

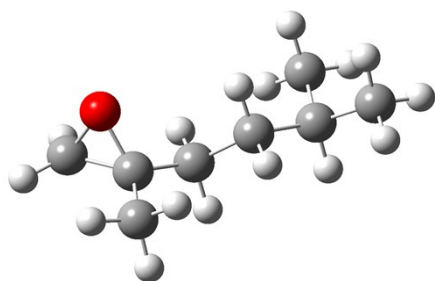
**P4<sub>p</sub>**



C,0,-0.0568013381,0.0127945096,0.0446625135  
H,0,-0.0983473064,-0.6077028762,0.9480982326  
C,0,1.3176475889,0.0426815357,-0.659752665  
C,0,1.3361238371,1.5270848095,-0.2266683257  
H,0,1.3601411866,2.2692586983,-1.0308732256  
C,0,2.4077893459,-0.8732077126,-0.1140948193  
H,0,2.4849167007,-0.7274625424,0.9714940206  
C,0,3.7769519266,-0.6292812441,-0.7624853697  
H,0,3.7121203768,-0.8426861532,-1.8382790415  
H,0,4.020197221,0.4375526246,-0.6799338688  
C,0,4.9432830502,-1.4375135891,-0.1628255767  
H,0,4.9661170034,-1.2334892804,0.9165897984  
C,0,6.2808870178,-0.971657318,-0.7545035791  
H,0,6.4401788718,0.0978418381,-0.5883694787  
H,0,7.1213647982,-1.5090382908,-0.3059194166  
H,0,6.3129217409,-1.1492757233,-1.8350766038

H,0,4.9363355111,-1.4330207336,0.7904971023  
H,0,5.7062156373,-1.2304990065,-0.7884638864  
H,0,6.5303115469,-0.689973013,0.6780871863  
H,0,1.1106229355,-0.6279278801,-1.5742894012  
H,0,2.756003001,-1.2121387861,0.2752888592  
H,0,-0.9241209851,0.3507625414,-0.6865309152

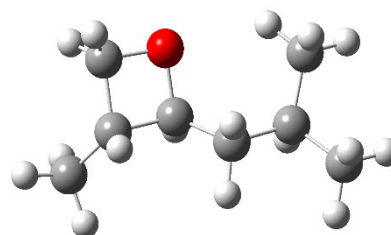
**P6<sub>p</sub>**



C,0,-0.0209408417,0.0328316324,-0.0079290394  
H,0,-0.0268127727,0.0475429704,1.0800077038  
H,0,0.9660535907,0.0432535439,-0.4659615876  
C,0,-1.1549852848,-0.559625527,-0.734550803  
C,0,-0.9262993449,-1.1190350283,-2.1227899689  
H,0,-1.7873423975,-0.9289767422,-2.7683707304  
H,0,-0.0538458279,-0.6518078868,-2.5826937519  
C,0,-2.3333328018,-1.1064082659,0.0559829409  
H,0,-2.2215701923,-2.1944387837,0.1505144953  
C,0,-3.6975293664,-0.775305382,-0.5661742123  
H,0,-3.7761547988,0.3128212755,-0.6789334813  
H,0,-3.7470432631,-1.1960450995,-1.5764880028

C,0,4.7681375667,-2.9511593823,-0.352347645  
H,0,3.8594898372,-3.3243130763,0.1260918607  
H,0,4.7150296636,-3.2056066352,-1.4169648284  
H,0,5.6126849947,-3.49836359,0.0763148416  
H,0,1.2358636291,-0.0755572716,-1.7437372262  
H,0,2.0975317807,1.781370347,0.5211236424  
H,0,2.0989042244,-1.9139566332,-0.2642472875  
O,0,0.0198298555,1.4218274681,0.3650657141  
H,0,-0.9214658328,-0.2129839737,-0.5877531496

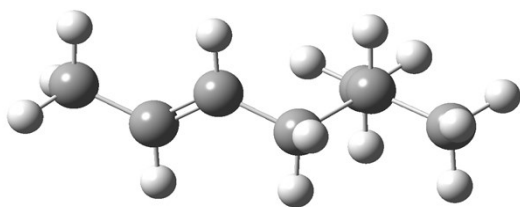
**P7<sub>p</sub>**



C,0,-0.0137515835,0.0162310034,-0.0179586478  
H,0,0.0205206099,0.0055384047,1.0790693768  
H,0,1.0069844226,0.0371959865,-0.4105678305  
C,0,-0.9830655396,-1.0158799913,-0.6292686098  
C,0,-1.5491919523,-2.1057614232,0.2674326262  
H,0,-2.3566202806,-2.6498753578,-0.2323146065  
H,0,-0.7798385249,-2.8354683026,0.5379551406  
C,0,-1.865067976,0.2170967858,-0.9464674009  
H,0,-2.7231936664,0.2995668593,-0.2625152423  
C,0,-2.3212822573,0.4281655031,-2.3797044373  
H,0,-1.4365985516,0.4481611363,-3.0289034818  
H,0,-2.9012567602,-0.4614690389,-2.6624111982

C,0,-4.9134498028,-1.2927034615,0.2272153562  
 H,0,-4.7773838981,-2.3726700861,0.3799787095  
 C,0,-6.2014335109,-1.0953148389,-0.5846910109  
 H,0,-6.1439619564,-1.6006979248,-1.5533017735  
 H,0,-7.0711679106,-1.4904025592,-0.0517694794  
 H,0,-6.3829748504,-0.0318553825,-0.7744624095  
 C,0,-5.0436146854,-0.6333649405,1.6078589458  
 H,0,-4.1786798911,-0.8309825693,2.2454926788  
 H,0,-5.1450969082,0.4530545574,1.5102664357  
 H,0,-5.9282598528,-1.0040038506,2.1337396026  
 H,0,-0.7631752821,-2.200581331,-2.0843051539  
 H,0,-2.2790608302,-0.6927217598,1.0661565843  
 O,0,-0.9973676335,0.8719239619,-0.6388709849

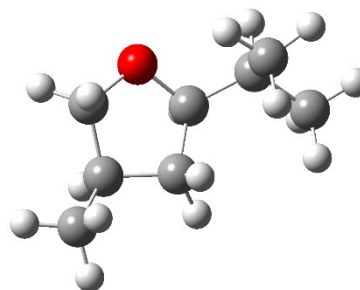
**P8<sub>p</sub>**



C,0,-0.0149567493,0.2062094639,-0.0457375128  
 H,0,-0.0276005428,0.6315719948,0.9589756832  
 C,0,1.1566350863,-0.1434453556,-0.574425991  
 H,0,1.1694062487,-0.568456833,-1.5779302818  
 C,0,-1.3538868234,0.0748590735,-0.7157110734  
 H,0,-1.2245134916,-0.3233020012,-1.7296180659  
 H,0,-1.7932298408,1.0753736419,-0.8283348877  
 C,0,-2.367181352,-0.8061799813,0.0522197036  
 H,0,-2.4319322188,-0.4150842928,1.0769132871  
 C,0,2.4913686089,0.0044688823,0.0962512847

C,0,-3.18163039,1.6816469594,-2.6300373332  
 H,0,-4.0089924603,1.6588966204,-1.9068981448  
 C,0,-3.7923963491,1.6413652828,-4.0378973994  
 H,0,-4.4031471773,0.7456581391,-4.1869663875  
 H,0,-4.4274468938,2.5138829995,-4.2165046112  
 H,0,-3.007995834,1.641794029,-4.8027062615  
 C,0,-2.3986443935,2.9851220217,-2.4129949018  
 H,0,-1.9635674439,3.0353850125,-1.4143695206  
 H,0,-1.5755632237,3.0626301894,-3.131765108  
 H,0,-3.0490923615,3.8534257813,-2.5563875123  
 H,0,-1.9516110645,-1.6845952422,1.1937315268  
 O,0,-0.8039381307,1.1192858026,-0.5166591836  
 H,0,-0.5791489162,-1.4506670129,-1.5483373271

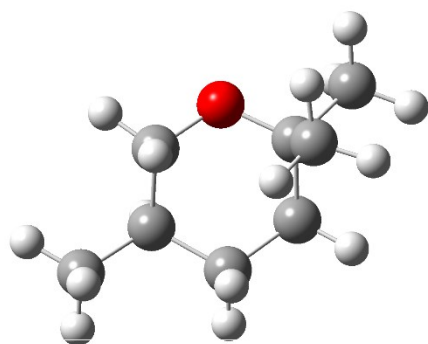
**P9<sub>p</sub>**



C,0,-0.1802362131,0.1753649422,0.0041680612  
 H,0,-0.2813570872,0.3150740112,1.0847188319  
 H,0,0.8750670262,0.3113211734,-0.2477748101  
 C,0,-0.6800914392,-1.2011124336,-0.4277179746  
 C,0,-2.160696532,-1.4616981348,-0.1151634796  
 H,0,-2.3226464308,-1.8399742232,0.8988891291  
 C,0,-0.6481798263,-1.4708335765,-1.9407312518  
 H,0,-1.0029156492,-0.587261168,-2.4818160022  
 C,0,-1.6312442928,-2.6391455374,-2.088162822

H,0,2.9983565517,-0.9626275186,0.1897573357  
H,0,3.1577725787,0.6515442163,-0.48548261  
H,0,2.3923743235,0.4332008156,1.0965116347  
C,0,-3.7615528469,-0.7009587404,-0.57891455  
H,0,-3.7512466684,-1.0678846542,-1.6111798144  
H,0,-4.4933678548,-1.2954497318,-0.0242758296  
H,0,-4.1154753607,0.3341642604,-0.5970625862  
C,0,-1.9070990304,-2.2669523351,0.131760188  
H,0,-1.8442150846,-2.7079492554,-0.8695638821  
H,0,-0.9207821621,-2.3517576199,0.5935449269  
H,0,-2.6092581085,-2.8686773457,0.7161474712

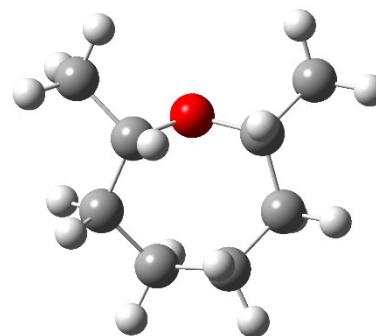
**P10<sub>p</sub>**



C,0,-0.0342178321,-0.0143161897,-0.0203146401  
C,0,-0.0481572096,-0.0564781079,1.514753082

H,0,-1.0988401057,-3.5777674682,-1.8699811487  
C,0,-2.3472687237,-2.8164456844,-3.4366024017  
H,0,-3.0225111365,-3.6687196708,-3.2913566899  
C,0,-1.3501283004,-3.1866241541,-4.5427689274  
H,0,-0.747289616,-4.0572047605,-4.265991343  
H,0,-1.8731507947,-3.4278184442,-5.4720432471  
H,0,-0.6657958418,-2.3591967642,-4.7566271308  
C,0,-3.2119397536,-1.6112978058,-3.8250905031  
H,0,-3.8827786919,-1.342567452,-3.0071310135  
H,0,-2.6045005223,-0.7362588803,-4.0765501019  
H,0,-3.8210212879,-1.8460011731,-4.7026036275  
H,0,-0.0807734315,-1.9720521575,0.0719386699  
H,0,-2.74747986,-0.5393902827,-0.2345317509  
H,0,0.3505840925,-1.715158604,-2.3085817767  
H,0,-0.7486568349,0.9699707525,-0.4898936256  
O,0,-2.6159849734,-2.4406519113,-1.0530948147

**P11<sub>p</sub>**



C,0,1.1700396973,1.223874818,-0.0901261186  
C,0,1.593528659,-0.2151332714,-0.4100723448  
C,0,0.7851259441,-1.3205930376,0.2875705605



C,0,1.3717656685,0.088233231,2.0796618362	C,0,-0.6811629489,-1.3976815092,-0.1752843295
C,0,2.1207985265,1.3148330347,1.5167456505	C,0,-1.0861181218,0.9969747422,0.760737034
C,0,0.7265488567,1.2354739724,-0.4746601899	C,0,-1.6529737808,-0.4100786561,0.49619686
H,0,1.3473221431,0.1449775323,3.1729930073	H,0,1.3966233472,1.4271822025,0.9690388889
H,0,-0.6931949101,0.7476424473,1.8908871422	H,0,1.5215339384,-0.3629295354,-1.4949300371
H,0,-0.4929983967,-0.9945101584,1.8635078311	H,0,0.8378529709,-1.2032509468,1.3776336709
H,0,0.5326261053,-0.8839515368,-0.3781684092	H,0,-0.7036340519,-1.2382120402,-1.2580480636
H,0,0.1427856407,2.1348223718,-0.2234010993	H,0,1.2703466231,-2.2772370355,0.0674417004
H,0,0.8693250025,1.2313988195,-1.5581153278	H,0,-1.0614847767,-2.4111323175,-0.0104168757
H,0,1.948844112,-0.8062713697,1.8198637897	H,0,-1.9881559942,-0.8149095062,1.4590757214
C,0,3.6183085472,1.2052652857,1.802828721	O,0,-0.2293128109,1.4433403379,-0.2952347382
H,0,4.1469071387,2.067373265,1.389248365	H,0,-0.4947005337,0.9670097055,1.6870357598
H,0,3.8073788489,1.1619266133,2.8787789323	C,0,1.9037540313,2.2406591608,-0.9565774206
H,0,4.0219644316,0.3033212765,1.3377124606	H,0,2.9867263642,2.1405525472,-0.8448031745
C,0,1.5765458292,2.636350378,2.085375002	H,0,1.6485584271,2.0901531382,-2.0088948805
H,0,1.7709966498,2.6964546183,3.1596613136	H,0,1.615010363,3.2559576259,-0.6779055239
H,0,2.0730185145,3.4785307685,1.5974910174	C,0,-2.1917554372,2.0345349353,0.9221898863
H,0,0.5003724378,2.7470149847,1.9398000556	H,0,-2.9081971552,1.7264697892,1.6892465809
C,0,-1.4402450576,-0.0602789818,-0.622554272	H,0,-1.7736438576,3.0034754147,1.2031158613
H,0,-1.4072722218,-0.0493595393,-1.7162586985	H,0,-2.7279430685,2.1538021505,-0.0231077656
H,0,-1.9701177091,-0.9663184501,-0.3151377364	H,0,-2.5493585443,-0.3251697944,-0.1285630247
H,0,-2.0376499023,0.7985903947,-0.2983022079	H,0,2.653991096,-0.3186574178,-0.1498518972
O,0,2.0366025111,1.3107041058,0.0744591177	

**CH<sub>2</sub>O**

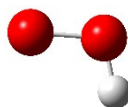
**OH**



O,0,0.,0.,-0.0076044417

H,0,0.,0.,0.9676044417

**HO<sub>2</sub>**

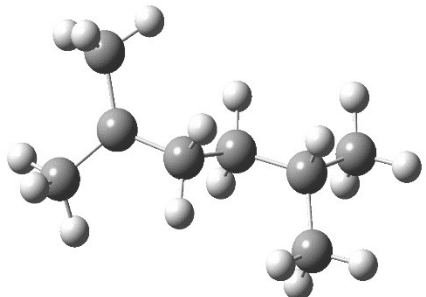
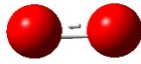
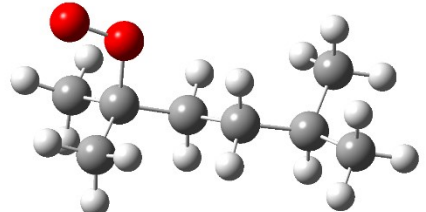


O,0,-0.0196500749,0.,-0.0154687204

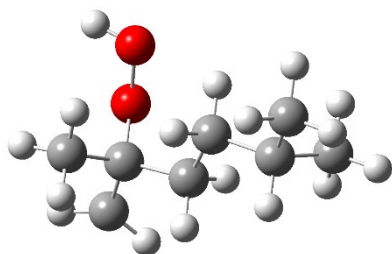
H,0,0.0204702082,0.,0.9593821961

O,0,1.2436878016,0.,-0.4239134757

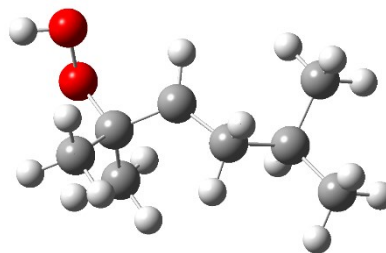
**Table S2:** Optimized geometries of reactants, intermediates, transition states and products for 2,5-dimethylhexyl-2-yl + O<sub>2</sub> reaction obtained using the B3LYP/CBSB7.

<b>2,5-Dimethylhexyl-2-yl Radical</b>	<b>O<sub>2</sub></b>
	
<p>C,0,0.0923327324,-0.0571185985,-0.4947866469  H,0,0.098777216,0.364566098,0.5265771127  H,0,1.1422703639,-0.1663706189,-0.7877698763  C,0,-0.641654613,-1.3578235661,-0.5598218318  C,0,0.0498544238,-2.6021764798,-0.100843386  H,0,-0.4657746086,-3.5066553725,-0.4375282751  H,0,1.0844681612,-2.6514326055,-0.4579346959  H,0,0.0989008669,-2.6596329718,1.001140511  C,0,-2.13020539,-1.3773058115,-0.7601944711  H,0,-2.5237937786,-0.3587838045,-0.6847825627  H,0,-2.6104042027,-1.9548369849,0.0460127016  C,0,-2.5653470785,-1.9955106344,-2.1102893944  H,0,-2.1678732414,-1.3824112502,-2.9292602304  H,0,-2.0928231899,-2.9793425349,-2.2104850335  C,0,-4.0863129794,-2.1614646638,-2.2921504972  H,0,-4.4601633617,-2.739412156,-1.4354557531  C,0,-4.3904639828,-2.9623174172,-3.5660828438  H,0,-3.9075375086,-3.9437334917,-3.5455365154  H,0,-5.466113673,-3.1206046797,-3.6883948153</p>	<p>O,0,0.,0.,0.  O,0,0.,0.,1.205752</p> <p><b>2,5-Dimethylhexyl-2-peroxy Radical (ROO-2)</b></p>  <p>C,0,0.0691058014,-0.0321052137,0.1304478773  H,0,0.1856725772,-0.1075801278,1.2143616621  H,0,1.0580681391,0.051003142,-0.322061199  C,0,-0.6486210343,-1.2679202129,-0.4057830359  C,0,0.1298964206,-2.546793466,-0.1139311838  H,0,-0.3307797738,-3.412549711,-0.5910792414  H,0,1.1504594559,-2.4520872796,-0.4857126304  C,0,-2.1199733036,-1.2970863905,0.0316355758  H,0,-2.1353602046,-1.2710378072,1.1277171382  C,0,-2.9514994976,-2.4861850225,-0.4665645912  H,0,-2.8896227398,-2.5417942117,-1.5593117727  H,0,-2.518960058,-3.4161339719,-0.083201933  C,0,-4.4350205336,-2.44243291,-0.0483921632  H,0,-4.4714800914,-2.3044373743,1.0414354556  C,0,-5.1170765698,-3.7791442572,-0.3726007334</p>

H,0,-4.0301330576,-2.4327883692,-4.4548839697	H,0,-4.6163982501,-4.6145136392,0.1256664037
C,0,-4.8271689135,-0.8167287385,-2.3124665449	H,0,-6.1635014185,-3.7776118522,-0.0543729235
H,0,-4.6934947468,-0.2582778176,-1.3829297963	H,0,-5.0980999334,-3.974177171,-1.4503192541
H,0,-4.4671974132,-0.1886516819,-3.1353082999	C,0,-5.2008883373,-1.2805119058,-0.6981176439
H,0,-5.9017224203,-0.9645578132,-2.4549533912	H,0,-4.787254204,-0.3058999679,-0.428241439
H,0,-0.3632806908,0.7000310076,-1.1406307475	H,0,-5.1758788066,-1.3628881706,-1.7901255266
	H,0,-6.2500851324,-1.2858657653,-0.3889471522
	H,0,0.1645134293,-2.7214300334,0.9645669921
	H,0,-2.5705522731,-0.3590047534,-0.3056626717
	H,0,-0.4972849707,0.8744526376,-0.095077626
	O,0,-0.7459601115,-1.1138162885,-1.897488641
	O,0,0.4224968496,-1.0686376612,-2.4955064094

QOOH-1<sub>t</sub>

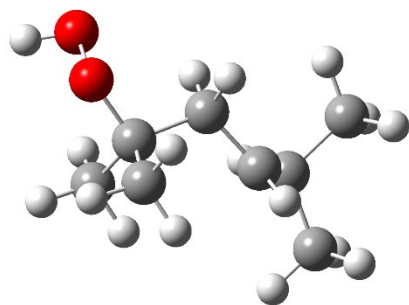
C,0,0.0010892332,-0.0446156894,-0.0107540808  
 H,0,0.002053087,-0.1373276656,1.0679770767  
 H,0,0.9498112333,0.0204705329,-0.5291150661  
 C,0,-1.2712431602,0.2017224202,-0.7579483289  
 C,0,-1.2288727647,-0.4750849234,-2.1322974136  
 H,0,-2.0839162254,-0.1785707965,-2.7388625087  
 H,0,-0.3131127314,-0.194024466,-2.6590828286  
 C,0,-2.4761396848,-0.2123134104,0.1133430539  
 H,0,-2.3074274868,-1.2530009408,0.4215865075  
 C,0,-3.8754183781,-0.0992172873,-0.5045880725  
 H,0,-4.0700304058,0.9381093672,-0.7898219683  
 H,0,-3.9111108038,-0.6844513131,-1.4300064771  
 C,0,-5.0081098566,-0.5959828236,0.4166836308  
 H,0,-4.7624542546,-1.6206782617,0.7299523042  
 C,0,-6.3350153845,-0.6486660391,-0.3539498647  
 H,0,-6.2600317782,-1.2933184149,-1.2347718844  
 H,0,-7.1446464482,-1.0319903668,0.2741256341  
 H,0,-6.6249117312,0.3505138382,-0.6966441506  
 C,0,-5.1600864327,0.2607204714,1.6822645837  
 H,0,-4.2589403554,0.252212318,2.3000113808  
 H,0,-5.3744037174,1.3025700319,1.4200709754  
 H,0,-5.9852444125,-0.1027429932,2.3018565849  
 H,0,-1.2400011933,-1.5618850175,-2.020394731

QOOH-2<sub>t</sub>

C,0,0.0239439582,0.1334467942,-0.4347128316  
 H,0,-0.1325363653,0.4510256988,0.59803111  
 H,0,1.0968390668,0.0125129262,-0.60245375  
 C,0,-0.7115472905,-1.1920841185,-0.6980190582  
 C,0,-0.1064979641,-2.3303293537,0.1447250071  
 H,0,-0.5717265717,-3.2811263739,-0.1179066995  
 H,0,0.9714704298,-2.3963675862,-0.0308265626  
 C,0,-2.1972905576,-1.0667418172,-0.5062612949  
 H,0,-2.8169691938,-1.3848341347,-1.3347872798  
 C,0,-2.8338772266,-0.6581378987,0.7808457105  
 H,0,-3.528567635,-1.4444779587,1.1179517634  
 H,0,-2.0771991494,-0.568552647,1.5683820443  
 C,0,-3.6380820014,0.6725910619,0.7341410408  
 H,0,-2.9516143057,1.4572683684,0.3924240089  
 C,0,-4.1282993315,1.0452540415,2.1390898046  
 H,0,-3.2958949384,1.1361260416,2.8435226447  
 H,0,-4.6638326918,1.9989702296,2.1298767596  
 H,0,-4.813190192,0.2841719917,2.5288817122  
 C,0,-4.807778697,0.6017642187,-0.2548026717  
 H,0,-4.4658113646,0.3941099607,-1.271173751  
 H,0,-5.5126289266,-0.1870101966,0.0317085068  
 H,0,-5.3584946812,1.5466343541,-0.2755833537  
 H,0,-0.2710359499,-2.155106246,1.2103241818

O,0,-1.2151306871,1.6615176248,-0.9113263332  
O,0,-2.2619537186,2.1295343015,-1.8254247718  
H,0,-1.7143865041,2.4545404124,-2.5522453346  
H,0,-2.4172211252,0.3952408794,1.0210983629

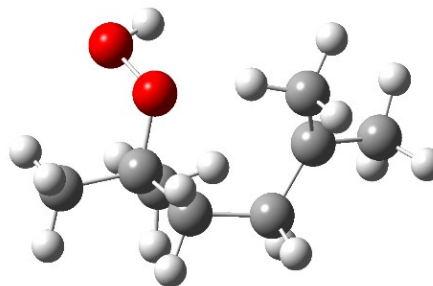
**QOOH-3<sub>t</sub>**



C,0,0.5520353041,-0.4887140356,0.0495161456  
H,0,0.5318283536,-0.4886708744,1.1415560787  
H,0,1.5362281907,-0.8338223659,-0.2792250984  
C,0,-0.5423811147,-1.4025126036,-0.5036505925  
C,0,-0.3019932429,-2.8636336379,-0.1206092484  
H,0,-1.0679696171,-3.5061723464,-0.5601444306  
H,0,0.6750918292,-3.1953192898,-0.4785574757  
C,0,-1.9663800608,-0.9242971993,-0.1033299277  
H,0,-2.6658182137,-1.6024532615,-0.6123000363  
C,0,-2.2400201552,-0.8797448526,1.3639637297  
H,0,-2.3379236702,-1.8182129261,1.9048779051  
C,0,-2.6219118785,0.3808464987,2.0807809721  
H,0,-2.0322223866,1.2051945911,1.6545588232  
C,0,-2.3163768279,0.2997551517,3.5839877827  
H,0,-1.2541664092,0.1142085095,3.764402039  
H,0,-2.5896693931,1.2287195449,4.0926743832

H,0,-0.3516014536,0.9106506005,-1.1020360441  
O,0,-0.4106696385,-1.4088300951,-2.1009656822  
O,0,-1.0548699369,-2.6326888309,-2.5531306104  
H,0,-0.2795471347,-3.1906378341,-2.6994715478

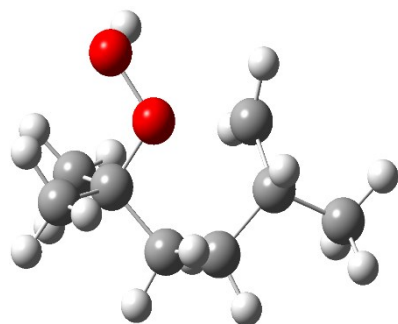
**QOOH-4<sub>t</sub>**



C,0,0.2048323073,-0.3893715544,0.3621511646  
H,0,-0.0728182136,-0.5069805624,1.4253052816  
H,0,1.2792459998,-0.5840956211,0.2949606402  
C,0,-0.571416709,-1.3211135813,-0.5140297725  
C,0,-0.0698997484,-2.7227704445,-0.6704475944  
H,0,-0.5331654509,-3.2320926404,-1.5216734251  
H,0,1.0164297439,-2.7510280665,-0.8047580416  
C,0,-2.0328679952,-1.0688375134,-0.7529216288  
H,0,-2.5850652217,-1.2417845442,0.1909119448  
C,0,-2.4548790933,0.3325311759,-1.2393726193  
H,0,-3.5493672461,0.3594572102,-1.2701129167  
H,0,-2.1561211017,1.0927393222,-0.5114977221  
C,0,-1.9621843493,0.8034615305,-2.6254478558  
C,0,-2.708651827,2.0763401006,-3.0395438266  
H,0,-2.6593878705,2.8210724248,-2.2415933463  
H,0,-2.2558971115,2.5018438079,-3.9358885092  
H,0,-3.7592814788,1.8586049573,-3.2499371336

H,0,-2.8820900446,-0.5135281698,4.05083265  
C,0,-4.1124092442,0.7321276888,1.8471284342  
H,0,-4.3370578781,0.8189126847,0.7811580236  
H,0,-4.7614482573,-0.0426668504,2.2667514105  
H,0,-4.3654146627,1.6837796241,2.3257225173  
H,0,-0.3299304092,-2.9752820741,0.9649602304  
H,0,0.4065500938,0.5373596527,-0.2927701611  
O,0,-0.461749667,-1.4665629142,-1.9508138287  
O,0,-0.6756396752,-0.1421911469,-2.5150809196  
H,0,0.2102000111,0.0445164136,-2.8530206945  
H,0,-2.1101886847,0.0646834391,-0.5462385269

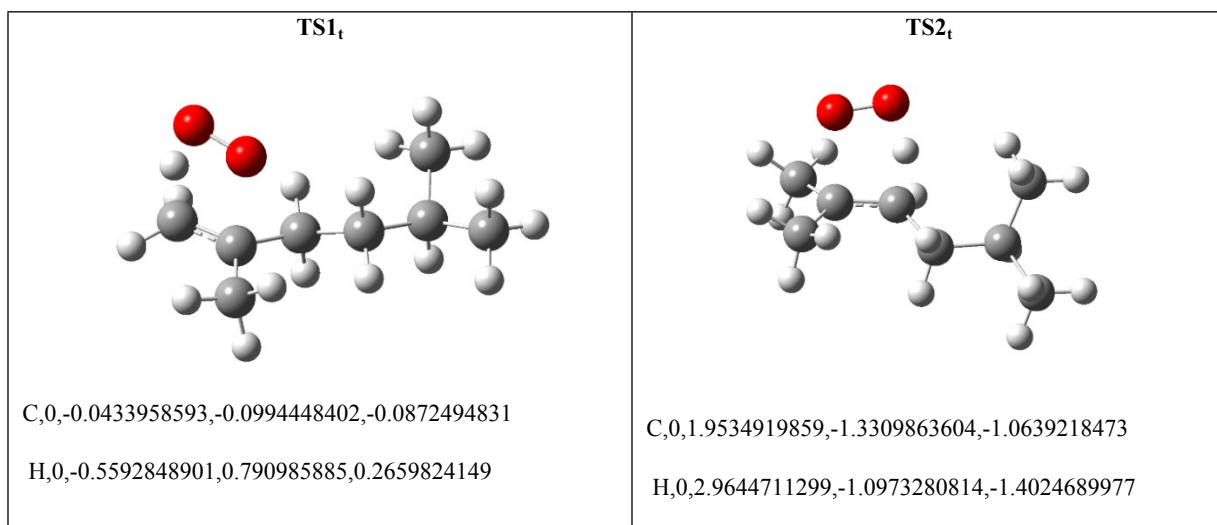
**QOOH-5<sub>t</sub>**



C,0,-0.155890573,-0.6199120165,-0.0182719191  
C,0,-0.0721245416,-0.0429295019,2.4595182544  
H,0,0.7090584958,-0.0364068974,3.2280670549  
C,0,-1.0376856289,1.0960738061,2.8340732984  
H,0,-1.3121007545,0.9726075076,3.8877882965  
H,0,-0.5034882013,2.0507432525,2.7704761513  
C,0,-2.3616404238,1.2669285103,2.0605942127  
C,0,-3.2247317894,2.3444599383,2.726307303

C,0,-2.0712398827,-0.2800070971,-3.7012890722  
H,0,-1.4343396326,-1.1329592935,-3.4582058898  
H,0,-3.1023837005,-0.6327923613,-3.7884827299  
H,0,-1.7666194896,0.1168338576,-4.6706848889  
H,0,-0.2875749097,-3.3406809937,0.2199973895  
H,0,0.0408439404,0.6576413626,0.0993062079  
O,0,-0.5702793287,1.1317019602,-2.376174226  
H,0,-2.4211924736,-1.8236514698,-1.4448276717  
O,0,0.0452083247,1.6152884783,-3.6028336108  
H,0,0.6415156748,0.8794172713,-3.7948545988

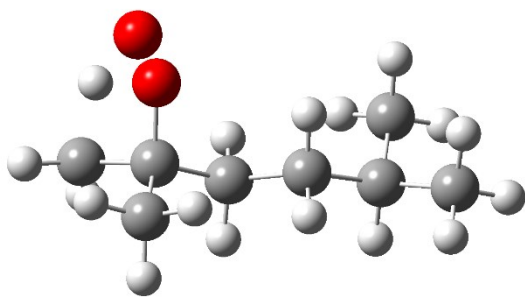
H,0,-2.6448624644,3.2585542448,2.8740052861	
H,0,-4.0810954376,2.5791674362,2.0925087307	
H,0,-3.5943305376,2.0034261722,3.6973274843	
C,0,-3.1395403705,-0.0430501036,1.9103643352	
H,0,-2.5726418929,-0.7712494381,1.3279545053	
H,0,-3.3480853664,-0.4735209647,2.8935551117	
H,0,-4.0930996455,0.1357311583,1.4115277382	
O,0,-1.9089359172,1.7590345863,0.772413813	
H,0,-0.5686133302,-1.0151805641,2.5562494216	
O,0,-3.042636019,1.9263558998,-0.1200360823	
H,0,-2.9035280413,1.1753661994,-0.7132630602	
C,0,0.621578456,0.0446093945,1.07250137	
H,0,0.7369543333,1.1027917039,0.8169030067	
C,0,2.0407610073,-0.5743719642,1.1546889748	
H,0,2.5488112044,-0.526231177,0.1883601214	
H,0,2.6537201506,-0.0419636935,1.8893567028	
H,0,1.9894701154,-1.6261497812,1.4539122323	
H,0,-0.4826614776,-1.6487440471,0.1027585797	
H,0,-0.2109933334,-0.1888101327,-1.0104133057	





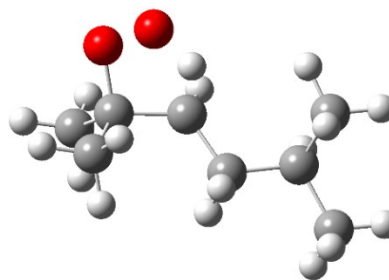
C,0,1.3515556944,-0.09242357,-0.0900698864	H,0,1.9005495781,-2.4166551604,-0.8994003904
C,0,2.1024930395,1.1863911471,0.1406495434	C,0,1.6316526633,-0.6170609583,0.215821694
H,0,2.9559330615,1.2870891747,-0.5310687967	C,0,2.7359798405,-0.5399969025,1.2302031494
H,0,1.4546357039,2.0545910133,0.0116824164	H,0,2.4739734404,0.112376693,2.065026953
C,0,2.1007364582,-1.4021090058,-0.0133707395	H,0,2.9309305344,-1.5422540517,1.6358090719
H,0,2.1846136634,-1.6461147367,1.0584842122	C,0,0.3225323849,-0.2783598908,0.5759222327
C,0,3.5032947056,-1.4493461163,-0.6347322273	H,0,0.1714451743,-0.138671818,1.6491120698
H,0,3.4350426587,-1.2075364852,-1.7001649452	C,0,-0.9048478737,-0.8145128003,-0.1627569855
H,0,4.1268105404,-0.6738546005,-0.1772571661	H,0,-0.8616134339,-0.5390015449,-1.223564223
C,0,4.2237634726,-2.801813635,-0.4651238075	H,0,-0.8976813107,-1.9115754817,-0.1344577609
H,0,4.2264136555,-3.0489140515,0.605941102	C,0,-2.2476619693,-0.3261498376,0.414454209
C,0,5.6849846057,-2.6836742672,-0.9209809183	H,0,-2.2628318221,-0.5884012435,1.4815307997
H,0,6.2158490977,-1.9054470924,-0.3646878418	C,0,-3.4153260421,-1.0570222615,-0.2622635665
H,0,6.2227929883,-3.6250228714,-0.7761319986	H,0,-3.3281495679,-2.1418322047,-0.1504168409
H,0,5.7408862134,-2.4294534927,-1.9848939026	H,0,-4.3738226676,-0.7522354417,0.1670523324
C,0,3.5212210727,-3.9450477678,-1.2124279659	H,0,-3.4464745623,-0.8333923222,-1.3341846956
H,0,2.5030364412,-4.1130198719,-0.8531882917	C,0,-2.4202726144,1.1948176119,0.2990890343
H,0,3.4658247466,-3.7297840009,-2.2849952544	H,0,-1.6467522777,1.7420606706,0.8427542937
H,0,4.069059946,-4.8836981554,-1.0894694409	H,0,-2.3768029728,1.5131401785,-0.7480149152
H,0,2.4897619474,1.2026465477,1.168512449	H,0,-3.3879609874,1.5071191514,0.7020250719
H,0,-0.5499783539,-1.0387059189,0.127171827	H,0,1.2535727863,-1.0871646435,-1.8629557387
O,0,1.4411647976,0.0947168482,-2.4068236666	H,0,3.6651056032,-0.1810577973,0.7822324638
H,0,1.4662244411,-2.1801476783,-0.4452825948	O,0,0.9801846517,2.0142435451,-0.3632330235
O,0,0.1804009403,0.0925708011,-2.622321828	O,0,2.093493322,1.4617168567,-0.6617657183
H,0,-0.2075716118,-0.0037310303,-1.4202941465	H,0,0.4307310672,1.0000508753,0.193735758

**TSQ1<sub>t</sub>**



C,0,-0.0106630178,0.0170704241,-0.0123523759  
 H,0,-0.0130531007,0.0345561206,1.0747118743  
 H,0,0.9818541116,0.0178276559,-0.4606071803  
 C,0,-1.0763693203,-0.8306132364,-0.7273798548  
 C,0,-0.5199397437,-2.1295223751,-1.3016713765  
 H,0,-1.257542622,-2.624448935,-1.936219668  
 H,0,0.3669595022,-1.9264757611,-1.9042106115  
 C,0,-2.3085598639,-1.0125752264,0.178889096  
 H,0,-2.0028263106,-1.5837633297,1.0643556885  
 C,0,-3.5060790195,-1.691517835,-0.4943179056  
 H,0,-3.7407407176,-1.1551020074,-1.4208481038  
 H,0,-3.2326549425,-2.7115594931,-0.7858264888  
 C,0,-4.7722893112,-1.7693005839,0.3822592688  
 H,0,-4.4919282414,-2.2377751695,1.3362769993  
 C,0,-5.8259339685,-2.6649670008,-0.2846815404  
 H,0,-5.4380015538,-3.6717509565,-0.4659238294  
 H,0,-6.7198469126,-2.7574642433,0.3388922133  
 H,0,-6.1358152256,-2.2487478108,-1.2493268712  
 C,0,-5.3637622943,-0.3860424995,0.6905383456  
 H,0,-4.6635107421,0.2535005856,1.232864358  
 H,0,-5.6390105726,0.1318254221,-0.2344245137  
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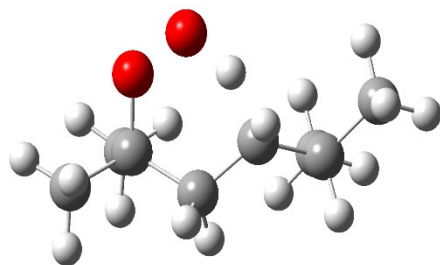
**TSQ2<sub>t</sub>**



C,0,0.00243  
 6501,0.0008609233,-0.0060528963  
 H,0,0.0059835537,0.0086655836,1.086905662  
 H,0,1.0404029614,-0.0030878365,-0.348779635  
 C,0,-0.7311386668,-1.2314777184,-0.5265239614  
 C,0,-0.0410922533,-2.533084388,-0.1154626141  
 H,0,-0.5384763484,-3.3893641753,-0.5720474383  
 H,0,0.9948250301,-2.5142200725,-0.4604686539  
 C,0,-2.2476941405,-1.2151382565,-0.2175711984  
 H,0,-2.6859328636,-0.2337350492,-0.4221816337  
 C,0,-2.8255882715,-1.9066680783,0.985670835  
 H,0,-2.5484597485,-2.9677663345,0.9873266712  
 H,0,-2.358436819,-1.4799396017,1.8890676818  
 C,0,-4.3561197479,-1.778015454,1.1271242654  
 H,0,-4.5987935925,-0.706947261,1.1172605686  
 C,0,-4.8222025054,-2.354302017,2.4703377328  
 H,0,-4.3332630246,-1.8555805322,3.3124409403  
 H,0,-5.9023543057,-2.238233123,2.5944324147  
 H,0,-4.5942924923,-3.4235605164,2.5371095746  
 C,0,-5.0964144218,-2.4432977458,-0.0414599689  
 H,0,-4.8244405696,-2.0008950446,-1.0030244209  
 H,0,-4.8651480568,-3.5130839267,-0.0890573481  
 H,0,-6.1789829629,-2.3425043274,0.0750722415

H,0,-0.2483027489,-2.8136734115,-0.4935443778  
H,0,-0.6328473739,1.131957145,-0.5230554693  
O,0,-1.4043014931,-0.0026430957,-1.8835844782  
H,0,-2.5943192089,-0.017163742,0.5273929813  
O,0,-1.4717141939,1.3154543534,-1.3565385198

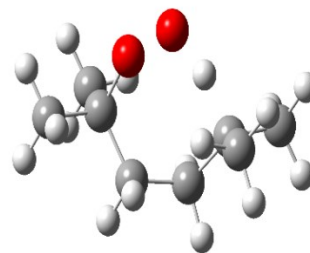
**TSQ3<sub>t</sub>**



C,0,0.0094768815,-0.0125073144,0.0411447676  
H,0,0.0001300713,-0.0292156747,1.1342807767  
H,0,1.0479911244,-0.0165113752,-0.2980386477  
C,0,-0.7173082867,-1.2401390063,-0.5123180142  
C,0,-0.029189774,-2.5340494448,-0.0827605392  
H,0,-0.4837841737,-3.3905000302,-0.585503013  
H,0,1.032634511,-2.5055962251,-0.335491237  
C,0,-2.2443534594,-1.2575943047,-0.1201587846  
H,0,-2.5298323842,-2.3049390602,0.0147800212  
C,0,-3.1820280239,-0.6281352137,-1.1381213008  
H,0,-2.2557878305,-0.1626256039,-2.0417055957  
H,0,-3.6587820896,-1.3659073557,-1.7865195824  
C,0,-4.116002829,0.5004261344,-0.7365459292  
H,0,-4.7363706902,0.1186906514,0.0925361411  
C,0,-5.0616695636,0.8649949226,-1.8903337095  
H,0,-5.6311597058,-0.0051139915,-2.2289068057

H,0,-0.0393452742,-2.6609731577,0.9700597656  
H,0,-0.4778027412,0.9130686297,-0.3645541962  
O,0,-0.7329561314,-1.1065659443,-1.9754066682  
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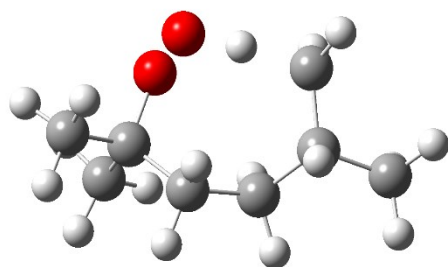
**TSQ4<sub>t</sub>**



C,0,0.0124954933,-0.0103871255,-0.0119291555  
H,0,0.0163204023,-0.0113171138,1.0885030832  
H,0,1.0552595979,-0.0198943527,-0.3404207183  
C,0,-0.0726625314,-2.5475475731,-0.271642092  
H,0,-0.2012065492,-2.7903173082,0.7949100301  
C,0,-0.5858396072,-3.7509673805,-1.0898671287  
H,0,-0.0956259932,-4.6513852017,-0.7030089325  
H,0,-1.6560239396,-3.8863872233,-0.9060137737  
C,0,-0.3739925542,-3.7362573661,-2.6214808088  
C,0,-1.0942414829,-4.932771263,-3.2482808064  
H,0,-2.1646932965,-4.8909964018,-3.03408298  
H,0,-0.9599977692,-4.9302996311,-4.3316061742  
H,0,-0.6967246735,-5.8684760145,-2.8479370909  
C,0,1.0992598052,-3.7095228992,-3.0295241393  
H,0,1.6011194741,-2.8169248639,-2.6599565133  
H,0,1.6123018626,-4.5919385812,-2.6376920274

H,0,-5.7751032572,1.6350202175,-1.5847636338  
 H,0,-4.4992170078,1.2505632613,-2.746588631  
 C,0,-3.3805233057,1.7470676164,-0.2185838766  
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 H,0,-2.7706949955,2.1930732561,-1.0098202111  
 H,0,-4.0969148674,2.5001603928,0.1202764408  
 H,0,-0.1262080673,-2.6719740226,0.99687337  
 H,0,-0.4555752341,0.9102072897,-0.301146236  
 O,0,-0.6290563127,-1.2757528075,-1.9533788519  
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 H,0,-2.3467226008,-0.7663317258,0.8520695495

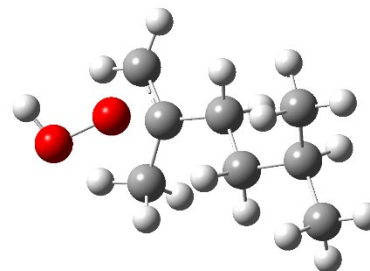
**TSQ5<sub>t</sub>**



C,0,0.0218446986,0.119806549,0.047559459  
 C,0,-0.0046595966,0.003885671,2.597793612  
 H,0,0.7028615744,-0.0654584036,3.4295287599  
 C,0,-1.096034649,1.0408157353,2.9549786705  
 H,0,-1.0070125215,1.3202941703,4.0093653165  
 H,0,-0.9243201283,1.9594462101,2.3873716653  
 C,0,-2.5653185175,0.6200880245,2.7360993909  
 C,0,-3.495675782,1.8255945805,2.8966174742  
 H,0,-3.275861631,2.5710561036,2.1312395255  
 H,0,-4.5380118419,1.5168172602,2.7890352519  
 H,0,-3.3690772435,2.2857093186,3.8804433618

H,0,1.1828925903,-3.713628937,-4.1184477625  
 H,0,-0.4409214677,0.9303068539,-0.3347488621  
 O,0,-1.092164536,-2.6086457611,-3.2148920397  
 H,0,1.0060456155,-2.4338430417,-0.4203624698  
 O,0,-0.4110709396,-1.3933341608,-3.0126065944  
 C,0,-0.748927622,-1.2070213209,-0.5397539974  
 H,0,-0.6156756596,-1.1390990563,-1.87716081  
 C,0,-2.247455038,-1.1573349855,-0.3292037198  
 H,0,-2.7715821698,-1.8951760113,-0.9400393796  
 H,0,-2.4956633326,-1.3598361547,0.7235200655  
 H,0,-2.6476191023,-0.1719330363,-0.5792220886

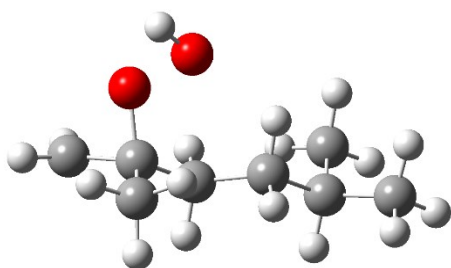
**TS3<sub>t</sub>**



C,0,-0.0059524046,0.0178109571,0.0007352444  
 H,0,-0.0095231595,0.0215409148,1.0842615828  
 H,0,0.9550907639,0.0296962503,-0.499882536  
 C,0,-1.1908217532,0.1396262539,-0.720137585  
 C,0,-1.1594035702,-0.1171911591,-2.2062735382  
 H,0,-1.9452933157,0.4316131379,-2.7241383456  
 H,0,-0.2008165211,0.181346054,-2.6307605673  
 C,0,-2.4930958847,-0.1109333008,0.027674151  
 H,0,-2.5284369969,-1.1832368029,0.2642952254  
 C,0,-3.788842186,0.2825556857,-0.6924668767  
 H,0,-3.7375872107,1.3389191936,-0.9732806441

C,0,-2.9916976056,-0.5303330245,3.6499108934  
 H,0,-2.3226343484,-1.3876860237,3.558730787  
 H,0,-2.9921325266,-0.1983711006,4.6909017787  
 H,0,-4.000781119,-0.857418246,3.3908449539  
 O,0,-2.7491814144,0.0491085121,1.4089361047  
 H,0,-0.4407696231,-0.994498194,2.4877755471  
 C,0,0.8045933807,0.3309799122,1.3210969408  
 H,0,1.1043083554,1.385049668,1.3755597161  
 O,0,-2.3424152956,0.9653154398,0.4161390637  
 H,0,-1.2758758349,0.6560378571,0.1969453511  
 H,0,-0.290530805,-0.9080860206,-0.1455369937  
 H,0,0.3894526892,0.6315536819,-0.8414753466  
 C,0,2.0981478215,-0.514635712,1.2704790878  
 H,0,2.6860969406,-0.2904760001,0.3768111517  
 H,0,2.722444744,-0.3137257092,2.1465765168  
 H,0,1.8633464849,-1.5833726852,1.2592587591

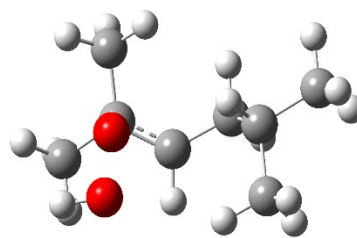
**TS4<sub>t</sub>**



C,0,-0.0029010046,0.0170805846,0.0117775229  
 H,0,-0.0064726751,0.0104960758,1.0936497251  
 H,0,0.9443831853,0.0328213272,-0.5101861065  
 C,0,-1.2696663633,0.1996394896,-0.7416586185  
 C,0,-1.1958767568,-0.205695394,-2.2094257634  
 H,0,-1.9861106029,0.2942975696,-2.7681879365

H,0,-3.8701930041,-0.287328564,-1.6244730629  
 C,0,-5.0673362518,0.0324098678,0.1321114262  
 H,0,-5.0501438468,-1.0131989686,0.4711740041  
 C,0,-6.3118452042,0.2158415242,-0.7480475603  
 H,0,-6.2920557245,-0.4551776762,-1.6119187391  
 H,0,-7.2287858077,0.0130037643,-0.1869257194  
 H,0,-6.3734406603,1.2423358617,-1.1254872644  
 C,0,-5.1551575661,0.9302284783,1.3751488512  
 H,0,-4.3209065887,0.771029096,2.0625488259  
 H,0,-5.1536191647,1.9875736639,1.0891734537  
 H,0,-6.0776829827,0.736679474,1.9303467403  
 H,0,-1.3040011503,-1.1865009439,-2.3975213887  
 O,0,-1.3136751074,2.0589434075,-0.6630176942  
 O,0,-0.5753199565,2.6598902389,-1.6886148365  
 H,0,0.1722121576,3.0461155771,-1.210879163  
 H,0,-2.4208614415,0.4099180362,0.9864071462

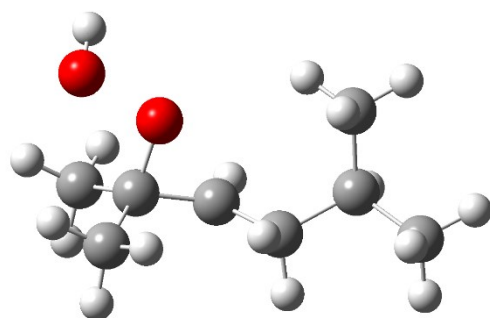
**TS5<sub>t</sub>**



C,0,-0.0126461891,0.0245820276,-0.0604276272  
 H,0,0.1123207995,0.0023292361,1.0279779486  
 H,0,0.9781943158,0.0666925821,-0.5152181855  
 C,0,-0.745994481,-1.2102474413,-0.5272321945  
 C,0,0.0581491666,-2.4886770435,-0.4951191359  
 H,0,-0.4599775927,-3.2915717177,-1.0237306913

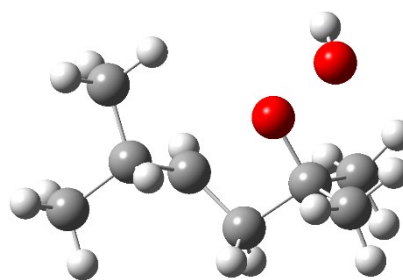
H,0,-0.2370198394,0.0968370319,-2.6364007767  
C,0,-2.5109531604,-0.2969238836,0.0116889573  
H,0,-2.4459711056,-1.3914433875,0.0797215274  
C,0,-3.8617312358,0.1021397828,-0.5959307093  
H,0,-3.9052731464,1.191340651,-0.6880838589  
H,0,-3.9305606311,-0.2964475818,-1.6139605585  
C,0,-5.0847011596,-0.3996922756,0.1974119418  
H,0,-4.9828620183,-1.4871983389,0.3227894396  
C,0,-6.3735976705,-0.1398332362,-0.5955886914  
H,0,-6.3419994992,-0.6201230361,-1.5780888902  
H,0,-7.2508637201,-0.5205332766,-0.0641403398  
H,0,-6.520713881,0.9337488612,-0.7549179086  
C,0,-5.1828698393,0.2292529397,1.5950958293  
H,0,-4.3175262935,-0.0083899802,2.2185118074  
H,0,-5.252788252,1.3200259259,1.5240962455  
H,0,-6.0730018427,-0.1283297038,2.1210659663  
H,0,-1.3049338664,-1.2878400842,-2.3212042441  
O,0,-1.0062161863,1.5835336379,-0.5420080451  
O,0,-2.0680625552,2.5595890617,-1.4829336183  
H,0,-1.3545758748,3.1225963727,-1.8139191061  
H,0,-2.4334395845,0.0903662787,1.0314604885

**TS6<sub>t</sub>**



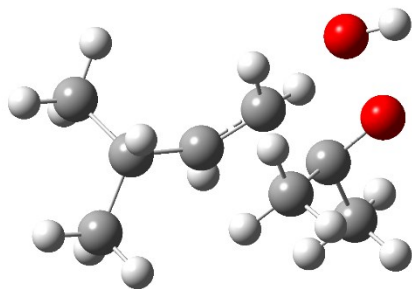
H,0,1.0422914493,-2.3410350519,-0.9472140044  
C,0,-2.1342962341,-1.3098355923,-0.4260486946  
H,0,-2.564732349,-2.2835306218,-0.6433169331  
C,0,-3.0986759125,-0.1835333913,-0.2355894552  
H,0,-3.9558993197,-0.5508679587,0.3445465986  
H,0,-2.6465147234,0.6204434808,0.3527558709  
C,0,-3.6486187174,0.4278861385,-1.5584344944  
H,0,-2.7875432042,0.8149548857,-2.1120865782  
C,0,-4.5994355262,1.5880343665,-1.2413742116  
H,0,-4.1098471908,2.3558950762,-0.634422269  
H,0,-4.9536103506,2.0648407483,-2.1599517779  
H,0,-5.4788100189,1.2367738863,-0.6898681674  
C,0,-4.329382247,-0.6268968332,-2.4394222653  
H,0,-3.6208530522,-1.3918764988,-2.7631795423  
H,0,-5.1523752329,-1.1168275835,-1.9054655555  
H,0,-4.748292304,-0.1639839665,-3.3376986607  
H,0,0.2152859427,-2.8167555766,0.5381388279  
H,0,-0.5434540314,0.938995223,-0.3244726644  
O,0,-0.5863099361,-0.7474434323,-2.4082215934  
O,0,-0.9185896214,-1.8072470472,-3.2626145619  
H,0,-0.0972999078,-2.3182862598,-3.3106192559

**TS7<sub>t</sub>**

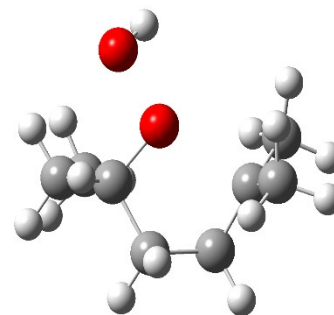


C,0,0.0154385249,-0.0280794658,-0.0121027848	C,0,-0.001138701,0.0052003947,-0.0052191205
H,0,0.1167290573,-0.0635549799,1.0760879911	H,0,0.005297291,0.0074844049,1.0882358238
H,0,1.009137436,-0.0162797628,-0.4619353967	H,0,1.0304719433,0.0045918471,-0.3591217676
C,0,-0.7520546568,-1.2398276968,-0.5368663632	C,0,-0.72607018,-1.2281317286,-0.5378432468
C,0,-0.0768316997,-2.5552165824,-0.1634329449	C,0,-2.1016374464,-1.4581859873,0.1336638076
H,0,-0.6110559221,-3.4090939053,-0.5798733442	H,0,-2.835452388,-1.8093244581,-0.5966426532
H,0,0.9323593446,-2.5591942108,-0.5783206602	C,0,-1.7811418671,-2.5392740188,1.1291596837
C,0,-2.229924214,-1.1400903105,-0.3647139998	H,0,-1.3848426012,-2.2383263347,2.0952698695
C,0,-3.1986674978,-2.2662675252,-0.3655546757	C,0,-2.3080963594,-3.9343458589,1.0218528765
H,0,-2.73910085,-3.1691518276,-0.7776882931	H,0,-2.4426822674,-4.1596898477,-0.0427005276
H,0,-3.4301225155,-2.5012957744,0.6881984124	C,0,-3.6921368004,-4.0442366719,1.7049463225
C,0,-4.5292344309,-1.9764080918,-1.0973474335	H,0,-4.4108931423,-3.3415206174,1.2747257199
H,0,-4.9227571418,-1.030807697,-0.7000198753	H,0,-4.0959971744,-5.0542544663,1.5857915581
C,0,-5.5560789706,-3.0755304198,-0.7972431371	H,0,-3.6157704391,-3.8364047255,2.7766244756
H,0,-5.750280725,-3.1636806079,0.2760059471	C,0,-1.3176396045,-4.951556241,1.6072449951
H,0,-6.5079837411,-2.8685777442,-1.293795944	H,0,-0.3585691525,-4.8888100392,1.0906297072
H,0,-5.2019939175,-4.0485187545,-1.1543276221	H,0,-1.1483722466,-4.7631668221,2.6729344584
C,0,-4.3174874605,-1.8109306112,-2.6075463736	H,0,-1.7019736093,-5.9705339075,1.5063952476
H,0,-3.5806714516,-1.0366545556,-2.8280033239	H,0,-0.4904499658,0.9214372537,-0.3491220582
H,0,-3.9504444858,-2.7429685699,-3.0499106334	H,0,-2.4897659947,-0.5446910969,0.5963252618
H,0,-5.2565387662,-1.5505577315,-3.1042516976	C,0,-0.7854217008,-1.249497882,-2.0607592903
H,0,-0.0117503243,-2.6692937121,0.9224436325	H,0,-1.3971118102,-0.4165532836,-2.4222899837
H,0,-0.4978613657,0.8964351456,-0.2877746513	H,0,0.2136873912,-1.1658287896,-2.487968516
O,0,-1.0258969701,-1.1404934663,-1.9250104515	H,0,-1.2310369352,-2.1848076208,-2.4067795784
H,0,-2.6286036736,-0.1318952893,-0.2976503186	O,0,-0.0811682314,-2.4425548389,-0.0182182624
O,0,0.4736451901,-1.1331053741,-2.7996278999	O,0,1.4016440639,-2.5068830214,-0.7910489278
H,0,0.270314325,-0.3002573905,-3.2469723547	H,0,1.9110892311,-2.5619677124,0.0279577672
	<b>TS9<sub>t</sub></b>

**TS8<sub>t</sub>**


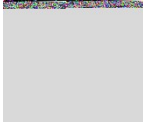
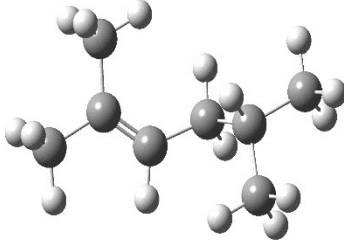


C,0,0.0020651361,-0.0267528126,0.0273453897  
H,0,0.0427628489,-0.0676794786,1.1175997697  
H,0,1.0259508487,-0.0123614685,-0.3587173146  
C,0,-0.7283845184,-1.2284442278,-0.5688412207  
C,0,-0.1407265023,-2.5857701294,-0.1648517496  
H,0,-0.7181109231,-3.4019150554,-0.6009710337  
H,0,0.8895574974,-2.6623165876,-0.522449921  
C,0,-2.4006023705,-1.257487493,0.0644976349  
H,0,-2.773040517,-2.1157258259,-0.4915868533  
C,0,-2.5158783828,-1.3621172969,1.4714370243  
H,0,-2.5526556365,-2.3518678158,1.9251050592  
C,0,-2.6149020543,-0.2027777908,2.415131009  
H,0,-2.2840886935,0.7010829768,1.8915766584  
C,0,-1.7467605899,-0.3982041254,3.6704933136  
H,0,-0.6890627133,-0.5048996849,3.417100486  
H,0,-1.8468739622,0.4551575811,4.3470067278  
H,0,-2.052893575,-1.2956402535,4.2179903361  
C,0,-4.096404658,0.0107639837,2.8142205616  
H,0,-4.7189406651,0.1961752017,1.936390792  
H,0,-4.4910395511,-0.8689641283,3.3314526111  
H,0,-4.1865207283,0.8685903571,3.4875072997  
H,0,-0.1456533816,-2.6783288923,0.9255401097



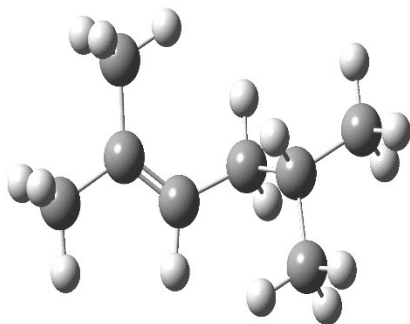
C,0,0.1849288448,-0.1913820223,0.223238921  
H,0,0.4060841811,-0.3479297212,1.2916042946  
H,0,1.1337875815,-0.2678141684,-0.3155853321  
C,0,-0.7901749069,-1.2120245718,-0.2696280641  
C,0,-0.3545113256,-2.6399060995,-0.2346394204  
H,0,-1.0125268569,-3.2805646122,-0.8257241576  
H,0,0.6670235364,-2.7500398915,-0.6112743497  
C,0,-2.2506296769,-0.8762123412,-0.3095844115  
H,0,-2.5812558168,-0.4516208179,0.6510059387  
C,0,-2.5309187595,0.1450626664,-1.422693143  
H,0,-3.6049121668,0.3369781522,-1.5211292067  
H,0,-2.0613032675,1.0980911499,-1.1631247063  
C,0,-1.9690912805,-0.3182493567,-2.7883617737  
C,0,-1.8609389511,0.8910967778,-3.7238988896  
H,0,-1.1695593923,1.6260188278,-3.3056810978  
H,0,-1.4889216009,0.5870327846,-4.701075754  
H,0,-2.8407923876,1.3621947371,-3.8473394416  
C,0,-2.8212188629,-1.4271166107,-3.4176200748  
H,0,-2.9409852786,-2.2721211732,-2.7353523896  
H,0,-3.8153147203,-1.0553626474,-3.6822964985  
H,0,-2.3306031475,-1.784174614,-4.323503648  
H,0,-0.355315567,-3.0288081401,0.7968315636



H,0,-0.4908599187,0.891641617,-0.2913847981	H,0,-0.1842835801,0.8293987708,0.1104846979
O,0,-0.8381777591,-1.192143212,-1.8891442517	O,0,-0.6525344363,-0.8316091664,-2.4772360585
O,0,-1.9285859559,0.1937983008,-2.3346351642	H,0,-2.8413606961,-1.7825103268,-0.4689323204
H,0,-1.5986205542,0.1326639349,-3.2406652669	O,0,0.0768181056,-1.0847250725,-3.9476676629
	H,0,0.3307670588,-1.9943011328,-3.744801115
<b>TS10<sub>t</sub></b>	<b>OH</b>
C,0,0.0189974533,0.044877427,-0.0010930878	
C,0,-0.0030696974,0.0012508968,2.4909159506	O,0,0.,0.,-0.0076044417
H,0,0.6569156936,-0.0048385927,3.3658836292	H,0,0.,0.,0.9676044417
C,0,-1.0009072966,1.1508388697,2.6553523441	<b>HO<sub>2</sub></b>
H,0,-1.4010102495,1.1238993405,3.6746763982	
H,0,-0.4623652046,2.1002216428,2.5600576314	O,0,-0.0196500749,0.,-0.0154687204
C,0,-2.2373466165,1.213123071,1.7242842595	H,0,0.0204702082,0.,0.9593821961
C,0,-2.9809730898,2.5203758901,2.0357125628	O,0,1.2436878016,0.,-0.4239134757
H,0,-2.3426536166,3.3771138549,1.8091975368	
H,0,-3.8871131252,2.6009944605,1.4392404764	<b>P1<sub>t</sub>,P3<sub>t</sub></b>
H,0,-3.2481022304,2.5528815686,3.0960114722	
C,0,-3.1642886849,0.0045614662,1.8943735259	
H,0,-2.6422793439,-0.9322048578,1.6870496141	C,0,-0.0482874076,0.5913234482,-0.2243140338
H,0,-3.5659295282,-0.0443061226,2.9107102798	H,0,-0.0793146166,1.0073800727,0.7774139428
H,0,-3.9978102145,0.093829975,1.196545284	H,0,0.9016502328,0.6449141777,-0.7459850316
O,0,-1.7499719676,1.2570787263,0.3552848008	C,0,-1.1257686736,0.0398760355,-0.7846011033
H,0,-0.5187028439,-0.9662945155,2.4922211998	
O,0,-3.0531981892,1.7345148886,-0.5759836923	
H,0,-2.9588173905,1.0066490953,-1.2043845122	
C,0,0.8655568875,0.1171741203,1.2241410718	
H,0,1.3616853883,1.0950341982,1.2478111443	
C,0,1.9632743189,-0.9702688852,1.2029422091	

H,0,2.6020498775,-0.8733401075,0.3215481207  
H,0,2.5977922299,-0.8930591355,2.0918205299  
H,0,1.5205733641,-1.9710150141,1.1894889272  
H,0,-0.5368092465,-0.868806596,-0.1847118784  
H,0,0.2588799727,0.6425149097,-0.8702217025

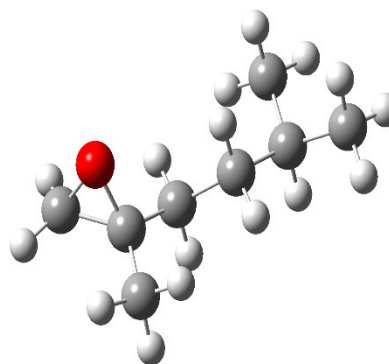
**P2<sub>t</sub>, P5<sub>t</sub>**



C,0,-0.0030266924,0.0020375898,-0.0065771211  
H,0,-0.0113722596,0.0105846359,1.0899743438  
H,0,1.0509367042,-0.0057319208,-0.3097420431  
C,0,-0.7292438718,-1.2067428899,-0.5448907028  
C,0,-0.1572707482,-2.5274112774,-0.0937175432  
H,0,-0.6971466556,-3.3879520131,-0.4875749885  
H,0,0.8925087371,-2.6170598598,-0.3975047872  
C,0,-1.7870177432,-1.0698033515,-1.3544787569  
C,0,-2.6243109129,-2.155363873,-1.9772801133  
H,0,-2.077234451,-3.102061976,-1.995011559  
C,0,-3.9920872716,-2.3955334136,-1.2896913641  
H,0,-3.7871048062,-2.6538613446,-0.2428796391  
C,0,-4.7158096174,-3.580960076,-1.9414384614  
H,0,-4.1089055047,-4.4906031049,-1.9026147499  
H,0,-5.6649975563,-3.7906318881,-1.4395348788  
H,0,-4.9360862812,-3.3727799793,-2.9943133088

C,0,-1.081809882,-0.5563045469,-2.169825691  
H,0,-1.7960849797,-0.0692521587,-2.8418176606  
H,0,-0.0883526289,-0.4677957913,-2.6131829292  
C,0,-2.4522492325,-0.0248218131,-0.0570145188  
H,0,-2.8398154375,-1.0517738555,-0.1091719404  
C,0,-3.5187904577,0.9319245222,-0.6262993092  
H,0,-3.1619819346,1.9644351801,-0.5208352962  
H,0,-3.625471015,0.753682576,-1.701961785  
C,0,-4.9113569298,0.8080467958,0.0215389545  
H,0,-5.2250885184,-0.2414973818,-0.0661480522  
C,0,-5.9326964532,1.6665067786,-0.7379394941  
H,0,-5.9833342526,1.3862320549,-1.7942283976  
H,0,-6.9353668186,1.5580147468,-0.3142020265  
H,0,-5.6643542224,2.7274275143,-0.6875707989  
C,0,-4.9040461007,1.1748900076,1.5125876311  
H,0,-4.2460730083,0.5253802084,2.09471796  
H,0,-4.5672247082,2.2077828967,1.6557536947  
H,0,-5.90780317,1.0919894179,1.9394296997  
H,0,-1.3509937779,-1.618714383,-2.1426443664  
H,0,-2.2863179739,0.1955756995,1.0004227927

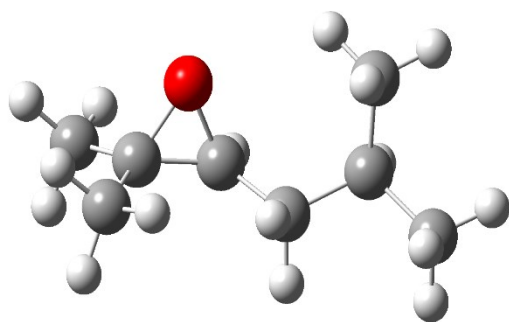
**P4<sub>t</sub>**



C,0,-0.0079673125,0.239445734,0.021856845

C,0,-4.8771007058,-1.1422873178,-1.3011226902  
H,0,-4.4013137752,-0.3062705357,-0.7832161567  
H,0,-5.0904095094,-0.8254392193,-2.3284593565  
H,0,-5.8348249443,-1.3359661159,-0.8092671112  
H,0,-0.4505807141,0.9339949354,-0.3573247203  
H,0,-0.1702046723,-2.5961593141,1.0003571065  
H,0,-2.0922125909,-0.053154678,-1.5953153701  
H,0,-2.8144533245,-1.8957096165,-3.0278420794

**P6<sub>t</sub>**



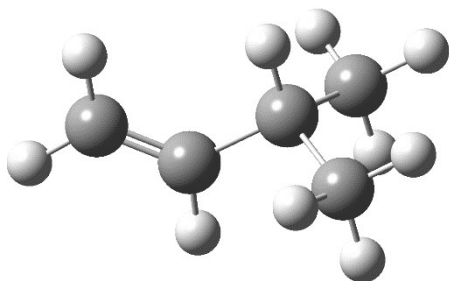
C,0,0.2833065776,-0.0350293558,0.1513406751  
H,0,1.1516913595,-0.2361619717,0.7862978585  
H,0,0.6490281246,0.3001159229,-0.8241339208  
C,0,-0.572439031,-1.2747753687,-0.0076836504

H,0,-0.0766955916,-0.0420084136,1.070628839  
H,0,0.9114367168,-0.0583549991,-0.4782237614  
C,0,-1.2376665273,0.4256468858,-0.7643838053  
C,0,-1.1877765963,0.2239590033,-2.2641457864  
H,0,-1.8366040789,0.9381767297,-2.7772106927  
H,0,-0.1715057265,0.3696531656,-2.6341836794  
C,0,-2.5844315023,0.2565767474,-0.0787555707  
H,0,-2.9658675981,-0.7505926964,-0.2916741983  
C,0,-3.6236573488,1.3062527537,-0.4981721605  
H,0,-3.2115422477,2.3039730779,-0.3042112658  
H,0,-3.7867483265,1.2431074853,-1.579660631  
C,0,-4.9918172679,1.1775292769,0.1998249944  
H,0,-5.351613621,0.1509317796,0.0423350585  
C,0,-6.0085894781,2.1316282904,-0.4427636319  
H,0,-6.1152968879,1.9383457027,-1.5142844311  
H,0,-6.9959358648,2.0275016614,0.0163884005  
H,0,-5.694453168,3.1740812241,-0.3223153049  
C,0,-4.9095804172,1.421884644,1.7135495502  
H,0,-4.2614116232,0.6999584373,2.2159710337  
H,0,-4.5192324833,2.4237005275,1.9235640206  
H,0,-5.8991949488,1.3474872759,2.1735799616  
H,0,-1.5153405718,-0.78535464,-2.532072584  
O,0,-0.4764522609,1.5574872745,-0.2925573923  
H,0,-2.4195954695,0.3121152211,1.0002455739

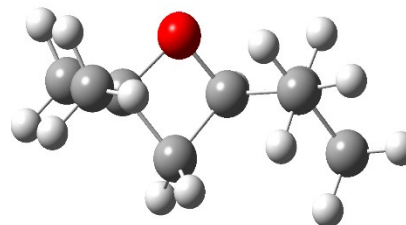
C,0,0.1276699859,-2.44858479,-0.6577488706  
 H,0,-0.546474342,-3.2902148264,-0.8094639073  
 H,0,0.5175898275,-2.1499740487,-1.6356518434  
 C,0,-1.7470330876,-1.4455178802,0.8721023684  
 H,0,-1.9138174351,-0.6433817347,1.5948584116  
 C,0,-2.3657871964,-2.7600466029,1.2852777343  
 H,0,-2.2125950117,-3.5128415676,0.506519204  
 H,0,-1.8342020056,-3.1123696956,2.1791770177  
 C,0,-3.8719357558,-2.6631342672,1.6065641112  
 H,0,-4.001104512,-1.8541933321,2.3390402592  
 C,0,-4.3686560045,-3.9623696453,2.2544618658  
 H,0,-3.815548662,-4.1920162398,3.1702780535  
 H,0,-5.4293937076,-3.89331092,2.5119996766  
 H,0,-4.2491136574,-4.8099106444,1.570686743  
 C,0,-4.7042596286,-2.3148371268,0.3642167006  
 H,0,-4.6194281909,-3.1050981816,-0.3896021429  
 H,0,-5.7623370464,-2.2131519783,0.6233704697  
 H,0,-0.29292931,0.7783831321,0.5955846525  
 H,0,0.9732497789,-2.781886973,-0.0480292443  
 O,0,-1.9059691222,-1.006951429,-0.4915950694  
 H,0,-4.3721800206,-1.3849826619,-0.0997444255

**P8<sub>t</sub>**

**3-methyl butene-1**



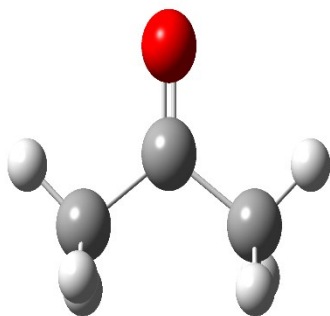
**P7<sub>t</sub>**



C,0,0.3655224546,-0.1625768857,0.2214659281  
 H,0,0.5446867656,-0.4449347383,1.2636455352  
 H,0,1.3019924982,-0.2714027957,-0.3322670835  
 C,0,-0.7155222815,-1.0386611443,-0.402664777  
 C,0,-0.3273859213,-2.5085205919,-0.4041207714  
 H,0,-1.1089887961,-3.1170961668,-0.862290419  
 H,0,0.595946199,-2.6532758377,-0.9723498105  
 C,0,-2.1602472078,-0.6950556498,0.04212517  
 H,0,-2.2552378786,-0.0306319539,0.9017924701  
 C,0,-2.2964436116,-0.0409771455,-1.3488111743  
 H,0,-2.2395800302,1.0547032199,-1.291763854  
 C,0,-3.4439389403,-0.4094754477,-2.2910037485  
 H,0,-3.1986329226,0.0673716973,-3.2494031812  
 C,0,-4.7578924836,0.1964288117,-1.778322689  
 H,0,-4.6774788893,1.2794388052,-1.6444105616  
 H,0,-5.574541644,0.0073499174,-2.4799584997  
 H,0,-5.0435182984,-0.2398253026,-0.8151553121  
 C,0,-3.5711316516,-1.9153939974,-2.5455286428  
 H,0,-2.6197581142,-2.3309024638,-2.881574604  
 H,0,-3.8842595553,-2.4537224904,-1.6453518503  
 H,0,-4.3210736118,-2.1094576439,-3.3173301598  
 H,0,-0.1609994422,-2.8650045053,0.6172719986

C,0,0.0225800813,0.1695866601,-0.0942923174  
 H,0,0.0117579973,0.5861321434,0.9137384312  
 C,0,1.1763985977,-0.2439875271,-0.6094110058  
 H,0,2.1056131077,-0.1780853323,-0.0543405217  
 H,0,1.2339474496,-0.6652250116,-1.6090069582  
 C,0,-1.3161435021,0.1194199686,-0.7851537865  
 H,0,-1.1661109112,-0.3158943198,-1.7804689202  
 C,0,-2.2967468306,-0.7788032711,-0.0097860547  
 H,0,-3.2659758473,-0.8248269676,-0.5152285848  
 H,0,-1.9108225796,-1.7969188079,0.0827200592  
 H,0,-2.4658953126,-0.3907436288,1.0002694415  
 C,0,-1.8924856588,1.5358981937,-0.9612146425  
 H,0,-2.0451671491,2.0184106229,0.0100132835  
 H,0,-1.2186133237,2.1664387511,-1.5463389296  
 H,0,-2.8595015826,1.5024503744,-1.4718550552

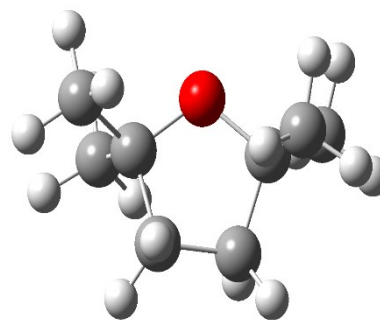
**Acetone**



C,0,-0.0037331857,-0.1788271373,0.0192758867  
 O,0,-0.006708308,-0.5150753888,1.1806891534  
 C,0,1.2870272102,-0.0368120229,-0.7690054177  
 H,0,2.1284017862,-0.3572353025,-0.1562756713  
 H,0,1.2482901155,-0.6285875479,-1.6886726405  
 H,0,1.4302600417,1.0070044584,-1.0673760211

H,0,0.0766347668,0.8908071071,0.1943800893  
 O,0,-1.0122655391,-0.576619127,-1.7628411439  
 H,0,-2.790207971,-1.572788994,0.1924522941

**P9<sub>t</sub>**

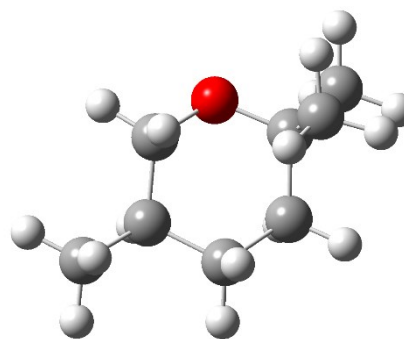


C,0,0.8348521649,-2.1917820623,-0.0599531038  
 H,0,1.6827685221,-2.5050984602,-0.6766704937  
 H,0,1.0317968236,-2.4824157251,0.9745170738  
 C,0,0.6234337124,-0.6734240445,-0.1404337248  
 C,0,1.8901522122,0.0697519383,0.2832762714  
 H,0,1.7191625572,1.1484542263,0.2751534273  
 H,0,2.1801314079,-0.2211433606,1.2959419724  
 C,0,0.0969492194,-0.236437521,-1.5248592835  
 H,0,0.488443852,-0.859527577,-2.3319218087  
 C,0,-1.4233137306,-0.3380672327,-1.3679281378  
 H,0,-1.9710033025,0.3021893763,-2.0628846613  
 H,0,-1.7592225083,-1.3661584302,-1.5313996243  
 C,0,-1.6527005403,0.0662727697,0.1047106317  
 C,0,-2.8068944735,-0.6892427126,0.7630805071  
 H,0,-2.643812864,-1.7670866915,0.6955858745  
 H,0,-2.8816215879,-0.4219786325,1.8200506042  
 H,0,-3.7583926193,-0.4484462704,0.27936991

C,0,-1.2905600587,0.1240256656,-0.7290346022  
H,0,-1.248294694,1.1155615278,-1.1900773945  
H,0,-1.4309350664,-0.5987203607,-1.5396050522  
H,0,-2.1352629822,0.0686663143,-0.0438829396

C,0,-1.8394817504,1.5819339333,0.261229679  
H,0,-1.0385115863,2.1316736944,-0.2390410687  
H,0,-2.7953566651,1.9071238459,-0.1606985905  
H,0,-1.8187969113,1.8486629984,1.3203857691  
H,0,2.7212066783,-0.1577880463,-0.3911727049  
H,0,-0.0531511232,-2.7319724779,-0.397111793  
O,0,-0.4312861216,-0.312694026,0.7835463437  
H,0,0.3944818844,0.795865198,-1.730637049

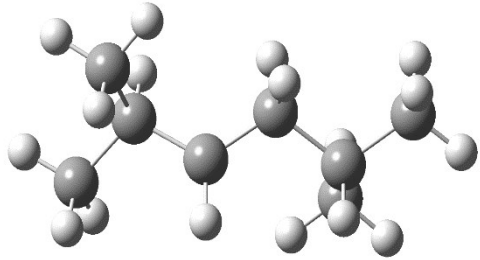
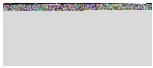
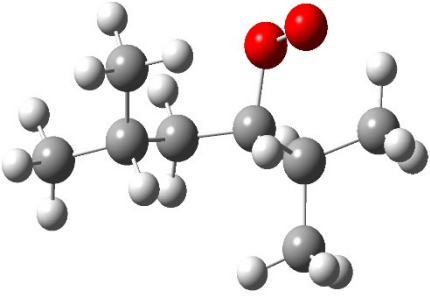
**P10<sub>t</sub>**



C,0,0.0095826825,-0.024997722,0.0302092218  
C,0,0.0683454099,-0.0140136161,2.5249038169  
H,0,0.7051851998,0.0736626492,3.4115636385  
C,0,-0.92279395,1.157164625,2.4776963148  
H,0,-1.5925149398,1.1300381681,3.3436803809  
H,0,-0.3629109344,2.0971857537,2.5372305246  
C,0,-1.7588681882,1.1854893251,1.1805265066  
C,0,-2.437052846,2.5447147288,1.0103596802  
H,0,-1.6837003451,3.3338254419,0.9599761891  
H,0,-3.0150409452,2.566117859,0.0834470559  
H,0,-3.1095190615,2.7521957344,1.8470409207  
C,0,-2.8152562056,0.0679153556,1.1484141098  
H,0,-2.3856236203,-0.9235310835,1.3034550354

	H,0,-3.5622873973,0.2285949744,1.930489029
	H,0,-3.3230392308,0.0698466974,0.1809760555
	O,0,-0.8798165257,1.0851078479,0.0383845741
	H,0,-0.4686652451,-0.9656683561,2.625567348
	C,0,0.9301899588,-0.0541827726,1.2544648152
	H,0,1.5337585926,0.8625964141,1.225176013
	C,0,1.8675960938,-1.2631695274,1.217879626
	H,0,2.4861553092,-1.2622966335,0.3152282259
	H,0,2.5393199786,-1.2659983076,2.0809882474
	H,0,1.3033241118,-2.2017886282,1.2346089256
	H,0,-0.5461192612,-0.9733996497,-0.0366286418
	H,0,0.5896255233,0.0787812259,-0.8901477216

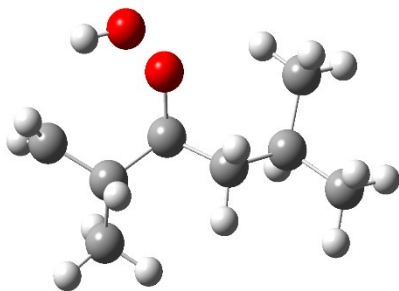
**Table S3:** Optimized geometries of reactants, intermediates, transition states and products for 2,5-dimethylhex-3-yl + O<sub>2</sub> reaction obtained using the B3LYP/CBSB7.

2,5-Dimethylhex-3-yl Radical	O <sub>2</sub>
	 O,0,0.,0.,0. O,0,0.,0.,1.205752
C,0,-0.2243255974,0.0685378828,-0.3039473497 H,0,0.2535955215,0.2900234989,0.6562817711 H,0,0.5240651828,0.2128997924,-1.0886048475 C,0,-0.7744766737,-1.3660338476,-0.3183311409 C,0,0.3786220698,-2.3907230363,-0.1752060412 H,0,0.007095173,-3.4175276808,-0.2215645426 H,0,1.1138394492,-2.2614189408,-0.9760479266 C,0,-1.8267543791,-1.5659033471,0.7302559546 H,0,-1.7117130217,-1.0313966145,1.6721681518 C,0,-2.8177722517,-2.6818417722,0.6798575262 H,0,-3.0427760862,-2.9335119146,-0.3667131386 H,0,-2.3742755761,-3.5991461604,1.1080411255 C,0,-4.1400216174,-2.4051401791,1.4290929992 H,0,-3.8782261128,-2.1130162701,2.455194458 C,0,-5.0020576086,-3.6715454987,1.5054889339 H,0,-4.4713417902,-4.4879575503,2.0042640561 H,0,-5.9281594213,-3.4872455772,2.0577092645 H,0,-5.2780871605,-4.0166458349,0.5029309197 C,0,-4.9183629509,-1.2473312824,0.7912246094 H,0,-4.3134978305,-0.3381443246,0.7463605778	<b>2,5-Dimethylhexyl-3-peroxy Radical (ROO-3)</b>  C,0,0.1934856173,-0.0760938343,-0.2073179335 H,0,0.0624944832,0.2780344238,0.8196400704 H,0,1.2594406347,-0.2596446025,-0.3665917322 C,0,-0.6002967366,-1.3670691856,-0.4531444802 C,0,-0.0467150182,-2.5008817243,0.4263782722 H,0,-0.5622147867,-3.4508596988,0.2690513304 H,0,1.0121373255,-2.6630121924,0.2101771487 C,0,-2.1118119462,-1.1930023964,-0.1975953859 H,0,-2.2959061956,-1.0480607514,0.8703572075 C,0,-2.9831715493,-2.299687381,-0.7950763594 H,0,-3.150398364,-2.053366523,-1.8511142132 H,0,-2.4124204789,-3.2326190732,-0.7894767768 C,0,-4.3343456757,-2.5523740043,-0.097145932



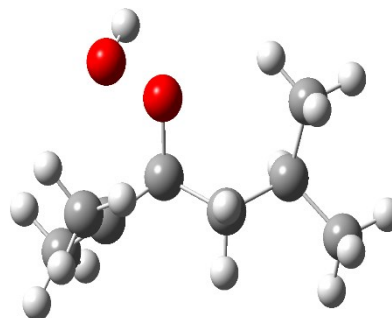
H,0,-5.2170396169,-1.4999557853,-0.2324130344	H,0,-4.1189097442,-2.7792239555,0.9561856257
H,0,-5.8272920933,-1.0234086841,1.3572615212	C,0,-5.0143102722,-3.7850008385,-0.7097352695
H,0,-1.022437511,0.7995846783,-0.4568947066	H,0,-4.3757839589,-4.6712664234,-0.6454880864
H,0,-1.237270914,-1.5449802988,-1.2998080676	H,0,-5.9531794859,-4.011252888,-0.1970044071
H,0,0.8937079144,-2.2613597909,0.7818063274	H,0,-5.2466813295,-3.6168223691,-1.766878956
	C,0,-5.2755872277,-1.3401249541,-0.1354292851
	H,0,-4.8536228659,-0.4691745933,0.3684117206
	H,0,-5.4949149526,-1.0493288123,-1.1680028294
	H,0,-6.2245019834,-1.5800448014,0.3528801345
	H,0,-0.1140054622,0.7272259769,-0.8770579339
	H,0,-0.4775708196,-1.6520475384,-1.5058795367
	H,0,-0.1319370365,-2.2430345639,1.4870412391
	O,0,-2.5649219089,0.0616430288,-0.8350930275
	O,0,-2.6464288164,1.0702046573,0.0079093957

**QOOH-1,**



C,0,0.0224565071,-0.0855516495,0.0255006638  
H,0,0.524988717,-0.1046400169,0.9866293024  
H,0,0.1554282892,0.7897539171,-0.5995223012  
C,0,-0.7163187857,-1.2871646736,-0.4682241125  
C,0,0.0094330991,-2.5747071189,-0.0295185259  
H,0,-0.5043050576,-3.4740981724,-0.3768258283  
H,0,1.0274718268,-2.5976788894,-0.4241193315  
C,0,-2.2160828447,-1.3379728452,-0.0099409602  
H,0,-2.2559530719,-1.6371335106,1.0432750331  
C,0,-3.0679708131,-2.2694385266,-0.8821002148  
H,0,-3.3979387839,-1.691216776,-1.7544677557  
H,0,-2.4314321492,-3.0699585304,-1.2707415332  
C,0,-4.2864384501,-2.908233454,-0.1872182948  
H,0,-3.9101017036,-3.4583360355,0.6865405012  
C,0,-4.9501069633,-3.9257623853,-1.1263743152  
H,0,-4.2451472374,-4.6991230632,-1.4467266335  
H,0,-5.7915069375,-4.4228304406,-0.6355150408  
H,0,-5.3357584067,-3.4325169481,-2.0251995479  
C,0,-5.311262136,-1.8790883408,0.308918072  
H,0,-4.8760334704,-1.1729775756,1.0169467535  
H,0,-5.709992741,-1.2956640772,-0.5272734262

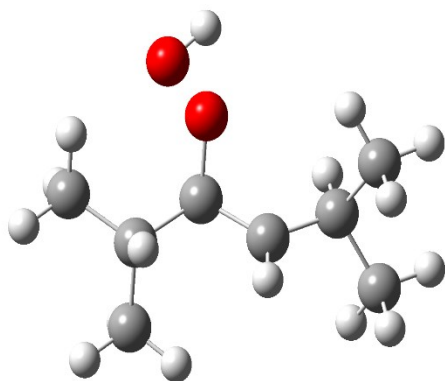
**QOOH-2,**



C,0,0.0291841707,-0.0066524366,-0.0330568221  
H,0,-0.0465460827,0.0517631361,1.0640352738  
H,0,1.0966030653,-0.0670334552,-0.2739711707  
C,0,-0.7160464933,-1.1916383866,-0.5564352928  
C,0,-0.1764553566,-2.5581078818,-0.2878136235  
H,0,-0.6649260203,-3.3223300041,-0.8997528102  
H,0,0.902025928,-2.6125943883,-0.4722340828  
C,0,-2.1407134811,-1.0254377392,-0.9972429169  
H,0,-2.6128002161,-2.0130476387,-1.0928908948  
C,0,-2.2885271136,-0.2765104237,-2.3366080804  
H,0,-1.9135285416,0.7463320561,-2.2196597625  
H,0,-1.6016143723,-0.7784247058,-3.0259553849  
C,0,-3.6973875044,-0.2516080912,-2.9696911308  
H,0,-4.150885495,-1.2394423613,-2.8091883032  
C,0,-3.5869521786,-0.0322017388,-4.486550626  
H,0,-2.9956608421,-0.8183841894,-4.9653181851  
H,0,-4.5748749324,-0.022086308,-4.9559129022  
H,0,-3.1070970493,0.9277011121,-4.7070014631  
C,0,-4.6214164662,0.8052394253,-2.3467672206  
H,0,-4.7307385581,0.660626573,-1.2723676247  
H,0,-4.2159644816,1.8103529955,-2.5076040814

H,0,-6.1504303175,-2.3829543847,0.7981816218  
H,0,-0.7405395181,-1.2438321557,-1.564276917  
H,0,0.0721646051,-2.624725472,1.0621736895  
O,0,-2.8465006425,-0.0540441328,-0.1188524231  
O,0,-2.5567977549,0.718028089,1.0682561291  
H,0,-1.6982652441,1.1097698847,0.8328110832

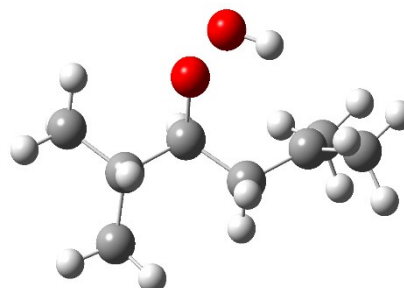
### QOOH-3<sub>s</sub>



C,0,-0.0233760902,0.0323310108,-0.0569480496  
H,0,-0.0132481578,0.0732995874,1.0367379655  
H,0,1.0141583396,0.0507612308,-0.4032892489  
C,0,-0.7213458735,-1.2381106305,-0.556925432  
C,0,0.0194793669,-2.4937484638,-0.0710244881  
H,0,-0.4326896808,-3.41417521,-0.448656495  
H,0,1.0627506202,-2.4745344267,-0.3974682884  
C,0,-2.2034070569,-1.3061172533,-0.1476363767  
H,0,-2.288959268,-1.373556506,0.9458907874  
C,0,-2.9587379329,-2.4112239584,-0.8002237042  
H,0,-2.5487462566,-2.8618603279,-1.7012147603  
C,0,-4.3512555408,-2.7877570926,-0.4005592582  
H,0,-4.5782448211,-2.2954924669,0.5533846987  
C,0,-4.4796301113,-4.3107688533,-0.1963507592

H,0,-5.6137113132,0.7716716993,-2.8070551126  
H,0,-0.3618431899,0.9354063982,-0.4226785242  
H,0,-0.3324573337,-2.8441318704,0.7660747385  
O,0,-2.9081150919,-0.258618471,-0.0375462408  
O,0,-2.8646797388,-0.973564512,1.229983853  
H,0,-3.7864528961,-1.25744671,1.2984092131

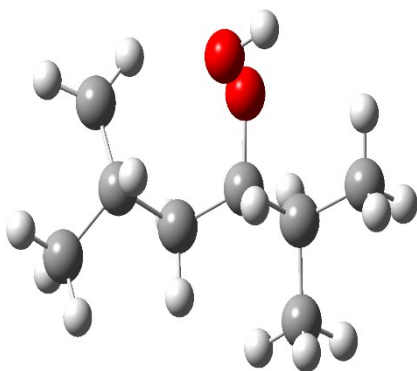
### QOOH-4<sub>s</sub>



C,0,0.0922609895,-0.2879150653,0.5312884382  
H,0,0.1899444114,-0.8184795901,1.4847677058  
H,0,1.0987508546,-0.1329861671,0.1327809908  
C,0,-0.7587699359,-1.0995611485,-0.4566796901  
C,0,-0.1222357588,-2.4744249094,-0.7111903314  
H,0,-0.6100003469,-3.0219598233,-1.5199269225  
H,0,0.9288837096,-2.3530606396,-0.9860476831  
C,0,-2.2141215189,-1.2099693818,0.0420306818  
H,0,-2.2173426737,-1.6096390715,1.0626207996  
C,0,-3.1349195807,-2.0485135066,-0.8747548693  
H,0,-3.0326285102,-1.6544752702,-1.8915718368  
H,0,-2.7423507712,-3.0774934694,-0.8927140705  
C,0,-4.5905237519,-2.0929728015,-0.4899542456  
C,0,-4.98557199,-2.8779587892,0.7246879916

H,0,-3.792529238,-4.6690728177,0.5743151827  
H,0,-5.4974463175,-4.5780079244,0.1034133078  
H,0,-4.2529499332,-4.8460940686,-1.1239984774  
C,0,-5.3828710179,-2.2920396015,-1.4392874163  
H,0,-5.3097842374,-1.2113286439,-1.5720573048  
H,0,-5.2099962467,-2.7652459045,-2.4111106573  
H,0,-6.4009014603,-2.5395641742,-1.1217286735  
H,0,-0.5232189147,0.931007706,-0.4177641783  
H,0,0.0168623122,-2.5451049916,1.0233377988  
O,0,-2.9300047313,-0.0939551693,-0.5267560374  
O,0,-2.8082269832,0.8931726288,0.5469682334  
H,0,-3.7370498771,0.9688176493,0.8038220498  
H,0,-0.7023830538,-1.2252551798,-1.6545152218

**QOOH-5,**

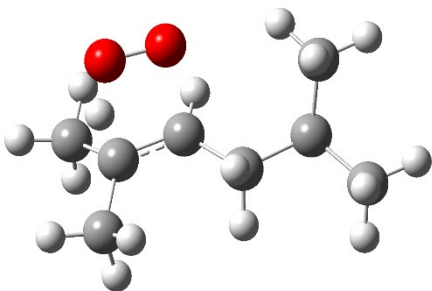


C,0,0.0379228261,-0.0788520077,0.1724465087  
H,0,0.1472210962,-0.2514106943,1.2490543721  
H,0,1.0423515868,-0.00346537,-0.2529779448  
C,0,-0.744776525,-1.223197225,-0.4874162995  
C,0,-0.0056230219,-2.5564747694,-0.294752378  
H,0,-0.4527107519,-3.3697892634,-0.8685488479  
H,0,1.0338689704,-2.4578243858,-0.6187159286

H,0,-4.2794127893,-2.7497525279,1.5486622786  
H,0,-5.9792509549,-2.5956324152,1.0856212349  
H,0,-5.0262468933,-3.9583750987,0.5020901488  
H,0,-0.3557293335,0.6853848453,0.7296805676  
H,0,-0.1553699917,-3.0973123271,0.1893709721  
O,0,-2.6895489103,0.1444933169,0.1039260584  
O,0,-3.7527901087,0.2283177666,1.0802777509  
H,0,-4.5017488187,-0.1279085441,0.5694286728  
C,0,-5.6191825442,-1.8735309819,-1.5567626655  
H,0,-5.3443859008,-1.0514501182,-2.2242621088  
H,0,-5.7372277615,-2.7688854833,-2.1928333704  
H,0,-6.6066002205,-1.6616247996,-1.1350992615  
H,0,-0.7928229396,-0.5546934405,-1.4090074318

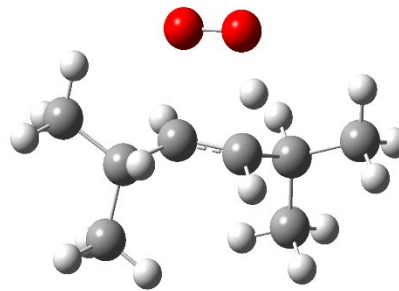
C,0,-2.1975547474,-1.2774973423,0.0364442127	
H,0,-2.1842088679,-1.3126466598,1.1324287043	
C,0,-3.0142109085,-2.4552251464,-0.5093421212	
H,0,-2.8910726386,-2.506666475,-1.5979811393	
H,0,-2.5679704494,-3.3674887358,-0.1011465245	
C,0,-4.5268274645,-2.4709664837,-0.1744732885	
H,0,-4.639037998,-2.098115981,0.8581686421	
C,0,-5.0653671466,-3.9146146034,-0.1954395029	
H,0,-4.5549382723,-4.5393528876,0.5437386466	
H,0,-6.1354667136,-3.9345465814,0.0292177915	
H,0,-4.9238046994,-4.3684173248,-1.1813254324	
C,0,-5.3282673759,-1.5928830682,-1.0801258501	
H,0,-4.905631144,-0.6874196123,-1.4915892281	
H,0,-6.3970404205,-1.751528379,-1.1738444283	
H,0,-0.4630582403,0.8788598696,0.027235904	
H,0,-0.8074816794,-1.0196372002,-1.5642128983	
H,0,0.0055920645,-2.851544057,0.7603021874	
O,0,-2.7693069957,-0.0028189902,-0.3336474209	
O,0,-3.7422323123,0.3876561386,0.6745019462	
H,0,-3.2939731793,1.158796841,1.0486669845	

**TS1<sub>s</sub>**



C,0,-0.049687816,0.0736358731,0.0458169024  
 H,0,0.4901505844,-0.0220988468,0.9913339016  
 H,0,0.6924624547,0.2716354405,-0.7363550026  
 C,0,-0.8362645421,-1.2017117431,-0.2539839196  
 C,0,-0.0256034843,-2.4933486791,-0.1162831707  
 H,0,-0.6448307028,-3.3736039226,-0.3052634699  
 H,0,0.8095994971,-2.5090577083,-0.8250550877  
 C,0,-1.8646009734,-1.1754830862,-1.2046622066  
 H,0,-2.1851084834,-2.125876263,-1.6206998541  
 C,0,-2.3880691492,0.0583212737,-1.8816062556  
 H,0,-2.8145573724,0.7427385225,-1.1369267185  
 H,0,-1.5285681826,0.5957640982,-2.3084238117  
 C,0,-3.4156140878,-0.1901296155,-3.0035180846  
 H,0,-2.9732858193,-0.9214993745,-3.6940581067  
 C,0,-3.660641904,1.1042831615,-3.7909561563  
 H,0,-2.7326029468,1.5000436107,-4.2144155966  
 H,0,-4.3596062667,0.936510122,-4.6148674784  
 H,0,-4.0902120641,1.877483078,-3.1448722862  
 C,0,-4.737758384,-0.7676645484,-2.4818693371  
 H,0,-4.5956025352,-1.7068272232,-1.9447422911  
 H,0,-5.2201768593,-0.0696123026,-1.7902856301  
 H,0,-5.4286346954,-0.952139515,-3.3096101544

**TS2<sub>s</sub>**

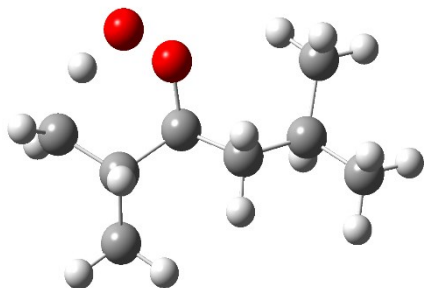


C,0,0.0273

879862,-0.1650851652,0.104925826  
 H,0,0.0224406054,-0.243507141,1.1973337968  
 H,0,1.068378131,-0.2165873162,-0.2255032888  
 C,0,-0.7922310979,-1.299406839,-0.5245464482  
 C,0,-0.1656661136,-2.6735680122,-0.1905035554  
 H,0,-0.7069202895,-3.4898254169,-0.6738816842  
 H,0,0.8743306866,-2.7043064469,-0.527646483  
 C,0,-2.2313255822,-1.3013225524,-0.0823226665  
 H,0,-2.4125301229,-1.049355045,0.9602518221  
 C,0,-3.2772996901,-1.8287894729,-0.8341121576  
 H,0,-2.9871188362,-2.3579942772,-1.7470461095  
 C,0,-4.5549109349,-2.3561801924,-0.1703859429  
 H,0,-4.7720342225,-1.7029884596,0.6843027468  
 C,0,-4.3514217169,-3.7844309798,0.3612904307  
 H,0,-3.5335288689,-3.8265965216,1.0854658697  
 H,0,-5.2577769225,-4.1549204153,0.8497491574  
 H,0,-4.1093480483,-4.4721816979,-0.4560384636  
 C,0,-5.7535310305,-2.2967872255,-1.128565095  
 H,0,-5.9493295838,-1.2746893681,-1.4627244511  
 H,0,-5.5729154594,-2.9123128566,-2.016521442  
 H,0,-6.6600289773,-2.6717176444,-0.6456119238  
 H,0,-0.3721620339,0.8119067199,-0.166331459

H,0,-0.6965478103,0.9494746423,0.1229598137  
H,0,0.3952287225,-2.5905485405,0.8884454822  
O,0,-3.5419329977,-1.4263050525,0.3476540708  
O,0,-2.804521171,-1.4083507733,1.384916591  
H,0,-1.654325306,-1.2933991106,0.7596199664

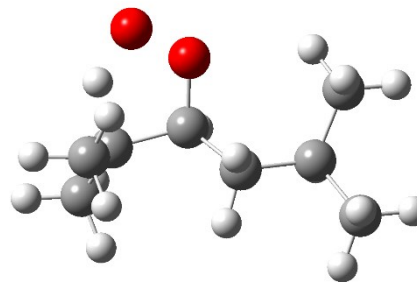
**TSQ1,**



C,0,-0.0233760902,0.0323310108,-0.0569480496  
H,0,-0.0132481578,0.0732995874,1.0367379655  
H,0,1.0141583396,0.0507612308,-0.4032892489  
C,0,-0.7213458735,-1.2381106305,-0.556925432  
C,0,0.0194793669,-2.4937484638,-0.0710244881  
H,0,-0.4326896808,-3.41417521,-0.448656495  
H,0,1.0627506202,-2.4745344267,-0.3974682884  
C,0,-2.2034070569,-1.3061172533,-0.1476363767  
H,0,-2.288959268,-1.373556506,0.9458907874  
C,0,-2.9587379329,-2.4112239584,-0.8002237042  
H,0,-2.5487462566,-2.8618603279,-1.7012147603  
C,0,-4.3512555408,-2.7877570926,-0.4005592582  
H,0,-4.5782448211,-2.2954924669,0.5533846987  
C,0,-4.4796301113,-4.3107688533,-0.1963507592  
H,0,-3.792529238,-4.6690728177,0.5743151827  
H,0,-5.4974463175,-4.5780079244,0.1034133078  
H,0,-4.2529499332,-4.8460940686,-1.1239984774

H,0,-0.1723313604,-2.8551551042,0.8888616312  
O,0,-2.7498271209,0.8759076009,-0.5860924977  
H,0,-0.7760724792,-1.1854534444,-1.6152859462  
O,0,-3.6718464036,0.6281539255,-1.4299570484  
H,0,-3.645314852,-0.6586480758,-1.3423330104

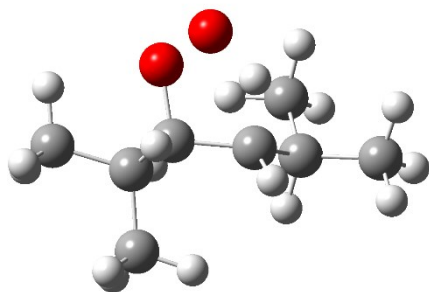
**TSQ2,**



C,0,-0.4759996921,-0.3162715925,-0.9824814006  
H,0,0.5064583879,0.1601852993,-0.9275676463  
H,0,-0.4874134103,-0.9290031407,-1.8945144706  
C,0,-0.732417451,-1.1639646382,0.2417925359  
C,0,0.3202196538,-2.1895312236,0.571127917  
H,0,0.1442284479,-2.651086405,1.5463157748  
H,0,0.3330492402,-2.9954764305,-0.1772538723  
C,0,-2.2074547111,-1.5798263763,0.4869740663  
H,0,-2.2193003065,-2.284805474,1.329407126  
C,0,-2.9641545363,-2.1571416189,-0.7059314232  
H,0,-3.1450899805,-1.3569047806,-1.4324033887  
H,0,-2.2953057368,-2.8765840832,-1.1939487419  
C,0,-4.2893493293,-2.8729435364,-0.3710653462  
H,0,-4.0760437063,-3.5990718277,0.425251417  
C,0,-4.7896281696,-3.6544156441,-1.5944825088  
H,0,-4.0525915644,-4.3884623277,-1.9340853723  
H,0,-5.7146744353,-4.1905293806,-1.3651901756

C,0,-5.3828710179,-2.2920396015,-1.4392874163  
 H,0,-5.3097842374,-1.2113286439,-1.5720573048  
 H,0,-5.2099962467,-2.7652459045,-2.4111106573  
 H,0,-6.4009014603,-2.5395641742,-1.1217286735  
 H,0,-0.5232189147,0.931007706,-0.4177641783  
 H,0,0.0168623122,-2.5451049916,1.0233377988  
 O,0,-2.9300047313,-0.0939551693,-0.5267560374  
 O,0,-2.8082269832,0.8931726288,0.5469682334  
 H,0,-3.7370498771,0.9688176493,0.8038220498  
 H,0,-0.7023830538,-1.2252551798,-1.6545152218

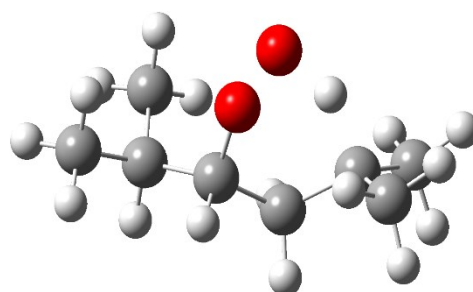
**TSQ3<sub>s</sub>**



C,0,0.0189791601,-0.0435681002,-0.1629648073  
 H,0,0.0034211673,0.0604734863,0.9277109015  
 H,0,1.0647986966,-0.0387566938,-0.4820718829  
 C,0,-0.6699926846,-1.3420931039,-0.6001762375  
 C,0,0.0391302535,-2.5654104294,-0.000452846  
 H,0,-0.4017757934,-3.5106307765,-0.327673798  
 H,0,1.0928041378,-2.5770420038,-0.2907273676  
 C,0,-2.159728918,-1.3281915014,-0.2112406222  
 H,0,-2.2570213981,-1.3352294476,0.8823598098

H,0,-4.9986317435,-2.9782961051,-2.430593002  
 C,0,-5.3723253303,-1.9124335846,0.1395236272  
 H,0,-5.0464491759,-1.3639858458,1.0240104834  
 H,0,-5.6275772594,-1.1755212582,-0.6296793956  
 H,0,-6.2845345088,-2.4618531191,0.3899556998  
 H,0,-1.2352065687,0.4608484616,-1.0893135121  
 H,0,1.3193455556,-1.7449480781,0.5723383503  
 O,0,-2.8224590817,-0.3520072578,0.9081539162  
 H,0,-0.9160507702,-0.298335832,1.2547384566  
 O,0,-1.90112577,0.156908789,1.8617393542

**TSQ4<sub>s</sub>**

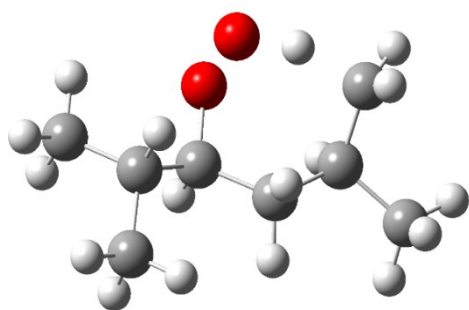


C,0,0.0120919001,-0.0160102674,0.0084771476  
 H,0,0.0048117254,-0.0215587833,1.101348723  
 H,0,1.0532994001,-0.0282925838,-0.3243392065  
 C,0,-0.7525654436,-1.2302454838,-0.5379867215  
 C,0,-0.0362697259,-2.5349530261,-0.1609220475  
 H,0,-0.5399223333,-3.420569925,-0.5550950791  
 H,0,0.9812091643,-2.5272325119,-0.5624409673  
 C,0,-2.2313688224,-1.1676350471,-0.1012021827  
 C,0,-3.1575083487,-2.1780966526,-0.8423475938



C,0,-2.9827016104,-2.4427285752,-0.8835751223  
 H,0,-3.3119194423,-1.536862779,-1.8391586631  
 H,0,-2.3904051695,-3.2003655327,-1.3972541762  
 C,0,-4.2153590503,-2.9974572874,-0.2042011672  
 H,0,-3.8505987308,-3.5148365819,0.7016965669  
 C,0,-4.9035891638,-4.0485578391,-1.0890187592  
 H,0,-4.2142705403,-4.8486479491,-1.3735395934  
 H,0,-5.7495593065,-4.5026968166,-0.5669754296  
 H,0,-5.2849676231,-3.5894307569,-2.0062811467  
 C,0,-5.2113609871,-1.9181613746,0.2495816602  
 H,0,-4.7520644679,-1.1853406666,0.9147274735  
 H,0,-5.6023348393,-1.3714680423,-0.6128488678  
 H,0,-6.0522280732,-2.3785538792,0.774984856  
 H,0,-0.4775910266,0.8274718927,-0.5911892354  
 H,0,-0.6245277301,-1.4045684197,-1.6936687128  
 H,0,0.0002508773,-2.5396467696,1.0941424288  
 O,0,-2.8303386433,-0.1121186011,-0.6151239512  
 O,0,-3.1515233503,-0.3342248404,-1.9843921965

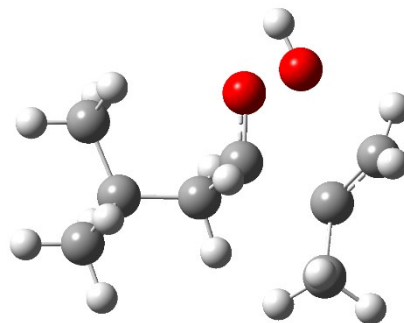
**TSQ5<sub>s</sub>**



C,0,-0.1793356671,0.1271737034,-0.360436784  
 H,0,0.0229506348,0.2458174262,0.710119755  
 H,0,0.7789115273,0.1701018084,-0.8855451637

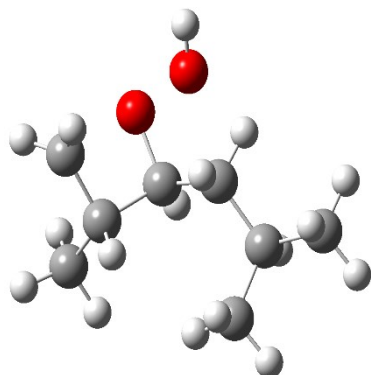
H,0,-3.6551999463,-1.6377603001,-1.6589733559  
 H,0,-2.547375464,-2.9550182859,-1.3077916444  
 C,0,-4.2023312341,-2.8424339117,0.0460243577  
 H,0,-3.3853924667,-2.9727525941,1.1162305489  
 C,0,-4.6227678392,-4.2323583924,-0.3780384314  
 H,0,-3.7601883259,-4.883475079,-0.5434240977  
 H,0,-5.2676822729,-4.6998815464,0.3705806938  
 H,0,-5.1907667289,-4.1959615244,-1.3193966951  
 C,0,-5.3170718336,-1.9429324802,0.5351414334  
 H,0,-4.9229704955,-1.0469489699,1.0193876189  
 H,0,-5.9461427607,-1.6198058707,-0.3076437457  
 H,0,-5.9636280525,-2.4616209205,1.2474296146  
 H,0,-0.435886805,0.9244872392,-0.3267209415  
 H,0,-0.7728959617,-1.1546400926,-1.6349477534  
 H,0,0.0217671388,-2.6467224041,0.922745625  
 H,0,-2.5865435548,-0.1479201091,-0.2827902348  
 O,0,-2.4009100446,-1.2648598458,1.3292495946  
 O,0,-2.4149537236,-2.6227491003,1.7200457109

**TS3<sub>s</sub>**

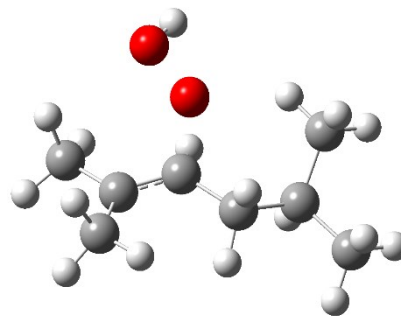


C,0,-0.0323641488,-0.0481471855,0.1714056302  
 H,0,-0.0275786366,-0.1784175,1.2494014526  
 H,0,0.8427786628,0.3810733014,-0.2955774298

C,0,-0.8879217725,-1.2048374662,-0.63943316	C,0,-1.2085559176,-0.2379476163,-0.573936385
C,0,-0.0282056612,-2.3876661321,-0.1686534217	C,0,-2.2882596296,-1.1184534101,0.0407548215
H,0,-0.4541527715,-3.3532569499,-0.4502200276	H,0,-3.2559668529,-1.001679971,-0.4510143102
H,0,0.9704296749,-2.3286616726,-0.609510284	H,0,-2.0095235373,-2.1734318078,-0.0363626063
C,0,-2.2864272543,-1.2304854223,0.0016124632	C,0,-1.9953632811,1.452857095,-0.87893492
H,0,-2.193243352,-1.0473650962,1.0801135934	H,0,-2.4981881473,1.5032771086,0.0932488216
C,0,-3.0685367533,-2.5415353734,-0.2188803782	C,0,-2.9125518506,1.3041554377,-2.0892095666
H,0,-2.8440184743,-2.9480912325,-1.2114236628	H,0,-2.2816424093,1.407852095,-2.9775525115
H,0,-2.6987807131,-3.2728929554,0.5053011333	H,0,-3.3486427661,0.3015178839,-2.115449183
C,0,-4.6040247735,-2.4080249143,-0.066182574	C,0,-4.0658344282,2.3333099543,-2.1337127645
H,0,-4.8093778838,-1.7019683855,0.7453961586	H,0,-4.6011383608,2.2745390182,-1.1753313046
C,0,-5.2396686913,-3.7631464835,0.3105046248	C,0,-5.0593672414,1.9580212151,-3.2433795904
H,0,-4.8481341712,-4.1187986128,1.2685801268	H,0,-5.4678151527,0.9539348192,-3.095041528
H,0,-6.3261867015,-3.6814023481,0.3989656243	H,0,-5.8976126643,2.6600940199,-3.274559099
H,0,-5.0204540939,-4.5212190536,-0.4477563498	H,0,-4.5718495789,1.9788938932,-4.2238892996
C,0,-5.2374082943,-1.8739057402,-1.3336303428	C,0,-3.5723705435,3.7750711862,-2.3138017187
H,0,-5.1699176726,-2.5288987796,-2.2039166043	H,0,-2.8842583558,4.0727353671,-1.5215072841
H,0,-6.1999071649,-1.3739158525,-1.2365752794	H,0,-3.0424105561,3.8831198988,-3.2663726521
H,0,-0.7868235815,0.9727043758,-0.6842848805	H,0,-4.4149597087,4.473120549,-2.3186171234
H,0,-1.0435673048,-1.2930766959,-1.7208452217	H,0,-1.022496585,-0.4179984536,-1.632677865
H,0,0.0938081771,-2.3767385865,0.920432774	H,0,-2.4204497368,-0.8879862147,1.1019460786
O,0,-3.0670041224,-0.0780383868,-0.3929907051	O,0,-1.0889765245,2.4064551769,-0.9459989805
H,0,-4.3559036591,-0.8457439668,-1.7029042641	O,0,0.1441128295,1.877599213,-2.0836265386
O,0,-3.4267677497,-0.1907993264,-1.7559228702	H,0,0.4070949031,2.78990867,-2.265357184

**TS4<sub>s</sub>**

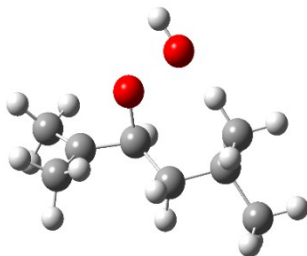
C,0,0.1631397278,0.284823811,0.3436533971  
 H,0,0.1469357367,0.653791323,1.3730749526  
 H,0,1.2065138962,0.206796643,0.0250048233  
 H,0,-0.2672244406,-0.7202526999,0.3385382645  
 C,0,-0.6224827651,1.2265567579,-0.5701313642  
 C,0,-2.0692077355,1.4825800134,-0.0836887714  
 C,0,-0.1065702204,2.6427731985,-0.5251745857  
 H,0,-0.2728737367,3.312862334,-1.3591095313  
 C,0,-3.1647428988,1.552781134,-1.1473786435  
 H,0,-3.9222211706,2.2319992074,-0.7484691212  
 C,0,-3.8502579144,0.2162499175,-1.4920433698  
 H,0,-4.226591333,-0.2055009327,-0.5503210232  
 H,0,-2.3676509018,0.8027985771,0.7214055195  
 H,0,-2.765695733,2.013883764,-2.0610631592  
 H,0,0.6611323416,2.9257511069,0.1836603777  
 O,0,-1.8274046874,2.7932714566,0.5027780389  
 H,0,-0.6192848946,0.8418959168,-1.5951829956  
 O,0,-3.1760682641,3.0131006286,1.4797549342  
 H,0,-3.2613841066,3.9570816863,1.2907296491  
 C,0,-2.9057911935,-0.817204084,-2.1232602003

**TS5<sub>s</sub>**

C,0,-0.015592562,0.0044768574,0.0234843662  
 H,0,-0.0848137782,0.0202119229,1.1191687882  
 H,0,1.052805928,-0.001411779,-0.2219579671  
 C,0,-0.6966447829,-1.216257147,-0.5160995402  
 C,0,-0.1417269068,-2.5397447896,-0.085278364  
 H,0,-0.494247042,-3.3572649433,-0.7180712318  
 H,0,0.9532177187,-2.5401466641,-0.0921457927  
 C,0,-1.9202980624,-1.161599376,-1.1782086177  
 H,0,-2.2584690761,-2.1021429097,-1.6073896992  
 C,0,-2.4681885253,0.0836438798,-1.8422998579  
 H,0,-2.9496209198,0.7107197767,-1.0808745844  
 H,0,-1.6342911896,0.6711861913,-2.2414013615  
 C,0,-3.4643437284,-0.1856625441,-2.9878610222  
 H,0,-2.9757121515,-0.8727105942,-3.6928636211  
 C,0,-3.7699996887,1.1153575863,-3.7423867013  
 H,0,-2.8592836056,1.5698649203,-4.1437728698  
 H,0,-4.4513540564,0.9354900931,-4.5787665412  
 H,0,-4.2446061164,1.8472005419,-3.079819126  
 C,0,-4.7620496853,-0.8461845013,-2.5037459341

H,0,-2.4697241657,-0.4338038199,-3.0525806402  
H,0,-2.0850477565,-1.0913623115,-1.4557915809  
H,0,-3.4465246754,-1.73611405,-2.3681671538  
C,0,-5.0586085531,0.4643651661,-2.4061175388  
H,0,-5.5956630549,-0.4658406654,-2.6135060886  
H,0,-5.7633055216,1.1656737221,-1.9508126308  
H,0,-4.742054922,0.8857243861,-3.366626779

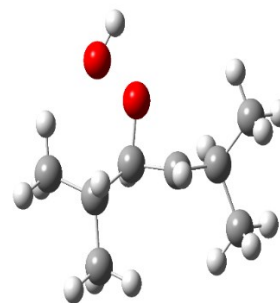
**TS6<sub>s</sub>**



C,0,0.,0.,0. H,0,0.,0.,1.09321432 H,0,1.052456366,0.,-  
0.3224543439  
C,0,-0.7155852937,-1.1929807862,-0.5408637423  
C,0,-0.7410510613,-2.4465427043,0.267386666  
H,0,0.2616711046,-2.8985763687,0.2962294316  
H,0,-1.0235802056,-2.2504280527,1.3073184056  
C,0,-1.4610553453,-1.1503536852,-1.8308056075  
H,0,-1.6279657595,-2.1574631191,-2.2333058586  
C,0,-0.9507311958,-0.2283530082,-2.9363189814  
H,0,-0.6968897024,0.7539122974,-2.5250703172  
H,0,-0.0075288234,-0.6754774427,-3.2779388883  
C,0,-1.8887887911,-0.0362227479,-4.1515512718  
H,0,-2.4679546319,-0.9573673817,-4.2829073809  
C,0,-1.0684380167,0.1985649547,-5.4286484024

H,0,-4.5721847318,-1.7854470414,-1.9808716203  
H,0,-5.2930835935,-0.1910991312,-1.8064855726  
H,0,-5.4268888211,-1.0557936375,-3.3470479281  
H,0,-0.4489772089,0.9336313938,-0.3456363624  
H,0,-0.4655077814,-2.7616441246,0.9412671107  
O,0,-3.1563554533,-1.1682244921,0.2961865313  
O,0,-3.0971703489,-2.3474119413,1.0542230035  
H,0,-3.6961534898,-2.9443563959,0.5818101464

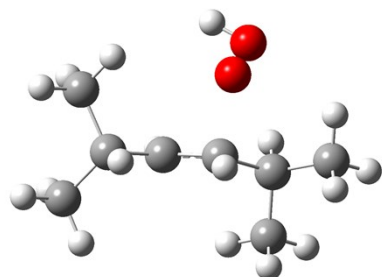
**TS7<sub>s</sub>**



C,0,-0.0037140391,-0.0107262931,0.0100992465  
H,0,0.0188787534,-0.0400536937,1.1047705697  
H,0,1.0309656544,0.0026169492,-0.3452264857  
C,0,-0.743815149,-1.2301549925,-0.5530686194  
C,0,-0.0681808942,-2.541476953,-0.1253976355  
H,0,-0.5572580477,-3.4173566474,-0.5621115589  
H,0,0.9792848048,-2.5546701376,-0.4376755683  
C,0,-2.2186142422,-1.2435615733,-0.1439148755  
H,0,-2.3341110174,-1.293047988,0.9467287091  
C,0,-3.1140726156,-2.1770762164,-0.8638784709  
H,0,-2.8754740899,-2.4009544227,-1.90051568  
C,0,-4.3844718716,-2.7120387845,-0.2909339429  
H,0,-4.5765390477,-2.1827747982,0.6486009179

H,0,-0.4086533101,-0.6473615885,-5.6460634936  
H,0,-1.7222528528,0.3439755192,-6.2935422345  
H,0,-0.4431145511,1.0938517538,-5.3346926349  
C,0,-2.8817751603,1.1134568087,-3.9276358959  
H,0,-3.4862790512,0.938078916,-3.0388790131  
H,0,-2.3478372705,2.0647658617,-3.8161031515  
H,0,-3.5566475756,1.2113947268,-4.7837423331  
H,0,-0.444136192,0.9334095001,-0.346679042  
H,0,-1.4303472667,-3.1819479297,-0.14862087  
O,0,-2.5929299529,-0.7392128966,-1.0912391838  
O,0,-4.0119762794,-1.0725702753,-2.0024729693  
H,0,-4.5427664589,-1.2532981873,-1.2149593376

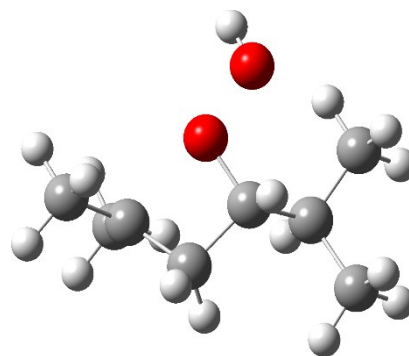
**TS8<sub>s</sub>**



C,0,-0.0173089723,0.0244291168,-0.0016141041  
H,0,-0.0117218551,0.0295225669,1.0941991744  
H,0,1.023111648,0.0449624487,-0.3377021122  
C,0,-0.7295984124,-1.2248325749,-0.5343761697  
C,0,-0.0056737601,-2.5048590621,-0.0726710442  
H,0,-0.4655597306,-3.4030189663,-0.4915292361  
H,0,1.0426988519,-2.4815618668,-0.3841849301

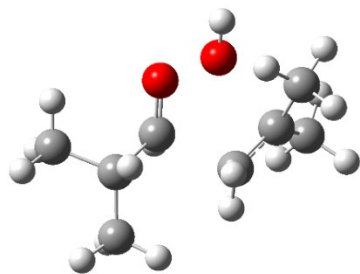
C,0,-4.2191994978,-4.2159690061,0.0324859624  
H,0,-3.4003345096,-4.3879573643,0.7350432922  
H,0,-5.1380512923,-4.6071544561,0.4785764518  
H,0,-4.0146623338,-4.7912593689,-0.8754541621  
C,0,-5.5773682957,-2.480877706,-1.2341077818  
H,0,-5.7073713038,-1.4162575672,-1.4364880502  
H,0,-5.4247057801,-2.992700808,-2.189838979  
H,0,-6.5002319175,-2.8665021519,-0.7915641291  
H,0,-0.4941740008,0.9158990638,-0.2854066125  
H,0,-0.0880672491,-2.6541855817,0.9640152512  
O,0,-3.0159727277,-0.2093352535,-0.6831445955  
O,0,-2.7957836645,1.2284983135,0.2404753236  
H,0,-3.6654480342,1.5804262201,0.0055232517  
H,0,-0.726459616,-1.1659694367,-1.6486365443

**TS9<sub>s</sub>**

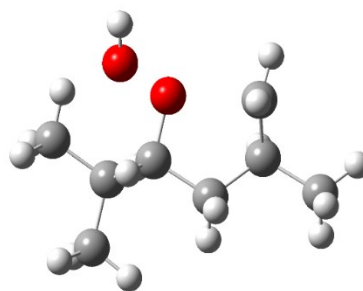


C,0,0.0093708501,-0.0060584959,-0.0005609556  
H,0,0.0361563926,-0.027137204,1.0920012533  
H,0,1.0400802949,0.0079989686,-0.3696110915  
C,0,-0.7283480906,-1.2272216669,-0.560989731  
C,0,0.0021926191,-2.5218495051,-0.1671128213

C,0,-2.1869630266,-1.2683702373,-0.1188311043	H,0,-0.4747202516,-3.4152892469,-0.5799252929
H,0,-2.3963890355,-0.902080525,0.8849305174	H,0,1.0352887864,-2.504608803,-0.5239339408
C,0,-3.0779892061,-2.1960668232,-0.6394050879	C,0,-2.2032355554,-1.3203746551,-0.1273520424
H,0,-2.829209716,-2.6785704311,-1.5850936017	H,0,-2.2576815445,-1.5449793795,0.9427696033
C,0,-4.4446626519,-2.475566371,-0.0858563239	C,0,-3.040470692,-2.2960497317,-0.9843885137
H,0,-4.5170858748,-1.9987068041,0.8985918837	H,0,-2.418750374,-2.9024229151,-1.6503326454
C,0,-4.6667875012,-3.9895708374,0.0925508859	H,0,-3.6268704778,-2.9755930604,-0.3607111607
H,0,-3.9227468398,-4.4249919645,0.7641842897	C,0,-3.939876337,-1.3504865634,-1.7505557798
H,0,-5.6587709199,-4.1889007117,0.508245928	C,0,-5.3762776424,-1.2389841643,-1.36296409
H,0,-4.5971511361,-4.5093951288,-0.8686833975	H,0,-5.5027100498,-1.3197294954,-0.2819370018
C,0,-5.5396431602,-1.8631470724,-0.9849201796	H,0,-5.8057453947,-0.2883015284,-1.6916303387
H,0,-5.4054688036,-0.7828007734,-1.0641741669	H,0,-5.9696554668,-2.0417905487,-1.8306591211
H,0,-5.5035997023,-2.2933799965,-1.9916789892	H,0,-0.4799115539,0.9211220989,-0.2948119908
H,0,-6.5339477119,-2.0617674606,-0.5735617128	H,0,0.0305307865,-2.6320922048,0.9220974029
H,0,-0.512162732,0.9325032625,-0.343689777	O,0,-2.9758667823,-0.1142734982,-0.3575468603
H,0,-0.026807052,-2.5954868887,1.0183378849	O,0,-2.6684365097,0.7981348418,1.0126630868
O,0,-2.8928694951,0.3630345655,-0.8523738861	H,0,-2.8766906823,1.643060253,0.5925165756
O,0,-2.4708680059,0.5326933566,-2.1789243723	C,0,-3.5432711063,-0.8843048899,-3.1126182716
H,0,-3.2555703389,0.2832509902,-2.6875227216	H,0,-2.4602638852,-0.8445885355,-3.2386318153
H,0,-0.7098072668,-1.1927980935,-1.62941774	H,0,-3.9390017505,-1.5649043908,-3.8851203858
	H,0,-3.9521691888,0.1080252314,-3.3250636341
	H,0,-0.7181774264,-1.1493584019,-1.6565970192

**TS10<sub>s</sub>**

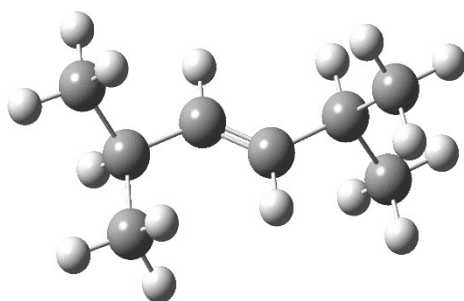
C,0,-0.0009051848,-0.0027815161,-0.0027462471  
 H,0,0.0022812666,-0.0019527007,1.0923571395  
 H,0,1.0392691545,-0.0022769313,-0.3406255479  
 C,0,-0.7415074587,-1.2385101662,-0.5497485552  
 C,0,-0.0505735034,-2.5290003787,-0.0941850676  
 H,0,-0.4506334425,-3.4168436487,-0.5874137415  
 H,0,1.0184101092,-2.4835894535,-0.3187320238  
 C,0,-2.2118523385,-1.1372645944,-0.1051576692  
 H,0,-2.3746937777,-1.4226394491,0.942360858  
 C,0,-3.0879017116,-2.7347607353,-0.8266528889  
 H,0,-2.642811715,-2.6755469832,-1.8157406838  
 H,0,-2.6849310839,-3.515082558,-0.1893268439  
 C,0,-4.4684095767,-2.515361777,-0.7548695317  
 C,0,-5.300576972,-3.2127309767,0.2754614726  
 H,0,-4.7278127313,-3.4016257991,1.184726157  
 H,0,-6.1891234816,-2.6364647583,0.5309040546  
 H,0,-5.6220098766,-4.1833312448,-0.1268320076  
 H,0,-0.4825003831,0.9154959245,-0.3394925908  
 H,0,-0.1519137994,-2.666200165,0.9877570468  
 O,0,-2.8472109735,-0.1119174547,-0.5308509287  
 O,0,-4.6318101301,-0.5965023012,0.4386532629  
 H,0,-5.0026640329,0.1162626617,-0.0982213461

**TS11<sub>s</sub>**

C,0,0.0058389431,-0.0053935731,-0.0020706998  
 H,0,0.0130209082,-0.0100251525,1.0913077501  
 H,0,1.0433902907,0.0010753099,-0.350735549  
 C,0,-0.7229840906,-1.2335824441,-0.5595272165  
 C,0,0.0198586931,-2.5183523249,-0.1539199248  
 H,0,-0.4018053029,-3.4127148957,-0.6185806884  
 H,0,1.0714861217,-2.459777364,-0.4467763198  
 C,0,-2.2083286594,-1.3196919461,-0.1464405483  
 H,0,-2.2839305217,-1.4415510201,0.9393333704  
 C,0,-2.9382351892,-2.4923659483,-0.8431449067  
 H,0,-2.4649444668,-2.6916265164,-1.8129050103  
 H,0,-2.8365605125,-3.4046542822,-0.2479061881  
 C,0,-4.4158213254,-2.1541618465,-1.0898058806  
 H,0,-4.9088843278,-2.0047559004,-0.1229696291  
 C,0,-5.1421291847,-3.2917204607,-1.8362041221  
 H,0,-5.1037240317,-4.2216830418,-1.2603916544  
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 H,0,-5.1898485276,-0.1079434039,-1.6269529039  
 H,0,-3.9114273791,-0.7832218792,-2.7761671277  
 H,0,-0.4703579242,0.9201853918,-0.3221869222

C,0,-5.1502029321,-1.8878364265,-1.9319218514  
H,0,-4.5489655049,-1.0509437051,-2.2965965092  
H,0,-5.2234092064,-2.6216654992,-2.7452016536  
H,0,-6.1558452901,-1.5408547373,-1.6924493562  
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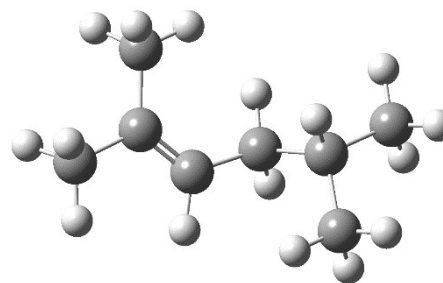
**P1<sub>s</sub>,P8<sub>s</sub>**



C,0,-0.0020050117,0.0016929138,-0.0031848172  
H,0,-0.0006165265,0.0035933535,1.0921121163  
H,0,1.0402203481,0.0032323436,-0.3366516464  
C,0,-0.7530723519,-1.2266321223,-0.5480667757  
C,0,-0.0521440305,-2.5285625095,-0.1194146518  
H,0,-0.5541612118,-3.4033220203,-0.5401581101  
H,0,0.9905612171,-2.5396789522,-0.4512077946  
C,0,-2.1938733426,-1.2186298325,-0.1006895384  
H,0,-2.34307279,-1.2570655181,0.977735187  
C,0,-3.2482180273,-1.1727450874,-0.9136108701  
H,0,-3.0636399039,-1.1346341326,-1.9882931338  
C,0,-4.7107761694,-1.1523806009,-0.5327301123  
H,0,-5.1717713978,-2.0306699891,-1.0087611783  
C,0,-5.397038238,0.0903663546,-1.133315661

H,0,-0.7121665763,-1.1617128239,-1.655720426  
H,0,-0.0109863644,-2.6569894741,0.932449889  
O,0,-2.9415503712,-0.1137802991,-0.4603772294  
O,0,-2.7231040551,0.8179830195,0.8802877597  
H,0,-2.8042835738,1.6624948741,0.4164496477

**P2<sub>s</sub>,P5<sub>s</sub>**

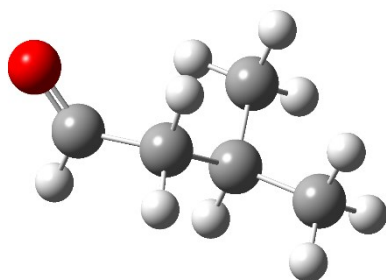


C,0,-0.0030266924,0.0020375898,-0.0065771211  
H,0,-0.0113722596,0.0105846359,1.0899743438  
H,0,1.0509367042,-0.0057319208,-0.3097420431  
C,0,-0.7292438718,-1.2067428899,-0.5448907028  
C,0,-0.1572707482,-2.5274112774,-0.0937175432  
H,0,-0.6971466556,-3.3879520131,-0.4875749885  
H,0,0.8925087371,-2.6170598598,-0.3975047872  
C,0,-1.7870177432,-1.0698033515,-1.3544787569  
C,0,-2.6243109129,-2.155363873,-1.9772801133  
H,0,-2.077234451,-3.102061976,-1.995011559  
C,0,-3.9920872716,-2.3955334136,-1.2896913641  
H,0,-3.7871048062,-2.6538613446,-0.2428796391  
C,0,-4.7158096174,-3.580960076,-1.9414384614  
H,0,-4.1089055047,-4.4906031049,-1.9026147499



H,0,-5.241247513,0.1477887926,-2.2143596951  
H,0,-6.4752271261,0.068480115,-0.9499650759  
H,0,-4.9944901448,1.0058000023,-0.6888401282  
C,0,-4.9744662608,-1.2513042163,0.9730981475  
H,0,-4.5377225362,-2.1575850725,1.4006389355  
H,0,-4.5568422638,-0.3911663441,1.5057559301  
H,0,-6.0495959927,-1.2731688867,1.1705894592  
H,0,-0.4695089272,0.9307432017,-0.3387745942  
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H,0,-0.738524004,-1.1764430734,-1.6436117148

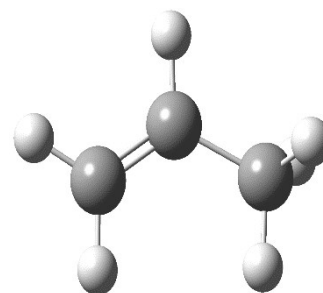
**P3<sub>s</sub>**



C,0,-0.0004050559,0.0655191478,0.0158091902  
H,0,0.0944757856,-0.4566440651,0.997158295  
C,0,1.2391549836,0.003234491,-0.8441472766  
H,0,2.0195081569,0.5717955838,-0.3193657904  
H,0,1.0321444081,0.5086751025,-1.7918825199  
C,0,1.7416351166,-1.4389935635,-1.0734216354  
H,0,1.8466017612,-1.914181244,-0.0885428636  
C,0,0.7334378074,-2.2570838724,-1.892243551  
H,0,-0.2496571173,-2.2907855975,-1.4145620286  
H,0,0.6005569656,-1.82325622,-2.8887262412  
H,0,1.0781820424,-3.2869170512,-2.0190758603  
C,0,3.1234539848,-1.4316227888,-1.7390095072

H,0,-5.6649975563,-3.7906318881,-1.4395348788  
H,0,-4.9360862812,-3.3727799793,-2.9943133088  
C,0,-4.8771007058,-1.1422873178,-1.3011226902  
H,0,-4.4013137752,-0.3062705357,-0.7832161567  
H,0,-5.0904095094,-0.8254392193,-2.3284593565  
H,0,-5.8348249443,-1.3359661159,-0.8092671112  
H,0,-0.4505807141,0.9339949354,-0.3573247203  
H,0,-0.1702046723,-2.5961593141,1.0003571065  
H,0,-2.0922125909,-0.053154678,-1.5953153701  
H,0,-2.8144533245,-1.8957096165,-3.0278420794

**P3<sub>s</sub>**

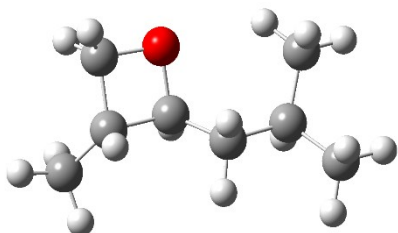


C,0,0.0053249208,0.1571552696,-0.0883882785  
H,0,-0.0192289544,0.5410506269,0.9302480173  
C,0,1.1787118407,-0.1689847089,-0.6213491893  
H,0,1.25605624,-0.5560585439,-1.6332872288  
H,0,2.1047693041,-0.0618017246,-0.067854745  
C,0,-1.3220444434,0.0422268962,-0.7784021874  
H,0,-1.9970120552,-0.6209572725,-0.2258996709  
H,0,-1.8203407493,1.0162689879,-0.8384078358  
H,0,-1.2142084929,-0.3488997261,-1.7928178562

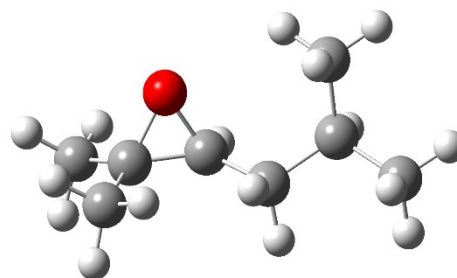
**P6<sub>s</sub>**

H,0,3.856887642,-0.8928872667,-1.1322801242  
H,0,3.4921707281,-2.4505937232,-1.885858672  
H,0,3.0812508769,-0.9484787405,-2.7206247366  
O,0,-1.0274634265,0.6191087194,-0.2832044505

**P4<sub>s</sub>**



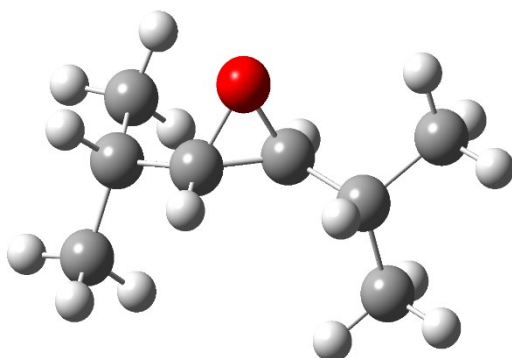
C,0,-0.0137515835,0.0162310034,-0.0179586478  
H,0,0.0205206099,0.0055384047,1.0790693768  
H,0,1.0069844226,0.0371959865,-0.4105678305  
C,0,-0.9830655396,-1.0158799913,-0.6292686098  
C,0,-1.5491919523,-2.1057614232,0.2674326262  
H,0,-2.3566202806,-2.6498753578,-0.2323146065  
H,0,-0.7798385249,-2.8354683026,0.5379551406  
C,0,-1.865067976,0.2170967858,-0.9464674009  
H,0,-2.7231936664,0.2995668593,-0.2625152423  
C,0,-2.3212822573,0.4281655031,-2.3797044373  
H,0,-1.4365985516,0.4481611363,-3.0289034818  
H,0,-2.9012567602,-0.4614690389,-2.6624111982  
C,0,-3.18163039,1.6816469594,-2.6300373332  
H,0,-4.0089924603,1.6588966204,-1.9068981448  
C,0,-3.7923963491,1.6413652828,-4.0378973994  
H,0,-4.4031471773,0.7456581391,-4.1869663875



C,0,0.2833065776,-0.0350293558,0.1513406751  
H,0,1.1516913595,-0.2361619717,0.7862978585  
H,0,0.6490281246,0.3001159229,-0.8241339208  
C,0,-0.572439031,-1.2747753687,-0.0076836504  
C,0,0.1276699859,-2.44858479,-0.6577488706  
H,0,-0.546474342,-3.2902148264,-0.8094639073  
H,0,0.5175898275,-2.1499740487,-1.6356518434  
C,0,-1.7470330876,-1.4455178802,0.8721023684  
H,0,-1.9138174351,-0.6433817347,1.5948584116  
C,0,-2.3657871964,-2.7600466029,1.2852777343  
H,0,-2.2125950117,-3.5128415676,0.506519204  
H,0,-1.8342020056,-3.1123696956,2.1791770177  
C,0,-3.8719357558,-2.6631342672,1.6065641112  
H,0,-4.001104512,-1.8541933321,2.3390402592  
C,0,-4.3686560045,-3.9623696453,2.2544618658  
H,0,-3.815548662,-4.1920162398,3.1702780535  
H,0,-5.4293937076,-3.89331092,2.5119996766  
H,0,-4.2491136574,-4.8099106444,1.570686743  
C,0,-4.7042596286,-2.3148371268,0.3642167006  
H,0,-4.6194281909,-3.1050981816,-0.3896021429  
H,0,-5.7623370464,-2.2131519783,0.6233704697  
H,0,-0.29292931,0.7783831321,0.5955846525  
H,0,0.9732497789,-2.781886973,-0.0480292443

H,0,-4.4274468938,2.5138829995,-4.2165046112  
H,0,-3.007995834,1.641794029,-4.8027062615  
C,0,-2.3986443935,2.9851220217,-2.4129949018  
H,0,-1.9635674439,3.0353850125,-1.4143695206  
H,0,-1.5755632237,3.0626301894,-3.131765108  
H,0,-3.0490923615,3.8534257813,-2.5563875123  
H,0,-1.9516110645,-1.6845952422,1.1937315268  
O,0,-0.8039381307,1.1192858026,-0.5166591836  
H,0,-0.5791489162,-1.4506670129,-1.5483373271

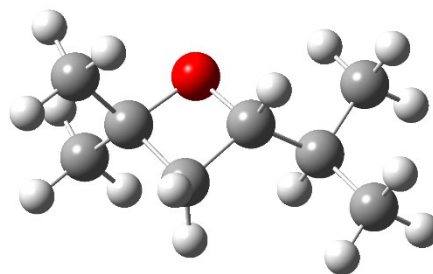
**P7<sub>s</sub>**



C,0,0.0188271363,0.0031653331,-0.012078904  
H,0,0.0260212196,0.0115811785,1.083064529  
H,0,1.0591506701,-0.0097319606,-0.3479735028  
C,0,-0.7432309939,-1.2164736974,-0.5484700801  
C,0,-0.0848620283,-2.5358704674,-0.1220860379  
H,0,-0.6478960588,-3.389023738,-0.5070399881  
H,0,0.9395548576,-2.6028006025,-0.498980548  
C,0,-2.1887119554,-1.1791550433,-0.0955350321  
H,0,-2.3268086134,-1.1811571525,0.9862907832  
C,0,-3.2709258181,-0.6332549614,-0.9283415723

O,0,-1.9059691222,-1.006951429,-0.4915950694  
H,0,-4.3721800206,-1.3849826619,-0.0997444255

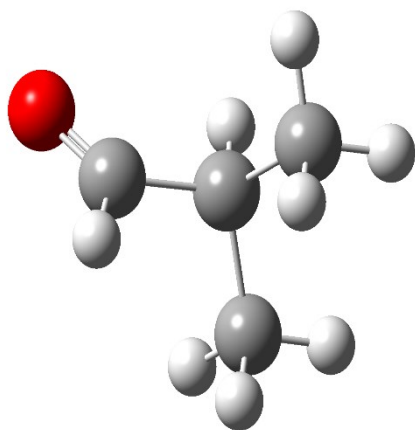
**P9<sub>s</sub>**



C,0,-0.0674023952,-0.2092868094,-0.8176579726  
H,0,0.1567485834,0.3596045501,0.0915347048  
H,0,0.8820410131,-0.4371004319,-1.3105830056  
C,0,-0.8363955625,-1.49337428,-0.4830030796  
C,0,-0.0520607102,-2.3958319494,0.4783095119  
H,0,-0.5897848352,-3.3231817654,0.6969024821  
H,0,0.917686582,-2.6672302249,0.0527210255  
C,0,-2.2059802374,-1.156324181,0.0975300014  
H,0,-2.0752410831,-0.6328707475,1.0554381434  
C,0,-3.2846428809,-2.2567782253,0.1453300608  
H,0,-3.004344189,-3.1780920724,-0.3696012554  
H,0,-3.6863658001,-2.5009299477,1.1293626094

H,0,-2.9795177808,-0.2707182535,-1.9159632509  
 C,0,-4.5589120512,-0.0133326392,-0.4099471541  
 H,0,-5.3338888354,-0.2841860074,-1.1401738809  
 C,0,-4.4340507675,1.5174695832,-0.402434257  
 H,0,-4.1576950352,1.9047187755,-1.3878212451  
 H,0,-5.3806711419,1.9837079281,-0.1166647175  
 H,0,-3.6716304768,1.8438723251,0.3120981092  
 C,0,-4.997467067,-0.5596535188,0.9528388161  
 H,0,-4.9900073406,-1.6513011366,0.952319635  
 H,0,-4.340150741,-0.2103261101,1.7550467962  
 H,0,-6.0102001092,-0.2230982839,1.1891861239  
 H,0,-0.4327847259,0.9396103624,-0.3514316538  
 H,0,-0.0446621396,-2.6196713511,0.9694061855  
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 O,0,-3.1010458,-2.0529916008,-0.7842317578

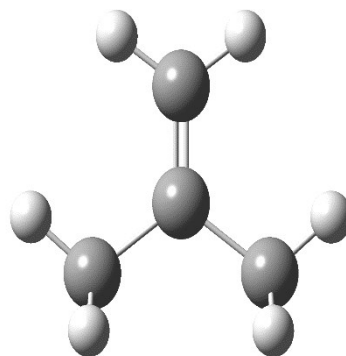
**P10<sub>s</sub>**



C,0,-0.0009962697,-0.0106515807,-0.0500603504  
 H,0,0.0292574534,-0.4825092337,0.9618300669  
 C,0,1.3293340455,-0.0218008175,-0.777362835

C,0,-4.1399404829,-1.28846297,-0.7106792523  
 C,0,-4.5381220852,-1.7794430484,-2.0944329839  
 H,0,-3.6820841975,-2.2212962117,-2.608445749  
 H,0,-5.3314405973,-2.5307747373,-2.0275310922  
 H,0,-4.9051608257,-0.9449628743,-2.6986981418  
 C,0,-5.3050516093,-0.6380656293,0.0253181404  
 H,0,-4.9893581162,-0.274728978,1.0061153568  
 H,0,-5.6815531057,0.214066645,-0.547100507  
 H,0,-6.1250181457,-1.3493519402,0.1667282181  
 H,0,-0.6561640816,0.4286668736,-1.4792746264  
 H,0,-1.0097223812,-2.042559235,-1.417613048  
 H,0,0.1354667595,-1.8853325924,1.4290350497  
 O,0,-3.0161231616,-0.3520216602,-0.8014775607

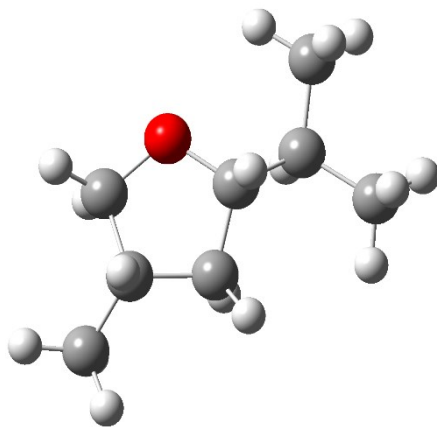
**P10<sub>s</sub>**



C,0,-0.00073284,-0.0359578168,-0.0025566991  
 H,0,-0.0012320772,-0.0827462072,1.0813030494  
 H,0,0.9678514806,-0.0051408891,-0.4902562194  
 C,0,-1.1356137457,-0.0171734341,-0.7014513293  
 C,0,-2.4879670068,-0.0595723089,-0.0373369421  
 H,0,-2.4047008666,-0.1053642603,1.0499495246  
 H,0,-3.0799153971,0.8250853547,-0.2996722687  
 H,0,-3.0617470444,-0.930536969,-0.3750773154

H,0,1.161179321,0.4640405716,-1.7426285806  
O,0,-1.0258478713,0.4521258501,-0.4796338355  
C,0,1.7818821298,-1.4753932442,-0.9970973966  
H,0,1.0648953594,-2.0296144647,-1.6078815226  
H,0,2.74896596,-1.4988003681,-1.505872891  
H,0,1.8953873074,-2.0023136127,-0.0439988392  
C,0,2.3642222555,0.7758397754,0.0343823247  
H,0,3.333935761,0.7620905219,-0.4697101397  
H,0,2.0604911871,1.8186640771,0.1549968761  
H,0,2.5022125208,0.3444706775,1.0312815616

**P11<sub>s</sub>**



C,0,-0.0479831032,0.0278538686,-0.1980635508  
H,0,0.1718088039,0.131416506,0.8705202967  
H,0,0.90136701,0.0793605852,-0.7390974446  
C,0,-0.7653001029,-1.2982785624,-0.4804947464  
C,0,0.0942526938,-2.4948687107,-0.0491765475  
H,0,-0.364443529,-3.4503802052,-0.3167369046  
H,0,1.0774431429,-2.4547955863,-0.5257782744  
C,0,-2.1402435415,-1.3345347287,0.1969421261  
H,0,-1.994053375,-1.2614075465,1.2864969872

C,0,-1.1497378087,0.047625113,-2.2073763228  
H,0,-1.6707006444,-0.8190004507,-2.6308645701  
H,0,-1.6886651759,0.9366358598,-2.5551951935  
H,0,-0.1403298217,0.0757754881,-2.6215476226

**OH**



O,0,0.,0.,-0.0076044417  
H,0,0.,0.,0.9676044417

**HO<sub>2</sub>**



O,0,-0.0196500749,0.,-0.0154687204  
H,0,0.0204702082,0.,0.9593821961  
O,0,1.2436878016,0.,-0.4239134757

C,0,-3.0161173085,-2.5524140479,-0.1250681039	
H,0,-2.8381643325,-2.8837500564,-1.1558617973	
H,0,-2.8252973454,-3.3977575758,0.5390042472	
C,0,-4.4421334087,-1.9969899743,0.0059235332	
H,0,-4.6874147657,-1.9236097204,1.0724883798	
C,0,-5.5268981108,-2.8061575659,-0.7008401287	
H,0,-5.6116386692,-3.8104738838,-0.2768833871	
H,0,-6.505941101,-2.3263301388,-0.6092782483	
H,0,-5.3039148614,-2.9100889569,-1.76762065	
C,0,-4.2506817262,-0.577825592,-0.5439628055	
H,0,-4.3858538827,-0.5658337801,-1.6355320134	
H,0,-4.9429498665,0.1482703463,-0.1072834254	
H,0,-0.666662895,0.8738584591,-0.4990281396	
H,0,-0.9459930469,-1.3670962342,-1.5613916034	
H,0,0.2543345874,-2.4907435371,1.034702738	
O,0,-2.9142794715,-0.1889956307,-0.2197149181	

**Table S4.** Arrhenius parameters for reactions on the  $R_1 + O_2$  surface (**Fig. S2**) in the high-pressure limit. The rate coefficients are in the form  $k(T) = A \times T^n \times \exp(-E_a/RT)$ , with  $A$  in  $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for bimolecular reaction, and  $\text{s}^{-1}$  for unimolecular reactions, and  $E_a$  in  $\text{kcal mol}^{-1}$ . Subscript p is used to indicate the relation to the primary alkylperoxy 2,5-dimethylhexyl-1-peroxy.

Reaction	Transition State	$A$	$n$	$E_a$
$R_1 + O_2 \rightarrow \text{ROO-1}$	-	$4.77 \times 10^{-16}$	1.033	-2.5
$\text{ROO-1} \rightarrow \text{P1}_p$	$\text{TS1}_p$	$1.01 \times 10^{13}$	0.030	30.3
$\text{ROO-1} \rightarrow \text{P2}_p$	$\text{TS2}_p$	$1.61 \times 10^{12}$	0.055	37.3
$\text{ROO-1} \rightarrow \text{QOOH-1}_p$	$\text{TSQ1}_p$	$8.76 \times 10^{11}$	0.019	21.9
$\text{ROO-1} \rightarrow \text{QOOH-2}_p$	$\text{TSQ2}_p$	$4.19 \times 10^{12}$	0.042	25.0
$\text{ROO-1} \rightarrow \text{QOOH-3}_p$	$\text{TSQ3}_p$	$5.05 \times 10^{11}$	0.025	17.4
$\text{ROO-1} \rightarrow \text{QOOH-4}_p$	$\text{TSQ4}_p$	$2.46 \times 10^{11}$	0.021	17.6
$\text{ROO-1} \rightarrow \text{QOOH-5}_p$	$\text{TSQ5}_p$	$8.61 \times 10^{10}$	0.029	16.2
$\text{ROO-1} \rightarrow \text{QOOH-6}_p$	$\text{TSQ6}_p$	$8.17 \times 10^{10}$	0.007	28.2
$\text{QOOH-1}_p \rightarrow \text{P3}_p$	$\text{TS3}_p$	$2.82 \times 10^{14}$	0.005	27.8
$\text{QOOH-1}_p \rightarrow \text{P4}_p$	$\text{TS4}_p$	$5.35 \times 10^{12}$	-0.001	20.5
$\text{QOOH-2}_p \rightarrow \text{P5}_p$	$\text{TS5}_p$	$4.29 \times 10^{12}$	-0.002	15.5
$\text{QOOH-2}_p \rightarrow \text{P6}_p$	$\text{TS6}_p$	$3.65 \times 10^{13}$	-0.032	11.0
$\text{QOOH-3}_p \rightarrow \text{P7}_p$	$\text{TS7}_p$	$1.68 \times 10^{12}$	0.003	16.4
$\text{QOOH-3}_p \rightarrow \text{P8}_p$	$\text{TS8}_p$	$3.00 \times 10^{13}$	0.005	25.8
$\text{QOOH-4}_p \rightarrow \text{P9}_p$	$\text{TS9}_p$	$7.07 \times 10^{11}$	0.002	7.6
$\text{QOOH-5}_p \rightarrow \text{P10}_p$	$\text{TS10}_p$	$1.0 \times 10^{12}$	0.002	7.3
$\text{QOOH-6}_p \rightarrow \text{P11}_p$	$\text{TS11}_p$	$1.92 \times 10^{10}$	0.346	11.1

**Table S5.** Arrhenius parameters for reactions on the R<sub>2</sub> + O<sub>2</sub> surface (**Fig. S3**) in the high-pressure limit. The rate coefficients are in the form  $k(T) = A \times T^n \times \exp(-E_a/RT)$ , with A in cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> for bimolecular reaction, and s<sup>-1</sup> for unimolecular reactions, and E<sub>a</sub> in kcal mol<sup>-1</sup>. Subscript t is used to indicate the relation to the tertiary alkylperoxy 2,5-dimethylhexyl-2-peroxy.

Reaction	Transition State	<i>A</i>	<i>n</i>	<i>E<sub>a</sub></i>
R <sub>2</sub> + O <sub>2</sub> → ROO-2	-	1.36×10 <sup>-17</sup>	1.900	-2.26
ROO-2 → P1 <sub>t</sub>	TS1 <sub>t</sub>	1.92×10 <sup>13</sup>	0.005	30.8
ROO-2 → P2 <sub>t</sub>	TS2 <sub>t</sub>	1.69×10 <sup>13</sup>	-0.009	29.7
ROO-2 → QOOH-1 <sub>t</sub>	TSQ1 <sub>t</sub>	6.00×10 <sup>11</sup>	0.071	31.3
ROO-2 → QOOH-2 <sub>t</sub>	TSQ2 <sub>t</sub>	3.46×10 <sup>11</sup>	0.061	27.5
ROO-2 → QOOH-3 <sub>t</sub>	TSQ3 <sub>t</sub>	5.92×10 <sup>11</sup>	0.025	20.8
ROO-2 → QOOH-4 <sub>t</sub>	TSQ4 <sub>t</sub>	3.37×10 <sup>11</sup>	0.020	16.4
ROO-2 → QOOH-5 <sub>t</sub>	TSQ5 <sub>t</sub>	1.98×10 <sup>11</sup>	0.001	22.0
QOOH-1 <sub>t</sub> → P3 <sub>t</sub>	TS3 <sub>t</sub>	1.03×10 <sup>13</sup>	-0.004	13.8
QOOH-1 <sub>t</sub> → P4 <sub>t</sub>	TS4 <sub>t</sub>	8.36×10 <sup>12</sup>	0.002	9.0
QOOH-2 <sub>t</sub> → P5 <sub>t</sub>	TS5 <sub>t</sub>	1.39×10 <sup>13</sup>	-0.003	14.1
QOOH-2 <sub>t</sub> → P6 <sub>t</sub>	TS6 <sub>t</sub>	1.14×10 <sup>13</sup>	0.007	7.6
QOOH-3 <sub>t</sub> → P7 <sub>t</sub>	TS7 <sub>t</sub>	2.24×10 <sup>12</sup>	-0.001	14.1
QOOH-3 <sub>t</sub> → P8 <sub>t</sub>	TS8 <sub>t</sub>	3.92×10 <sup>13</sup>	0.011	26.6
QOOH-4 <sub>t</sub> → P9 <sub>t</sub>	TS9 <sub>t</sub>	2.20×10 <sup>12</sup>	0.005	7.5
QOOH-5 <sub>t</sub> → P10 <sub>t</sub>	TS10 <sub>t</sub>	1.88×10 <sup>12</sup>	-0.007	14.2



**Table S6.** Arrhenius parameters for reactions on the  $R_3 + O_2$  surface (**Fig. S4**) in the high-pressure limit. The rate coefficients are in the form  $k(T) = A \times T^n \times \exp(-E_a/RT)$ , with  $A$  in  $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  for bimolecular reaction, and  $\text{s}^{-1}$  for unimolecular reactions, and  $E_a$  in  $\text{kcal mol}^{-1}$ . Subscript s is used to indicate the relation to the secondary alkylperoxy 2,5-dimethylhexyl-2-peroxy.

Reaction	Transition State	$A$	$n$	$E_a$
$R_3 + O_2 \rightarrow \text{ROO-3}$	-	$1.05 \times 10^{-17}$	1.589	-3.32
$\text{ROO-3} \rightarrow \text{P1}_s$	$\text{TS1}_s$	$3.19 \times 10^{12}$	0.061	24.0
$\text{ROO-3} \rightarrow \text{P2}_s$	$\text{TS2}_s$	$2.84 \times 10^{13}$	0.015	28.7
$\text{ROO-3} \rightarrow \text{QOOH-1}_s$	$\text{TSQ1}_s$	$1.68 \times 10^{12}$	0.002	21.5
$\text{ROO-3} \rightarrow \text{QOOH-2}_s$	$\text{TSQ2}_s$	$3.19 \times 10^{12}$	0.061	24.0
$\text{ROO-3} \rightarrow \text{QOOH-3}_s$	$\text{TSQ3}_s$	$1.14 \times 10^{12}$	0.043	28.0
$\text{ROO-3} \rightarrow \text{QOOH-4}_s$	$\text{TSQ4}_s$	$1.21 \times 10^{12}$	0.017	19.8
$\text{ROO-3} \rightarrow \text{QOOH-5}_s$	$\text{TSQ5}_s$	$8.48 \times 10^{11}$	0.007	20.6
$\text{QOOH-1} \rightarrow \text{P3}_s$	$\text{TS3}_s$	$5.02 \times 10^{13}$	0.008	27.0
$\text{QOOH-1} \rightarrow \text{P4}_s$	$\text{TS4}_s$	$6.06 \times 10^{12}$	-0.001	16.0
$\text{QOOH-2} \rightarrow \text{P5}_s$	$\text{TS5}_s$	$9.1 \times 10^{12}$	-0.005	14.3
$\text{QOOH-2} \rightarrow \text{P6}_s$	$\text{TS6}_s$	$4.7 \times 10^{14}$	0.058	10.5
$\text{QOOH-3} \rightarrow \text{P7}_s$	$\text{TS7}_s$	$2.14 \times 10^{13}$	0.019	10.9
$\text{QOOH-3} \rightarrow \text{P8}_s$	$\text{TS8}_s$	$1.77 \times 10^{12}$	0.0001	15.1
$\text{QOOH-4} \rightarrow \text{P9}_s$	$\text{TS9}_s$	$2.26 \times 10^{13}$	0.004	15.2
$\text{QOOH-4} \rightarrow \text{P10}_s$	$\text{TS10}_s$	$4.37 \times 10^{12}$	0.009	13.0
$\text{QOOH-5} \rightarrow \text{P11}_s$	$\text{TS11}_s$	$3.69 \times 10^{12}$	0.001	12.4

**Table S7:** Branching fractions of 2,5-dimethylhex-1-yl + O<sub>2</sub> calculated using RRKM/ME.

**Table S7-a** Temperature-dependent branching fractions for 2,5-dimethylhex-1-yl + O<sub>2</sub> at 0.001 atm.

T (K)	QOOH -1 <sub>p</sub>	QOOH -2 <sub>p</sub>	QOOH -3 <sub>p</sub>	QOOH -4 <sub>p</sub>	QOOH -5 <sub>p</sub>	QOOH -6 <sub>p</sub>	ROO -1 <sub>p</sub>	P10 p	P11 p	P1 p	P2 p	P3 p	P4 p	P5 <sub>p</sub>	P6 p	P7 p	P8 p	P9 <sub>p</sub>
400	0.00	0.00	0.00	0.00	0.00	0.00	0.16	0.67	0.00	0.0 0	0.0 0	0.0 0	0.0 0	0.00	0.0 0	0.0 1	0.0 0	0.15
450	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.70	0.00	0.0 0	0.0 0	0.0 0	0.0 0	0.00	0.0 0	0.0 1	0.0 0	0.20
500	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.69	0.00	0.0 0	0.0 0	0.0 0	0.0 0	0.00	0.0 1	0.0 2	0.0 0	0.24
550	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.67	0.00	0.0 0	0.0 0	0.0 0	0.0 0	0.00	0.0 1	0.0 3	0.0 0	0.27
600	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.63	0.00	0.0 1	0.0 0	0.0 0	0.0 0	0.00	0.0 1	0.0 5	0.0 0	0.30
650	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.00	0.0 1	0.0 0	0.0 0	0.0 0	0.00	0.0 1	0.0 6	0.0 0	0.31
700	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.56	0.00	0.0 1	0.0 0	0.0 0	0.0 0	0.00	0.0 2	0.0 8	0.0 0	0.33
750	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.53	0.00	0.0 1	0.0 0	0.0 0	0.0 0	0.00	0.0 2	0.1 0	0.0 0	0.34
800	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.49	0.00	0.0 2	0.0 0	0.0 0	0.0 0	0.00	0.0 2	0.1 2	0.0 0	0.34
850	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.47	0.00	0.0 2	0.0 0	0.0 0	0.0 0	0.00	0.0 2	0.1 4	0.0 1	0.34
900	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.44	0.00	0.0 2	0.0 0	0.0 0	0.0 0	0.00	0.0 3	0.1 5	0.0 1	0.34

**Table S7-b** Temperature-dependent branching fractions for 2,5-dimethylhex-1-yl + O<sub>2</sub> at 0.01 atm.

T (K)	QOOH- 1 <sub>p</sub>	QOOH- 2 <sub>p</sub>	QOOH- 3 <sub>p</sub>	QOOH- 4 <sub>p</sub>	QOOH- 5 <sub>p</sub>	QOOH- 6 <sub>p</sub>	ROO- 1 <sub>p</sub>	P10 <sub>p</sub>	P11 <sub>p</sub>	P1 <sub>p</sub>	P2 <sub>p</sub>	P3 <sub>p</sub>	P4 <sub>p</sub>	P5 <sub>p</sub>	P6 <sub>p</sub>	P7 <sub>p</sub>	P8 <sub>p</sub>	P9 <sub>p</sub>
400	0.00	0.00	0.00	0.00	0.00	0.00	0.70	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06
450	0.00	0.00	0.00	0.00	0.00	0.00	0.54	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
500	0.00	0.00	0.00	0.00	0.00	0.00	0.38	0.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
550	0.00	0.00	0.00	0.00	0.00	0.00	0.24	0.51	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.00
600	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.55	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.00
650	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.55	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.06	0.00
700	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.53	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.02	0.08	0.00
750	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.51	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.02	0.10	0.00
800	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.48	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.02	0.12	0.00
850	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.45	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.02	0.13	0.01

900	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.43	0.00	0.02	0.00	0.00	0.00	0.00	0.03	0.15	0.01	0.34
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**Table S7-c** Temperature-dependent branching fractions for 2,5-dimethylhex-1-yl + O<sub>2</sub> at 0.1 atm.

T (K)	QOOH-1 <sub>p</sub>	QOOH-2 <sub>p</sub>	QOOH-3 <sub>p</sub>	QOOH-4 <sub>p</sub>	QOOH-5 <sub>p</sub>	QOOH-6 <sub>p</sub>	ROO-1 <sub>p</sub>	P10 <sub>p</sub>	P11 <sub>p</sub>	P1 <sub>p</sub>	P2 <sub>p</sub>	P3 <sub>p</sub>	P4 <sub>p</sub>	P5 <sub>p</sub>	P6 <sub>p</sub>	P7 <sub>p</sub>	P8 <sub>p</sub>	P9 <sub>p</sub>
400	0.00	0.00	0.00	0.00	0.00	0.00	0.95	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
450	0.00	0.00	0.01	0.00	0.00	0.00	0.91	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02
500	0.00	0.00	0.01	0.00	0.00	0.00	0.84	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04
550	0.00	0.00	0.01	0.00	0.00	0.00	0.75	0.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.07
600	0.00	0.00	0.01	0.00	0.00	0.00	0.63	0.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.11
650	0.00	0.00	0.01	0.00	0.00	0.00	0.50	0.29	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.00	0.15
700	0.00	0.00	0.01	0.00	0.00	0.00	0.38	0.34	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.05	0.00	0.20
750	0.00	0.00	0.01	0.00	0.00	0.00	0.29	0.36	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.07	0.00	0.24
800	0.00	0.00	0.01	0.00	0.00	0.00	0.22	0.37	0.00	0.01	0.00	0.00	0.00	0.00	0.02	0.09	0.00	0.26
850	0.00	0.00	0.01	0.00	0.00	0.00	0.17	0.37	0.00	0.02	0.00	0.00	0.00	0.00	0.02	0.12	0.00	0.28
900	0.00	0.00	0.01	0.00	0.00	0.00	0.14	0.36	0.00	0.02	0.00	0.00	0.00	0.00	0.02	0.14	0.01	0.29

**Table S7-d** Temperature-dependent branching fractions for 2,5-dimethylhex-1-yl + O<sub>2</sub> at 1 atm.

T (K)	QOOH-1 <sub>p</sub>	QOOH-2 <sub>p</sub>	QOOH-3 <sub>p</sub>	QOOH-4 <sub>p</sub>	QOOH-5 <sub>p</sub>	QOOH-6 <sub>p</sub>	ROO-1 <sub>p</sub>	P10 <sub>p</sub>	P11 <sub>p</sub>	P1 <sub>p</sub>	P2 <sub>p</sub>	P3 <sub>p</sub>	P4 <sub>p</sub>	P5 <sub>p</sub>	P6 <sub>p</sub>	P7 <sub>p</sub>	P8 <sub>p</sub>	P9 <sub>p</sub>
400	0.00	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
450	0.00	0.00	0.01	0.00	0.00	0.00	0.99	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
500	0.00	0.00	0.01	0.00	0.00	0.00	0.97	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
550	0.00	0.00	0.01	0.00	0.00	0.00	0.96	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
600	0.00	0.00	0.02	0.00	0.00	0.00	0.94	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02
650	0.00	0.00	0.02	0.00	0.00	0.00	0.91	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.03
700	0.00	0.00	0.02	0.00	0.00	0.00	0.87	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.05
750	0.00	0.00	0.03	0.00	0.00	0.00	0.81	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.07
800	0.00	0.00	0.03	0.00	0.00	0.00	0.75	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.00	0.09
850	0.00	0.00	0.04	0.00	0.00	0.00	0.67	0.15	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.05	0.00	0.12
900	0.00	0.00	0.04	0.00	0.00	0.00	0.60	0.16	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.06	0.00	0.13

**Table S7-e** Temperature-dependent branching fractions for 2,5-dimethylhex-1-yl + O<sub>2</sub> at 20 atm.

T (K)	QOOH-1 <sub>p</sub>	QOOH-2 <sub>p</sub>	QOOH-3 <sub>p</sub>	QOOH-4 <sub>p</sub>	QOOH-5 <sub>p</sub>	QOOH-6 <sub>p</sub>	ROO-1 <sub>p</sub>	P10 <sub>p</sub>	P11 <sub>p</sub>	P1 <sub>p</sub>	P2 <sub>p</sub>	P3 <sub>p</sub>	P4 <sub>p</sub>	P5 <sub>p</sub>	P6 <sub>p</sub>	P7 <sub>p</sub>	P8 <sub>p</sub>	P9 <sub>p</sub>
400	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
450	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
500	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
550	0.00	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
600	0.00	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
650	0.00	0.00	0.01	0.00	0.00	0.00	0.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
700	0.00	0.00	0.01	0.00	0.00	0.00	0.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
750	0.00	0.00	0.02	0.00	0.00	0.00	0.97	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
800	0.00	0.00	0.02	0.00	0.00	0.00	0.95	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
850	0.00	0.00	0.03	0.00	0.00	0.00	0.94	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
900	0.00	0.00	0.04	0.00	0.00	0.00	0.93	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01

**Table S8:** Branching fractions of 2,5-dimethylhex-2-yl + O<sub>2</sub> calculated using RRKM/ME.

**Table S8-a** Temperature-dependent branching fractions for 2,5-dimethylhex-2-yl + O<sub>2</sub> at 0.001 atm.

T (K)	QOO H-1 <sub>t</sub>	QOO H-2 <sub>t</sub>	QOO H-3 <sub>t</sub>	QOO H-4 <sub>t</sub>	QOO H-5 <sub>t</sub>	ROO- 2 <sub>t</sub>	P10 <sub>t</sub>	P1 <sub>t</sub>	P2 <sub>t</sub>	P3 <sub>t</sub>	P4 <sub>t</sub>	P5 <sub>t</sub>	P6 <sub>t</sub>	P7 <sub>t</sub>	P8 <sub>t</sub>	P9 <sub>t</sub>
400	0.00	0.00	0.05	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.86
450	0.00	0.00	0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.94
500	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.97
550	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.97
600	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.96
650	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.03	0.00	0.95
700	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.03	0.00	0.94
750	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.93
800	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.91
850	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.05	0.00	0.90
900	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.02	0.03	0.00	0.00	0.00	0.00	0.05	0.00	0.88

**Table S8-b** Temperature-dependent branching fractions for 2,5-dimethylhex-2-yl + O<sub>2</sub> at 0.01 atm.

T (K)	QOOH -1 <sub>t</sub>	QOOH -2 <sub>t</sub>	QOOH -3 <sub>t</sub>	QOOH -4 <sub>t</sub>	QOOH -5 <sub>t</sub>	ROO- 2 <sub>t</sub>	P10 <sub>t</sub>	P1 <sub>t</sub>	P2 <sub>t</sub>	P3 <sub>t</sub>	P4 <sub>t</sub>	P5 <sub>t</sub>	P6 <sub>t</sub>	P7 <sub>t</sub>	P8 <sub>t</sub>	P9 <sub>t</sub>
400	0.00	0.00	0.00	0.00	0.00	0.48	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.51
450	0.00	0.00	0.00	0.00	0.00	0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.66
500	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.78
550	0.00	0.00	0.00	0.00	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.86
600	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.91
650	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.92
700	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.03	0.00	0.93
750	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.92
800	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.90
850	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.05	0.00	0.89
900	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.02	0.03	0.00	0.00	0.00	0.00	0.05	0.00	0.87

**Table S8-c** Temperature-dependent branching fractions for 2,5-dimethylhex-2-yl + O<sub>2</sub> at 0.1 atm.

T (K)	QOOH-1 <sub>t</sub>	QOOH-2 <sub>t</sub>	QOOH-3 <sub>t</sub>	QOOH-4 <sub>t</sub>	QOOH-5 <sub>t</sub>	ROO-2 <sub>t</sub>	P10 <sub>t</sub>	P1 <sub>t</sub>	P2 <sub>t</sub>	P3 <sub>t</sub>	P4 <sub>t</sub>	P5 <sub>t</sub>	P6 <sub>t</sub>	P7 <sub>t</sub>	P8 <sub>t</sub>	P9 <sub>t</sub>
400	0.00	0.00	0.00	0.00	0.00	0.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.09
450	0.00	0.00	0.00	0.00	0.00	0.84	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.16
500	0.00	0.00	0.00	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.24
550	0.00	0.00	0.00	0.00	0.00	0.63	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.36
600	0.00	0.00	0.00	0.00	0.00	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.48
650	0.00	0.00	0.00	0.00	0.00	0.38	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.59
700	0.00	0.00	0.00	0.00	0.00	0.28	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.68
750	0.00	0.00	0.00	0.00	0.00	0.22	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.03	0.00	0.73
800	0.00	0.00	0.00	0.00	0.00	0.17	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.76
850	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.77
900	0.00	0.00	0.00	0.00	0.00	0.13	0.00	0.02	0.02	0.00	0.00	0.00	0.00	0.05	0.00	0.78

**Table S8-d** Temperature-dependent branching fractions for 2,5-dimethylhex-2-yl + O<sub>2</sub> at 1 atm.

T (K)	QOOH-1 <sub>t</sub>	QOOH-2 <sub>t</sub>	QOOH-3 <sub>t</sub>	QOOH-4 <sub>t</sub>	QOOH-5 <sub>t</sub>	ROO-2 <sub>t</sub>	P10 <sub>t</sub>	P1 <sub>t</sub>	P2 <sub>t</sub>	P3 <sub>t</sub>	P4 <sub>t</sub>	P5 <sub>t</sub>	P6 <sub>t</sub>	P7 <sub>t</sub>	P8 <sub>t</sub>	P9 <sub>t</sub>
400	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
450	0.00	0.00	0.00	0.00	0.00	0.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02
500	0.00	0.00	0.00	0.00	0.00	0.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
550	0.00	0.00	0.00	0.00	0.00	0.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05
600	0.00	0.00	0.00	0.00	0.00	0.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08
650	0.00	0.00	0.00	0.00	0.00	0.87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12
700	0.00	0.00	0.00	0.00	0.00	0.81	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.17
750	0.00	0.00	0.00	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.23
800	0.00	0.00	0.00	0.00	0.00	0.69	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.28
850	0.00	0.00	0.01	0.00	0.00	0.62	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.33
900	0.00	0.00	0.01	0.00	0.00	0.57	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.38

**Table S8-e** Temperature-dependent branching fractions for 2,5-dimethylhex-2-yl + O<sub>2</sub> at 20 atm.

T (K)	QOOH-1 <sub>t</sub>	QOOH-2 <sub>t</sub>	QOOH-3 <sub>t</sub>	QOOH-4 <sub>t</sub>	QOOH-5 <sub>t</sub>	ROO-2 <sub>t</sub>	P10 <sub>t</sub>	P1 <sub>t</sub>	P2 <sub>t</sub>	P3 <sub>t</sub>	P4 <sub>t</sub>	P5 <sub>t</sub>	P6 <sub>t</sub>	P7 <sub>t</sub>	P8 <sub>t</sub>	P9 <sub>t</sub>
400	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
450	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
500	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
550	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
600	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
650	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
700	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01

<b>750</b>	0.00	0.00	0.00	0.00	0.00	0.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
<b>800</b>	0.00	0.00	0.00	0.00	0.00	0.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02
<b>850</b>	0.00	0.00	0.01	0.00	0.00	0.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02
<b>900</b>	0.00	0.00	0.01	0.00	0.00	0.96	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03

**Table S9-a** Temperature-dependent branching fractions for 2,5-dimethylhex-3-yl + O<sub>2</sub> at 0.001 atm.

T(K)	QOO H-1 <sub>s</sub>	QOO H-2 <sub>s</sub>	QOO H-3 <sub>s</sub>	QOO H-4 <sub>s</sub>	QOO H-5 <sub>s</sub>	ROO- 3 <sub>s</sub>	P10 <sub>s</sub>	P11 <sub>s</sub>	P1 <sub>s</sub>	P2 <sub>s</sub>	P3 <sub>s</sub>	P4 <sub>s</sub>	P5 <sub>s</sub>	P6 <sub>s</sub>	P7 <sub>s</sub>	P8 <sub>s</sub>	P9 <sub>s</sub>
400	0.00	0.00	0.00	0.00	0.00	0.29	0.38	0.00	0.00	0.01	0.00	0.00	0.00	0.05	0.00	0.00	0.27
450	0.00	0.00	0.00	0.00	0.00	0.17	0.42	0.00	0.00	0.02	0.00	0.00	0.00	0.06	0.00	0.00	0.33
500	0.00	0.00	0.00	0.00	0.00	0.09	0.43	0.00	0.00	0.03	0.00	0.00	0.00	0.06	0.00	0.00	0.38
550	0.00	0.00	0.00	0.00	0.00	0.04	0.43	0.00	0.01	0.04	0.00	0.00	0.00	0.07	0.00	0.00	0.41
600	0.00	0.00	0.00	0.00	0.00	0.02	0.41	0.00	0.01	0.05	0.00	0.00	0.00	0.08	0.00	0.00	0.43
650	0.00	0.00	0.00	0.00	0.00	0.01	0.39	0.00	0.01	0.06	0.00	0.00	0.00	0.08	0.01	0.00	0.43
700	0.00	0.00	0.00	0.00	0.00	0.00	0.36	0.01	0.02	0.07	0.00	0.00	0.00	0.09	0.01	0.00	0.44
750	0.00	0.00	0.00	0.00	0.00	0.00	0.34	0.01	0.02	0.09	0.00	0.00	0.00	0.09	0.01	0.00	0.43
800	0.00	0.00	0.00	0.00	0.00	0.00	0.32	0.01	0.02	0.10	0.00	0.00	0.00	0.10	0.01	0.00	0.43
850	0.00	0.00	0.00	0.00	0.00	0.00	0.30	0.01	0.03	0.11	0.00	0.00	0.00	0.10	0.01	0.00	0.42
900	0.00	0.00	0.00	0.00	0.00	0.00	0.29	0.01	0.03	0.13	0.00	0.00	0.01	0.10	0.01	0.00	0.42

**Table S9-b** Temperature-dependent branching fractions for 2,5-dimethylhex-3-yl + O<sub>2</sub> at 0.01 atm.

T(K)	QOOH -1 <sub>s</sub>	QOOH -2 <sub>s</sub>	QOOH -3 <sub>s</sub>	QOOH -4 <sub>s</sub>	QOOH -5 <sub>s</sub>	ROO -3 <sub>s</sub>	P10 <sub>s</sub>	P11 <sub>s</sub>	P1 <sub>s</sub>	P2 <sub>s</sub>	P3 <sub>s</sub>	P4 <sub>s</sub>	P5 <sub>s</sub>	P6 <sub>s</sub>	P7 <sub>s</sub>	P8 <sub>s</sub>	P9 <sub>s</sub>
400	0.00	0.00	0.00	0.00	0.00	0.78	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.08
450	0.00	0.00	0.00	0.00	0.00	0.63	0.17	0.00	0.00	0.01	0.00	0.00	0.00	0.03	0.00	0.00	0.15
500	0.00	0.00	0.00	0.00	0.00	0.47	0.24	0.00	0.00	0.02	0.00	0.00	0.00	0.04	0.00	0.00	0.22
550	0.00	0.00	0.00	0.00	0.00	0.31	0.30	0.00	0.01	0.03	0.00	0.00	0.00	0.05	0.00	0.00	0.29
600	0.00	0.00	0.00	0.00	0.00	0.19	0.33	0.00	0.01	0.04	0.00	0.00	0.00	0.06	0.00	0.00	0.35
650	0.00	0.00	0.00	0.00	0.00	0.11	0.35	0.00	0.01	0.06	0.00	0.00	0.00	0.07	0.00	0.00	0.39
700	0.00	0.00	0.00	0.00	0.00	0.07	0.34	0.01	0.02	0.07	0.00	0.00	0.00	0.08	0.01	0.00	0.41
750	0.00	0.00	0.00	0.00	0.00	0.04	0.33	0.01	0.02	0.09	0.00	0.00	0.00	0.09	0.01	0.00	0.42
800	0.00	0.00	0.00	0.00	0.00	0.03	0.31	0.01	0.02	0.10	0.00	0.00	0.00	0.09	0.01	0.00	0.42
850	0.00	0.00	0.00	0.00	0.00	0.03	0.29	0.01	0.03	0.11	0.00	0.00	0.00	0.10	0.01	0.00	0.41
900	0.00	0.00	0.00	0.00	0.00	0.02	0.28	0.01	0.03	0.12	0.00	0.00	0.01	0.10	0.01	0.00	0.41



**Table S9-c** Temperature-dependent branching fractions for 2,5-dimethylhex-3-yl + O<sub>2</sub> at 0.1 atm.

T(K)	QOOH-1 <sub>s</sub>	QOOH-2 <sub>s</sub>	QOOH-3 <sub>s</sub>	QOOH-4 <sub>s</sub>	QOOH-5 <sub>s</sub>	ROO-3 <sub>s</sub>	P10 <sub>s</sub>	P11 <sub>s</sub>	P1 <sub>s</sub>	P2 <sub>s</sub>	P3 <sub>s</sub>	P4 <sub>s</sub>	P5 <sub>s</sub>	P6 <sub>s</sub>	P7 <sub>s</sub>	P8 <sub>s</sub>	P9 <sub>s</sub>
400	0.00	0.00	0.00	0.00	0.00	0.97	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
450	0.00	0.00	0.00	0.00	0.00	0.93	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
500	0.00	0.00	0.00	0.01	0.00	0.87	0.06	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.06
550	0.00	0.00	0.00	0.01	0.00	0.77	0.09	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.10
600	0.00	0.00	0.00	0.00	0.00	0.65	0.14	0.00	0.00	0.02	0.00	0.00	0.00	0.03	0.00	0.00	0.15
650	0.00	0.00	0.00	0.00	0.00	0.52	0.18	0.00	0.01	0.03	0.00	0.00	0.00	0.04	0.00	0.00	0.21
700	0.00	0.00	0.00	0.00	0.00	0.39	0.21	0.00	0.01	0.05	0.00	0.00	0.00	0.05	0.00	0.00	0.26
750	0.00	0.00	0.00	0.00	0.00	0.29	0.24	0.01	0.02	0.07	0.00	0.00	0.00	0.07	0.01	0.00	0.30
800	0.00	0.00	0.00	0.00	0.00	0.22	0.24	0.01	0.02	0.08	0.00	0.00	0.00	0.08	0.01	0.00	0.33
850	0.00	0.00	0.00	0.00	0.00	0.17	0.25	0.01	0.02	0.10	0.00	0.00	0.00	0.08	0.01	0.00	0.35
900	0.00	0.00	0.00	0.00	0.00	0.14	0.24	0.01	0.03	0.11	0.00	0.00	0.00	0.09	0.01	0.00	0.36

**Table S9-d** Temperature-dependent branching fractions for 2,5-dimethylhex-3-yl + O<sub>2</sub> at 1 atm.

T(K)	QOOH-1 <sub>s</sub>	QOOH-2 <sub>s</sub>	QOOH-3 <sub>s</sub>	QOOH-4 <sub>s</sub>	QOOH-5 <sub>s</sub>	ROO-3 <sub>s</sub>	P10 <sub>s</sub>	P11 <sub>s</sub>	P1 <sub>s</sub>	P2 <sub>s</sub>	P3 <sub>s</sub>	P4 <sub>s</sub>	P5 <sub>s</sub>	P6 <sub>s</sub>	P7 <sub>s</sub>	P8 <sub>s</sub>	P9 <sub>s</sub>
400	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
450	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
500	0.00	0.00	0.00	0.00	0.00	0.98	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
550	0.00	0.00	0.00	0.00	0.00	0.97	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
600	0.00	0.00	0.00	0.01	0.00	0.94	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
650	0.00	0.00	0.00	0.01	0.00	0.89	0.04	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.04
700	0.00	0.00	0.00	0.01	0.00	0.84	0.05	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.07
750	0.00	0.00	0.00	0.01	0.00	0.77	0.07	0.00	0.01	0.02	0.00	0.00	0.00	0.02	0.00	0.00	0.10
800	0.00	0.00	0.00	0.00	0.00	0.69	0.09	0.00	0.01	0.03	0.00	0.00	0.00	0.03	0.00	0.00	0.13
850	0.00	0.00	0.00	0.00	0.00	0.61	0.11	0.00	0.01	0.05	0.00	0.00	0.00	0.04	0.00	0.00	0.16
900	0.00	0.00	0.00	0.00	0.00	0.55	0.12	0.01	0.02	0.06	0.00	0.00	0.00	0.05	0.01	0.00	0.18

**Table S9-e** Temperature-dependent branching fractions for 2,5-dimethylhex-3-yl + O<sub>2</sub> at 20 atm.

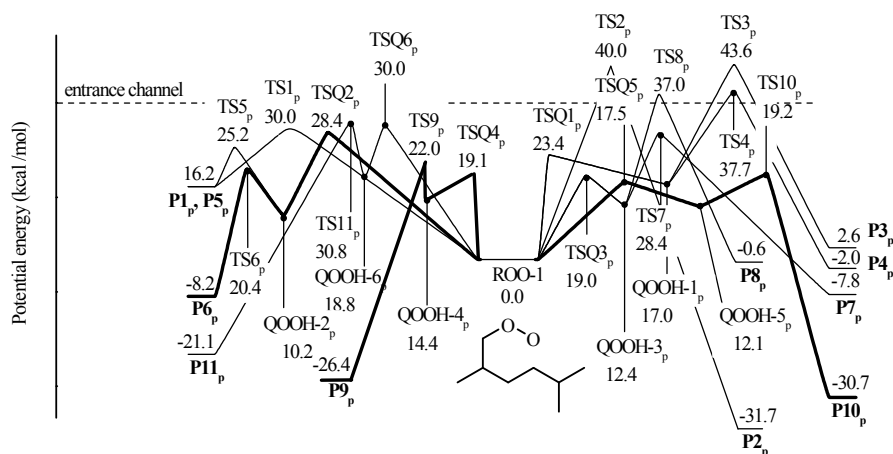
T(K)	QOOH-1 <sub>s</sub>	QOOH-2 <sub>s</sub>	QOOH-3 <sub>s</sub>	QOOH-4 <sub>s</sub>	QOOH-5 <sub>s</sub>	ROO-3 <sub>s</sub>	P10 <sub>s</sub>	P11 <sub>s</sub>	P1 <sub>s</sub>	P2 <sub>s</sub>	P3 <sub>s</sub>	P4 <sub>s</sub>	P5 <sub>s</sub>	P6 <sub>s</sub>	P7 <sub>s</sub>	P8 <sub>s</sub>	P9 <sub>s</sub>
400	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
450	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
500	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
550	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
600	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
650	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
700	0.00	0.00	0.00	0.00	0.00	0.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

<b>750</b>	0.00	0.00	0.00	0.01	0.00	0.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<b>800</b>	0.00	0.00	0.00	0.01	0.00	0.97	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
<b>850</b>	0.00	0.00	0.00	0.01	0.00	0.96	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
<b>900</b>	0.00	0.00	0.00	0.01	0.00	0.95	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.02

## PES for 2,5-dimethylhex-1-yl (primary) + O<sub>2</sub>

Six isomerization pathways to QOOH species exist for the 2,5-dimethylhexyl-1-peroxy radical, denoted ROO-1: QOOH-1<sub>p</sub> via 1,5-hydrogen transfer (TSQ1<sub>p</sub>), QOOH-2<sub>p</sub> via 1,4-hydrogen transfer (TSQ2<sub>p</sub>), QOOH-3<sub>p</sub> via 1,5-hydrogen transfer (TSQ3<sub>p</sub>), QOOH-4<sub>p</sub> via 1,6-hydrogen transfer (TSQ4<sub>p</sub>), QOOH-5<sub>p</sub> via 1,7-hydrogen transfer (TSQ5<sub>p</sub>), and QOOH-6<sub>p</sub> via 1,8-hydrogen transfer (TSQ6<sub>p</sub>). **Fig. 2** depicts the reaction pathways and the corresponding zero-point-energy-corrected barrier heights for the 17 distinct transition states. The transition states of three types of pathways were considered: OH-loss from unimolecular decomposition of QOOH, HO<sub>2</sub>-elimination channels from ROO-1 and QOOH, and unimolecular QOOH decomposition channels via C–C β-scission yielding carbonyl + alkene + OH.

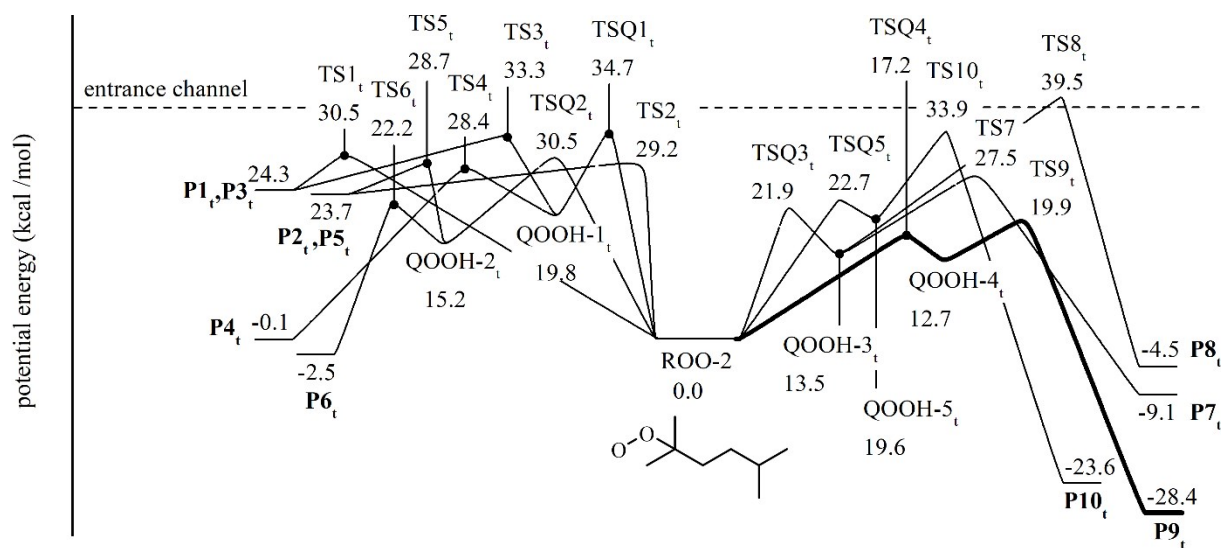
The well depth of the primary alkylperoxy, ROO-1 is 34.8 kcal mol<sup>-1</sup> below the entrance channel and is similar to smaller alkylperoxy systems, e.g. CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub> + O<sub>2</sub> in Goldsmith et al.[51] (33.3 kcal mol<sup>-1</sup>), Merle et al.[36] (34.8 kcal mol<sup>-1</sup>), Asatryan et al.[54] (35.3 kcal mol<sup>-1</sup>), and Huynh et al.[52] (34.8 kcal mol<sup>-1</sup>). The well depth of QOOH-1<sub>p</sub> obtained on the 2,5-dimethylhex-1-yl + O<sub>2</sub> surface is consistent with the analogous QOOH in *n*-propyl + O<sub>2</sub> reaction obtained by Goldsmith et al.[51] and Merle et al.[56] Among the isomerization channels of ROO-1, the barrier height to QOOH-5<sub>p</sub> is the lowest, which is a 1,7-hydrogen-transfer from a tertiary carbon to the O–O group on what was initially a primary carbon. The three most energetically favorable unimolecular decomposition pathways on the 2,5-dimethylhex-1-yl + O<sub>2</sub> surface are (1) QOOH-2<sub>p</sub> → 2-methyl-2-*iso*-pentyl-oxirane + OH (P6<sub>p</sub>, via TS6<sub>p</sub> in **Fig. S1**), (2) QOOH-4<sub>p</sub> → 2-*iso*-propyl-4-methyl-tetrahydrofuran + OH (P9<sub>p</sub>, via TS9<sub>p</sub> in **Fig. S2**), and (3) QOOH-5<sub>p</sub> → 2,2,5-trimethyltetrahydropyran + OH (P10<sub>p</sub>, via TS10<sub>p</sub> in **Fig. S1**). Conversely, the pathways with the highest energy barriers relative to the entrance channel are ROO-1 → 2,5-dimethylhexanal + OH (P2<sub>p</sub>, via TS2<sub>p</sub> in **Fig. S1** OH, 39.7 kcal mol<sup>-1</sup>, and QOOH-1<sub>p</sub> → 5-methylhex-1-ene + OH + CH<sub>2</sub>O (P3<sub>p</sub>, via TS3<sub>p</sub> in **Fig. S1**), 43.3 kcal mol<sup>-1</sup>, which were neglected in the branching fraction calculations given the focus on rate coefficients at temperatures below 1000 K.



**Figure S1.** CBS-QB3-calculated stationary point energies at 0 K for OH-loss, HO<sub>2</sub>-elimination, and C–C β-scission reactions from QOOH for 2,5-dimethylhex-1-yl + O<sub>2</sub>. The energy of the entrance channel is 34.8 kcal mol<sup>-1</sup> relative to ROO-1. Bold lines correspond to the energetically most favorable pathways.

## PES for 2,5-dimethylhex-2-yl (tertiary) + O<sub>2</sub>

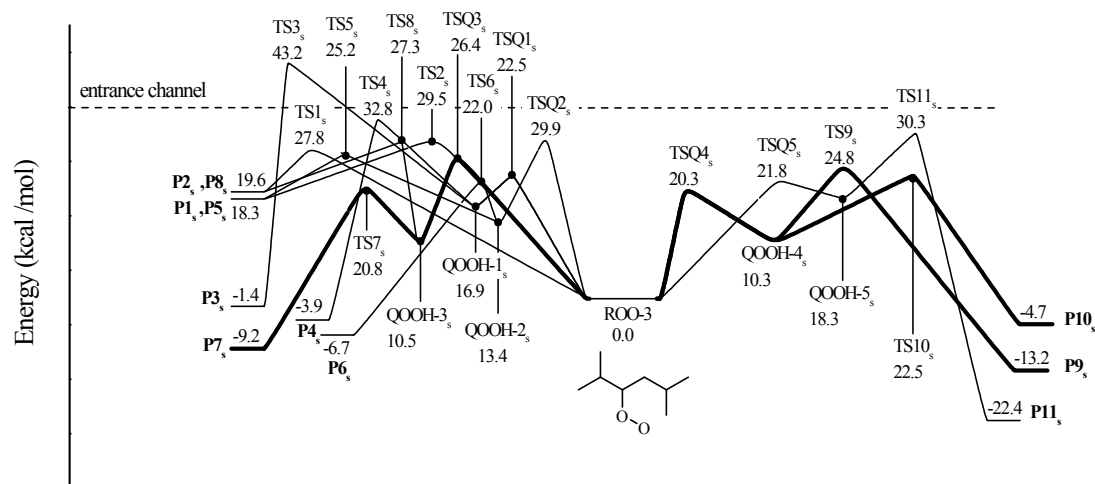
Five isomerization pathways to QOOH species exist for the 2,5-dimethylhexyl-2-peroxy radical, denoted ROO-2: QOOH-1<sub>t</sub> via 1,4-hydrogen transfer (TSQ1<sub>t</sub>), QOOH-2<sub>t</sub> via 1,4-hydrogen transfer (TSQ2<sub>t</sub>), QOOH-3<sub>t</sub> via 1,5-hydrogen transfer (TSQ3<sub>t</sub>), QOOH-4<sub>t</sub> via 1,6-hydrogen transfer (TSQ4<sub>t</sub>), and QOOH-5<sub>t</sub> via 1,7-hydrogen transfer (TSQ5<sub>t</sub>). The potential energy surface of 2,5-dimethylhex-2-yl + O<sub>2</sub> is depicted in **Fig. S2**. The optimized geometries of other transition states are listed in the Supplemental Material (**Table S2** and **Fig. S4-b**). The well depth of the 2,5-dimethylhexyl-2-peroxy radical, relative to the energy of 2,5-dimethylhex-2-yl + O<sub>2</sub> entrance channel, is 37.9 kcal mol<sup>-1</sup>, which is similar to the peroxy radical from 2-pentyl + O<sub>2</sub> calculated in Asatryan et al. [54] (37.5 kcal mol<sup>-1</sup>) and experimentally reported by Knyazev et al. [57] (37.6 kcal mol<sup>-1</sup>). Among the isomerization channels of ROO-2, the barrier height QOOH-4<sub>t</sub> is the lowest, which is a 1,6 H-transfer from a tertiary carbon to the O–O group on what was initially the other tertiary carbon. The most energetically favorable unimolecular decomposition pathways for ROO-2 are (1) QOOH-1<sub>t</sub> → 2-methyl-2-*iso*-pentyl-oxirane + OH (P4<sub>t</sub>, via TS4<sub>t</sub> in **Fig. S2**), (2) QOOH-2<sub>t</sub> → 2-*iso*-butyl-3,3-dimethyloxirane + OH (P6<sub>t</sub>, via TS6<sub>t</sub> in **Fig. S2**), and (3) QOOH-4<sub>t</sub> → 2,2,5,5-tetramethyl-tetrahydrofuran + OH (P9<sub>t</sub>, via TS9<sub>t</sub> in **Fig. S2**). Concerted C–C and O–O bond-scission of the secondary 2-hydroperoxy-2,5-dimethylhex-4-yl (QOOH-5<sub>t</sub>), to acetone + *iso*-pentene + OH, is energetically disfavored (P8<sub>t</sub>, via TS8<sub>t</sub> in **Fig. S2**).



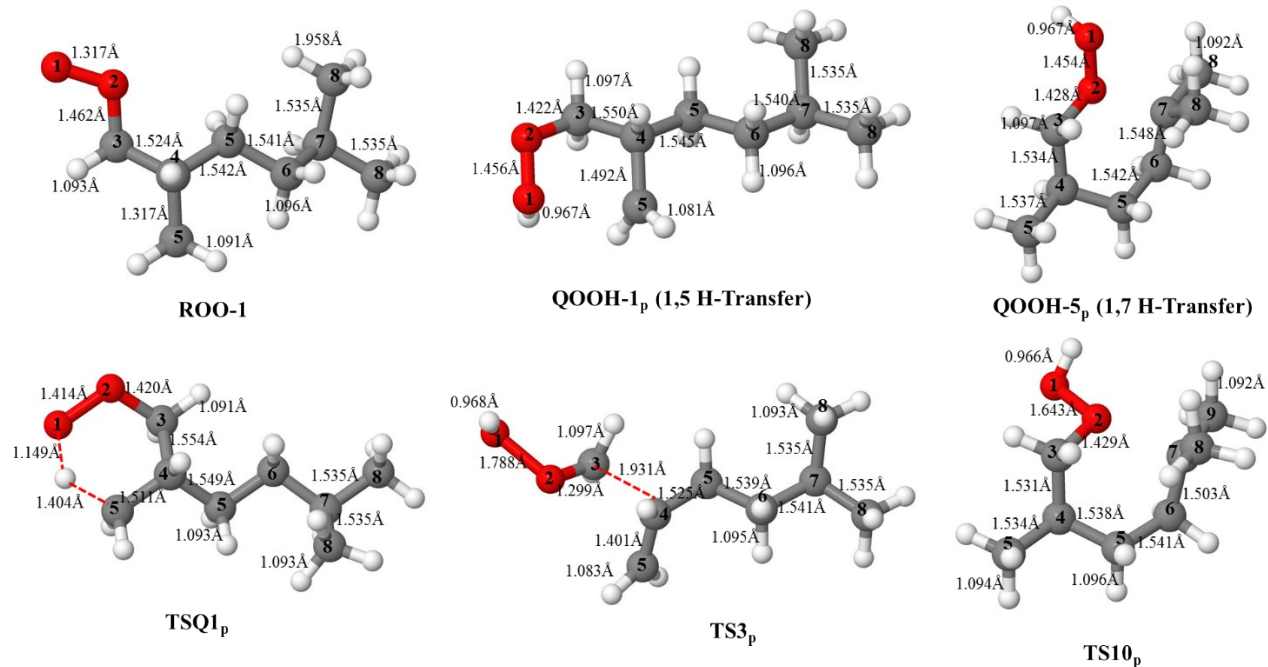
**Figure S2.** CBS-QB3-calculated stationary point energies at 0 K for OH-loss and HO<sub>2</sub>-elimination channels from QOOH, and QOOH decomposition yielding carbonyl + alkene + OH for 2,5-dimethylhex-2-yl + O<sub>2</sub>.

## PES for 2,5-dimethylhex-3-yl (secondary) + O<sub>2</sub>

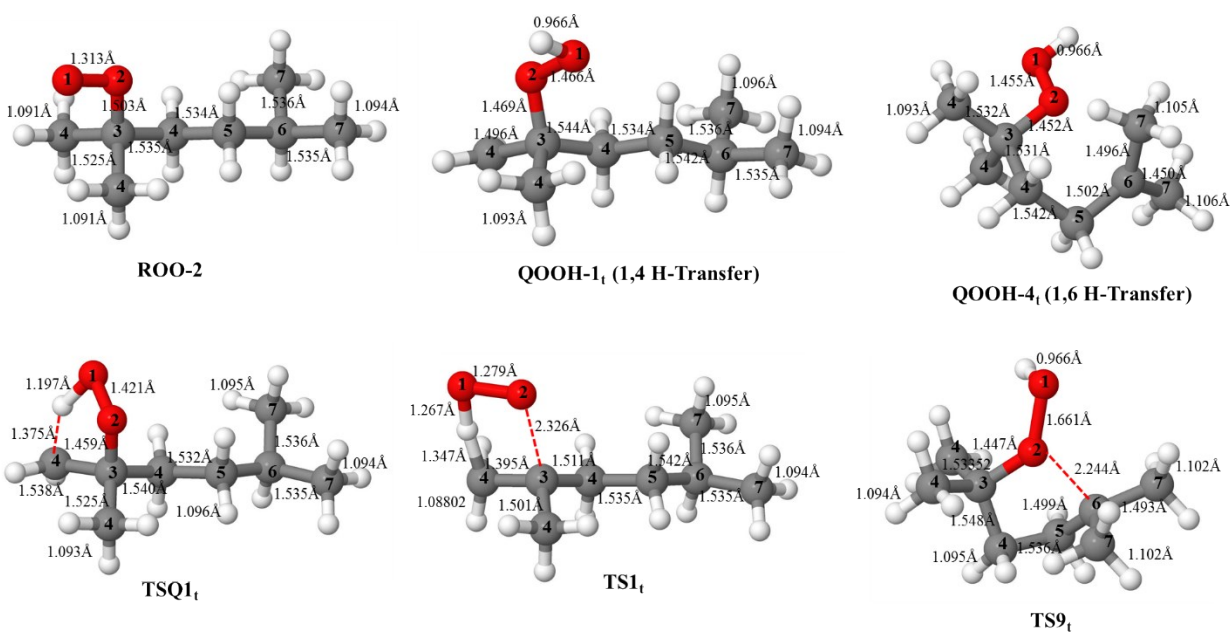
Five isomerization pathways to QOOH species exist for the 2,5-dimethylhexyl-3-peroxy radical, denoted ROO-3: QOOH-1<sub>s</sub> via 1,5-hydrogen transfer (TSQ1<sub>s</sub>), QOOH-2<sub>s</sub> via 1,4-hydrogen transfer (TSQ2<sub>s</sub>), QOOH-3<sub>s</sub> via 1,4-hydrogen transfer (TSQ3<sub>s</sub>), QOOH-4<sub>s</sub> via 1,5-hydrogen transfer (TSQ4<sub>s</sub>), and QOOH-5<sub>s</sub> via 1,6-hydrogen transfer (TSQ5<sub>s</sub>). The potential energy surface of 2,5-dimethylhex-3-yl + O<sub>2</sub> is depicted in **Fig. 6**. The optimized geometries of transition states corresponding to direct HO<sub>2</sub> loss (TS<sub>1</sub>), sequential HO<sub>2</sub> loss and OH-loss are listed in the Supplemental Material (**Table S3** and **Fig. S4-c**). Among the isomerization channels of ROO-3, the barrier height to QOOH-4<sub>s</sub> is the lowest, and arises from a 1,5 H-transfer from secondary carbon to the O–O group on an initially tertiary carbon (**Fig. S3**). The most energetically favorable unimolecular decomposition pathways of ROO-3 are (1) QOOH-4<sub>s</sub> → methylpropanal + *iso*-butene + OH (P10<sub>s</sub>, via TS10<sub>s</sub> in **Fig. S3**) and (2) QOOH-3 → 2,3-di-*iso*-propyloxirane + OH (P7<sub>s</sub>, via TS7<sub>s</sub> in **Fig. S3**). Two HO<sub>2</sub>-elimination pathways exist: 2,5-dimethylhex-2-ene + HO<sub>2</sub> (P2<sub>s</sub>) and 2,5-dimethylhex-3-ene + HO<sub>2</sub> (P8<sub>s</sub>). Similar to the results calculated for primary + O<sub>2</sub> and tertiary alkyl + O<sub>2</sub> surfaces, direct HO<sub>2</sub>-elimination is energetically preferred over sequential formation via C–O bond-scission in QOOH. The barrier height to form 2,5-dimethylhex-2-ene + HO<sub>2</sub> directly from ROO-3 (TS2<sub>s</sub>) is slightly lower (1.7 kcal mol<sup>-1</sup>) than the barrier leading to 2,5-dimethylhex-3-ene + HO<sub>2</sub> (TS1<sub>s</sub>). Unlike the surfaces for reactions of primary and tertiary 2,5-dimethylhexyl with O<sub>2</sub>, the reactions leading to direct conjugate alkene + HO<sub>2</sub> are more competitive on the surface of 2,5-dimethylhex-3-yl + O<sub>2</sub> due to the fewer number of pathways with comparatively lower barrier heights



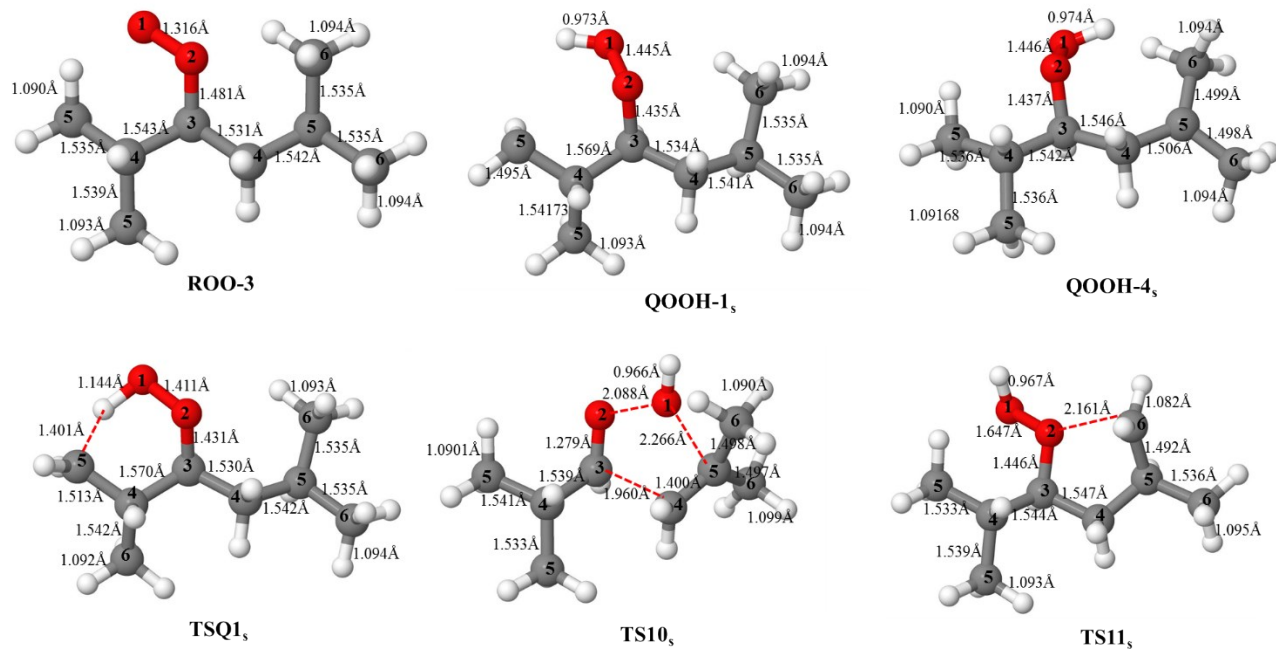
**Figure S3.** CBS-QB3-calculated stationary point energies at 0 K for OH-loss and HO<sub>2</sub>-elimination channels from QOOH, and QOOH decomposition yielding carbonyl + alkene + OH for 2,5-dimethyl-3-hexyl + O<sub>2</sub>. The energy of the entrance channel is 35.2 kcal mol<sup>-1</sup> relative to ROO-3. Bold lines correspond to the most energetically favorable pathways (Section 3.2 and 3.3).



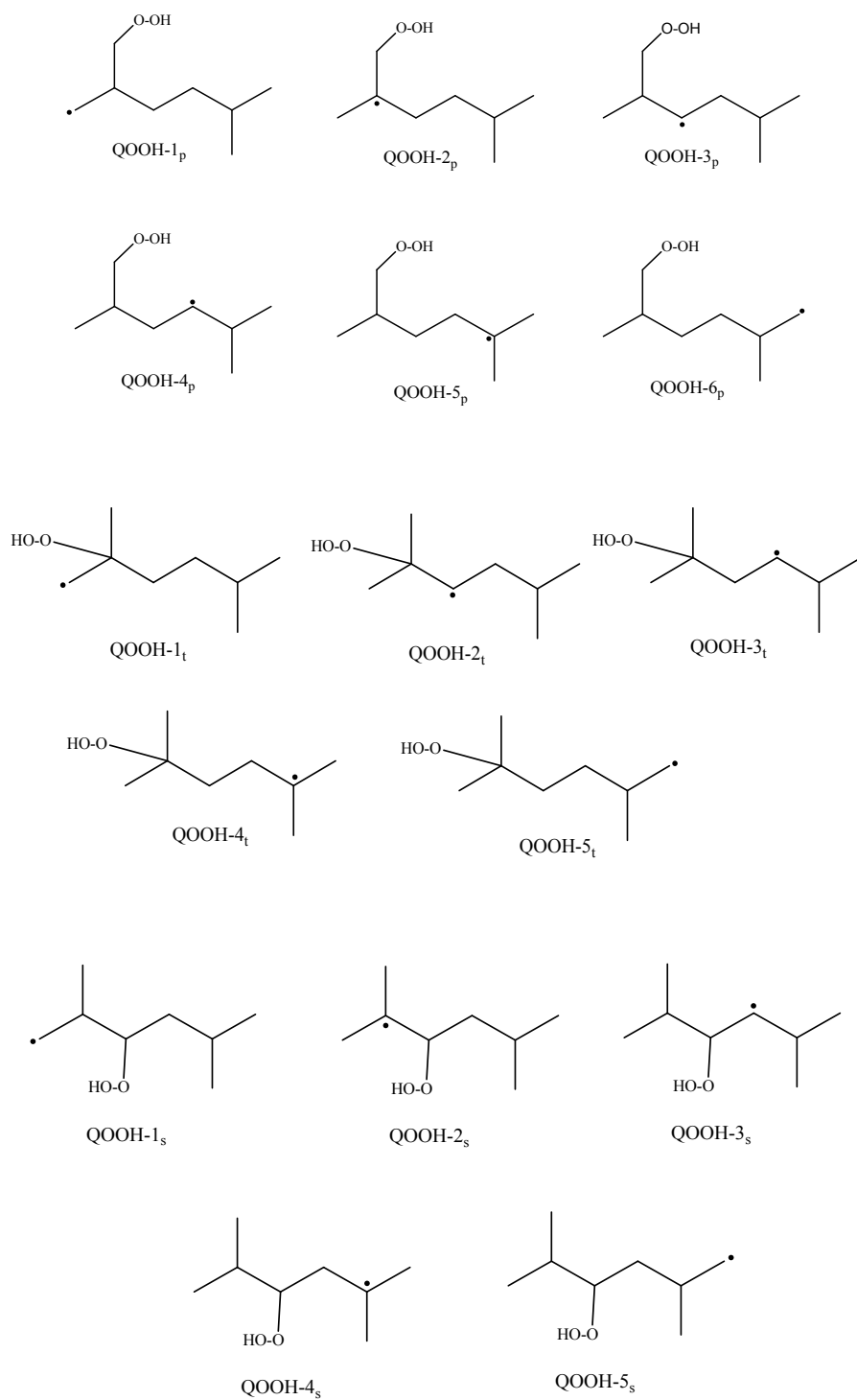
**Figure S4-a.** Optimized geometries of ROO, some QOOHs and some transition states with atom numbers for 2,5-dimethylhex-1-yl + O<sub>2</sub> reaction.



**Figure S4-b.** Optimized geometries of ROO, some QOOHs and some transition states with atom numbers for 2,5-dimethylhex-2-yl + O<sub>2</sub> reaction.

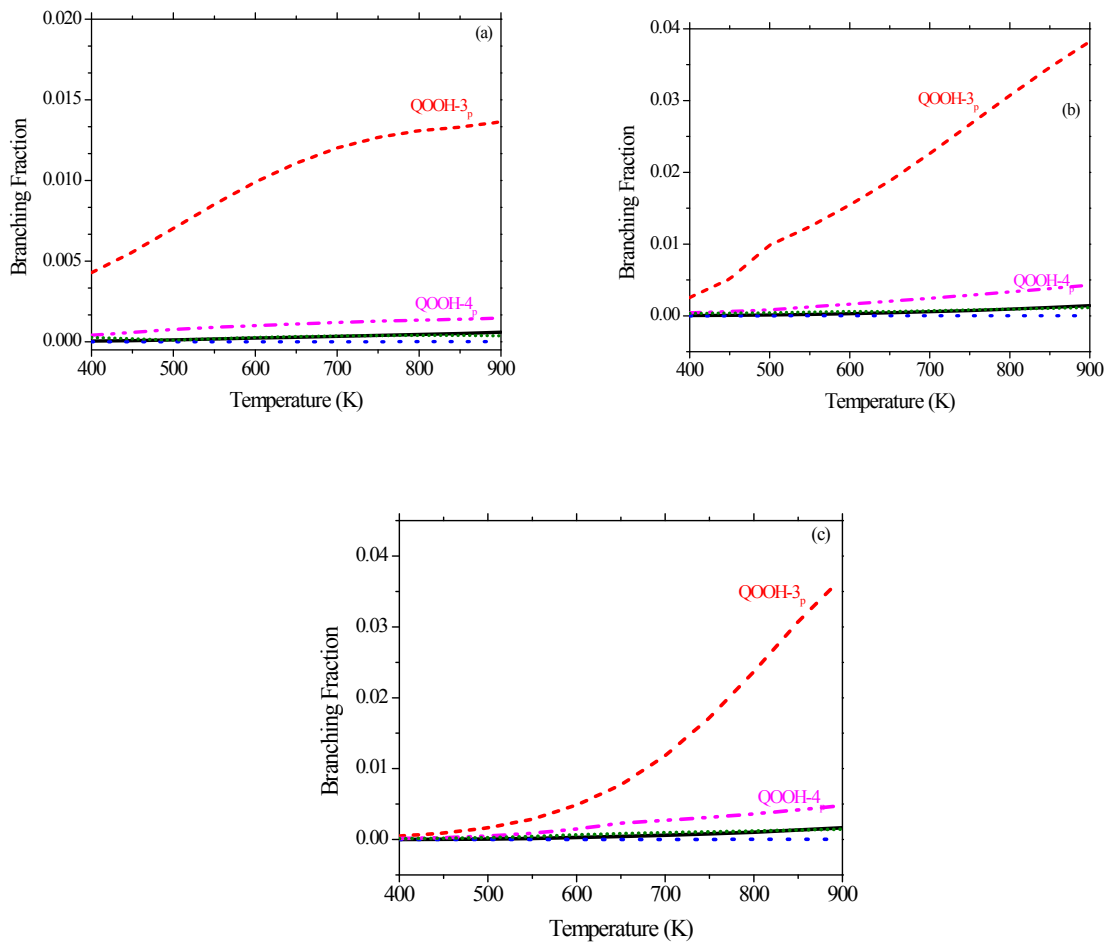


**Figure S4-c.** Optimized geometries of ROO, some QOOHs and some transition states with atom numbers for 2,5-dimethylhex-3-yl + O<sub>2</sub> reaction.

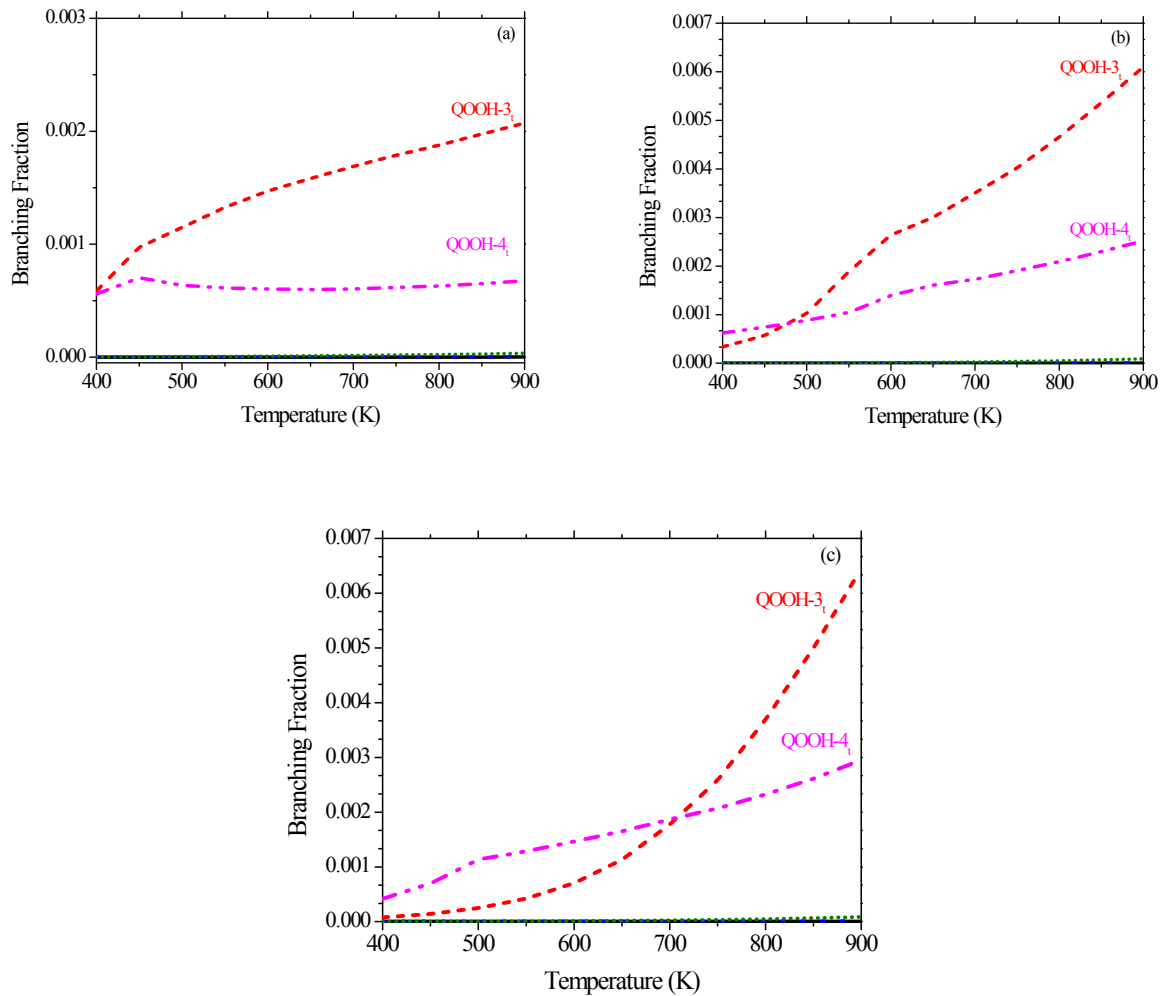


**Figure S5:** Nomenclature of QOOHs.

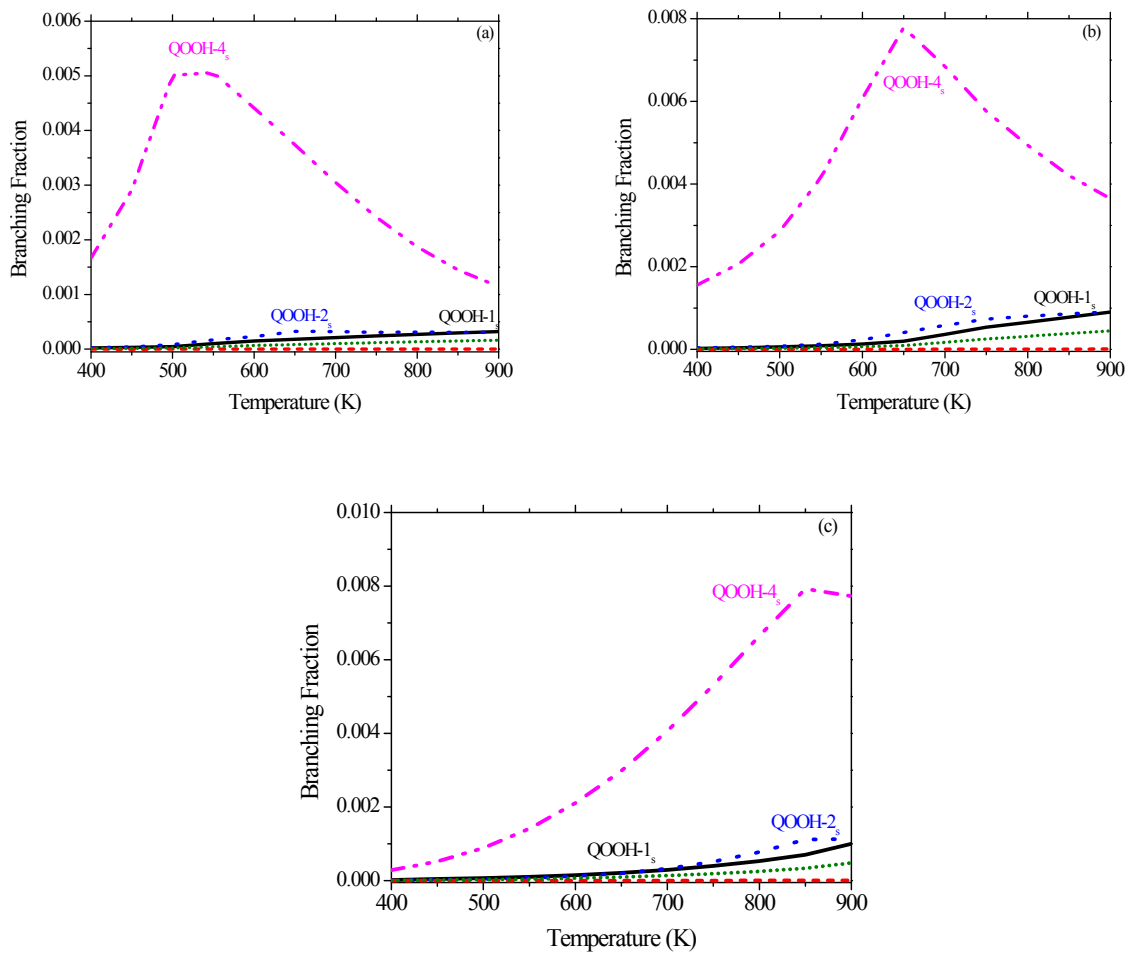




**Figure S6-a.** Temperature-dependent branching fractions for the formation of QOOH<sub>p</sub> from 2,5-dimethylhex-1-yl + O<sub>2</sub> at (a) 0.1 atm, (b) 1 atm, and (c) 20 atm.



**Figure S6-b.** Temperature-dependent branching fractions for the formation of QOOH<sub>t</sub> from 2,5-dimethylhex-2-yl + O<sub>2</sub> at (a) 0.1 atm, (b) 1 atm, and (c) 20 atm.



**Figure S6-c.** Temperature-dependent branching fractions for the formation of QOOH<sub>s</sub> from 2,5-dimethylhex-3-yl + O<sub>2</sub> at (a) 0.1 atm, (b) 1 atm, and (c) 20 atm.

### **Full Reference of Gaussian09 suites of Program**

Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

### **Full Reference of Multiwell**

Multiwell, Software 2016, Barker, J. R.; Nguyen, T. L.; Stanton, J. F.; Aieta, Ceotto, C. M.; Gabas, F.; Kumar, T. J. D.; Li, C. G. L.; Lohr, L. L.; Maranzana, A.; Ortiz, N. F.; Preses, J. M.; Stimac, P. J, <http://aoss-research.engin.umich.edu/multiwell> (accessed April 20, 2016).

### **Full Reference of MESMER**

Robertson, S. H.; Glowacki, D. R.; Liang, C.-H.; Morley, C. M.; Pilling, J.; et al. MESMER (Master Equation Solver for Multi Energy well Reactions); University of Leeds: Leeds, U.K., 2008. <http://www.chem.leeds.ac.uk/mesmer.html>

### **Rate Coefficients**

The Rate coefficients were computed from 400 to 900 K and fitted to the modified Arrhenius Equation

$$k_{\infty}(T) = A \times T^n \times \exp\left(\frac{-E_a}{RT}\right)$$

to calculate the Pressure-dependent rate coefficients and branching fractions at 400 to 900 between 0.001 atm to 20 atm.

### **Quantum Composite CBS-QB3 Calculations:**

Single-point energy calculations were carried out using the composite CBS-QB3 method[67, 68] with B3LYP-optimized geometries.[69, 70] Results using the CBS-QB3 are accurate within ~ 1-2 kcal mol<sup>-1</sup>. [43] Previous studies on reaction systems analogous to the present work report similar accuracy. The composite method determines geometries and frequencies at the B3LYP/ CBSB7, which are then followed by a series of single-point energy calculations with higher-order levels of theory: CCSD(T)/6-31+G(d), MP4SDQ/CBSB4, and MP2/CBSB7

The lower-frequency normal mode vibrations in R + O<sub>2</sub> reactions can be approximately described as large amplitude torsions, which were identified visually using GaussView. These were treated as one-dimensional (1-D) unsymmetrical hindered internal rotations with hindrance potentials and mass factors obtained using the B3LYP level of theory. For unsymmetrical

internal rotors, the 1-D torsional potentials were computed by carrying out constrained geometry optimizations at fixed dihedral angles (“relaxed” as explained in the MultiWell User Manual), and the torsional potential needed to compute the eigenstates for unsymmetrical hindered rotors was fitted to a Fourier cosine expansion.

We estimated the error in our calculation. The relative error in the high-pressure limit rate coefficients are estimated to be a factor of  $\sim 5$  (at 500 K) and  $\sim 7$  (600 K), which reflects the estimated  $\sim 2$  kcal mol<sup>-1</sup> uncertainty in the enthalpies of reaction computed using electronic structure methods. Additional uncertainties arise from possible errors in optimized geometries, harmonic frequencies, rotational constants, tunneling corrections, and treatment of hindered rotors, but the dominant error is usually in the computed energies. For pressure-dependent reactions the collisional energy transfer parameters are a further source of error.”

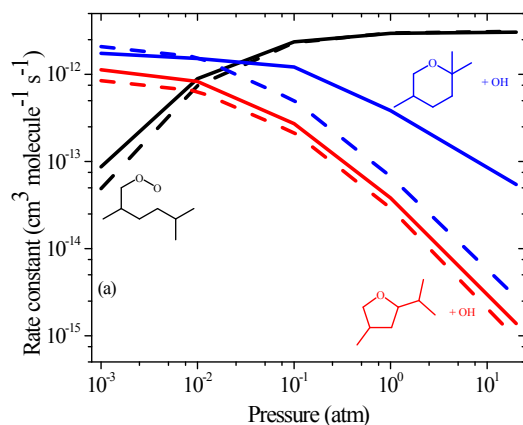
### Comparison between MESMER ME codes and MultiWell rate coefficients

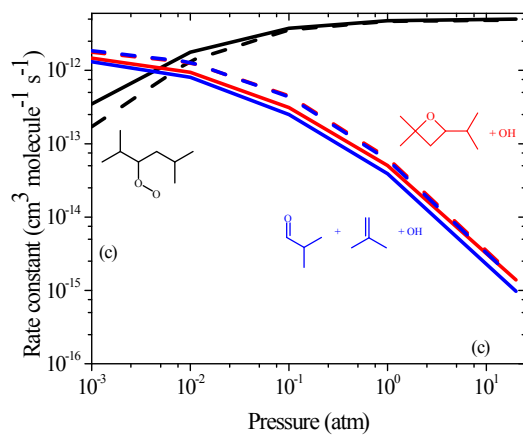
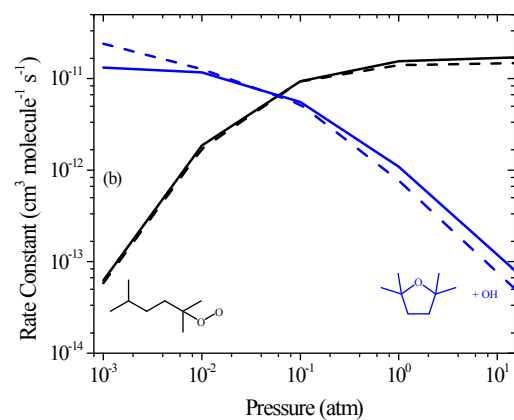
**MultiWell:** MultiWell ME code is stochastic simulation program that accurately solves the Master Equation numerically. The details of these codes are given in MultiWell manual.

**MESMER:** MESMER ME code is based on Eigenvalue methods (i.e. Barts-Widom) which accurately solves the Master Equation. The details are given in MESMER manual.

In short, Eigen value and stochastic methods both can predict the rate coefficients for all types of reactions.

We have also compared the pressure-dependent rate coefficients for 2,5-dimethylhexyl + O<sub>2</sub> at 550 K. The results are shown in **Figure S7**. Our computed results using both codes are in very good agreement each other, however some disagreement were observed at higher pressure (**Fig 7 a**). In addition, we have also compared the complete temperature-dependent rate branching ratio using both codes and results are consistent with each other. Therefore, we believe our calculation are reasonably accurate for the prediction oxidation of larger fuel such as 2,5-dimethylhexyl + O<sub>2</sub> reaction.





**Figure S7.** Pressure-dependent rate coefficients for (a) 2,5-dimethylhex-1-yl + O<sub>2</sub>, (b) 2,5-dimethylhex-2-yl + O<sub>2</sub>, and (c) 2,5-dimethylhex-3-yl + O<sub>2</sub>. Solid lines: *MultiWell ME* codes, dashed lines: *MESMER ME* codes.