Electronic Supplementary Material for PCCP

Allylic H-abstraction
Hydrogen Abstraction from 1,4 type Polyalkenes as a Model for Free Radical Trapping by Polyunsaturated Fatty Acids (PUFAs)

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SUPPORTING INFORMATION

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Table S1 Optimized geometries (Cartesian coordinates in Angstrom), their harmonic vibrational frequencies (cm^{-1}) and rotational constants (GHz) of stable species.

(Z,Z)-hepta-2,5-diene	*(E,E)*-hepta-2,5-diene
GEOMETRY	**GEOMETRY**
C,0,0.9108361842,0.1643882316,-2.2215599275	C,0,-0.6021017281,-0.7044151827,-2.1829635393
C,0,0.8831825586,0.2538145967,-0.8981448791	C,0,-0.5042312210,-0.7604248911,-0.8638110061
H,0,1.8796923325,0.0486835286,-2.6888666756	H,0,0.2980814498,-0.5521735287,-2.7657907384
H,0,1.8252539763,0.1942681669,-0.3702615710	H,0,-1.3998471501,-0.9055745290,-0.2727126630
C,0,-0.3172985607,0.4084194366,-0.0062335991	C,0,0.7724285838,-0.6154500354,-0.0860091252
H,0,-0.2139266740,1.3233250921,0.5734959225	H,0,0.9535236145,-1.5173630818,0.4998902582
H,0,-1.2206674122,0.5232670137,-0.6016832011	H,0,1.6045100143,-0.5208136776,-0.7847235405
C,0,-0.4776367962,-0.7758419887,0.9061137184	C,0,0.7444406816,0.5690348168,0.8370641910
C,0,-0.4174015516,-0.7995360411,2.2312550625	C,0,0.8476315562,0.5087793352,2.1556240540
H,0,-0.6451644190,-1.7132930579,0.3934489499	H,0,0.6131579970,1.5323955507,0.3603099771
H,0,-0.5518570446,-1.7578680273,2.7149563438	H,0,0.9719095897,-0.4597344837,2.6243785928
C,0,-0.2419004047,0.2060137644,-3.1743169003	C,0,-1.8731723972,-0.8387970148,-2.9581555459
H,0,-0.2728529774,-0.6995654669,-3.7792898579	H,0,-1.8279508850,-1.6820273900,-3.6467477578
H,0,-1.2002436394,0.3042815272,-2.6756491449	H,0,-2.7251500355,-0.9871182431,-2.2999608433
H,0,-0.1395962327,1.0409606845,-3.8668558057	H,0,-2.0630999925,0.0488313038,-3.5609281145
C,0,-0.1866826012,0.3456699814,3.1658951016	C,0,0.8102429818,1.6857119950,3.0765112890
H,0,-1.0311151469,0.4659952863,3.8438833707	H,0,0.6822503269,2.6148065277,2.5274333617
H,0,0.6893912323,0.1634590443,3.7874399401	H,0,-0.0075990949,1.6010523010,3.7915343966
H,0,-0.0375069656,1.2889183252,2.6513302709	H,0,1.7287834219,1.7610851114,3.6577551603
FREQUENCIES	**FREQUENCIES**
40.0811 49.2507 130.6955	61.1062 78.1177 143.9305
140.8473 202.4524 229.8342	214.6409 218.3030 245.8214
347.6975 405.5326 529.2321	259.7195 318.3103 376.5205
576.6041 587.0515 752.9902	511.3483 561.5942 814.5093
766.2036 916.1286 955.7715	839.7714 907.1203 976.3881
1002.0152 1031.3868 1065.8417	1005.7094 1058.8816 1059.9812
1069.6493 1072.1735 1121.3820	1101.2925 1125.2651 1125.5369
1121.5734 1155.7506 1201.1011	1141.1278 1154.1578 1210.1135
1286.6684 1346.8901 1359.2209	1284.1206 1348.1762 1388.4800
1379.9894 1479.3266 1484.5703	1391.2674 1410.5916 1434.9290
1512.1099 1512.5828 1559.8833	1498.0099 1499.0067 1555.2528
1565.6050 1566.1250 1573.7672	1562.0786 1562.2440 1574.9993
1580.5975 1821.4855 1833.4052	1575.2550 1830.9831 1842.7384
3132.7003 3132.9456 3152.9931	3119.5801 3128.0340 3128.4476
3179.4737 3179.4850 3186.5971	3158.0082 3178.4432 3178.4640
3230.2693 3231.1398 3243.1970	3212.6220 3212.6228 3240.1843
3243.8329 3266.0435 3266.3258	3240.8467 3246.6123 3246.8303
ROTATIONAL CONSTANTS	**ROTATIONAL CONSTANTS**
8.1941670 1.0087775 0.9809069	9.4165856 0.8605792 0.8279154

•OH	•CH_3
GEOMETRY O,0,0.,0.,-0.1077298879 H,0,0.,0.,0.8618391036 **FREQUENCY** 3826.7494 **ROTATIONAL CONSTANTS** 0.0000000 567.0372597 567.0372597	**GEOMETRY** C,0,-0.0000012602,-0.0000021828,-0.0000008911 H,0,-0.1790807927,-0.3101768566,1.0130494048 H,0,0.8954186015,-0.3101769267,-0.5065219754 H,0,-0.7163302473,0.6203668801,-0.5065220826 **FREQUENCIES** 443.8912 1481.5331 1481.5347 3234.3582 3413.8455 3413.8471 **ROTATIONAL CONSTANTS** 289.55331 289.55331 144.77666
•iso-C_3H_7	•OOH
GEOMETRY C,0,0.3682956569,-1.2509624094,0.1099571931 H,0,-0.1560007741,-1.6074139691,1.0039262909 H,0,1.3963174277,-1.0540116122,0.4149213615 H,0,0.3803171378,-2.0738385248,-0.60049999 C,0,-0.2694889455,-0.0353025279,-0.4618417667 H,0,-1.0432368396,-0.1605848235,-1.2033493578 C,0,-0.141588984,1.2833117791,0.2137817627 H,0,-0.4588602583,2.1001639283,-0.429736416 H,0,-0.7491617899,1.3384216132,1.124239305 H,0,0.8873187321,1.474982337,0.5191156721 **FREQUENCIES** 113.7346 135.7012 365.0931 424.4032 919.4744 981.5685 990.8445 1087.8946 1194.3548 1237.4693 1436.8799 1496.2487 1498.2520 1553.9673 1563.8631 1564.9679 1574.8220 3066.2194 3071.2209 3146.1724 3148.4256 3203.3570 3203.9629 3281.9855 **ROTATIONAL CONSTANTS** 37.7676762 8.3729821 7.4900561	**GEOMETRY** O,0,-0.6011180458,0.,0.0550349912 H,0,-0.6866693661,0.,1.0191261756 O,0,0.6869517166,0.,-0.1824257631 **FREQUENCIES** 1265.0182 1535.1615 3766.1951 **ROTATIONAL CONSTANTS** 632.26886 34.64803 32.84798

C_7H_{12}×OH	*(Z,Z)*-hepta-2,5-diene-OH complex	*(E,E)*-hepta-2,5-diene-OH complex
Terminal position	**GEOMETRY** C,0,0.7402664852,-0.0969957483,-1.9110372056 C,0,0.7401948762,-0.0969282017,-0.5801409506 H,0,1.703970915,-0.0977600111,-2.4034841352 H,0,1.6982322069,-0.1133758197,-0.0781419647 C,0,-0.4458290186,-0.1237513652,0.3444155716 H,0,-0.4141782316,0.7510871576,0.9900553282 H,0,-1.3716349259,-0.054746378,-0.2226076717 C,0,-0.4612670282,-1.3826054438,1.1668332727 C,0,-0.3622704014,-1.4939512884,2.4850623714 H,0,-0.5505998044,-2.2922344337,0.5889155652 H,0,-0.3879214709,-2.4932714197,2.8983961719 C,0,-0.4358760638,-0.0874652353,-2.8366501823 H,0,-0.3645601547,-0.9060458363,-3.5505476885 H,0,-1.3836850749,-0.1781085376,-2.3171631428 C,0,-0.2225528086,-0.4017675969,3.497487427 H,0,-1.0514983576,-0.425120989,4.2039190237 H,0,0.6883612636,-0.5334376871,4.0802965097 H,0,-0.1927649289,0.5877894774,3.0540908709 H,0,-0.4554762716,0.8381669097,-3.4098880166 O,0,0.5103225206,3.10077962,-1.909638027 H,0,0.6831784253,2.2116098853,-1.5525584585 **FREQUENCIES** 16.9833 34.0447 46.3684 75.5779 129.7187 144.9563 150.9906 204.5152 233.6662 342.5567 351.5020 406.2736 442.8016 530.8579 577.8292 587.0044 757.9015 777.9501 915.6695 955.4149 1000.9190 1032.1498 1066.1118 1070.1645 1077.7606 1121.9974 1126.2252 1156.9440 1201.3459 1287.9267 1345.7722 1358.8414 1378.8716 1480.2598 1484.7816 1512.5452 1513.1153 1558.1084 1565.7808 1567.5882 1573.5615 1580.2231 1808.1821 1829.3622 3134.6698 3140.6339 3155.8714 3182.3210 3190.4614 3194.6270 3231.6182 3233.3789 3244.5685 3245.5568 3265.8579 3268.0242 3752.4147 **ROTATIONAL CONSTANTS** 2.9400870 0.7703075 0.6568100	**GEOMETRY** C,0,-1.0834425091,-0.8409008447,-2.4992954896 C,0,-1.083293091,-0.8408915268,-1.175378288 H,0,-0.1338836251,-0.8407622134,-3.0201605528 H,0,-2.0270085528,-0.8353934002,-0.6448100403 C,0,0.1482483163,-0.8287691799,-0.3152280633 H,0,0.1627573062,-1.7108254114,0.3258203269 H,0,1.0288964374,-0.887185642,-0.9550998635 C,0,0.2207266209,0.4025891638,0.5432638373 C,0,0.1898855713,0.4122291986,1.8709679955 H,0,0.2641933831,1.3446650515,0.0105791351 H,0,0.1280874705,-0.534428366,2.3942355063 C,0,-2.3059235417,-0.8461392834,-3.3590460653 H,0,-2.327829788,-1.7225297921,-4.0058169454 H,0,-3.2125655856,-0.8464907385,-2.7600253904 H,0,-2.3318224227,0.0262370798,-4.0111489975 C,0,0.2371864175,1.6363171323,2.7291704456 H,0,0.2483898766,2.5420578426,2.1286919654 H,0,-0.6244544162,1.6802468852,3.39320363 H,0,1.1277832007,1.6341409586,3.3553192297 O,0,3.404547306,0.6355102637,1.9341190727 H,0,2.5207515616,0.4995776766,1.5495331809 **FREQUENCIES** 26.4994 43.7078 66.6462 95.6163 127.0096 153.7502 216.7901 223.9245 251.7521 259.3583 315.2194 343.4330 380.1179 441.1320 514.5155 559.8898 819.4620 844.7427 905.3504 975.6542 1006.5422 1058.9362 1068.9841 1100.7466 1126.1125 1130.4300 1139.0964 1153.6980 1209.7857 1284.4946 1348.9110 1387.6820 1391.1949 1411.5361 1434.3293 1498.1553 1499.1539 1555.1326 1561.5477 1563.5272 1573.2929 1574.6102 1818.1671 1838.1639 3123.7249 3130.3014 3136.2811 3163.3828 3181.4340 3194.8431 3214.9765 3216.5539 3239.6345 3242.2833 3246.7224 3248.9411 3758.2828 **ROTATIONAL CONSTANTS** 3.6627802 0.6250957 0.5620157

C_7H_{12}×OH	*(Z,Z)*-hepta-2,5-diene-OH complex	*(E,E)*-hepta-2,5-diene-OH complex
Central position	**GEOMETRY** C,0,0.,0.,0. C,0,0.2152436737,-1.3000526729,-0.1537001105 H,0,-0.3369204907,0.3323683654,0.9727941556 H,0,0.0505801953,-1.9429602814,0.700272617 C,0,0.6872159271,-2.0130096663,-1.3896147052 H,0,-0.0602800364,-2.7451855707,-1.6881685324 C,0,2.0149385914,-2.6822567914,-1.1606254183 C,0,2.319744719,-3.9714190621,-1.2884316462 H,0,2.8014250988,-2.0117098102,-0.8401069232 H,0,3.3385336279,-4.2617889904,-1.0683321796 C,0,0.1585507921,1.088148842,-1.0138420238 H,0,0.8706863418,1.8356096862,-0.6659510747 H,0,0.5015932127,0.7245976691,-1.9763530174 H,0,-0.7866648687,1.6065922203,-1.1706926081 C,0,1.4185345804,-5.0981247925,-1.6858535034 H,0,1.7978546622,-5.601400783,-2.5741316504 H,0,1.378311276,-5.8470246326,-0.8960049738 H,0,0.4038172939,-4.7763168086,-1.8925187654 H,0,0.7885901692,-1.320559996,-2.2219106357 O,0,2.5336008221,-2.165363498,-4.2736449807 H,0,2.5838183147,-2.6305953513,-3.4197365571 **FREQUENCIES** 24.9594 38.2146 41.8529 69.7709 134.9797 136.1672 150.9033 201.7770 234.6006 335.7583 348.7668 406.2501 449.1225 527.6494 577.0966 590.0207 758.0752 775.0633 917.6405 956.1843 1001.1824 1031.2534 1067.1655 1071.7052 1078.3486 1122.6215 1122.9677 1161.5771 1200.2312 1291.1734 1345.1023 1359.6481 1382.2908 1481.0546 1486.5543 1513.0894 1513.9913 1557.5889 1565.6390 1566.2332 1573.3545 1578.9552 1808.7014 1829.5508 3134.5321 3137.5788 3156.1628 3181.7582 3186.0391 3193.8215 3233.6674 3235.7845 3244.5989 3245.6799 3265.1549 3266.7104 3752.0236 **ROTATIONAL CONSTANTS** 2.3539223 0.9245367 0.7186118	**GEOMETRY** C,0,1.6780221611,-0.9486399213,-0.4066386253 C,0,0.8461470566,-0.2392354283,0.3464730561 H,0,1.5981993187,-0.8696966415,-1.4840170313 H,0,0.9133229012,-0.3291407529,1.4243768491 C,0,-0.2142931057,0.6926968103,-0.1699023765 H,0,-0.217833087,0.6815088157,-1.2581210695 C,0,-1.5798411185,0.3481208798,0.3505124696 C,0,-2.6212052387,0.0316534971,-0.4022086483 H,0,-1.6957804307,0.3667606491,1.4273697719 H,0,-2.4996386351,0.0123161786,-1.4781079331 C,0,2.7202891883,-1.8889305872,0.1098174684 H,0,3.7133677408,-1.61283032,-0.2417300252 H,0,2.7382779782,-1.9051930736,1.1961927566 H,0,2.5337524712,-2.9034902193,-0.2398612266 C,0,-3.9834871958,-0.3054495827,0.1122305038 H,0,-4.0191344708,-0.2662170579,1.1976950108 H,0,-4.7324032039,0.3846777372,-0.274815002 H,0,-4.2857442078,-1.3046049102,-0.1997740424 H,0,0.0420302505,1.7102613409,0.1336328348 O,0,2.7912017943,2.3138495591,0.0225501622 H,0,2.5081785359,1.383557775,-0.0249452781 **FREQUENCIES** 31.8376 46.0882 59.8226 101.7268 124.4813 133.5728 213.2142 217.8266 244.7875 268.3817 310.6305 346.3663 395.9886 449.3287 502.0851 557.9422 802.8991 820.5287 952.3735 965.9950 1010.1246 1056.8859 1068.9952 1102.4862 1114.7488 1125.6164 1126.9878 1149.0618 1222.8489 1275.2133 1361.0561 1392.1205 1393.5116 1398.8849 1445.0693 1498.1215 1499.9594 1555.0720 1561.4136 1561.7387 1574.9252 1575.1097 1823.2133 1841.6535 3113.0862 3129.5708 3133.2607 3177.1104 3180.6161 3186.4639 3213.5705 3216.3735 3233.5417 3239.1597 3244.2013 3246.2237 3754.8957 **ROTATIONAL CONSTANTS** 2.6378066 0.7384279 0.6056010

C_7H_{12}×iso-C_3H_7	*(Z,Z)*-hepta-2,5-diene-C_3H_7 complex	*(E,E)*-hepta-2,5-diene-C_3H_7 complex
Terminal position	**GEOMETRY** C,0,-0.8982024068,-0.1175509535,1.2647133322 C,0,0.40288006,0.14208342,1.2147458983 H,0,-1.2087909657,-0.9672878533,1.8582790398 H,0,1.0664246425,-0.5010728727,1.7768203769 C,0,1.0950543452,1.2586935799,0.4832948675 H,0,1.7994413058,0.8344467042,-0.2291416769 H,0,0.3774550226,1.8323955803,-0.0995127695 C,0,1.8038049731,2.1804313962,1.436387264 C,0,3.1042557641,2.4313031757,1.5144991972 H,0,1.1528823709,2.6751566549,2.1444293457 H,0,3.4286180144,3.1255735105,2.2781808472 C,0,-2.0150993607,0.617066697,0.5930984798 H,0,-2.7436120524,0.9604135997,1.3268581493 H,0,-1.6758383152,1.4816458993,0.0324871322 C,0,4.2049950039,1.8742064943,0.6681087919 H,0,4.7357838858,2.6735195996,0.1518368124 H,0,4.9404060533,1.3584996584,1.2847881594 H,0,3.8508274486,1.1740192097,-0.0809374295 H,0,-2.5444468442,-0.0415274583,-0.0947753315 C,0,-2.4921005363,-2.5823790225,-1.6140675213 H,0,-2.637777935,-2.872036526,-0.5843852627 C,0,-1.1120786694,-2.2558317385,-2.0629052892 H,0,-0.565933178,-3.1499259077,-2.3851895766 H,0,-1.1231353187,-1.5775719015,-2.9161076957 H,0,-0.5309426294,-1.7931423175,-1.2691784863 C,0,-3.5589923918,-2.9132189568,-2.5963738109 H,0,-3.4195159774,-3.9094890677,-3.0314017624 H,0,-4.546628872,-2.9011113465,-2.1417867844 H,0,-3.5623173446,-2.2113297171,-3.4302703446 **FREQUENCIES** 13.4301 18.7134 28.3679 33.6001 42.4297 49.4871 58.1146 69.8718 132.9669 141.2206 161.2907 165.5861 203.7267 232.2006 346.1081 375.3740 404.6656 453.3544 528.2647 577.3238 586.0242 753.3273 766.1214 916.6977 920.0137 956.1194 983.9051 990.1095 1001.2788 1032.3796 1066.1514 1069.1945 1072.2699 1094.2521 1121.5994 1124.7052 1156.7707 1193.2860 1201.0478 1238.3433 1285.0040 1346.2369 1358.4808 1376.7163 1438.1857 1480.2671 1485.1509 1496.1572 1499.1326 1512.9292 1513.4474 1555.7030 1558.6661 1564.0611 1566.3320 1566.7922 1568.6665 1574.9735 1575.5769 1581.2282 1818.9884 1831.6325 3064.5141 3069.8498 3131.9883 3132.8719 3148.3898 3150.9062 3152.6337 3179.4785 3181.3820 3186.3992 3203.3604 3208.7358 3229.8457 3231.2387 3241.9853 3243.5881 3264.6969 3266.0710 3275.8419 **ROTATIONAL CONSTANTS** 2.2753942 0.3360529 0.3063098	**GEOMETRY** C,0,-1.5768046154,-1.6923897303,-3.4209762842 C,0,-1.6480822757,-1.6361746799,-2.1001377885 H,0,-0.6310492057,-1.4726817636,-3.9010952911 H,0,-2.591095466,-1.847861407,-1.6117012567 C,0,-0.5098215915,-1.2746192424,-1.1893638785 H,0,-0.3019949766,-2.1021928585,-0.5100269624 H,0,0.3892084681,-1.1249563681,-1.7882707692 C,0,-0.7973141237,-0.04092313,-0.381925032 C,0,-0.8634716383,0.0049914952,0.9405592544 H,0,-0.9805053123,0.8614048769,-0.9518413429 H,0,-0.6887242427,-0.9055826909,1.5008590671 C,0,-2.710200263,-2.0438153504,-4.3300366166 H,0,-2.4780025083,-2.9251787472,-4.9271408912 H,0,-3.6193487685,-2.2466344855,-3.7702181659 H,0,-2.9187125987,-1.2359929253,-5.0308926475 C,0,-1.1598255742,1.2274750394,1.7481800685 H,0,-1.3424539073,2.0885492867,1.1106069505 H,0,-2.0377375916,1.0802022468,2.3765326904 H,0,-0.3295798554,1.4677238261,2.4114971291 C,0,2.5925720381,1.2478173214,2.8375644674 H,0,2.2005048958,0.2735747019,3.0874885876 C,0,2.7736280123,1.5842773846,1.4000674922 H,0,2.0145346579,1.1148222349,0.7795097091 H,0,2.7285380486,2.6610003252,1.2364854348 H,0,3.7489875802,1.2545988585,1.0238446014 C,0,3.2935170338,2.0188420605,3.8990565142 H,0,2.8890785317,1.8095363028,4.8864019227 H,0,4.3635896638,1.7845795594,3.9356409639 H,0,3.2195805717,3.092202018,3.7243910883 **FREQUENCIES** 12.4685 21.5497 27.0895 32.5135 50.3991 56.6719 73.0279 88.2622 130.3672 152.0162 156.9751 216.5797 228.6649 248.6322 260.6085 319.2786 374.7610 377.0525 451.0252 511.6207 561.0109 815.3024 839.9020 906.8682 919.8764 977.0117 984.0504 990.0145 1006.2402 1059.2994 1060.4932 1093.8492 1100.9573 1125.4695 1128.9009 1140.8121 1154.2780 1193.4270 1209.9630 1238.2360 1283.6545 1347.2969 1388.2499 1391.2745 1410.3415 1434.3844 1438.2916 1495.4982 1498.6356 1498.8187 1499.7588 1554.9190 1555.4805 1562.3220 1562.4719 1564.1730 1568.2087 1574.6657 1575.2237 1577.0909 1828.3015 1840.7352 3064.4863 3069.7737 3119.8294 3128.0367 3128.5582 3148.4545 3150.9154 3158.1076 3178.6011 3181.3540 3203.2894 3209.4622 3211.8893 3213.1057 3237.9998 3240.3399 3246.0408 3246.3506 3275.9634 **ROTATIONAL CONSTANTS** 2.8070611 0.2930481 0.2753281

C_7H_{12}×iso-C_3H_7	*(Z,Z)*-hepta-2,5-diene-C_3H_7 complex	*(E,E)*-hepta-2,5-diene-C_3H_7 complex
Central position	**GEOMETRY** C,0,-1.076199448,-1.9835480125,1.201828621 C,0,-0.0660305768,-1.163851843,1.4662485382 H,0,-1.0552919623,-2.9600594544,1.6671586741 H,0,0.7045819845,-1.5180164903,2.137564137 C,0,0.1403006591,0.2407177501,0.9707913716 H,0,1.1100964019,0.3043560061,0.482533484 C,0,0.0512622069,1.2346146547,2.0955153514 C,0,0.9970800803,2.0519303979,2.540165636 H,0,-0.9072706016,1.2556967334,2.596103966 H,0,0.7427744927,2.6964540067,3.3710778265 C,0,-2.2677810668,-1.7292548407,0.3332484892 H,0,-3.1878454988,-1.8073606923,0.9118597231 H,0,-2.2492811419,-0.7502177881,-0.1330619112 H,0,-2.3332472911,-2.4747704988,-0.4586993754 C,0,2.3959628529,2.2078655208,2.0332016507 H,0,2.5699714944,3.2272921144,1.6900514717 H,0,3.1164292547,2.0188560277,2.8283865275 H,0,2.6255269253,1.5378996341,1.2115193077 H,0,-0.5979165028,0.4897245639,0.2114928442 C,0,-0.5374671231,-0.3684431607,-2.9799988893 H,0,-1.5234839096,-0.7452938788,-2.7548772937 C,0,0.6372060772,-1.1771293974,-2.5573846025 H,0,0.4581108886,-1.6882849178,-1.6144676495 H,0,0.8924006973,-1.9448256715,-3.2969721495 H,0,1.5243605632,-0.5546267992,-2.4411926781 C,0,-0.4065815071,0.6877409702,-4.0190612709 H,0,0.4664431956,1.3152115279,-3.8393932406 H,0,-0.2808225474,0.2625967037,-5.0213890859 H,0,-1.2820493703,1.3315166371,-4.0550239498 **FREQUENCIES** 15.3825 17.8890 26.7666 33.7631 43.4908 49.9648 56.2491 57.6070 130.9455 140.3552 148.8650 161.5356 204.2622 229.0413 347.6453 374.8493 404.9404 450.4080 529.4470 578.3185 585.2064 752.9475 768.0372 914.8390 918.9605 954.6688 983.3797 989.9264 1001.4607 1032.0554 1065.9444 1069.2083 1071.3143 1093.0796 1121.3389 1121.5867 1154.3889 1193.7096 1201.2416 1237.5270 1286.5432 1347.2901 1359.2647 1378.9823 1438.5081 1480.0100 1484.7334 1496.0720 1498.9024 1512.9120 1513.4071 1554.2152 1557.4767 1563.8727 1564.9703 1566.4352 1567.9100 1574.0598 1574.6347 1580.0349 1819.4324 1831.6762 3064.9039 3070.0019 3131.6038 3132.4852 3147.9373 3150.2765 3155.4203 3177.3953 3178.8749 3188.9738 3203.3452 3205.2024 3230.7324 3233.3036 3242.8060 3244.1454 3265.3815 3265.5506 3278.7023 **ROTATIONAL CONSTANTS** 0.8989802 0.8153388 0.4846373	**GEOMETRY** C,0,-0.3629895759,2.078415813,-0.3157267813 C,0,0.5957581765,1.4352133509,0.3338578082 H,0,-1.0660566249,1.5027797764,-0.904895176 H,0,1.3099642273,2.0015119111,0.9187567839 C,0,0.8043285414,-0.0522028321,0.3102760687 H,0,0.7471012474,-0.4490459663,1.3245470248 C,0,2.129242945,-0.4299306609,-0.2876896848 C,0,3.094352126,-1.0768011272,0.3472235676 H,0,2.284708839,-0.1242413292,-1.3148683477 H,0,2.9326490322,-1.3729023706,1.3765249974 C,0,-0.5631281051,3.5600141907,-0.3067233517 H,0,-1.5474513148,3.8236154027,0.079085361 H,0,0.1829964523,4.0572226508,0.3075191378 H,0,-0.500151714,3.9724310678,-1.3133466403 C,0,4.4164686039,-1.4471735776,-0.243997458 H,0,5.2381826273,-1.0051841268,0.3188498064 H,0,4.568485706,-2.5260200923,-0.2260171782 H,0,4.4972848079,-1.1133966599,-1.2751315564 H,0,-0.0058654518,-0.5140728947,-0.2548070191 C,0,-3.1107666085,-0.8974065726,-0.2600577468 H,0,-3.3137841579,-0.0341291894,-0.8759796101 C,0,-2.8919046063,-0.6829277627,1.195515492 H,0,-2.3528986216,0.2416119325,1.3878538551 H,0,-3.837249582,-0.6269128152,1.7472312159 H,0,-2.3243549529,-1.5025044726,1.6352310836 C,0,-3.4643600922,-2.2397086178,-0.7945571038 H,0,-2.8359811149,-3.0174780747,-0.3610789354 H,0,-4.5001186504,-2.5128100961,-0.5623683508 H,0,-3.3594691823,-2.2854278767,-1.8758313123 **FREQUENCIES** 13.1684 18.3632 25.5887 33.8578 53.1184 59.0414 65.1927 87.1461 133.7939 149.0151 161.0759 216.8791 221.5886 246.8244 260.0811 319.8765 376.0470 377.9571 462.6059 511.8789 561.0972 816.6696 840.5081 906.6170 918.4522 976.0079 983.1257 988.6759 1005.6615 1059.6089 1061.1989 1094.9319 1100.8010 1125.2729 1125.8824 1140.8720 1153.3059 1193.7420 1209.7025 1237.5569 1283.9401 1348.2430 1389.0295 1392.5494 1411.5055 1434.8839 1438.7146 1495.3947 1497.4853 1498.3426 1498.6924 1553.5037 1557.1113 1562.2843 1562.4830 1564.0224 1567.7789 1573.9162 1575.1200 1575.4180 1828.6902 1840.9532 3065.5843 3070.4176 3120.5955 3127.8203 3128.2865 3150.9471 3154.4336 3160.2211 3177.9112 3178.1683 3203.6001 3206.3805 3212.1154 3212.6831 3239.2497 3241.4775 3245.5247 3247.5718 3272.8141 **ROTATIONAL CONSTANTS** 0.8075801 0.5684834 0.3471575

C_7H_{12}×OOH	*(Z,Z)*-hepta-2,5-diene-OOH complex	*(E,E)*-hepta-2,5-diene-OOH complex
Terminal position	**GEOMETRY** C,0,0.6181723946,-0.4239656541,-1.6627342479 C,0,0.6181723946,-0.4239656541,-0.3299676879 H,0,1.5816552611,-0.4239656541,-2.155335595 H,0,1.5769010773,-0.444211369,0.1715971456 C,0,-0.5688329697,-0.4625957218,0.59395175 H,0,-0.5325836467,0.3963179703,1.2602386038 H,0,-1.4930562443,-0.3742429184,0.0273438744 C,0,-0.5915869023,-1.7406628776,1.3859800712 C,0,-0.4955090767,-1.8834109752,2.7013678163 H,0,-0.6841573035,-2.6356760849,0.7862634169 H,0,-0.526817744,-2.8922102984,3.0904690944 C,0,-0.5569794087,-0.4322292285,-2.5884981694 H,0,-0.5149434776,-1.3031772987,-3.2408820475 H,0,-1.5077199364,-0.450746113,-2.0670184898 C,0,-0.3529761507,-0.8168411047,3.7401933632 H,0,-1.1840384433,-0.8533990091,4.4435083042 H,0,0.555504773,-0.9675974279,4.3220969319 H,0,-0.3171291104,0.1833052676,3.3216868787 H,0,-0.536032233,0.4487828562,-3.2259013287 O,0,0.5583722942,2.8492474837,-2.4406792216 O,0,0.7890310559,2.731761331,-1.1577525672 H,0,0.7804285413,1.7707768581,-0.9883698517 **FREQUENCIES** 10.4734 25.7070 32.5445 46.7985 74.2592 100.8211 137.0222 156.6897 174.4227 208.7671 236.7990 345.8349 407.0885 488.0975 533.4334 577.8851 585.1749 758.4217 783.5734 914.6837 953.9182 1001.2191 1032.3867 1065.9796 1069.7757 1076.9327 1122.1182 1127.2910 1157.4563 1201.6353 1283.7207 1287.9613 1345.8711 1358.9031 1379.7658 1480.1923 1484.7786 1512.7925 1513.4487 1558.1416 1565.1934 1565.8265 1575.0609 1580.6682 1595.8075 1801.4506 1828.9435 3135.0901 3144.1681 3157.0579 3182.9994 3191.6171 3202.8286 3231.6721 3236.6676 3245.3709 3246.2527 3265.5791 3268.7581 3626.4895 **ROTATIONAL CONSTANTS** 2.3285067 0.6037739 0.5079744	**GEOMETRY** C,0,0.5333196705,1.6629146963,-2.7097497782 C,0,0.1587241559,0.5422472172,-2.1127244068 H,0,1.246165165,2.3066992313,-2.2093844208 H,0,-0.5572613263,-0.1061588736,-2.601579548 C,0,0.6390538016,0.0832141218,-0.7654118268 H,0,1.1275724182,-0.887500169,-0.8546789795 H,0,1.389949813,0.783600954,-0.3991988893 C,0,-0.4910037009,-0.024760138,0.2210862858 C,0,-0.9135300789,-1.1552344621,0.7796819977 H,0,-1.0147361004,0.8979379346,0.4396884463 H,0,-0.3972958684,-2.0764550905,0.5394593779 C,0,0.0527884203,2.1269234528,-4.0465984575 H,0,0.8819731481,2.2421216908,-4.7436709446 H,0,-0.6563581382,1.4262285644,-4.4788899871 H,0,-0.4337400835,3.098948403,-3.9735764776 C,0,-2.0647913922,-1.2761123152,1.7255528508 H,0,-2.5218312346,-0.3104219701,1.9239740752 H,0,-2.829879401,-1.9354660919,1.3181261667 H,0,-1.7402511276,-1.7063262022,2.6704205236 O,0,0.9133819282,-1.5241336343,3.4916341728 O,0,1.2525067488,-0.3755352746,2.9643411301 H,0,0.6912180615,-0.2910125458,2.1704882444 **FREQUENCIES** 27.2219 31.8204 41.7436 65.6118 95.7176 103.0507 150.3904 172.9332 216.8636 234.7435 254.9214 262.6034 319.1498 381.5797 486.9119 518.6165 560.0455 819.5839 844.3315 905.1397 975.4504 1007.0251 1058.5569 1068.3260 1100.4926 1126.1875 1129.6884 1138.5315 1154.7199 1210.8382 1283.4255 1285.6775 1350.3919 1388.3014 1391.8871 1412.2280 1434.7205 1495.8873 1498.9138 1556.5421 1561.2894 1561.8267 1574.4039 1577.0405 1594.5107 1811.9706 1837.8251 3124.3431 3130.8364 3138.5120 3163.7330 3182.2539 3199.0849 3215.4233 3221.3135 3242.0805 3242.8893 3249.4876 3250.9454 3624.2907 **ROTATIONAL CONSTANTS** 2.8786809 0.5058732 0.4481163

C_7H_{12}×OOH	*(Z,Z)*-hepta-2,5-diene-OOH complex	*(E,E)*-hepta-2,5-diene-OOH complex
Central position	**GEOMETRY** C,0,0.,0.,0. C,0,0.2254493393,-1.294379599,-0.1840195403 H,0,-0.4903431776,0.288821447,0.9200421916 H,0,-0.0821930228,-1.9766837236,0.5966670944 C,0,0.8884680096,-1.9498767226,-1.3635446868 H,0,0.2069615347,-2.6768501782,-1.8001096358 C,0,2.1762283788,-2.6130314568,-0.9588299854 C,0,2.491112978,-3.9066248715,-1.0184826547 H,0,2.9135664105,-1.9376218108,-0.5454241775 H,0,3.4682433428,-4.1944232545,-0.6524308474 C,0,0.3346877573,1.1349414678,-0.9148325502 H,0,0.9762370314,1.8562874296,-0.4100597702 H,0,0.8407401614,0.8170653352,-1.8199158829 H,0,-0.5677708252,1.6707984014,-1.2069395551 C,0,1.6433411431,-5.0403511582,-1.505242755 H,0,2.1416734747,-5.5804090354,-2.3088567175 H,0,1.4773898391,-5.7577167117,-0.7027307893 H,0,0.674805872,-4.7174083646,-1.8702967478 H,0,1.105584202,-1.2218741399,-2.1398982633 O,0,3.0612180628,-1.3761350047,-3.9937389934 O,0,3.6182323628,-2.5451105375,-3.8042991162 H,0,3.287474028,-2.8457672117,-2.9368221968 **FREQUENCIES** 16.2220 27.8222 35.2052 46.0591 68.1682 100.4396 135.2907 141.6278 172.5113 206.0022 235.0141 346.3222 407.4610 486.0911 532.3401 577.6174 588.1213 759.0558 782.8537 916.1326 954.1293 1002.0880 1031.3895 1066.4846 1070.8389 1078.4663 1122.7364 1123.1316 1158.5231 1201.5940 1284.2758 1289.2712 1345.5708 1358.5077 1380.6116 1481.1319 1486.3008 1513.3060 1515.1427 1560.6195 1565.6532 1566.2900 1573.0384 1580.6979 1594.7555 1801.7617 1828.4935 3134.7229 3138.8238 3161.4761 3181.9121 3188.0973 3206.4055 3234.2734 3235.7227 3244.8713 3246.5216 3265.0137 3266.9461 3626.3725 **ROTATIONAL CONSTANTS** 1.5709615 0.8349111 0.5815638	**GEOMETRY** C,0,-0.587495747,-0.0058227786,-1.7491913573 C,0,-0.587495747,-0.0058227786,-0.4199045573 H,0,0.3637640287,-0.0058227786,-2.2674672365 H,0,-1.5367423934,0.0129386227,0.1017660016 C,0,0.6384187028,-0.006531037,0.4491152406 H,0,1.5323959217,-0.0471063714,-0.1700139056 C,0,0.6923559343,1.1950181417,1.3489858961 C,0,1.6581933637,2.0996597176,1.3483101089 H,0,-0.1329933769,1.3061500533,2.0414378311 H,0,2.48010876,1.9840583545,0.6527127772 C,0,-1.8100670501,0.0343551638,-2.6116825614 H,0,-1.8434632377,-0.8104243457,-3.2982247816 H,0,-2.7182544143,0.0221747743,-2.0153539001 H,0,-1.8198035553,0.9356795091,-3.2229398355 C,0,1.7192340076,3.2926538914,2.2467048287 H,0,0.8594066487,3.3348610715,2.9099332633 H,0,2.6186740779,3.277003518,2.8612219113 H,0,1.747691831,4.2172200784,1.671072461 H,0,0.6271216428,-0.9117170656,1.0587510997 O,0,-0.767145689,-3.1930214964,0.4694587907 O,0,-0.7158454471,-3.1490837273,-0.8374930981 H,0,-0.6528376297,-2.1992355518,-1.0526468161 **FREQUENCIES** 22.0375 32.7023 37.9900 60.3438 92.2339 104.2139 137.3389 162.4939 214.4610 221.1598 249.4925 269.2932 313.0912 398.8079 486.2465 510.6849 555.8644 806.1311 821.5662 951.3912 964.3848 1011.1657 1055.9103 1069.7785 1102.2863 1112.2908 1125.5316 1126.7142 1148.4765 1222.9066 1276.2624 1283.7360 1361.5263 1392.1288 1393.7557 1399.3958 1443.8893 1498.1531 1500.6776 1557.2081 1561.4417 1561.6527 1574.8869 1575.0695 1595.5355 1816.7295 1840.9606 3124.2409 3129.8473 3133.9358 3180.3163 3181.0785 3187.2225 3214.0270 3218.1377 3238.2449 3241.5490 3245.0906 3248.6284 3623.7220 **ROTATIONAL CONSTANTS** 2.0081415 0.6103514 0.4908732

(Z,Z)-hepta-2,5-diene-1-yl radical	*(E,E)*-hepta-2,5-diene-1-yl radical
GEOMETRY	**GEOMETRY**
C,0.8802489174,0.3111606972,-2.3126224448	C,-0.4670224977,-0.7380857538,-2.1308913508
C,0.8789902587,0.3690060556,-0.9299099994	C,-0.5156926035,-0.7023110605,-0.8082958720
H,1.8514059672,0.2486877251,-2.7841698059	H,0.5012870314,-0.7512842357,-2.6159883432
H,1.8302413715,0.3268918813,-0.4211997770	H,-1.4787317996,-0.6819474113,-0.3140881481
C,-0.3274883781,0.4424344604,-0.0444633137	C,0.6842392087,-0.6639425724,0.0968368788
H,-0.2469049852,1.3150178174,0.6011131114	H,0.6758922720,-1.5313071491,0.7581930853
H,-1.2260151946,0.5855285875,-0.6412667960	H,1.5863160959,-0.7443913990,-0.5128968095
C,-0.4763959302,-0.8079048617,0.7797317396	C,0.7343605507,0.5828581481,0.9235758134
C,-0.4174548948,-0.9251227284,2.1000136082	C,0.7256563515,0.6079066622,2.3033908740
H,-0.6305499479,-1.7074493107,0.1998923815	H,0.7639537068,1.5207697342,0.3864657690
H,-0.5396771080,-1.9174467289,2.5132229631	H,0.6883021244,-0.3443232750,2.8170930470
C,-0.2139843380,0.3250111521,-3.1507362835	C,-1.6568785672,-0.7658853184,-3.0351704170
H,-0.0894070067,0.2782848594,-4.2188568072	H,-1.6566161916,-1.6589334733,-3.6593375508
H,-1.2241503058,0.3814962893,-2.7823535246	H,-2.5850608363,-0.7502713074,-2.4701496663
C,-0.2039810730,0.1529372500,3.1149268191	H,-1.6584504821,0.0892075340,-3.7104525961
H,-1.0484104405,0.2083793121,3.8011824664	C,0.7630576357,1.7497779300,3.0751464759
H,0.6769395516,-0.0584316997,3.7201967918	H,0.8009532205,2.7279131354,2.6231943946
H,-0.0730792734 ,1.1339091158,2.6705982443	H,0.7558343897,1.7026596359,4.1504124046
FREQUENCIES	**FREQUENCIES**
26.6761 47.8571 132.8395	52.6177 74.5867 145.7549
191.9195 217.0296 340.7268	215.7268 231.3790 258.7935
352.3391 496.7696 559.6239	314.5225 371.6226 501.0443
575.9311 586.7703 744.1017	559.6391 567.5165 776.7339
762.8777 801.3543 909.8474	811.1101 828.2202 905.6480
959.4043 1021.5873 1033.5288	973.9172 1005.6660 1035.2468
1064.5381 1066.2951 1082.6361	1058.9122 1105.7957 1125.5069
1121.2940 1168.6170 1229.8929	1145.9986 1190.5984 1237.2648
1275.8475 1294.1970 1351.8231	1268.2943 1336.5666 1343.2808
1372.0481 1480.6902 1496.4666	1390.9259 1412.0294 1438.4151
1511.6096 1541.7495 1562.8260	1498.3540 1552.1875 1561.9637
1565.8466 1577.7839 1601.5263	1568.5647 1574.7516 1588.4104
1825.1284 3132.9265 3149.2807	1835.0784 3109.8428 3128.9303
3179.8253 3184.8353 3230.3623	3150.7675 3179.4897 3213.2165
3244.9758 3251.7357 3268.2286	3241.3471 3243.6909 3248.5826
3276.2388 3283.5205 3365.8977	3261.7643 3268.5760 3361.7761
ROTATIONAL CONSTANTS	**ROTATIONAL CONSTANTS**
8.5730095 1.0468595 1.0139640	10.1486350 0.8814535 0.8511363

(Z,Z)-hepta-2,5-diene-4-yl radical	*(E,E)*-hepta-2,5-diene-4-yl radical
GEOMETRY	**GEOMETRY**
C,1.3585779328,0.0785799543,-2.1055258879	C,-0.7542608349,-0.0000299306,-2.3678066896
C,1.3423731147,0.0557062791,-0.7444637485	C,-0.7573686115,-0.0000087323,-1.0092270855
H,2.3232294011,0.1177414001,-2.5898920669	H,0.1976642722,-0.0000467272,-2.8816244012
H,2.3025908947,0.0786433651,-0.2463646166	H,-1.7143116224,0.0000080101,-0.5018580759
C,0.2138135162,0.0053161605,0.0976611927	C,0.3945582347,-0.0000067586,-0.1999206275
H,-0.7659223906,-0.0191297652,-0.3499039619	H,1.3591098346,-0.0000232809,-0.6886602246
C,0.3175577764,-0.0143541729,1.5027410975	C,0.3658951080,0.0000154382,1.2075917357
C,-0.6991742630,-0.0621393863,2.4067341689	C,1.4632257568,0.0000177866,2.0085928497
H,1.3226547263,0.0116796866,1.9024258622	H,-0.6091922679,0.0000336146,1.6791518725
H,-0.4327568256,-0.0706724805,3.4534632032	H,2.4405548930,0.0000015368,1.5449157206
C,0.1786888147,0.0553612627,-3.0190956562	C,-1.9780395605,-0.0000318942,-3.2190400650
H,-0.7657875797,0.0162060472,-2.4870602636	H,-2.0098956952,-0.8739247041,-3.8705770421
H,0.1640103707,0.9396895367,-3.6564515374	H,-2.8821669873,-0.0000095306,-2.6156973904
H,0.2203961963,-0.8068688657,-3.6848973868	H,-2.0098746313,0.8738349318,-3.8706116799
C,-2.1618084693,-0.1047578035,2.1131990217	C,1.4258028859,0.0000413534,3.4988387269
H,-2.6164058353,-1.0009749474,2.5358184919	H,0.4045541727,0.0000493184,3.8710216015
H,-2.6731166318,0.7455591058,2.5648529475	H,1.9323377202,-0.8738339634,3.9098967207
H,-2.3790628615,-0.0941468460,1.0505081993	H,1.9323424412,0.8739254169,3.9098698307
FREQUENCIES	**FREQUENCIES**
77.6564 78.4910 106.3216	86.3009 110.0099 148.6978
121.9630 156.4836 283.8489	186.4258 192.7921 276.0691
364.5186 366.2741 441.8063	297.0720 325.2307 377.7647
602.0825 640.6596 731.4594	488.9242 586.5321 803.9229
767.5852 852.3555 938.6970	805.2931 870.4599 961.5960
973.4987 1005.3823 1043.1516	987.4108 1002.2884 1049.3248
1070.0036 1089.4624 1092.2826	1093.2646 1094.5462 1140.0070
1136.4194 1204.9142 1256.3647	1153.5634 1192.8981 1274.4404
1279.1670 1344.1886 1363.8353	1296.7661 1357.5207 1365.7534
1483.6424 1492.7004 1522.0193	1393.5294 1489.4301 1498.1526
1532.8981 1560.4940 1561.6792	1526.6810 1558.4590 1558.5498
1563.4603 1567.5463 1604.1138	1563.1311 1570.9308 1599.7093
1662.9843 3125.4902 3125.8746	1682.2806 3118.3949 3118.9749
3169.0724 3169.2199 3230.2032	3163.7183 3163.7829 3209.9368
3231.3513 3242.8345 3248.1072	3209.9715 3235.9065 3240.9852
3274.0570 3275.3376 3305.2949	3252.6554 3255.3471 3263.5665
ROTATIONAL CONSTANTS	**ROTATIONAL CONSTANTS**
6.3532210 1.1027256 0.9505143	18.9134209 0.7852476 0.7609348

H_2O	CH_4
GEOMETRY O,0,-0.0955762179,0.,-0.0675465926 H,0,-0.0544709293,0.,0.8882098342 H,0,0.8190806727,0.,-0.3478370931 **FREQUENCIES** 1759.5624 3906.3530 4026.5386 **ROTATIONAL CONSTANTS** 824.46215 437.77916 285.94560	**GEOMETRY** C,0,0.,0.,0. H,0,0.0000000216,-0.0000000229,1.0851236587 H,0,1.0230643894,-0.0000000104,-0.3617079066 H,0,-0.5115321899,0.8859997739,-0.3617078573 H,0,-0.5115322212,-0.8859997405,-0.3617078947 **FREQUENCIES** 1422.9347 1422.9347 1422.9347 1644.0616 1644.0616 3142.0735 3255.9786 3255.9786 3255.9786 **ROTATIONAL CONSTANTS** 159.69998 159.69998 159.69998
C_3H_8	H_2O_2
GEOMETRY C,0,0.4913362442,-1.1946118853,0.0685158614 H,0,0.33236155,-1.3833141688,1.1288062664 H,0,1.5442025473,-0.9533849819,-0.0671234186 H,0,0.2915541328,-2.1201257302,-0.4666209542 C,0,-0.3972868992,-0.0611120199,-0.4243329669 H,0,-0.2410783979,0.0836329046,-1.4929271091 H,0,-1.443275062,-0.3426925381,-0.3063506628 C,0,-0.1395068558,1.2487304817,0.3072705319 H,0,0.8922932915,1.5715214759,0.1795553448 H,0,-0.783750136,2.044467456,-0.0596260178 H,0,-0.3195628612,1.1418561234,1.3755659934 **FREQUENCIES** 227.1913 282.3283 378.1727 781.4574 913.9592 950.3024 973.8895 1107.3944 1235.3470 1275.8603 1379.5274 1440.4359 1491.4124 1503.6007 1571.5499 1572.8706 1579.8718 1589.4249 1596.2936 3133.1557 3134.3694 3137.2807 3160.4729 3196.4275 3206.3854 3208.1531 3208.8748 **ROTATIONAL CONSTANTS** 29.7762406 8.4926559 7.5198460	**GEOMETRY** O,0,-0.7038846587,0.0479803686,0.097410328 H,0,-0.7175873711,0.0239891857,1.0574413645 O,0,0.6943859055,0.0467647836,-0.1512804339 H,0,0.7935773961,-0.7819504036,-0.6264805171 **FREQUENCIES** 379.0368 1058.7347 1410.0184 1547.9952 3898.3898 3900.6895 **ROTATIONAL CONSTANTS** 308.60862 27.58704 26.54596

OH transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
terminal	**GEOMETRY** C,0,1.5758157833,-0.8681881756,0.719724279 C,0,0.3154859098,-0.4405641496,0.8412100569 H,0,2.0331209718,-1.3185840283,1.5892507536 H,0,-0.1797733624,-0.596975076,1.789335722 C,0,-0.5346067505,0.2162045704,-0.207889225 H,0,-0.8335313238,1.2006318414,0.1467484031 H,0,0.0402147436,0.3795620878,-1.1170066929 C,0,-1.7458596043,-0.6162306382,-0.5273856281 C,0,-3.0206675882,-0.3057190944,-0.3315166788 H,0,-1.5220534573,-1.5849266009,-0.9525003503 H,0,-3.7575389151,-1.0423956309,-0.622059129 C,0,2.4369261093,-0.7637226494,-0.4643694286 H,0,3.1395848409,-1.5843284152,-0.5652394307 H,0,1.9274496782,-0.5729739832,-1.4004409311 C,0,-3.5880981146,0.952646136,0.244513819 H,0,-4.2489789821,1.4391316998,-0.4719260232 H,0,-4.1899041122,0.733487978,1.1257717109 H,0,-2.8265242691,1.6693174666,0.5329956113 H,0,3.1990896224,0.181774572,-0.3475229307 O,0,3.9132056754,1.2843015119,-0.2101471494 H,0,3.2792246932,1.775309998,0.328047316 **FREQUENCIES** -1719.5329 27.0775 39.5916 47.4182 77.9710 110.5652 146.8538 206.7945 233.3971 347.4394 349.5670 401.2085 518.3535 578.5681 587.3081 674.7464 747.5528 761.5331 851.6615 919.7326 968.3916 1018.9929 1033.2564 1058.3623 1067.6778 1071.4043 1121.8638 1136.9003 1162.3668 1203.4720 1285.2112 1332.2722 1341.1441 1356.5843 1376.5403 1481.9752 1494.4338 1511.8800 1512.8577 1552.1122 1565.5013 1566.7690 1579.0486 1753.3206 1827.6367 3134.5526 3152.3564 3182.2361 3186.7348 3198.9048 3231.6849 3246.3086 3252.6249 3268.9960 3270.5052 3281.4539 3858.8096 **ROTATIONAL CONSTANTS** 4.3150976 0.6414577 0.6073022	**GEOMETRY** C,0,-1.0899090366,-0.9431437155,-2.7229308367 C,0,-1.0953979731,-0.9409294625,-1.3990260751 H,0,-0.1402517426,-1.0094801389,-3.2395363118 H,0,-2.0387125962,-0.8697083434,-0.8726178283 C,0,0.1311452529,-1.0127874255,-0.5340861992 H,0,0.0851697025,-1.8938341192,0.1064899678 H,0,1.0079583405,-1.1309150821,-1.1722256339 C,0,0.2933488582,0.207637788,0.3224925232 C,0,0.3080241505,0.2105842171,1.6557860438 H,0,0.3793169791,1.1479300501,-0.207241991 H,0,0.2165183511,-0.7312841309,2.1803625703 C,0,-2.3057565329,-0.8654312584,-3.5885378672 H,0,-2.3853053499,-1.7394409681,-4.2340293463 H,0,-3.2131426374,-0.8019007388,-2.9940127181 H,0,-2.2683290947,0.0053951473,-4.2421770002 C,0,0.4765835234,1.4097056241,2.4828317475 H,0,0.3789115057,2.344318677,1.9417660753 H,0,-0.1168376426,1.4167832976,3.3918389553 H,0,1.6039164745,1.4363258249,2.9503833609 O,0,2.8645074673,1.5140240973,3.3275637193 H,0,3.2664985174,1.3198031419,2.4713141284 **FREQUENCIES** -1713.4442 33.5278 49.9743 61.3200 98.0868 112.9535 178.3372 217.3377 244.9853 261.8296 315.4875 373.1802 379.1110 514.5682 558.0007 672.3916 799.4803 828.2378 884.0244 921.0338 981.1968 1006.7986 1048.1975 1058.4412 1105.2697 1118.6890 1125.8026 1146.1716 1165.2066 1213.7669 1282.2349 1337.7765 1352.4125 1386.1250 1391.7923 1413.2648 1436.6183 1498.8999 1509.1591 1547.7258 1552.7747 1562.0844 1574.6665 1767.2611 1836.7420 3120.6304 3130.2881 3160.5963 3181.2566 3187.0172 3214.7971 3241.6827 3247.5047 3249.3044 3251.3378 3267.5448 3859.7008 **ROTATIONAL CONSTANTS** 6.8437932 0.5062406 0.4960990

OH transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
central	**GEOMETRY** C,0,-2.319483455478,-0.807545884003,-0.264280187105 C,0,-1.178161510178,-0.902596809503,-0.938613624805 H,0,-3.135646070478,-1.442888266703,-0.579672990405 H,0,-1.140523577478,-1.585910432303,-1.775381048805 C,0,0.088416524422,-0.160075489603,-0.664485415205 H,0,0.739529621222,-0.167992819403,-1.531642497005 C,0,0.806150901622,-0.539364259703,0.579151432895 C,0,2.124384444922,-0.533739300703,0.775707342495 H,0,0.174150504122,-0.836360797803,1.403019111295 H,0,2.479414629822,-0.836370655903,1.751341628995 C,0,-2.611437226278, 0.098589769697,0.889095437295 H,0,-2.676890811578,-0.464424693303,1.820916774895 H,0,-1.863065637778,0.874984934797,1.000268983595 H,0,-3.574942788178,0.585740110497,0.750957490995 C,0,3.195154624222,-0.165081858003,-0.200112049005 H,0,3.785252804722,0.670562483697,0.175145846195 H,0,3.886906259622,-0.994634311603,-0.341760874505 H,0,2.805036150722,0.116744798797,-1.172099271905 H,0,-0.196262560578,1.000501638397,-0.568580281605 O,0,-0.294801316878,2.345809796397,-0.290219475705 H,0,0.445306191322,2.372452630597,0.330465314495 **FREQUENCIES** -1317.6379 32.5597 59.4330 94.0885 120.5104 138.2293 162.3606 202.9043 213.5835 226.4095 343.4561 411.0558 490.4935 572.5340 595.4810 667.1420 736.5753 777.1640 867.0346 927.2102 959.4729 995.4181 1025.0141 1042.1567 1061.8160 1104.1820 1116.0839 1123.4216 1160.0055 1207.3571 1323.9575 1345.6465 1373.7086 1409.9646 1440.5687 1478.4127 1491.8844 1512.5104 1514.8560 1564.0642 1566.6327 1571.3272 1580.7848 1776.2477 1800.0313 3128.9622 3134.0765 3180.8253 3182.5762 3212.0564 3237.1923 3243.1864 3253.6233 3255.3659 3272.1576 3282.3152 3854.0633 **ROTATIONAL CONSTANTS** 2.7197039 1.0409808 0.9067496	**GEOMETRY** C,0,-0.860355790302,-0.217962671003,-2.218885518094 C,0,-0.858696990202,-0.247934820403,-0.891082017894 H,0,0.087829764898,-0.166839851603,-2.739286642494 H,0,-1.803677647102,-0.294648970403,-0.364449516094 C,0,0.361352724398,-0.248028637303,-0.046662431394 H,0,1.260278949398,-0.055660006703,-0.626241408894 C,0,0.298088052398,0.581940398397,1.178162133106 C,0,1.298118467698,1.325982364097,1.637629580306 H,0,-0.630268281202,0.544978263697,1.733525924906 H,0,2.225265836498,1.353099225397,1.079542438806 C,0,-2.083432880802,-0.236846181503,-3.076247521994 H,0,-2.076686829402,-1.090850519503,-3.753003887494 H,0,-2.988536369202,-0.288247390303,-2.477195297094 H,0,-2.139781742502,0.655394785297,-3.698775747694 C,0,1.253280601998,2.145771190397,2.884789580406 H,0,0.289243708698,2.065215798097,3.379530275306 H,0,2.021776406498,1.827889179897,3.588755858206 H,0,1.438586595898,3.197984393097,2.671368271406 H,0,0.511515847198,-1.363815763903,0.336935004406 O,0,0.640400707398,-2.748135618703,0.544001620906 H,0,0.231122989998,-3.016944049503,-0.288941067194 **FREQUENCIES** -1068.4057 52.7799 62.4816 86.2080 110.6717 120.1186 147.5142 209.0330 212.3093 250.1811 272.3345 324.7910 390.1405 472.0426 554.9863 635.7764 789.1115 834.8025 883.9781 964.6033 970.5253 998.2737 1046.9134 1056.8708 1113.5172 1121.1018 1122.7390 1151.3711 1170.6360 1230.4312 1285.1607 1385.0745 1387.0976 1397.8945 1399.8425 1425.9692 1468.8102 1497.9356 1499.5273 1560.3539 1560.6553 1572.8921 1573.7511 1791.6036 1820.1074 3129.3644 3129.6955 3180.2787 3180.3765 3192.1034 3215.6543 3216.1432 3241.9962 3246.7826 3249.1237 3253.6573 3854.4546 **ROTATIONAL CONSTANTS** 2.4253748 0.8194307 0.6460216

CH_3 transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
terminal	**GEOMETRY** C,0,1.019086585692,-0.249892804787,-1.632997459492 C,0,0.972195097992,-0.172703942987,-0.300030301192 H,0,1.998150785792,-0.325941118787,-2.086016205092 H,0,1.906015233192,-0.216570442287,0.242864095208 C,0,-0.251420649208,-0.055019379487,0.563280429908 H,0,-0.210473989308,0.882906640413,1.114060339308 H,0,-1.145579266308,-0.006181482187,-0.055113135392 C,0,-0.369396788408,-1.215547426687,1.511860250608 C,0,-0.346399208408,-1.191253974787,2.838182124908 H,0,-0.467701060308,-2.177868935287,1.028160200908 H,0,-0.438321093108,-2.139197496787,3.351397677208 C,0,-0.105152874108,-0.191820485487,-2.572674137492 H,0,0.056153114392,-0.754754934687,-3.485731576892 H,0,-1.080094850008,-0.410332714287,-2.153727106192 C,0,-0.211304729908,-0.003873289987,3.738253125508 H,0,-1.077537525408,0.083088954013,4.393420318608 H,0,0.659588090992,-0.108660199287,4.384512872208 H,0,-0.110943410508,0.930130909813,3.195700725508 H,0,-0.239526983108,1.000320150313,-3.007528097792 C,0,-0.443676120108,2.332268725213,-3.503798763992 H,0,-0.644708628808,2.905510617013,-2.609874170592 H,0,0.494102148692,2.573532434413,-3.984191689892 H,0,-1.282710447408,2.251073091613,-4.180385859692 **FREQUENCIES** -1915.0599 25.9846 28.4803 40.8702 47.1622 100.0577 144.6929 204.7083 239.6313 339.1877 358.6621 406.8477 479.4781 515.1935 571.9792 584.0975 610.7592 746.4181 760.7773 793.7680 923.8705 970.9429 1017.2514 1046.2828 1052.2226 1068.8025 1080.9630 1121.3746 1133.0096 1158.5526 1185.6885 1206.9182 1286.4222 1339.6287 1355.8873 1375.5956 1473.4896 1477.4364 1482.0070 1498.0593 1512.8809 1519.3904 1520.6031 1551.6445 1565.3734 1566.7859 1578.3971 1753.4186 1827.6805 3132.5242 3148.2443 3179.2193 3181.4312 3184.8791 3194.7017 3230.7754 3243.4226 3243.7349 3263.2606 3266.1669 3273.2769 3325.4423 3326.9645 **ROTATIONAL CONSTANTS** 4.0510095 0.6471175 0.6072204	**GEOMETRY** C,0,-0.858864811397,-0.943698892911,-2.850215196197 C,0,-0.977476862397,-0.950730884611,-1.531591181297 H,0,0.132820292703,-0.984847751111,-3.283878581397 H,0,-1.964359914697,-0.902950198611,-1.088609927497 C,0,0.169666860303,-0.999939834411,-0.562820036497 H,0,0.090302435203,-1.891789373711,0.059977215703 H,0,1.101542802903,-1.089454969511,-1.123216393797 C,0,0.221743872503,0.210397244189,0.322763252603 C,0,0.122478812503,0.189268692889,1.651975594503 H,0,0.329753897603,1.161454610689,-0.183120094497 H,0,0.008741019903,-0.768483583411,2.144427392003 C,0,-1.997873991197,-0.886184934011,-3.816575192797 H,0,-2.003037585097,-1.756453807711,-4.472188718597 H,0,-2.953770925897,-0.847656339511,-3.300985645897 H,0,-1.925694291797,-0.009387361211,-4.459456905897 C,0,0.205913516803,1.365243699789,2.522214799103 H,0,0.105806945703,2.313079058389,2.003960459303 H,0,-0.433739090697,1.326821447289,3.397892398703 H,0,1.372401291903,1.433597464389,3.040699372003 C,0,2.677926364503,1.560973360889,3.615731881003 H,0,2.788075271403,0.667327486689,4.214010656303 H,0,3.328080673803,1.599718609989,2.753167614003 H,0,2.641994607303,2.477053996489,4.188417637003 **FREQUENCIES** -1920.5754 33.2450 38.4197 55.3277 74.3001 100.1334 187.0658 217.8653 251.9077 260.8424 315.6377 368.1531 375.0596 476.3361 510.1480 565.4971 604.3073 745.8962 823.6669 854.3111 917.4358 990.7794 1027.5382 1049.9009 1059.5393 1106.2488 1125.3182 1135.2026 1146.3203 1158.8548 1190.8591 1216.2055 1282.8452 1347.1953 1382.6193 1390.6963 1411.7000 1434.4374 1477.7367 1479.9366 1498.6057 1520.1805 1521.9627 1546.5859 1553.3482 1562.1989 1575.3632 1768.4367 1836.7392 3116.5221 3128.5309 3155.1505 3178.6370 3183.5336 3184.4018 3213.1829 3237.0931 3240.4830 3246.3812 3247.1538 3259.6392 3323.9878 3326.3029 **ROTATIONAL CONSTANTS** 6.5672429 0.5095228 0.4989985

CH_3 transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
central	**GEOMETRY** C,0,1.621503789397,0.251706381208,-1.834003347206 C,0,1.682571799797,0.257326000908,-0.505441734206 H,0,2.553606608697,0.320957827308,-2.377890280006 H,0,2.660360813597,0.356119309708,-0.054720607506 C,0,0.539308685097,0.161514574008,0.445774143494 H,0,0.854830732997,0.411829090208,1.453196553794 C,0,-0.259261920703,-1.086761159392,0.407589018394 C,0,-1.018349438303,-1.580202757692,1.385744429394 H,0,-0.224466278103,-1.634148222192,-0.522568144706 H,0,-1.546612676803,-2.502940245492,1.189012610794 C,0,0.391164953697,0.169859753208,-2.681182200606 H,0,0.379320521697,-0.749264018092,-3.267463203606 H,0,-0.520286190803,0.203459168908,-2.094035325706 H,0,0.361910676797,0.993261526708,-3.394035477206 C,0,-1.233231002903,-1.000406507492,2.746842794694 H,0,-2.281848223803,-0.743028399792,2.895837335894 H,0,-0.976127515103,-1.721875737892,3.521901964694 H,0,-0.648399516703,-0.102426527092,2.917159453094 H,0,-0.235057517703,1.110716153908,0.197719134894 C,0,-1.140895449903,2.271963467408,-0.016276007106 H,0,-1.170898964803,2.757306757908,0.948280157394 H,0,-0.637972695903,2.830534976708,-0.791656256606 H,0,-2.065228271103,1.799499826208,-0.315020496306 **FREQUENCIES** -1751.5939 32.6248 43.7616 66.4357 80.0648 128.3924 141.0283 178.7527 197.7312 226.8045 324.7139 417.8259 456.5420 468.4726 545.9177 581.0484 594.2826 731.2208 747.2079 771.5899 928.7741 968.2808 1019.3540 1042.8975 1043.5100 1058.6448 1102.4887 1112.6070 1117.3002 1150.0268 1160.0265 1209.3674 1324.4722 1345.6512 1364.6399 1424.4135 1473.4101 1489.7668 1500.0410 1508.9398 1511.1571 1515.9661 1524.6975 1566.2754 1569.6856 1572.5538 1573.3771 1772.6312 1797.6849 3129.1821 3130.0195 3174.5750 3175.4541 3190.1708 3200.3953 3231.2107 3235.1658 3247.0320 3253.0770 3268.8312 3280.6701 3334.3500 3338.8445 **ROTATIONAL CONSTANTS** 2.5338547 1.0483969 0.9104620	**GEOMETRY** C,0,-1.507994099006,-0.015829517294,-1.449908217883 C,0,-0.692358302606,-0.939517333994,-0.953156941683 H,0,-1.557689299106,0.955110519106,-0.977234870083 H,0,-0.670497745506,-1.913048908894,-1.427389707483 C,0,0.230851829794,-0.783717257994,0.195845947117 H,0,0.114172368794,-1.588041243894,0.920281814917 C,0,0.327779910794,0.537726387906,0.844213727317 C,0,0.368553127294,0.740417541706,2.157140931517 H,0,0.414531610194,1.391162417906,0.183914988817 H,0,0.283808996994,-0.112541049494,2.818729560517 C,0,-2.400063215706,-0.218182476694,-2.631907188983 H,0,-2.168219797906,0.489111966106,-3.428199697683 H,0,-2.302229554006,-1.222185096594,-3.036697863483 H,0,-3.445856639206,-0.060930228894,-2.369075894983 C,0,0.522622844694,2.072763884106,2.815343004017 H,0,0.595657475094,2.871769629506,2.082158379317 H,0,-0.321568429706,2.290615863706,3.469076103417 H,0,1.416636640094,2.104741276306,3.437967871517 H,0,1.370108341394,-1.046355028294,-0.261964112983 C,0,2.721551877094,-1.374374687994,-0.779696289583 H,0,2.652307733194,-2.413413927794,-1.067665555383 H,0,2.834863136194,-0.682755046194,-1.601808736483 H,0,3.358311329394,-1.178960381094,0.070657889017 **FREQUENCIES** -1767.4029 36.2673 60.9767 64.6073 92.6192 116.4019 141.7492 210.3008 215.1885 256.8333 279.1040 311.3922 365.7928 434.6731 499.9494 549.4393 623.0792 660.5694 819.9840 855.0643 934.6899 977.3609 1041.9417 1047.1899 1060.2843 1080.4053 1120.9049 1121.2197 1155.2950 1165.2755 1165.7184 1219.0684 1313.7771 1380.2528 1391.7261 1398.1564 1408.1420 1474.9568 1492.6938 1497.6836 1500.8260 1511.1545 1517.7315 1561.0188 1561.5917 1574.9336 1575.5478 1801.3635 1807.4881 3125.4310 3126.2940 3163.2844 3174.4509 3175.3354 3188.6147 3211.4248 3211.8885 3237.2598 3242.0387 3247.8485 3266.1579 3332.6764 3335.6597 **ROTATIONAL CONSTANTS** 1.9531092 0.9708206 0.6974386

iso-C_3H_7 transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
terminal	**GEOMETRY** C,0,1.303885580397,-0.693720233003,-1.054288535708 C,0,1.272837103997,-0.664614290003,0.283985953992 H,0,2.279940827897,-0.677118841203,-1.520221237008 H,0,2.215515563497,-0.651050984703,0.812798471192 C,0,0.056000143397,-0.676781891703,1.164642529292 H,0,0.017950358297,0.248606233797,1.736666466692 H,0,-0.846901949303,-0.696054909703,0.557160496292 C,0,0.055185469697,-1.864004770303,2.086954805092 C,0,0.083969479797,-1.867441507903,3.413450841992 H,0,0.046141006997,-2.820242767603,1.581711341392 H,0,0.086484714297,-2.830976762803,3.905453915292 C,0,0.170351314797,-0.689775574303,-1.975998409208 H,0,0.364186922497,-1.180133309603,-2.923358971408 H,0,-0.781302032803,-1.001372570803,-1.562417187708 C,0,0.109944617797,-0.692552229803,4.339449277792 H,0,-0.757059530103,-0.703093509103,4.999306962492 H,0,0.990487935997,-0.727283358403,4.980197481892 H,0,0.117118596997,0.258085724797,3.817014401092 H,0,-0.075152739303,0.541249741697,-2.355020261708 C,0,-0.388646435203,1.854228830097,-2.717917119808 H,0,0.483013623397,2.109984022697,-3.313280927508 C,0,-0.456161127503,2.594259833097,-1.410612444208 H,0,-0.624002608003,3.662664615397,-1.564312246008 H,0,-1.274326823503,2.225002993597,-0.793939593608 H,0,0.465463764997,2.483053556697,-0.844522444908 C,0,-1.659821909803,1.778522904297,-3.518227273508 H,0,-1.979383371903,2.768129279697,-3.852936842508 H,0,-1.540301779503,1.158708683197,-4.403935838008 H,0,-2.473137904703,1.363115739497,-2.925001740308 **FREQUENCIES** -2014.1257 19.2663 22.7835 36.8611 48.4524 74.6430 139.3743 149.9931 160.3964 194.0923 211.2584 229.7431 263.1901 341.6193 369.9549 412.8428 489.9751 548.9218 562.4246 581.9907 640.7624 758.2534 781.3042 892.5100 920.7101 941.5343 969.6587 972.2751 994.5958 1019.6363 1044.2685 1050.9236 1069.2482 1083.2828 1121.2867 1122.9237 1160.7358 1182.1649 1203.9085 1230.7873 1246.4436 1287.0188 1337.4701 1354.8990 1374.2984 1421.2927 1479.4030 1481.3901 1493.8330 1496.2787 1511.1093 1512.5779 1515.2142 1551.5248 1562.0258 1564.7576 1566.2410 1569.3095 1577.2734 1578.2459 1578.9382 1735.9127 1827.1341 3106.8825 3111.0003 3132.3767 3146.8874 3169.4772 3170.6294 3179.0150 3179.9086 3191.0174 3196.4728 3206.2923 3214.1402 3230.9886 3241.7034 3243.6541 3264.2217 3266.1609 3273.1583 **ROTATIONAL CONSTANTS** 2.1666177 0.4247707 0.3901964	**GEOMETRY** C,0,-1.708045388990,-1.511143257889,-3.376059289497 C,0,-1.723931488490,-1.506630811389,-2.052174485997 H,0,-0.752017533490,-1.518252679389,-3.885193893697 H,0,-2.674813710490,-1.492350612289,-1.534364762297 C,0,-0.504776028490,-1.497642063589,-1.174303467597 H,0,-0.499439929090,-2.385322440189,-0.540418475697 H,0,-0.383965526510,1.556381928089,-1.804625588197 C,0,-0.436913714590,-0.276732474589,-0.304448602897 C,0,-0.446916158290,-0.288105511489,1.031435199103 H,0,-0.401018772490, 0.672583633111,-0.823594235097 H,0,-0.492029267290,-1.246519549289,1.534077851403 C,0,-2.919840854790,-1.510636629889,-4.251395935497 H,0,-2.941306663090,-2.388922593389,-4.895943783297 H,0,-3.833684642890,-1.502556999589,-3.663253292297 H,0,-2.932773823390,-0.640128204689,-4.906670055797 C,0,-0.346471705290, 0.890706488711,1.887218089103 H,0,-0.536607599090,1.833325743411,1.384993430403 H,0,-0.884810313690,0.823485759311,2.826302379403 H,0,0.893885803110,1.025929944811,2.296302300503 C,0,2.219053425410,1.224595682811,2.683539034303 H,0,2.406330420410,0.306455344811,3.232994231303 C,0,2.978933183810,1.309349755111,1.388473344303 H,0,2.806645312810,0.432253085011,0.769383548203 H,0,2.679562223410,2.186102741611,0.816149077603 H,0,4.054835837210,1.387538897411,1.560518079303 C,0,2.226273980210,2.453448077011,3.551043486603 H,0,1.589970527710,2.332034754211,4.424752127703 H,0,3.232616102010,2.682552176411,3.909099692103 H,0,1.876498998810,3.324917397911,2.999527136903 **FREQUENCIES** -2018.0804 12.4233 25.8709 47.3369 62.9367 92.5647 135.0653 155.1370 197.5289 202.4067 217.8524 221.2861 261.8406 271.3535 316.1881 375.3988 397.7672 486.6185 536.6333 554.4256 628.0002 822.8439 850.3640 887.2423 915.0848 934.8154 969.3214 990.0483 996.7817 1028.3705 1051.2876 1060.4167 1106.8787 1123.5560 1125.5637 1147.4888 1162.5892 1182.0597 1212.1563 1231.8821 1246.6805 1283.5701 1347.1037 1379.7475 1390.2246 1412.1906 1421.5993 1434.4336 1480.1074 1496.1191 1498.3447 1511.4620 1514.1055 1545.8657 1553.5245 1562.0671 1562.3101 1569.7260 1575.3181 1577.8609 1579.0845 1751.6316 1836.4080 3106.9525 3111.1386 3115.1121 3128.2580 3153.6313 3169.6240 3171.2725 3178.2993 3185.4491 3189.8658 3205.8951 3212.8023 3213.7601 3234.2975 3239.8593 3246.0641 3246.7012 3261.4905 **ROTATIONAL CONSTANTS** 3.4226919 0.3180855 0.3066212

iso-C_3H_7 transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
central	**GEOMETRY** C,0,2.007336436486,-0.341495110501,-1.811798179999 C,0,1.932357467186,-0.305646056901,-0.482339403599 H,0,2.988919029186,-0.250935479401,-2.256396181699 H,0,2.858410819186,-0.155718419501,0.055505930101 C,0,0.714274815786,-0.415932589601,0.363182717301 H,0,0.939733246786,-0.182852060101,1.398390714201 C,0,-0.104347046314,-1.638080147201,0.230891323701 C,0,-0.906125470814,-2.175143071501,1.153423538401 H,0,-0.048621927314,-2.136288402801,-0.725203178499 H,0,-1.445047132714,-3.072035365001,0.880894797901 C,0,0.879563867286,-0.487922132001,-2.784327865299 H,0,0.940429149486,-1.436812044401,-3.318225447799 H,0,-0.092096506114,-0.437119282201,-2.305213013299 H,0,0.922528427386, 0.296229108199,-3.539408997199 C,0,-1.152403057314,-1.682566274901,2.543484307601 H,0,-2.186576838614,-1.359654209601,2.665118820701 H,0,-0.985242497314,-2.476364447001,3.270662218401 H,0,-0.515758830314,-0.845401248601,2.810997050501 H,0,-0.030642578914,0.579428186899,0.060529311701 C,0,-0.819117186714,1.770536614599,-0.191072958499 H,0,-1.007339137914,1.648250474099,-1.252629404599 C,0,0.109221832886,2.905434392599,0.132836001601 H,0,1.020643229086,2.852443935999,-0.457631866099 H,0,-0.357588943314,3.873250811499,-0.066484695499 H,0,0.388754947886,2.895989603099,1.185495626201 C,0,-2.042807195714,1.615551685799,0.665136358701 H,0,-1.783338171014,1.595859971699,1.722593580201 H,0,-2.738408196214,2.446319007199,0.520806620201 H,0,-2.576484865814,0.696985997599,0.433703075101 **FREQUENCIES** -1904.9832 19.7124 52.3153 65.3314 67.8993 107.4412 112.1035 151.4245 166.5115 173.1282 197.9043 213.3366 229.5752 235.6971 333.4235 389.7544 438.6645 470.8297 547.6824 588.5632 707.2323 744.0400 763.9559 874.0215 924.5785 928.9876 968.9909 970.9119 994.0920 1020.3479 1040.9471 1049.1629 1056.9574 1106.5417 1111.3086 1115.4682 1154.2449 1176.3508 1210.5715 1223.1278 1244.7398 1328.8925 1348.1659 1379.0450 1421.3288 1453.1542 1475.7545 1488.4134 1494.6228 1497.1647 1511.0256 1520.0320 1528.5032 1559.7864 1565.2374 1568.2439 1569.1228 1570.8827 1574.7676 1576.9928 1577.6920 1759.9532 1786.6791 3101.2617 3106.0750 3127.4350 3128.4973 3167.3279 3168.5837 3173.2081 3174.5874 3199.9889 3200.8466 3208.6921 3220.0625 3228.4306 3233.3285 3244.9121 3253.2250 3267.1805 3284.6209 **ROTATIONAL CONSTANTS** 1.0931827 0.9317769 0.6088614	**GEOMETRY** C,0,-1.144091622403,0.427274496804,-2.394314604897 C,0,-1.144912125003,0.505203507004,-1.065861638897 H,0,-0.195200200103,0.361506239304,-2.911673591997 H,0,-2.096620924103,0.578107036704,-0.552628209897 C,0,0.051708385897,0.462221573704,-0.205137886397 H,0,0.976431903897,0.574232936204,-0.765875189597 C,0,0.018122488497,1.296682068004,1.010239677103 C,0,1.061452568597,1.928153410004,1.542750284203 H,0,-0.939644039003,1.365499091404,1.512654164603 H,0,2.018694245097,1.868025730204,1.040302831503 C,0,-2.366788992203,0.432222402004,-3.253406323397 H,0,-2.435148977203,-0.475860945696,-3.852524431697 H,0,-3.271207458603,0.507218431804,-2.655079424597 H,0,-2.356265273303,1.267882032704,-3.952898283997 C,0,1.022886506297,2.738924781504,2.797427213803 H,0,0.026116490897,2.751108774004,3.230893107003 H,0,1.709745337997,2.344778931104,3.546496593703 H,0,1.321400449697,3.770535945904,2.611968376903 H,0,0.147364523197,-0.742250972696,0.200468970103 C,0,0.335050357097,-2.130083945596,0.624337345503 H,0,-0.582855643903,-2.261709132496,1.188857002303 C,0,1.574647955997,-2.108869747796,1.470914041603 H,0,1.782449371197,-3.092198695596,1.901106682303 H,0,2.446538709997,-1.826977715396,0.882327146803 H,0,1.483680243297,-1.403271290596,2.292915802003 C,0,0.384852612197,-2.918246005896,-0.652402550897 H,0,0.460698167097,-3.991331154996,-0.457676009697 H,0,-0.504791630603,-2.755949779696,-1.255746096097 H,0,1.251045894597,-2.640240700596,-1.251162785997 **FREQUENCIES** -1882.1508 18.9891 53.4414 61.1818 87.5851 115.7585 117.1614 153.9437 168.8394 190.6446 203.4531 209.9758 217.3841 271.9253 284.5063 316.0008 375.2776 395.3616 481.1774 569.8126 580.6626 807.7820 829.0344 882.9650 929.6451 963.5031 971.0131 984.7143 995.9168 1044.9447 1046.8301 1057.9618 1111.6208 1118.2393 1118.5583 1148.3221 1169.8566 1182.1624 1216.7490 1236.8080 1244.6871 1284.7420 1383.6952 1386.9157 1398.5058 1408.7053 1437.6054 1476.4306 1495.3232 1495.3977 1498.6239 1501.4390 1520.2430 1560.3943 1561.1887 1561.3170 1567.6563 1575.2088 1575.7244 1576.2041 1577.7745 1779.1433 1801.2231 3098.7355 3102.9514 3124.1525 3124.5664 3166.8391 3167.7704 3172.5813 3172.6561 3182.3649 3196.1849 3209.6560 3209.8097 3209.8595 3217.5673 3227.7576 3233.9950 3244.0859 3245.1714 **ROTATIONAL CONSTANTS** 1.0430813 0.7319893 0.4518485

H_2O_2 transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
terminal	**GEOMETRY** C,0,0.654108922397,-0.675146668404,-1.443450306504 C,0,0.776238947297,-0.448440323204,-0.120023507204 H,0,1.564830228097,-0.825522147404,-2.003566229804 H,0,1.769421279197,-0.471484052604,0.305447491096 C,0,-0.329428494403,-0.209249945904,0.866052996796 H,0,-0.170149257903,0.751575295396,1.351720737296 H,0,-1.286906433103,-0.138908501404,0.354468617896 C,0,-0.389931770603,-1.308915459504,1.891061430596 C,0,-0.192821206803,-1.212318182504,3.199397763896 H,0,-0.606721870803,-2.286720355404,1.483741016496 H,0,-0.273184412403,-2.122783273704,3.777869028196 C,0,-0.568855111303,-0.676962353904,-2.213580462804 H,0,-0.537321308703,-1.239945419404,-3.137751425104 H,0,-1.496992827103,-0.810817597004,-1.673672522704 C,0,0.126075316097,0.010499585396,3.999468748396 H,0,-0.639294462903,0.184967999296,4.754717957596 H,0,1.067953672297,-0.114743781304,4.532313287796 H,0,0.204128835197,0.906967370096,3.393584668696 H,0,-0.680459576103,0.546307048896,-2.670977005604 O,0,-0.655596036803,1.725985662196,-2.977915419104 O,0,0.654679026597,2.069814858896,-2.736615833804 H,0,0.639712599797,2.377903333996,-1.825205577604 **FREQUENCIES** -2368.5292 22.5055 34.1603 41.2867 67.4229 83.8985 142.9166 199.5945 216.8446 307.8960 340.3784 373.8405 438.5459 509.9990 533.2041 580.6635 583.8441 606.9526 760.0527 799.4923 918.1269 968.3326 1024.3732 1041.4912 1053.7281 1067.5613 1075.0291 1094.6512 1121.7251 1139.4067 1158.9512 1201.0924 1266.3321 1293.9531 1332.2798 1354.3604 1373.1850 1481.4513 1493.3811 1496.7769 1512.2719 1525.8020 1556.3352 1565.0603 1571.6142 1579.0291 1679.2495 1826.5388 3134.9483 3151.7229 3183.0065 3187.1198 3215.5689 3231.1705 3246.8478 3262.3614 3269.6630 3282.4811 3298.2830 3857.4193 **ROTATIONAL CONSTANTS** 3.1267590 0.5424601 0.5040341	**GEOMETRY** C,0,-1.328540037508,-1.022429748910,-2.975282593583 C,0,-1.345132479008,-1.034150277510,-1.651539710883 H,0,-0.373234146808,-0.981540310510,-3.484049965783 H,0,-2.294705378608,-1.070093688610,-1.133017637683 C,0,-0.124737582808,-0.982867013810,-0.775619819683 H,0,-0.080127119808,-1.870525470110,-0.144335390383 H,0,0.764082136792,-0.999524584510,-1.408221613083 C,0,-0.104469787608,0.238491865790,0.093012164017 C,0,-0.121023857808,0.226867725690,1.437835411617 H,0,-0.109360073008,1.189689054490,-0.423615512483 H,0,-0.119367584508,-0.727390104510,1.945668845317 C,0,-2.538934247108,-1.067012066710,-3.850754720783 H,0,-2.519659512508,-1.938742283110,-4.503826667183 H,0,-3.452413253708,-1.105816536810,-3.263550804183 H,0,-2.589287859808,-0.191299053610,-4.496906228983 C,0,-0.081344052008,1.409944284990,2.265821039317 H,0,-0.311709977308,2.345343209890,1.769749146217 H,0,-0.534179102908,1.324793187190,3.245839248817 H,0,1.180182204592,1.555624284990,2.591664642317 O,0,2.385737470392,1.579031709290,2.768269329817 O,0,2.778842446392,0.340436061590,2.313661463817 H,0,2.988232596492,0.500671510990,1.388324967917 **FREQUENCIES** -2354.9828 32.6500 52.4647 62.2773 71.0067 101.9099 174.4653 213.4426 222.0225 260.2626 312.1011 334.0008 378.2167 424.2594 486.8416 551.1815 573.4639 586.7943 824.3946 855.8937 916.2174 989.2806 1015.9653 1036.1107 1058.7820 1096.0258 1106.5547 1126.0013 1138.0416 1149.1510 1180.3579 1213.8635 1268.2790 1285.1371 1347.7638 1375.6658 1391.3553 1413.8574 1435.7967 1493.1158 1499.4124 1524.9123 1552.4798 1560.0747 1561.9881 1574.8272 1697.3676 1835.9203 3119.2477 3130.6591 3160.5143 3181.8416 3204.3192 3215.4967 3242.2687 3250.0670 3251.0390 3266.5125 3289.3892 3857.5471 **ROTATIONAL CONSTANTS** 4.3184359 0.4430572 0.4202758

H_2O_2 transition state	*(Z,Z)-hepta-2,5-diene*	*(E,E)-hepta-2,5-diene*
central	**GEOMETRY** C,0,1.911216155599,0.041210125506,-1.798521383894 C,0,1.992415068099,0.003916667106,-0.466882908394 H,0,2.842943688199,0.096524335106,-2.344344011094 H,0,2.977347859699,0.084676749806,-0.029464614294 C,0,0.880571161699,-0.096224174294,0.500584617906 H,0, 1.219311232299,0.023975722106,1.523981270106 C,0,-0.107836907401,-1.173542648694,0.353083395806 C,0,-1.014384216601,-1.527756859594,1.274388775506 H,0,-0.100590883801,-1.709873904194,-0.582811297194 H,0,-1.663558956701,-2.360654053994,1.044497159206 C,0, 0.675451481499,0.049683136806,-2.639557288194 H,0, 0.585676529799,-0.874109076194,-3.212623766694 H,0,-0.228875649701,0.188719487506,-2.058560987494 H,0, 0.727691465899,0.859755527906,-3.365373159694 C,0,-1.200802388701,-0.899365774094,2.620275047706 H,0,-2.257350381201,-0.836544211094,2.873430905406 H,0,-0.730326405901,-1.498292437294,3.401009695506 H,0,-0.787375479101,0.102743355506,2.667943813306 H,0, 0.183872389899,0.968930420006,0.390859442006 O,0,-0.716272772901,1.866185309906,0.425845227906 O,0,-1.704184610201,1.353433618106,-0.375127751294 H,0,-2.224888469701,0.809673824306,0.225494199406 **FREQUENCIES** -2285.4090 49.5305 59.3575 78.2789 93.6727 102.6311 142.1752 161.8024 197.1315 218.9421 279.5778 349.2176 409.6718 465.6137 481.0002 527.4822 600.6550 720.4485 749.9790 765.8440 925.8312 970.7845 1027.1496 1030.6124 1037.9144 1053.5073 1105.5129 1109.0387 1117.6997 1124.8343 1162.9335 1209.3855 1269.9146 1322.5465 1341.0013 1412.7940 1481.1758 1487.5592 1502.0875 1511.2377 1514.7258 1518.9050 1563.7244 1568.5851 1577.9708 1579.4286 1712.5099 1762.1048 3127.1643 3129.9583 3178.3401 3183.5792 3208.3367 3234.7294 3244.3972 3255.8408 3264.0489 3273.3552 3296.9366 3844.9635 **ROTATIONAL CONSTANTS** 1.9027707 1.0321450 0.8421977	**GEOMETRY** C,0,-0.786703354293,0.027860574297,-2.245492722301 C,0,-0.769447225793,0.157978489997,-0.915730131301 H,0,0.155541935807,0.013936806697,-2.778617603501 H,0,-1.709259285493,0.173572093797,-0.380208741101 C,0,0.446389847207,0.240889833097,-0.102656082501 H,0,1.345901230807,0.432471181597,-0.680860431801 C,0,0.382933525907,0.990303065697,1.157057520099 C,0,1.404254904007,1.655805097897,1.695835023599 H,0,-0.560962026993,0.960393100397,1.685963914899 H,0,2.347822633407,1.677906488697,1.165791188999 C,0,-2.021795432793,-0.076990181803,-3.078117888901 H,0,-2.027348853593,-0.995106433203,-3.665441934901 H,0,-2.917976344193,-0.063970547003,-2.463940477801 H,0,-2.086698563093,0.746447676597,-3.788800469501 C,0,1.356879354907,2.388753380697,2.995102723699 H,0,0.374856520807,2.320186988497,3.455002437699 H,0,2.087102014507,1.987420738597,3.697424594699 H,0,1.596556782007,3.443326328797,2.862051213299 H,0,0.629268826007,-0.966041574603,0.250552624899 O,0,0.708592710307,-2.233636581803,0.424803735499 O,0,-0.557597840793,-2.665459213503,0.127940519499 H,0,-0.517833540993,-2.845378045703,-0.816861010201 **FREQUENCIES** -2244.1279 51.6115 62.5120 72.8561 105.2710 117.8443 135.0684 196.3345 209.3851 211.4855 272.5818 275.2761 367.3877 396.6894 430.5413 484.5655 557.6994 589.5908 823.3172 838.3308 964.5578 983.8560 1017.2763 1038.1743 1047.1271 1108.1291 1114.8540 1117.2521 1128.4107 1153.0059 1181.3004 1236.8584 1270.5757 1310.0120 1381.2746 1388.7773 1397.8621 1464.6882 1497.0773 1498.8454 1499.0526 1511.5420 1559.6046 1559.7728 1572.3981 1573.0827 1736.2593 1781.6480 3127.1335 3128.3170 3176.0130 3178.2146 3198.6361 3216.4176 3216.6545 3246.0250 3247.3818 3252.7916 3260.9471 3849.7354 **ROTATIONAL CONSTANTS** 1.7949726 0.7412671 0.5603190

Table S2 Energy values in hartree for obtaining the G3MP2//BH energies for the critical points of the potential surface (continued)

Reactants and products	*cis – cis (Z,Z)*		*trans – trans (E,E)*	
R_1	$-C_4H_7$	$-CH_3$	$-C_4H_7$	$-CH_3$
R_2	-H	$-C_3H_5$	-H	$-C_3H_5$
	Terminal	central	terminal	central
E in hartree	Product			
Hcorr	0.17234	0.172206	0.171857	0.171809
ZPVE	0.162934	0.162518	0.162366	0.162203
MP2/6-31G(d)	-272.272495	-272.283587	-272.276705	-272.287449
QCISD(T)/6-31G(d)	-272.392343	-272.411628	-272.396271	-272.415317
MP2/G3MP2Large	-272.610346	-272.620371	-272.613036	-272.622603
E in hartree	Reactants			
Hcorr	0.186874		0.186413	
ZPVE	0.177192		0.17669	
MP2/6-31G(d)	-272.917384		-272.922369	
QCISD(T)/6-31G(d)	-273.028635		-273.033525	
MP2/G3MP2Large	-273.265266		-273.269026	
E in hartree	OH	CH_3	C_3H_7	OOH
Hcorr	0.012023	0.034741	0.097723	0.018753
ZPVE	0.008718	0.030685	0.091721	0.014959
MP2/6-31G(d)	-75.5209502	-39.668712	-118.005077	-150.4972144
QCISD(T)/6-31G(d)	-75.5369939	-39.6909037	-118.060745	-150.5249665
MP2/G3MP2Large	-75.6145014	-39.7302198	-118.169184	-150.6704185
E in hartree	H_2O	CH_4	C_3H_8	H_2O_2
Hcorr	0.025859	0.05043	0.112995	0.031929
ZPVE	0.022081	0.046627	0.107612	0.027782
MP2/6-31G(d)	-76.1965747	-40.332488	-118.660119	-151.128533
QCISD(T)/6-31G(d)	-76.2075241	-40.3557687	-118.715799	-151.1493745
MP2/G3MP2Large	-76.3149323	-40.4043085	-118.835122	-151.3225012

Pre-reaction complex	*cis – cis (Z,Z)*		*trans – trans (E,E)*	
R_1	$-C_4H_7$	$-CH_3$	$-C_4H_7$	$-CH_3$
R_2	-H	$-C_3H_5$	-H	$-C_3H_5$
	Terminal	central	terminal	central
E in hartree	OH			
Hcorr	0.200867	0.200871	0.200406	0.20033
ZPVE	0.188225	0.188218	0.187712	0.187604
MP2/6-31G(d)	-348.446129	-348.446413	-348.450955	-348.450141
QCISD(T)/6-31G(d)	-348.572748	-348.573088	-348.57749	-348.576789
MP2/G3MP2Large	-348.886562	-348.886582	-348.890148	-348.889237
E in hartree	iso-C_3H_7			
Hcorr	0.286629	0.286587	0.286168	0.286176
ZPVE	0.26973	0.269623	0.269183	0.269185
MP2/6-31G(d)	-390.925723	-390.925821	-390.930661	-390.930728
QCISD(T)/6-31G(d)	-391.092498	-391.092606	-391.097337	-391.097456
MP2/G3MP2Large	-391.43779	-391.438748	-391.441484	-391.441913
E in hartree	OOH			
Hcorr	0.208047	0.208045	0.207593	0.207513
ZPVE	0.194237	0.194205	0.193792	0.193612
MP2/6-31G(d)	-423.42669	-423.427003	-423.431601	-423.430677
QCISD(T)/6-31G(d)	-423.56469	-423.565042	-423.569484	-423.568664
MP2/G3MP2Large	-423.94725	-423.947542	-423.951067	-423.95019

(continued)

Transition state	*cis – cis (Z,Z)*		*trans – trans (E,E)*	
R_1	$-C_4H_7$	$-CH_3$	$-C_4H_7$	$-CH_3$
R_2	-H	$-C_3H_5$	-H	$-C_3H_5$
	Terminal	central	terminal	central
E in hartree	OH			
Hcorr	0.194801	0.195036	0.194362	0.194561
ZPVE	0.182874	0.183211	0.182332	0.182419
MP2/6-31G(d)	-348.418095	-348.418561	-348.422932	-348.422913
QCISD(T)/6-31G(d)	-348.553557	-348.558881	-348.558096	-348.562798
MP2/G3MP2Large	-348.869268	-348.868239	-348.872893	-348.872027
E in hartree	CH_3			
Hcorr	0.219314	0.219085	0.218875	0.218796
ZPVE	0.206956	0.206566	0.206434	0.206153
MP2/6-31G(d)	-312.553244	-312.55187	-312.55772	-312.558123
QCISD(T)/6-31G(d)	-312.695355	-312.69912	-312.6996	-312.704
MP2/G3MP2Large	-312.967424	-312.967868	-312.970579	-312.972604
E in hartree	iso-C_3H_7			
Hcorr	0.281765	0.281591	0.281302	0.281041
ZPVE	0.266922	0.266526	0.266312	0.265781
MP2/6-31G(d)	-390.890592	-390.889995	-390.894625	-390.895992
QCISD(T)/6-31G(d)	-391.065433	-391.070393	-391.069271	-391.076048
MP2/G3MP2Large	-391.407718	-391.408869	-391.410114	-391.412337
E in hartree	OOH			
Hcorr	0.201114	0.201138	0.200703	0.200638
ZPVE	0.188487	0.188396	0.188019	0.187698
MP2/6-31G(d)	-423.37392	-423.374154	-423.378476	-423.378742
QCISD(T)/6-31G(d)	-423.51772	-423.52628	-423.52197	-423.529955
MP2/G3MP2Large	-423.904	-423.902538	-423.907315	-423.907046

Table S3 Selected parameters of the complexes of all the H-abstraction reactions optimized at the BH&HLYP/6-31G(d) level of theory.

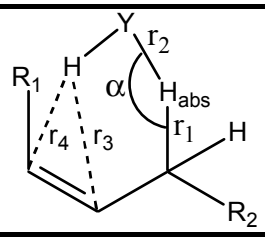
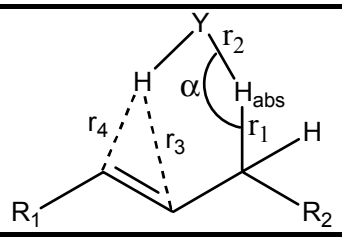
HY=X				
	cis – cis (Z,Z)		*trans – trans (E,E)*	
R_1	$-C_4H_7$	$-CH_3$	$-C_4H_7$	$-CH_3$
R_2	-H	$-C_3H_5$	-H	$-C_3H_5$
	Terminal	central	terminal	central
HY	$R_2(H_{abs}$-Y) in Å			
•OH	2.881	2.823	2.864	2.817
• CH_3	-	-	-	-
• iso-C_3H_7	2.961	3.305	2.961	3.128
•OOH	2.753	2.699	2.784	2.738
HY	r_3(H···C) in Å			
•OH	2.337	2.330	2.355	2.352
• CH_3	-	-	-	-
• iso-C_3H_7	3.060	3.169	3.089	3.351
•OOH	2.302	2.332	2.174	2.284
HY	r_4(H···C) in Å			
•OH	2.506	2.532	2.512	2.505
• CH_3	-	-	-	-
• iso-C_3H_7	3.284	3.221	3.254	3.199
•OOH	2.297	2.332	2.295	2.302
HY	α(C-H_{abs}-X) in degree			
•OH	112.8	115.0	111.4	114.7
• CH_3	-	-	-	-
• iso-C_3H_7	146.5	127.0	145.4	142.2
•OOH	123.2	126.7	121.0	125.2

Table S4 Selected parameters of the TSs of all the H-abstraction reactions optimized at the BH&HLYP/6-31G(d) level of theory.

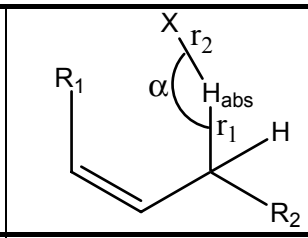
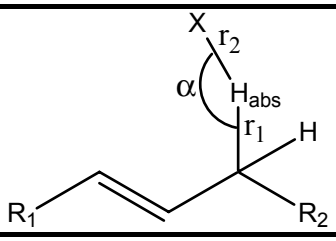
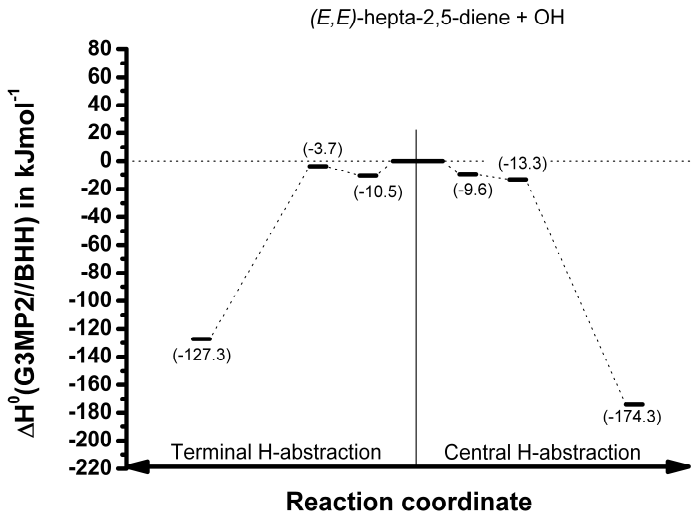
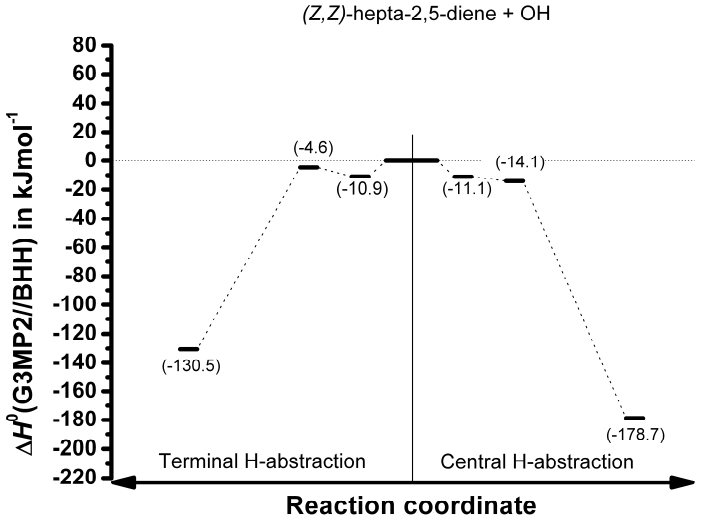
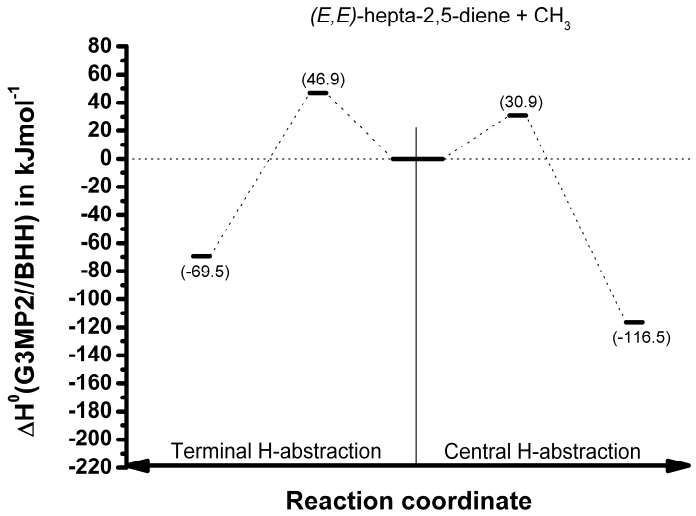
				
	cis – cis (Z,Z)		*trans – trans (E,E)*	
R_1	$-C_4H_7$	$-CH_3$	$-C_4H_7$	$-CH_3$
R_2	-H	$-C_3H_5$	-H	$-C_3H_5$
	terminal	central	terminal	central
X	$R_1(C\text{-}H_{abs})$ in Å			
•OH	1.220	1.199	1.221	1.189
$•CH_3$	1.276	1.250	1.278	1.256
• iso-C_3H_7	1.311	1.280	1.313	1.275
•OOH	1.311	1.277	1.311	1.271
	$R_2(H_{abs}\text{-}X)$ in Å			
•OH	1.321	1.377	1.318	1.406
$•CH_3$	1.436	1.488	1.432	1.484
• iso-C_3H_7	1.398	1.450	1.395	1.463
•OOH	1.219	1.271	1.219	1.282
	$\alpha(C\text{-}H_{abs}\text{-}X)$ in degree			
•OH	174.1	168.2	173.8	169.4
$•CH_3$	177.8	176.6	178.0	178.9
• iso-C_3H_7	177.3	175.1	177.0	176.5
•OOH	171.5	166.4	171.9	170.3

Figure S1 Enthalpy diagrams for the radical-molecule reactions studied.







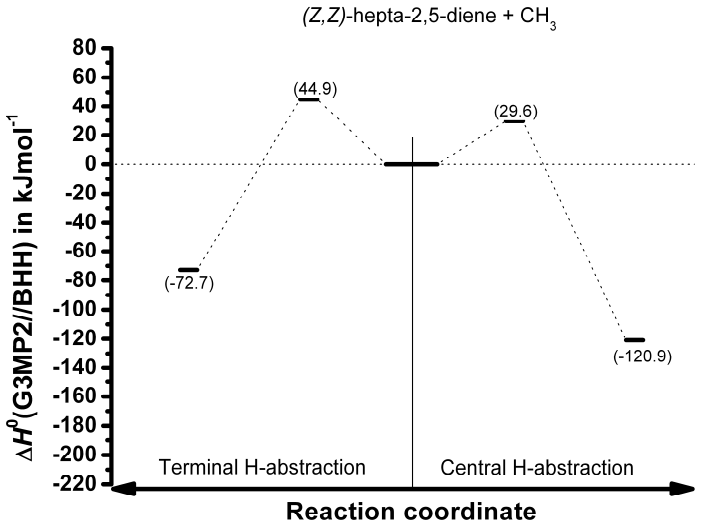


Figure S1 Enthalpy diagrams for the radical-molecule reactions studied.