

Supplementary Material

Contents

A: Cartesian coordinates (angstroms), vibrational frequencies (cm-1) and electronic energies (hartrees) for the stationary points on the cis-3-hexene + OH Potential Energy Surface	calculated	at	BHandHLYP/cc-pVDZ.....	2
B: Cartesian coordinates (angstroms), vibrational frequencies (cm-1) and electronic energies (hartrees) for the stationary points on the cis-3-hexene + OH Potential Energy Surface	calculated	at	BHandHLYP/aug-cc-pVDZ.....	15
C: Plot of the kinetic data for the reaction of cis-3-hexene with OH radicals using allyl ether as reference compound. $[S]_0$ and $[S]_t$ are the concentrations of the cis-3-hexene at times 0 and t, respectively, $[R]_0$ and $[R]_t$ are the concentrations of the reference compound at times 0 and t, respectively.....				28
D: Plot of the kinetic data for the reaction of cis-3-hexene with OH radicals using 3-buten-1-ol as reference compound. $[S]_0$ and $[S]_t$ are the concentrations of the cis-3-hexene at times 0 and t, respectively, $[R]_0$ and $[R]_t$ are the concentrations of the reference compound at times 0 and t, respectively.....				29

A: Cartesian coordinates (angstroms), vibrational frequencies (cm-1) and electronic energies (hartrees) for the stationary points on the cis-3-hexene + OH Potential Energy Surface calculated at BHandHLYP/cc-pVDZ

Reactant a BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	1.499313	-0.33923	-0.53763
C	0.624058	0.837341	-0.23017
C	-0.62408	0.837404	0.230092
H	0.954068	-1.27706	-0.40576
H	1.092786	1.80694	-0.39683
H	-1.09285	1.807057	0.396413
C	-1.49941	-0.33905	0.537828
C	-2.7674	-0.35756	-0.31133
H	-3.34278	0.56501	-0.18104
H	-0.95415	-1.27696	0.406438
H	-1.78531	-0.29558	1.596862
H	-3.41489	-1.19551	-0.0366
C	2.767511	-0.35745	0.311238
H	3.414919	-1.1955	0.036648
H	3.342857	0.565068	0.180435
H	2.526327	-0.44774	1.374695
H	1.784994	-0.29619	-1.59676
H	-2.52595	-0.44826	-1.37469

Frequencies

53.21 60.39 206.43 213.19 249.24 317.24 371.07 531.90 587.46
 786.28 806.99 837.37 878.03 942.82 1049.10 1069.94 1081.01 1105.37
 1128.78 1132.42 1218.03 1311.45 1325.97 1342.52 1371.02 1392.99 1447.88
 1448.01 1485.31 1509.97 1516.20 1521.67 1521.97 1534.51 1536.26 1817.80
 3105.42 3106.66 3116.40 3117.00 3164.97 3177.05 3192.31 3196.15 3198.01
 3199.79 3208.43 3233.72

E(BHandHLYP)..... -235.697484

Reactant b BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	1.593811	0.049687	0.565285
C	0.665141	0.906925	-0.23913
C	-0.6651	0.906868	-0.23913
H	2.18515	0.697167	1.226193
H	1.162521	1.609037	-0.90794
H	-1.16254	1.608951	-0.90794
C	-1.59372	0.049574	0.565301
C	-2.54784	-0.75566	-0.31209
H	-3.1373	-0.09883	-0.96042
H	-1.03571	-0.62521	1.219198
H	-2.18488	0.697002	1.226398
H	-3.24681	-1.33822	0.295208
C	2.547721	-0.75579	-0.31212
H	3.246675	-1.33838	0.295173
H	1.998132	-1.44861	-0.95665
H	3.137216	-0.09909	-0.96055
H	1.035831	-0.62492	1.21937
H	-1.99839	-1.44849	-0.95673

Frequencies

44.92 72.47 206.51 223.09 263.20 299.06 347.36 527.59 610.90 752.88
824.28 832.62
882.48 942.33 1058.56 1063.09 1080.78 1105.55
1130.12 1130.56 1217.00 1313.77 1323.26 1343.86 1369.69 1394.08 1446.77
1448.19 1486.39 1506.87 1517.31 1521.54 1521.84 1534.21 1534.82 1818.29
3103.11 3104.85 3116.07 3116.76 3164.49 3176.61 3192.04 3196.13 3197.03
3199.32 3208.16 3233.45

E(BHandHLYP)..... -235.6974783

PC π c BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.23698	-1.20069	-0.31187
C	-0.42042	-0.70178	0.841978
C	0.764146	-0.08869	0.815203
H	-0.72407	-1.01961	-1.25955
H	-0.86876	-0.87039	1.821062
H	1.201072	0.189278	1.774325
C	1.605577	0.254642	-0.37756
C	2.980993	-0.40321	-0.32289
H	3.518135	-0.12048	0.588333
H	1.099409	-0.02404	-1.30492
H	1.73324	1.344224	-0.41204
H	3.593563	-0.10242	-1.17741
O	-0.97872	2.531048	-0.06862
H	-0.68665	1.720875	0.385774
C	-2.63145	-0.57963	-0.35137
H	-3.21721	-0.9869	-1.18011
H	-3.17913	-0.78425	0.574779
H	-2.57256	0.505272	-0.4725
H	-1.33402	-2.28998	-0.21747
H	2.895548	-1.49386	-0.33221

Frequencies

42.54 55.21 64.06 103.96 125.02 208.15 222.04 260.91 313.85 334.47
376.04 438.55 530.68 589.16 795.25 810.34 840.79 878.47 943.97 1053.13
1074.21 1080.70 1106.75 1132.40 1138.25 1218.85 1311.21 1327.41 1343.41
1370.38 1394.85 1448.71 1452.80 1487.21 1511.81 1515.14 1522.09 1528.00
1535.19 1540.18 1801.34 3108.92 3110.45 3118.91 3120.38 3167.98 3180.31
3194.77 3199.96 3201.70 3208.93 3213.64 3233.47 3739.45

E(BHandHLYP)..... -311.409810

PC π d BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.63123	-0.03431	-0.35168
C	-0.69918	-0.0422	0.8225
C	0.632171	-0.12384	0.819082
H	-2.12029	0.947458	-0.40313
H	-1.19042	0.022953	1.793156
H	1.131665	-0.11691	1.787801
C	1.554747	-0.22374	-0.35865
C	2.536041	-1.38319	-0.22848
H	3.135214	-1.29319	0.683558
H	0.988797	-0.31938	-1.2887
H	2.114751	0.716449	-0.44086
H	3.22478	-1.41079	-1.07727
O	0.30287	2.943003	-0.23875
H	0.152753	2.117253	0.253932
C	-2.70193	-1.11544	-0.24744
H	-3.39578	-1.06337	-1.09099
H	-2.25337	-2.11331	-0.23732
H	-3.28613	-1.00521	0.672012
H	-1.07921	-0.14764	-1.28783
H	2.010583	-2.34202	-0.18631

Frequencies

18.35 38.65 54.51 70.43 137.06 201.82 223.33 268.96 289.26 330.08
 353.33 414.21 519.70 617.83 752.44 827.27 830.98 883.66 944.74 1061.91
 1068.45 1084.84 1105.70 1132.96 1135.41 1214.95 1313.55 1323.61 1343.74
 1370.24 1397.08 1448.88 1450.29 1487.38 1504.19 1517.59 1522.51 1522.74
 1534.01 1534.59 1801.40 3105.71 3114.06 3118.74 3119.39 3166.34 3178.73
 3195.09 3200.33 3201.08 3201.70 3209.82 3234.10 3746.07

E(BHandHLYP)..... -311.408542

PCπ e BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	1.596966	-0.83491	-0.42288
C	0.66709	-0.81227	0.75331
C	-0.66717	-0.81225	0.753323
H	2.061141	-1.82888	-0.47386
H	1.162986	-0.81679	1.724035
H	-1.16306	-0.81676	1.724054
C	-1.59705	-0.83485	-0.42287
C	-2.69561	0.219689	-0.3232
H	-3.29003	0.081688	0.586283
H	-1.04413	-0.71115	-1.3576
H	-2.0613	-1.82879	-0.47383
H	-3.3763	0.157348	-1.17665
O	0.000196	2.423066	0.168744
H	-0.00031	1.526348	0.549962
C	2.695602	0.219548	-0.32318
H	3.37641	0.157024	-1.17654
H	2.272815	1.22757	-0.29589
H	3.289889	0.081591	0.586391
H	1.044058	-0.71114	-1.35762
H	-2.27272	1.227664	-0.29572

Frequencies

56.46 72.89 96.28 112.43 119.52 207.51 245.80 278.51 292.98 343.92
 352.14 458.76 515.06 622.14 741.79 828.50 838.83 885.49 946.37 1061.56
 1067.23 1079.91 1107.09 1135.02 1139.54 1215.70 1313.73 1321.76 1341.97
 1365.86 1392.67 1450.59 1456.91 1487.03 1504.43 1516.02 1525.79 1527.93
 1538.07 1540.68 1799.48 3103.62 3105.11 3119.91 3120.42 3163.47 3176.41
 3193.82 3197.52 3207.20 3210.35 3211.26 3231.96 3731.15

E(BHandHLYP)..... -311.410766

TSf BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	1.746083	0.014055	-0.50548
C	0.815329	0.351604	0.613435
C	-0.49937	0.031836	0.698287
H	1.927085	0.924025	-1.09288
H	1.237337	0.962623	1.410659
H	-1.01921	0.315162	1.610327
C	-1.24183	-0.92081	-0.19462
C	-2.75148	-0.79347	-0.06449
H	-3.06506	0.220345	-0.31934
H	-0.93622	-1.94432	0.061783
H	-0.9453	-0.75509	-1.23264
H	-3.26358	-1.49732	-0.72606
O	-1.07931	1.772178	-0.39965
H	-0.67051	2.450917	0.150813
C	3.079951	-0.53634	-0.01172
H	3.754315	-0.74019	-0.84809
H	2.942325	-1.46775	0.54602
H	3.580333	0.175968	0.652772
H	1.278896	-0.69913	-1.18852
H	-3.07798	-1.00392	0.959888

Frequencies

-282.6342 29.74 81.83 108.72 161.32 175.35 206.05 233.01 261.06 305.31
 369.88 448.40 620.42 727.09 752.21 804.69 831.24 884.36 953.66 998.51
 1071.16 1085.21 1108.24 1120.64 1131.41 1211.83 1300.93 1319.88 1332.70
 1365.60 1387.53 1447.48 1449.47 1486.77 1500.26 1510.28 1520.92 1523.29
 1532.92 1539.88 1678.53 3100.76 3104.86 3117.35 3121.08 3171.78 3180.22
 3193.35 3198.78 3199.41 3218.17 3228.99 3250.87 3872.37

E(BHandHLYP)..... -311.4046259

TSg BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.29224	-1.12666	0.022554
C	-0.5204	-0.22797	0.933788
C	0.6427	0.413882	0.653805
H	-0.68605	-1.41121	-0.84054
H	-0.99618	-0.00658	1.88868
H	1.079867	1.008713	1.451738
C	1.554805	0.143201	-0.50432
C	2.644516	-0.86494	-0.15351
H	3.237272	-0.5287	0.703717
H	0.980692	-0.20599	-1.36507
H	2.00779	1.091227	-0.80417
H	3.329155	-1.00644	-0.99496
O	-0.31762	2.056685	-0.29217
H	-0.97707	2.282078	0.375254
C	-2.59094	-0.4787	-0.45557
H	-3.14667	-1.15007	-1.11665
H	-3.24167	-0.23041	0.39007
H	-2.36795	0.445915	-0.99282
H	-1.52701	-2.05528	0.558383
H	2.218123	-1.83955	0.103226

Frequencies

-280.9368 55.45 67.68 121.91 175.20 211.57 226.88 236.50 266.22 322.61
 393.93 502.71 582.22 733.53 792.24 814.87 839.52 875.09 941.53 1007.75
 1049.06 1081.40 1106.81 1121.13 1128.93 1219.76 1299.40 1323.01 1331.78
 1368.74 1384.23 1439.83 1447.03 1483.77 1510.61 1519.83 1521.01 1523.63
 1539.88 1542.93 1675.60 3109.10 3115.40 3117.70 3156.89 3175.27 3181.54
 3192.95 3196.48 3208.13 3218.05 3221.31 3255.69 3870.48

E(BHandHLYP)..... -311.4058426

TSh BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.59569	0.145889	-0.47655
C	-0.63905	0.472232	0.624052
C	0.709579	0.321783	0.611768
H	-2.00093	1.084802	-0.87648
H	-1.08285	0.930624	1.50757
H	1.23857	0.57029	1.528146
C	1.517053	-0.44002	-0.39536
C	1.76835	-1.8796	0.042252
H	2.268817	-1.91802	1.015553
H	1.024781	-0.42151	-1.36971
H	2.469135	0.080056	-0.52512
H	2.405417	-2.4001	-0.67889
O	1.067292	2.20178	-0.30175
H	0.48528	2.768667	0.218806
C	-2.75171	-0.7308	-0.00416
H	-3.45944	-0.91844	-0.81656
H	-2.39132	-1.69744	0.360785
H	-3.30237	-0.25365	0.813358
H	-1.07669	-0.33732	-1.30705
H	0.832041	-2.43912	0.131614

Frequencies

-284.5523 38.67 60.76 91.19 165.20 189.57 210.70 224.07 253.70 312.93
 365.39 510.58 588.36 733.69 768.21 815.75 834.36 877.77 941.69 1008.81
 1056.99 1081.85 1106.98 1120.22 1125.88 1219.15 1301.35 1320.50 1326.84
 1368.31 1383.10 1447.25 1449.86 1485.95 1507.70 1520.20 1521.34 1522.72
 1533.91 1539.22 1677.55 3104.23 3115.31 3117.13 3158.12 3177.14 3182.10
 3195.20 3197.62 3198.40 3210.11 3216.65 3256.45 3868.60

E(BHandHLYP)..... -311.4041443

TSi BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.42002	-0.75674	-0.32821
C	-0.57442	-0.22196	0.791288
C	0.767803	-0.36838	0.925563
H	-0.90193	-0.61564	-1.27946
H	-1.12469	0.111916	1.667865
H	1.218275	-0.03426	1.859441
C	1.721248	-0.85118	-0.11812
C	2.674198	0.250853	-0.57811
H	2.103617	1.086243	-0.99015
H	2.304382	-1.68489	0.294613
H	1.17703	-1.24978	-0.97731
H	3.366394	-0.11881	-1.3402
O	-0.35258	1.720975	-0.06979
H	0.138536	2.152955	0.639478
C	-2.79608	-0.11234	-0.38932
H	-3.3866	-0.52614	-1.21114
H	-3.3531	-0.28455	0.538196
H	-2.70018	0.965198	-0.53249
H	-1.529	-1.8407	-0.18777
H	3.271584	0.629089	0.258691

Frequencies

-283.62 63.32 90.53 122.54 176.92 215.08 225.36 240.37 285.42 295.64
 360.57 474.07 614.84 731.82 750.66 826.09 829.37 885.38 952.54 1000.93
 1059.51 1085.85 1107.94 1123.20 1132.46 1215.45 1300.59 1328.10 1333.55
 1368.96 1385.83 1440.62 1447.70 1487.30 1500.34 1514.20 1520.24 1522.27
 1538.95 1542.74 1676.70 3101.39 3105.49 3117.95 3121.64 3173.51 3180.17
 3192.52 3197.89 3218.84 3221.74 3230.55 3250.31 3873.71

E(BHandHLYP)..... -311.4063144

PRODj BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	1.772495	-0.30147	-0.44012
C	0.853403	-0.10317	0.715276
C	-0.58213	0.270642	0.528126
H	1.445912	0.336002	-1.26775
H	1.152414	-0.49161	1.686818
H	-0.9909	0.585026	1.50138
C	-1.43838	-0.88787	0.019828
C	-2.9106	-0.52902	-0.10213
H	-3.04332	0.317737	-0.77832
H	-1.30791	-1.73638	0.700384
H	-1.04615	-1.19827	-0.95516
H	-3.4909	-1.37309	-0.48558
O	-0.73242	1.319358	-0.41372
H	-0.23016	2.070461	-0.10103
C	3.234935	-0.03327	-0.10587
H	3.878669	-0.21788	-0.97058
H	3.578668	-0.67913	0.70891
H	3.384349	1.003635	0.21074
H	1.681158	-1.33699	-0.81058
H	-3.33021	-0.25021	0.870672

Frequencies

46.89 67.83 109.73 209.15 236.84 257.45 269.39 319.12 342.48 371.79
474.97 541.52 684.96 795.96 816.63 858.00 932.85 1013.70 1053.49 1079.84
1092.29 1102.97 1125.28 1186.86 1209.55 1293.26 1309.66 1347.17 1360.58
1365.17 1425.64 1443.51 1449.44 1452.34 1473.71 1505.59 1508.54 1519.33
1522.04 1530.09 1534.95 3034.04 3053.26 3115.97 3118.22 3123.72 3157.02
3163.34 3189.25 3190.55 3195.53 3221.68 3237.38 3956.60

E(BHandHLYP)..... -311.451903

PRODI BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.43302	-0.63386	-0.40381
C	-0.51015	-0.03868	0.602892
C	0.634011	0.83577	0.1981
H	-1.47566	0.022704	-1.27874
H	-0.5332	-0.42511	1.619159
H	1.060959	1.2929	1.104088
C	1.757011	0.090871	-0.52045
C	2.450604	-0.95065	0.340353
H	2.879085	-0.50127	1.242908
H	1.341203	-0.37147	-1.42242
H	2.475531	0.843429	-0.86124
H	3.266621	-1.42938	-0.20769
O	0.217999	1.850143	-0.7011
H	-0.50089	2.329257	-0.29104
C	-2.83462	-0.89278	0.135414
H	-3.47159	-1.35504	-0.62399
H	-2.80732	-1.56372	1.000421
H	-3.31302	0.037978	0.455702
H	-1.01564	-1.58789	-0.76925
H	1.759823	-1.73742	0.659298

Frequencies

47.54 69.59 114.90 207.73 226.36 250.76 265.04 338.08 369.98 372.07
458.47 540.52 654.67 794.42 823.58 860.66 930.59 1021.52 1069.79 1081.34
1095.29 1101.85 1127.46 1171.66 1213.42 1293.29 1312.07 1323.46 1349.93
1387.14 1429.35 1440.12 1449.48 1456.84 1474.14 1506.92 1519.94 1522.38
1523.27 1530.17 1534.71 3034.00 3058.93 3116.13 3116.45 3128.44 3155.37
3165.24 3190.63 3190.76 3196.10 3198.00 3244.34 3952.05

E(BHandHLYP)..... -311.450951

PRODm BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	1.707428	-0.59915	-0.19894
C	0.541142	-0.51016	0.726367
C	-0.86978	-0.62584	0.24407
H	2.367085	-1.42083	0.117926
H	0.717357	-0.21821	1.758679
H	-1.52142	-0.81101	1.112271
C	-1.38759	0.625403	-0.46316
C	-1.49885	1.840849	0.440756
H	-2.16196	1.645731	1.290673
H	-0.731	0.837975	-1.31435
H	-2.36698	0.373277	-0.8831
H	-1.90638	2.696492	-0.10448
O	-1.01232	-1.67599	-0.6972
H	-0.67349	-2.47681	-0.29936
C	2.540869	0.681679	-0.25712
H	3.403516	0.558282	-0.9191
H	1.948575	1.523523	-0.62844
H	2.917011	0.95287	0.734701
H	1.351729	-0.86603	-1.19831
H	-0.52501	2.137331	0.842359

Frequencies

39.88 63.19 117.28 213.62 228.51 256.96 282.00 325.75 367.35 373.35
464.56 542.89 648.98 774.47 832.49 862.19 924.95 1009.47 1060.74 1080.53
1089.88 1102.11 1129.41 1174.55 1211.43 1292.41 1314.69 1323.94 1352.87
1384.64 1429.64 1436.46 1443.50 1456.70 1470.66 1511.63 1518.14 1522.84
1523.94 1531.62 1535.47 3055.18 3071.00 3115.33 3116.82 3125.32 3163.58
3167.28 3190.45 3192.22 3196.50 3198.81 3247.64 3953.13

E(BHandHLYP)..... -311.450265

PRODn BHandHLYP/cc-pVDZ

Cartesian Coordinates

C	-1.48982	-0.83638	0.059615
C	-0.65953	0.410874	0.357347
C	0.775863	0.102386	0.640137
H	-1.07192	-1.31822	-0.83143
H	-1.09403	0.896152	1.245524
H	1.05773	-0.0909	1.67326
C	1.723052	-0.29508	-0.43871
C	3.174259	0.05458	-0.13198
H	3.304097	1.134802	-0.01361
H	1.652525	-1.38314	-0.60914
H	1.407601	0.169933	-1.37799
H	3.839507	-0.27916	-0.93339
O	-0.80132	1.260944	-0.76815
H	-0.31533	2.06548	-0.59282
C	-2.96321	-0.5309	-0.15697
H	-3.52425	-1.44131	-0.38635
H	-3.40814	-0.08129	0.737467
H	-3.09095	0.171538	-0.98288
H	-1.36433	-1.53944	0.890338
H	3.507205	-0.42079	0.796634

Frequencies

46.84 67.88 109.72 209.16 236.84 257.45 269.40 319.14 342.46 371.72
474.97 541.31 684.97 795.96 816.62 858.01 932.86 1013.69 1053.50 1079.83
1092.30 1102.98 1125.28 1186.85 1209.51 1293.26 1309.65 1347.15 1360.58
1365.18 1425.63 1443.50 1449.45 1452.34 1473.68 1505.59 1508.54 1519.33
1522.05 1530.10 1534.96 3033.99 3053.29 3115.96 3118.22 3123.73 3157.07
3163.35 3189.27 3190.53 3195.53 3221.67 3237.57 3956.58

E(BHandHLYP)..... -311.451903

B: Cartesian coordinates (angstroms), vibrational frequencies (cm-1) and electronic energies (hartrees) for the stationary points on the cis-3-hexene + OH Potential Energy Surface calculated at BHandHLYP/aug-cc-pVDZ.

Reactant a BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.59879	-0.24678	0.200982
C	-0.64856	0.58114	-0.60918
C	0.681889	0.576034	-0.57704
H	-1.06076	-0.8802	0.905958
H	-1.1244	1.256069	-1.3167
H	1.196377	1.252945	-1.255
C	1.585098	-0.23938	0.297049
C	2.489995	0.631934	1.165457
H	3.096132	1.300894	0.550805
H	1.009699	-0.91347	0.931254
H	2.212648	-0.87154	-0.33962
H	3.168048	0.018942	1.761789
C	-2.50405	-1.11046	-0.67462
H	-3.21572	-1.67213	-0.06702
H	-3.07347	-0.49561	-1.37493
H	-1.91742	-1.82213	-1.25794
H	-2.22484	0.42272	0.799837
H	1.900223	1.248565	1.84575

Frequencies

47.11 49.12 201.60 210.31 241.69 308.81 370.81 526.21 586.83 773.54
 798.15 831.32 875.57 941.33 1039.12 1064.14 1076.63 1104.55 1126.17
 1129.10 1215.96 1311.46 1322.71 1342.75 1366.18 1386.66 1443.74 1443.96
 1486.35 1512.27 1516.58 1523.16 1523.72 1533.64 1535.54 1802.81 3105.36
 3106.52 3114.93 3115.44 3164.96 3175.78 3188.58 3192.03 3193.36 3197.56
 3210.10 3234.18

E(BHandHLYP)..... -235.709965

Reactant b BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.35288	-0.34796	-0.95119
C	-0.47184	0.821893	-0.63568
C	0.780634	0.812052	-0.18584
H	-1.57145	-0.34363	-2.02421
H	-0.93314	1.793485	-0.79613
H	1.252069	1.776312	-0.01124
C	1.644696	-0.37148	0.125515
C	2.170956	-0.34296	1.558542
H	2.73817	0.570618	1.749199
H	1.107014	-1.30336	-0.04863
H	2.4974	-0.37407	-0.56153
H	2.829563	-1.19173	1.750559
C	-2.67162	-0.3032	-0.18294
H	-3.31335	-1.14204	-0.45782
H	-2.49739	-0.34636	0.893538
H	-3.21707	0.618912	-0.39485
H	-0.84115	-1.28802	-0.74565
H	1.349687	-0.38013	2.276288

Frequencies

40.40 59.37 202.65 221.64 260.44 291.18 346.38 521.97 611.35 737.42
819.54 823.83 879.80 940.59 1045.95 1059.01 1076.33 1104.41 1127.18
1127.70 1214.76 1313.72 1319.63 1343.26 1364.94 1389.40 1443.23 1444.67
1487.30 1508.10 1519.03 1523.62 1523.71 1533.12 1534.76 1802.84 3103.26
3105.02 3114.65 3115.30 3164.48 3175.07 3188.34 3191.95 3192.42 3196.79
3210.57 3234.43

E(BHandHLYP)..... -235.709996

PC π c BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.23035	-1.21599	-0.3629
C	-0.43274	-0.65814	0.77676
C	0.758885	-0.05951	0.738065
H	-0.73837	-1.01967	-1.31495
H	-0.89571	-0.77329	1.754151
H	1.181082	0.263849	1.686562
C	1.625407	0.204999	-0.45605
C	2.990791	-0.46815	-0.33258
H	3.51036	-0.13702	0.568862
H	1.136935	-0.1235	-1.3728
H	1.775243	1.28533	-0.55105
H	3.621094	-0.22766	-1.1899
O	-0.97446	2.69945	0.238244
H	-0.67485	1.809352	0.48606
C	-2.6568	-0.67177	-0.39948
H	-3.22687	-1.13499	-1.20601
H	-3.1777	-0.877	0.538119
H	-2.66256	0.40775	-0.55699
H	-1.27141	-2.30442	-0.25194
H	2.887289	-1.55301	-0.27896

Frequencies

36.11 44.70 49.63 59.03 119.91 197.55 215.50 244.12 302.87 327.91
 372.99 434.86 524.05 589.18 780.13 800.52 835.62 876.02 942.09 1045.48
 1070.10 1075.82 1105.43 1128.90 1132.18 1215.89 1312.49 1323.76 1344.21
 1367.38 1390.64 1444.37 1449.01 1489.05 1511.89 1516.20 1524.22 1527.62
 1534.65 1534.97 1790.34 3106.82 3107.73 3117.31 3117.74 3169.07 3179.36
 3192.02 3196.27 3198.00 3201.09 3211.32 3234.50 3744.84

E(BHandHLYP)..... -311.432899

PC π d BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.37162	-0.85688	-0.40818
C	-0.56887	-0.32805	0.741512
C	0.632368	0.251733	0.713394
H	-2.30061	-0.28261	-0.48117
H	-1.03355	-0.45502	1.716435
H	1.057254	0.554675	1.66746
C	1.501395	0.530066	-0.47543
C	2.884957	-0.09994	-0.33402
H	3.388239	0.258236	0.566385
H	1.029744	0.179845	-1.39307
H	1.6168	1.613545	-0.58017
H	3.51405	0.148306	-1.19
O	-1.3754	2.875173	0.178179
H	-0.9669	2.030297	0.429
C	-1.71913	-2.33339	-0.23368
H	-2.33747	-2.68709	-1.05991
H	-0.81656	-2.94551	-0.19737
H	-2.2723	-2.49871	0.693142
H	-0.84451	-0.71178	-1.35067
H	2.814411	-1.18676	-0.26705

Frequencies

30.33 34.88 39.64 56.41 120.20 202.69 220.11 261.29 291.25 330.42
 355.93 421.63 524.77 612.32 749.97 824.76 826.78 879.65 941.20 1054.63
 1059.94 1079.17 1105.22 1129.21 1130.54 1214.73 1315.43 1322.59 1344.49
 1367.62 1391.10 1444.30 1446.18 1488.90 1508.02 1519.80 1524.96 1525.17
 1533.75 1535.79 1790.52 3107.66 3111.71 3116.96 3117.56 3168.11 3178.51
 3192.05 3195.72 3196.12 3199.91 3211.90 3235.27 3743.39

E(BHandHLYP)..... -311.432928

PCπe BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	1.594798	-0.89724	-0.42157
C	0.666862	-0.8162	0.752534
C	-0.66712	-0.81628	0.75258
H	2.138033	-1.84602	-0.36473
H	1.161259	-0.76293	1.719983
H	-1.16146	-0.76311	1.720064
C	-1.59511	-0.89738	-0.42147
C	-2.60611	0.246755	-0.44737
H	-3.187	0.278182	0.476692
H	-1.03763	-0.91659	-1.35727
H	-2.13835	-1.84615	-0.36463
H	-3.30464	0.128068	-1.27678
O	0.001719	2.517017	0.836491
H	0.000294	1.546679	0.874628
C	2.605828	0.246868	-0.44748
H	3.304038	0.1284	-1.27719
H	2.107915	1.211162	-0.56345
H	3.187052	0.277997	0.476378
H	1.037298	-0.91646	-1.35735
H	-2.10819	1.210985	-0.5638

Frequencies

23.23 25.57 50.95 57.34 111.68 203.32 230.30 260.74 292.43 335.05
 349.23 440.91 522.84 613.49 741.60 822.17 825.86 880.86 940.49 1055.32
 1060.45 1074.65 1104.82 1128.89 1130.73 1214.05 1312.82 1318.44 1343.15
 1362.92 1387.79 1442.76 1448.30 1488.75 1509.09 1519.21 1519.88 1527.46
 1535.10 1536.89 1791.21 3107.32 3108.93 3115.59 3116.44 3167.70 3178.50
 3188.74 3193.71 3195.20 3199.82 3208.86 3232.35 3749.15

E(BHandHLYP)..... -311.432907

TSf BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	1.743855	-0.00333	-0.51178
C	0.807559	0.346075	0.599322
C	-0.49562	0.003826	0.696513
H	1.928854	0.894991	-1.10978
H	1.226501	0.956237	1.395447
H	-1.02073	0.298469	1.598268
C	-1.23943	-0.92355	-0.22056
C	-2.74936	-0.83574	-0.05305
H	-3.09898	0.171891	-0.27399
H	-0.91046	-1.9482	-0.01711
H	-0.97111	-0.70686	-1.25381
H	-3.25421	-1.53283	-0.72312
O	-1.0848	1.866033	-0.37393
H	-0.5829	2.518606	0.121078
C	3.077062	-0.54224	0.00124
H	3.751334	-0.76093	-0.82791
H	2.935843	-1.46035	0.574097
H	3.570399	0.18391	0.650856
H	1.284793	-0.72966	-1.18169
H	-3.04531	-1.08387	0.968946

Frequencies

-167.41 31.53 72.43 73.44 149.66 169.45 184.59 223.22 252.84 300.92
 364.66 455.76 620.42 665.04 744.36 803.25 832.69 882.31 952.06 1008.47
 1068.90 1084.39 1108.49 1120.30 1132.15 1209.59 1305.92 1321.93 1331.73
 1364.53 1385.70 1445.67 1447.59 1490.93 1506.75 1514.37 1525.27 1526.29
 1533.64 1538.29 1692.34 3101.48 3107.58 3116.41 3118.65 3168.81 3176.74
 3189.12 3195.18 3196.66 3215.46 3222.30 3260.24 3919.91

E(BHandHLYP)..... -311.43053

TSg BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.30113	-1.08221	-0.03377
C	-0.53815	-0.17332	0.873951
C	0.66607	0.396999	0.643027
H	-0.74366	-1.26579	-0.95116
H	-1.03324	0.071692	1.810428
H	1.090945	0.991191	1.443941
C	1.594922	0.102861	-0.49395
C	2.645408	-0.93908	-0.1137
H	3.222203	-0.6186	0.756529
H	1.035139	-0.23209	-1.36605
H	2.086725	1.032589	-0.77998
H	3.343987	-1.09918	-0.93654
O	-0.24764	2.163783	-0.31492
H	-0.94264	2.377845	0.312972
C	-2.68816	-0.54015	-0.37341
H	-3.239	-1.24757	-0.99509
H	-3.27358	-0.36589	0.53219
H	-2.60833	0.403211	-0.91403
H	-1.41282	-2.05181	0.463774
H	2.181579	-1.89653	0.129511

Frequencies

-171.16 44.79 52.34 84.83 154.86 185.75 213.66 219.21 247.35 311.79
 392.18 501.41 585.62 669.62 776.06 813.24 832.00 874.01 940.94 1014.00
 1051.83 1077.23 1106.62 1118.13 1125.96 1217.76 1302.16 1321.09 1330.54
 1367.54 1382.28 1440.19 1441.44 1488.04 1510.48 1520.94 1523.87 1524.79
 1536.22 1542.41 1690.69 3099.49 3114.57 3116.74 3154.16 3175.35 3178.87
 3191.14 3193.91 3204.19 3206.82 3220.16 3262.14 3917.62

E(BHandHLYP)..... -311.4309709

TSh BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.5988	0.124856	-0.49106
C	-0.63976	0.473038	0.600627
C	0.701102	0.293535	0.606519
H	-1.99753	1.051671	-0.91602
H	-1.0813	0.94562	1.474621
H	1.228189	0.556874	1.516379
C	1.511844	-0.45946	-0.40241
C	1.787506	-1.89279	0.048177
H	2.293375	-1.91138	1.015867
H	1.012671	-0.45977	-1.37015
H	2.454881	0.069011	-0.54145
H	2.42604	-2.40655	-0.67221
O	1.075158	2.268622	-0.28074
H	0.468201	2.821503	0.218082
C	-2.76176	-0.7275	0.013171
H	-3.46619	-0.9369	-0.79308
H	-2.40678	-1.68016	0.409674
H	-3.30708	-0.21716	0.809887
H	-1.0876	-0.39063	-1.30275
H	0.861079	-2.46121	0.146949

Frequencies

-186.96 35.56 58.29 81.46 151.58 182.99 206.06 216.30 248.05 306.70
 365.50 519.11 589.08 675.89 762.83 816.02 830.54 876.10 939.95 1015.39
 1052.29 1076.25 1106.42 1119.83 1123.96 1218.70 1304.41 1319.37 1329.59
 1367.53 1382.04 1441.70 1445.73 1488.78 1510.80 1521.68 1524.01 1525.06
 1534.54 1542.12 1687.86 3107.89 3114.69 3116.40 3155.99 3175.20 3179.35
 3191.97 3195.12 3195.69 3208.38 3220.33 3262.57 3918.96

E(BHandHLYP)..... -311.4305934

TSi BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.6886	-0.82696	-0.13612
C	-0.75304	-0.25617	0.878543
C	0.592756	-0.16941	0.783001
H	-1.14871	-1.0864	-1.04602
H	-1.21807	0.146459	1.774759
H	1.125272	0.231669	1.638381
C	1.448493	-0.77754	-0.28893
C	2.85371	-0.19493	-0.33032
H	2.816939	0.874588	-0.53219
H	1.507985	-1.85622	-0.10881
H	0.967077	-0.64984	-1.25799
H	3.448414	-0.67539	-1.10835
O	0.386496	1.802589	-0.20556
H	-0.14555	2.266246	0.445983
C	-2.8395	0.118657	-0.46956
H	-3.52768	-0.34296	-1.17918
H	-3.40798	0.376257	0.42694
H	-2.46046	1.04143	-0.90949
H	-2.10053	-1.76256	0.259218
H	3.368366	-0.34591	0.621509

Frequencies

-174.64 43.71 71.96 80.64 143.51 188.72 196.68 228.85 274.65 291.24
352.64 457.22 626.32 676.79 727.97 808.97 830.69 885.07 952.34 1007.42
1068.13 1084.69 1107.60 1120.75 1130.54 1210.53 1305.38 1323.70 1333.73
1365.74 1384.63 1441.34 1447.07 1491.78 1503.98 1509.90 1524.36 1526.11
1535.07 1538.14 1691.01 3093.93 3101.93 3116.60 3119.06 3169.72 3177.19
3188.59 3194.69 3204.41 3216.71 3222.52 3258.45 3920.83

E(BHandHLYP)..... -311.430996

PRODj BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	1.755273	-0.31253	-0.41876
C	0.847466	-0.02046	0.725303
C	-0.59683	0.308954	0.530184
H	1.46507	0.297674	-1.27666
H	1.172782	-0.29084	1.724639
H	-1.02511	0.589683	1.499816
C	-1.4053	-0.86261	-0.02101
C	-2.89418	-0.5687	-0.12333
H	-3.07902	0.273601	-0.7885
H	-1.23704	-1.72411	0.629734
H	-1.00558	-1.12079	-1.00403
H	-3.43333	-1.43548	-0.5091
O	-0.7721	1.387997	-0.38426
H	-0.26457	2.134043	-0.07826
C	3.228002	-0.09456	-0.09171
H	3.859912	-0.34712	-0.94451
H	3.53891	-0.71634	0.750661
H	3.42005	0.946421	0.174308
H	1.617144	-1.35593	-0.73923
H	-3.31259	-0.32441	0.85603

Frequencies

47.18 71.09 106.33 193.71 229.04 247.38 267.33 320.35 325.16 345.71
 470.77 523.31 684.34 790.64 808.95 854.19 932.70 1006.52 1053.29 1081.92
 1091.08 1099.03 1126.16 1176.27 1209.75 1292.19 1308.87 1348.85 1358.36
 1364.59 1419.87 1441.62 1447.06 1453.53 1471.58 1507.71 1512.62 1523.54
 1525.47 1530.77 1534.12 3036.71 3079.39 3114.74 3116.68 3125.08 3148.52
 3165.12 3184.38 3185.41 3191.29 3213.59 3244.65 3990.61

E(BHandHLYP)..... -311.475424

PRODI BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.39273	-0.62603	-0.40846
C	-0.52824	0.02721	0.613122
C	0.646385	0.870198	0.234075
H	-1.458	0.014613	-1.29065
H	-0.62746	-0.28068	1.648322
H	1.087874	1.284656	1.14766
C	1.736111	0.109098	-0.51557
C	2.376466	-0.99626	0.309584
H	2.81376	-0.60028	1.229055
H	1.305224	-0.29922	-1.43201
H	2.490302	0.837023	-0.82051
H	3.173801	-1.4844	-0.25199
O	0.264137	1.942153	-0.62571
H	-0.44703	2.425801	-0.21529
C	-2.78856	-0.95865	0.105434
H	-3.37878	-1.46204	-0.66168
H	-2.73912	-1.61703	0.975429
H	-3.32215	-0.054	0.402326
H	-0.91477	-1.55467	-0.75444
H	1.650531	-1.7617	0.589903

Frequencies

49.60 68.17 117.86 194.37 228.24 245.62 250.30 320.77 342.94 363.82
454.48 529.92 649.67 793.41 817.97 855.42 929.75 1022.07 1061.24 1077.25
1091.84 1096.46 1124.56 1162.94 1213.76 1292.83 1309.81 1320.75 1350.40
1382.59 1425.49 1439.62 1446.97 1453.23 1473.41 1507.69 1523.68 1525.04
1527.53 1530.90 1538.20 3036.48 3084.87 3115.04 3115.44 3131.73 3146.93
3166.36 3185.63 3188.88 3191.85 3194.17 3250.38 3987.90

E(BHandHLYP)..... -311.475097

PRODm BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	1.571688	0.117054	-0.46144
C	0.601617	-0.01815	0.660358
C	-0.78646	-0.53066	0.449152
H	1.401958	-0.68306	-1.18529
H	0.83642	0.455341	1.607436
H	-1.28721	-0.59334	1.422123
C	-1.63618	0.347317	-0.46515
C	-1.88066	1.740594	0.09315
H	-2.37148	1.695187	1.068088
H	-1.1476	0.406727	-1.43984
H	-2.58565	-0.16838	-0.62089
H	-2.52339	2.316282	-0.57385
O	-0.77985	-1.82278	-0.15479
H	-0.22453	-2.39986	0.361689
C	3.026048	0.114938	-0.00542
H	3.702112	0.245963	-0.8516
H	3.215699	0.92429	0.702955
H	3.280333	-0.82521	0.487288
H	1.375216	1.052638	-1.00603
H	-0.94818	2.2945	0.216279

Frequencies

49.67 68.27 117.89 194.44 228.27 245.70 250.39 320.84 343.42 363.87
454.49 529.93 649.65 793.38 818.00 855.44 929.75 1022.05 1061.25 1077.26
1091.85 1096.47 1124.56 1163.01 1213.74 1292.85 1309.82 1320.79 1350.40
1382.60 1425.52 1439.63 1446.98 1453.27 1473.41 1507.68 1523.69 1525.04
1527.53 1530.90 1538.21 3036.58 3084.72 3114.97 3115.37 3131.64 3146.91
3166.26 3185.55 3188.80 3191.76 3194.09 3250.38 3987.60

E(BHandHLYP)..... -311.475097

PRODn BHandHLYP/aug-cc-pVDZ

Cartesian Coordinates

C	-1.45973	-0.81188	0.008228
C	-0.6638	0.433207	0.390689
C	0.782708	0.148197	0.633461
H	-1.05415	-1.20225	-0.92766
H	-1.098	0.843756	1.310102
H	1.107236	0.025634	1.66169
C	1.69697	-0.29452	-0.45576
C	3.166489	-0.01771	-0.16019
H	3.347667	1.05235	-0.04436
H	1.569889	-1.37419	-0.62494
H	1.4038	0.184669	-1.39224
H	3.803586	-0.38253	-0.96727
O	-0.84553	1.370988	-0.66708
H	-0.34525	2.157157	-0.46843
C	-2.95082	-0.5494	-0.13793
H	-3.48067	-1.46689	-0.39924
H	-3.37501	-0.17381	0.796355
H	-3.14083	0.189211	-0.91538
H	-1.28609	-1.57145	0.774294
H	3.480525	-0.51046	0.762545

Frequencies

47.15 70.99 106.31 193.63 229.01 247.31 267.38 320.34 325.10 345.59
 470.75 523.19 684.27 790.62 808.95 854.19 932.70 1006.49 1053.26 1081.92
 1091.07 1099.03 1126.17 1176.25 1209.77 1292.19 1308.86 1348.87 1358.34
 1364.61 1419.83 1441.63 1447.03 1453.56 1471.59 1507.69 1512.62 1523.54
 1525.46 1530.75 1534.12 3036.73 3079.47 3114.75 3116.69 3125.07 3148.50
 3165.12 3184.38 3185.44 3191.32 3213.62 3244.71 3990.60

E(BHandHLYP)..... -311.475424

C: Plot of the kinetic data for the reaction of cis-3-hexene with OH radicals using allyl ether as reference compound. $[S]_0$ and $[S]_t$ are the concentrations of the cis-3-hexene at times 0 and t, respectively, $[R]_0$ and $[R]_t$ are the concentrations of the reference compound at times 0 and t, respectively.

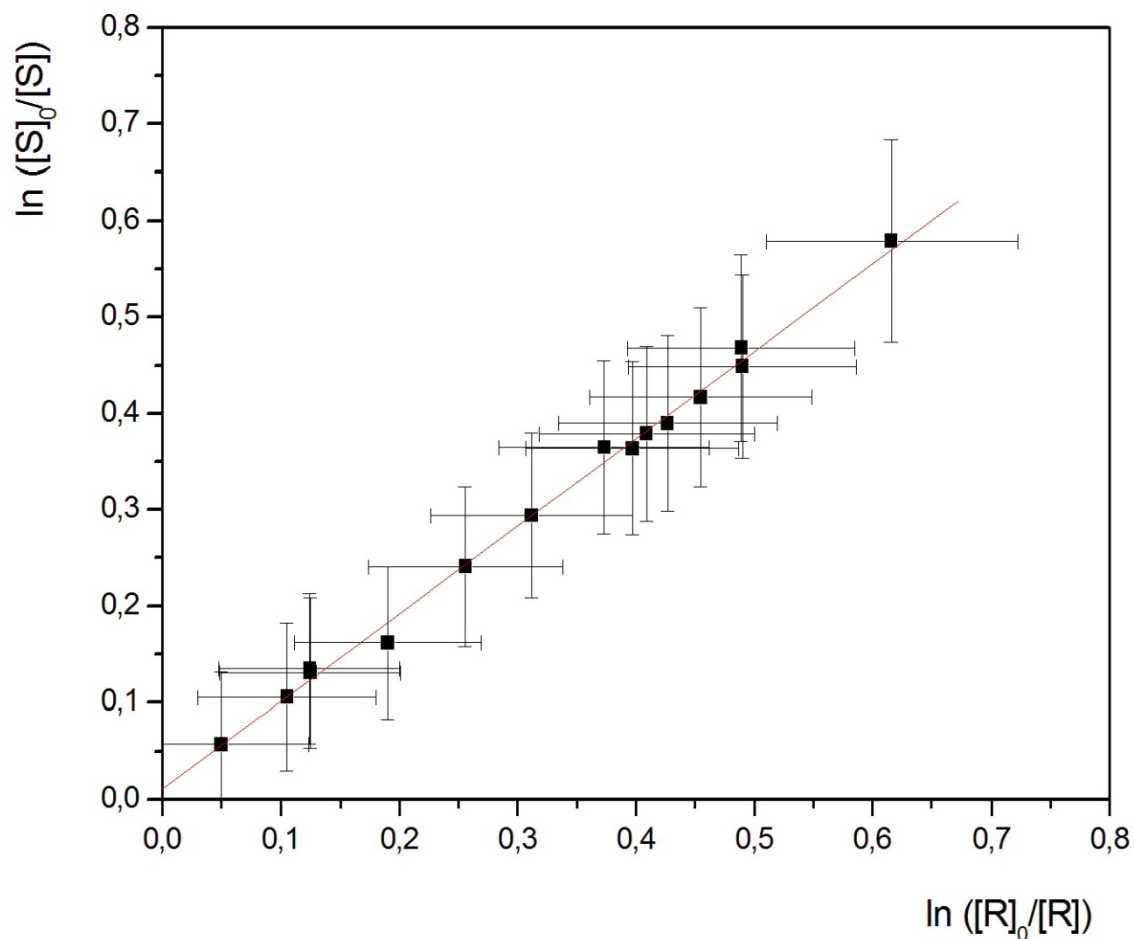


Figure 1. Plot of the kinetic data for the reaction of cis-3-hexene with OH radicals using allyl ether as reference compound. $[S]_0$ and $[S]_t$ are the concentrations of the cis-3-hexene at times 0 and t, respectively, $[R]_0$ and $[R]_t$ are the concentrations of the reference compound at times 0 and t, respectively.

D: Plot of the kinetic data for the reaction of cis-3-hexene with OH radicals using 3-buten-1-ol as reference compound. $[S]_0$ and $[S]_t$ are the concentrations of the cis-3-hexene at times 0 and t, respectively, $[R]_0$ and $[R]_t$ are the concentrations of the reference compound at times 0 and t, respectively.

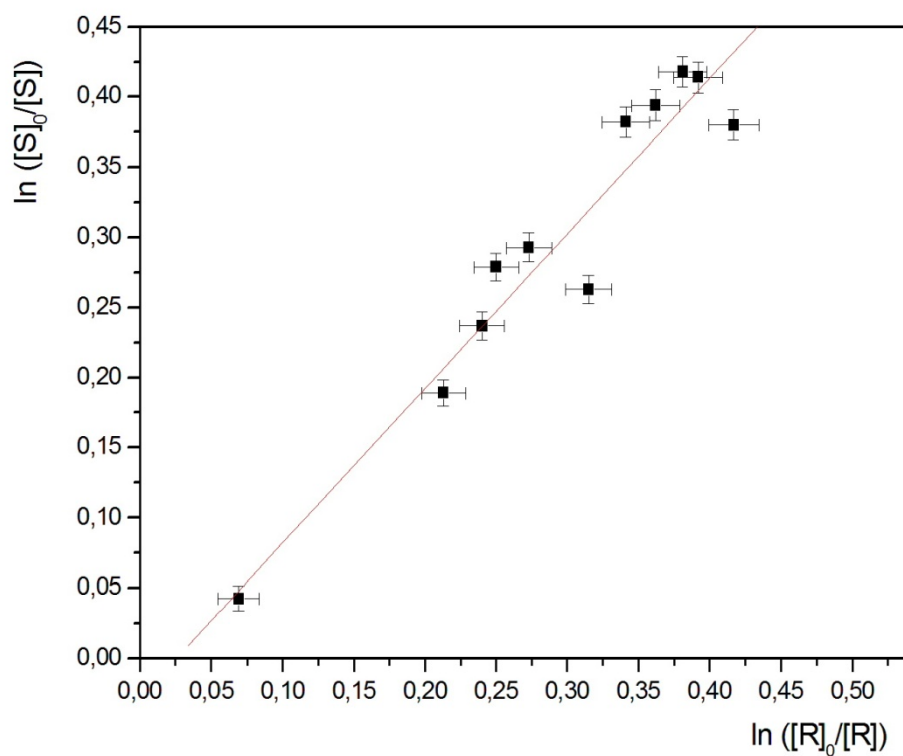


Figure 2. Plot of the kinetic data for the reaction of cis-3-hexene with OH radicals using 3-buten-1-ol as reference compound. $[S]_0$ and $[S]_t$ are the concentrations of the cis-3-hexene at times 0 and t, respectively, $[R]_0$ and $[R]_t$ are the concentrations of the reference compound at times 0 and t, respectively.