Kinetics of Hydrogen Abstraction and Addition Reactions of 3-Hexene by ȯH Radicals

Supplementary Information

Feiyu Yang, Fuquan Deng, Youshun Pan, Yingjia Zhang*, Chenglong Tang, Zuohua Huang*

State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China

Table S1. The Optimized geometries calculated at BHandHLYP/6-311G(d, p) level.

C_6H_{12}

Rotational constants (GHZ): 8.8456435 1.4822254 1.3752118

Zero-point correction= 0.170310 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

73.9457	116.2703	157.3060
191.4356	215.1044	273.1004
371.5494	413.2387	505.3840
615.1804	776.2208	820.8144
913.5389	929.3362	959.1751
1051.8126	1064.5007	1099.2177
1132.6848	1150.0876	1190.7816
1270.0142	1318.1852	1366.2841
1387.7025	1409.5175	1429.6482
1463.0630	1508.0325	1519.1658
1536.9119	1549.7042	1558.6665
1811.7087	3012.0965	3094.2035
3098.8567	3107.9471	3136.9439
3174.1425	3180.3656	3206.4256
3216.9693	3227.1705	3331.7674

Cartesian Coordinates (Å):

C	-0.55382100	-0.82285800	0.09528900
C	0.38769700	0.00777800	-0.31723000
C	1.83727100	-0.34016300	-0.45198800
C	-2.01405800	-0.52439800	0.25519200
C	2.73504400	0.52158400	0.43192000
C	-2.44514600	0.89150800	-0.08776800
H	-0.26581000	-1.83481800	0.34932300
H	0.12627300	1.02473700	-0.57454200
H	1.98287300	-1.39066700	-0.21291100
H	2.14156700	-0.21295100	-1.49074500
H	-2.57659500	-1.23147100	-0.35507800
H	-2.29850800	-0.74965000	1.28333200
H	3.78213100	0.26967900	0.29102000
H	2.61417100	1.57677500	0.20091900
H	2.49163900	0.38340000	1.48115900
H	-3.51368200	1.01051200	0.06128500
H	-1.93971100	1.62149600	0.53777900

H	-2.22627800	1.13225000	-1.12403300

TSdir

Rotational constants (GHZ): 3.36843 1.14043 0.98044

Zero-point correction= 0.176144 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

-1515.9714	45.5632	104.1403
109.2832	123.0973	161.4516
199.0296	218.1680	241.4917
311.5571	390.5381	424.6959
535.8279	575.8918	789.1228
811.4885	880.6627	909.0783
941.7773	974.9898	1046.2316
1064.3593	1079.0253	1137.8741
1140.6327	1161.9717	1207.7193
1314.8213	1320.2914	1364.1021
1381.9683	1398.6378	1420.7869
1445.3080	1458.4135	1465.6550
1537.8495	1538.2174	1545.2208
1550.0266	1559.0728	1804.4911
3095.0499	3099.1927	3110.5142
3132.1602	3139.1098	3166.9783
3177.3674	3178.6913	3182.3714
3197.6081	3224.4664	3924.2897

Cartesian Coordinates (Å):

C	-0.15710800	-0.53005700	-0.78327600
C	0.77542300	0.26457600	-0.24441600
C	2.25451900	0.18027900	-0.51304300
C	-1.62218800	-0.47777300	-0.47498500
C	3.07301000	-0.11963000	0.76017700
C	-2.10844600	-1.40845400	0.63783300
H	0.14678400	-1.29126400	-1.50257800
H	0.45439400	1.03801600	0.45028500
H	2.45182600	-0.58743600	-1.26679100
H	2.60328400	1.12967500	-0.93656400
H	-1.88375400	0.62788500	-0.06161800
H	-2.23323200	-0.57834000	-1.37618100
H	4.14239600	-0.13830400	0.54119200
H	2.90055700	0.63992200	1.52614900

H	2.79425000	-1.08700300	1.18158200
H	-3.17570200	-1.27858000	0.82100200
H	-1.93581200	-2.45478200	0.36304500
H	-1.57000200	-1.21557000	1.56614900
O	-2.04163800	1.91750000	0.35185900
H	-1.65314500	2.40214500	-0.41428700

H_2O

Rotational constants (GHZ): 837.49641 442.98009 289.73139

Zero-point correction= 0.022190 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

1682.8671	3980.5641	4077.0194

Cartesian Coordinates (Å):

H	0.75233100	-0.46448500	0.00000000
O	0.00000000	0.11612100	0.00000000
H	-0.75233100	-0.46448600	0.00000000

TSind

Rotational constants (GHZ): 3.50155 1.13592 0.96182

Zero-point correction= 0.176114 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

-1503.3455	32.1810	92.3897
117.4118	124.9757	165.3399
193.2193	217.0531	238.2176
282.5942	414.1288	420.9976
495.3643	666.1608	795.7314
810.1724	875.9437	935.9841
939.3955	966.6629	1047.5728
1061.6409	1095.3669	1134.5272
1138.1030	1155.4497	1215.8640
1241.3453	1315.6465	1357.6633
1382.6038	1396.8254	1426.1536
1462.8185	1463.7600	1481.8387
1536.6585	1541.8652	1546.1843
1550.0633	1558.6707	1800.2852
3097.3947	3100.8696	3108.9633
3124.8534	3139.3908	3162.6874
3176.3206	3179.0600	3180.6659
3192.8722	3222.3022	3924.8911

Cartesian Coordinates (Å):

C	-0.21713900	-0.83249000	-0.21534200
C	0.86180900	-0.09223700	-0.50408300
C	2.29086300	-0.53718600	-0.34331800
C	-1.63985600	-0.40161400	-0.39859100
C	3.09539900	0.35418500	0.62536600

C	-2.63809400	-1.00528400	0.58346700
H	-0.07532000	-1.83372000	0.19195600
H	0.71179800	0.92137400	-0.87085300
H	2.31932800	-1.57502200	0.00073500
H	2.78401000	-0.52145600	-1.32261100
H	-1.69661800	0.77953100	-0.30658300
H	-1.97709300	-0.52091100	-1.43494500
H	4.13483200	0.02606700	0.68609700
H	3.09272900	1.39588000	0.29575500
H	2.66987900	0.31977800	1.63016100
H	-3.63924600	-0.60475200	0.42297400
H	-2.68984600	-2.09300000	0.46613100
H	-2.35130000	-0.79865300	1.61658200
O	-1.59609900	2.17810000	-0.07450200
H	-1.03225700	2.16784300	0.73562500

OH

Rotational constants (GHZ): 0.0000000 575.6284200 575.6284200

Zero-point correction= 0.008845 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

3882.3805

Cartesian Coordinates (Å):

O	0.00000000	0.00000000	0.10692300
H	0.00000000	0.00000000	-0.85538400

P_1

Rotational constants (GHZ): 9.11888 1.53132 1.40777

Zero-point correction= 0.154770 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

73.9457	116.2703	157.3060
191.4356	215.1044	273.1004
371.5494	413.2387	505.3840
615.1804	776.2208	820.8144
913.5389	929.3362	959.1751
1051.8126	1064.5007	1099.2177
1132.6848	1150.0876	1190.7816
1270.0142	1318.1852	1366.2841
1387.7025	1409.5175	1429.6482
1463.0630	1508.0325	1519.1658
1536.9119	1549.7042	1558.6665
1811.7087	3012.0965	3094.2035
3098.8567	3107.9471	3136.9439
3174.1425	3180.3656	3206.4256
3216.9693	3227.1705	3331.7674

Cartesian Coordinates (Å):

C	-0.62200700	-0.78699300	0.14672100

C	0.33969400	-0.03155300	-0.35288300
C	1.78745200	-0.40643800	-0.39786600
C	-2.08538600	-0.44933000	0.20902800
C	2.67209200	0.56315800	0.38153000
C	-2.44595000	0.95951800	-0.08761800
H	-0.36146700	-1.75822800	0.54574100
H	0.08957300	0.93719800	-0.76287300
H	1.91529200	-1.41467200	-0.01166100
H	2.11909200	-0.42693500	-1.43576900
H	-2.62945900	-1.11891000	-0.45750300
H	-2.44312500	-0.71197900	1.21198400
H	3.71917900	0.28439600	0.30713200
H	2.57103500	1.57627600	0.00116000
H	2.39886100	0.57606300	1.43243900
H	-1.86781100	1.76740200	0.32559400
H	-3.38654500	1.19921500	-0.54971500

P_2

Rotational constants (GHZ): 9.78536 1.46254 1.36531

Zero-point correction= 0.155551 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

27.6002	67.3351	112.1050
183.1973	256.0173	351.1724
385.0675	404.9944	621.5349
687.7461	783.9593	814.2618
936.3997	939.0308	1008.2493
1045.9872	1062.8594	1106.2912
1112.1112	1207.2325	1247.5479
1265.6088	1322.8675	1372.2297
1431.8851	1460.7390	1463.8499
1505.4579	1535.2967	1536.4611
1548.1013	1555.9469	1562.9914
1570.0448	3077.4423	3086.4415
3108.3020	3135.1146	3140.6048
3174.5613	3180.8940	3189.5339
3209.2984	3235.2514	3249.5559

Cartesian Coordinates (Å):

C	0.61938500	0.80653000	0.10018000
C	-0.37426500	-0.04800100	-0.32147700
C	-1.81094300	0.33508000	-0.44213200
C	1.96602600	0.52605900	0.23509100
C	-2.73227700	-0.51905400	0.42831800
C	2.62244900	-0.78095900	-0.05075500
H	0.31435800	1.81172500	0.35669800
H	-0.12654300	-1.06647400	-0.57912900

H	-1.93218400	1.38442600	-0.18440200
H	-2.12713600	0.23535100	-1.48168800
H	2.60269200	1.31351700	0.60483800
H	-3.77166100	-0.23422100	0.29252300
H	-2.64073700	-1.57206600	0.17597100
H	-2.48479400	-0.40816700	1.47969100
H	3.57483000	-0.63304000	-0.55350000
H	2.83523200	-1.32523000	0.86986600
H	2.01369300	-1.42375600	-0.67621200

P_3

Rotational constants (GHZ): 10.24641 1.40532 1.33771

Zero-point correction= 0.156453 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

62.6161	98.3631	139.5773
203.1642	243.3313	299.0755
344.6688	390.5087	576.4169
771.5384	808.0338	856.8809
897.1661	941.2639	1025.6224
1092.0803	1097.4545	1131.4975
1144.3999	1178.6753	1312.1828
1328.9598	1354.5267	1394.2276
1410.1711	1455.0066	1462.5446
1529.6437	1538.0266	1546.6869
1548.8212	1557.2938	1557.7884
1827.6945	3098.5726	3103.0183
3105.3309	3108.8347	3117.0124
3128.0325	3153.2127	3175.9055
3182.2456	3186.4470	3190.4979

Cartesian Coordinates (Å):

C	-0.55878400	-0.68404900	0.09712600
C	0.43498900	0.03167500	-0.34841500
C	1.87131000	-0.40451000	-0.41697900
C	-2.01178600	-0.58939700	0.30818000
C	2.78890600	0.47202200	0.42934800
C	-2.60103800	0.76305400	-0.10058800
H	0.23346500	1.04427900	-0.69610200
H	1.94613700	-1.43941900	-0.09814000
H	2.20248000	-0.36962300	-1.45416600
H	-2.50396000	-1.38465200	-0.24900500
H	-2.23150900	-0.78043700	1.35712200
H	3.82381500	0.15478500	0.33950700
H	2.73264400	1.51228900	0.11916100
H	2.50949200	0.42378500	1.47749100
H	-3.67203500	0.77734600	0.07590400

H	-2.15307600	1.57005200	0.47033300
H	-2.42903800	0.95881500	-1.15414000

P_a

Rotational constants (GHZ): 4.04520 1.49570 1.28095

Zero-point correction= 0.184923 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

57.8496	77.9205	132.3473
174.0140	222.1969	239.2039
277.9106	330.5390	334.7239
394.4855	457.5742	564.3140
568.9470	784.9101	816.2622
897.7648	929.0761	1005.1668
1054.0769	1088.3783	1096.9860
1107.7465	1145.7841	1188.2791
1214.1529	1283.4059	1315.6294
1328.3833	1373.7494	1413.4388
1425.1940	1463.7702	1467.7097
1472.1175	1483.3997	1525.4775
1544.4854	1551.4646	1552.9336
1559.9461	1566.0043	3037.8370
3089.2948	3109.9055	3112.4715
3115.1761	3120.6034	3151.3497
3175.3254	3176.7866	3183.7717
3196.8199	3233.1607	3981.4213

Cartesian Coordinates (Å):

C	-0.40940300	-0.49257900	-0.69387100
C	0.40030600	0.40780600	0.17558400
C	1.89717100	0.30439200	-0.07805800
C	-1.89860900	-0.53213600	-0.62591100
C	2.49003200	-1.04668700	0.29373800
C	-2.47714100	-0.38822500	0.77809900
H	0.07621700	-0.97570900	-1.52774000
H	0.21387600	0.17537700	1.22264400
H	2.09093700	0.51890300	-1.12965700
H	2.37804900	1.09230000	0.49440200
H	-2.31121000	0.26709800	-1.24932800
H	-2.24851900	-1.45855600	-1.07702500
H	3.56193600	-1.06062500	0.12304700
H	2.32072400	-1.26856000	1.34436000
H	2.05247300	-1.85327400	-0.28665600
H	-3.56086900	-0.44528300	0.75127600
H	-2.11841200	-1.17686600	1.43379900
H	-2.20258400	0.56707500	1.21156100
H	0.03615800	2.01363800	-0.85848800

O	-0.03786400	1.76113100	0.05629000

PC

Rotational constants (GHZ): 2.88097 1.21548 0.91306

Zero-point correction= 0.179968 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

40.8578	42.1676	83.6508
103.7868	128.6876	161.4375
169.6009	195.6801	209.9653
226.2538	277.9804	342.4558
384.5781	452.4973	507.2910
757.7284	795.8281	823.7886
934.8473	956.5807	1017.3104
1051.9129	1066.9964	1117.7718
1123.7025	1208.2085	1225.9659
1308.2151	1332.5325	1357.6670
1395.7346	1465.5637	1465.9797
1502.1294	1527.4143	1536.7039
1549.8814	1554.8175	1571.0967
1578.4849	1692.3538	3082.1695
3088.2604	3107.5568	3129.1496
3138.3118	3172.3793	3179.1094
3197.0449	3199.6679	3210.6545
3227.2644	3961.3678	4057.7391

Cartesian Coordinates (Å):

C	0.77386200	-0.63831200	-0.18567400
C	-0.44771400	-0.87250700	0.44008600
C	-1.72593200	-1.19996100	-0.27668000
C	1.96829300	-0.31515900	0.45087400
C	-2.84945900	-0.17070700	-0.01298700
C	3.26569400	-0.06817800	-0.25454600
H	0.79576900	-0.71498400	-1.27182700
H	-0.49455200	-0.81487500	1.52600300
H	-1.53759200	-1.26357900	-1.35219100
H	-2.08061400	-2.19148500	0.03375200
H	-0.12424800	1.68509000	-0.12225100
H	1.97343100	-0.24011700	1.53542000
H	-3.75520200	-0.43281100	-0.56290000
H	-3.10352200	-0.13473900	1.04985800
H	-2.53104200	0.82543800	-0.32121300
H	3.65359600	0.93548900	-0.04766100
H	4.04136700	-0.77067100	0.07097100
H	3.16110300	-0.16665300	-1.33632900
O	-0.60774100	2.53028000	-0.11433000
H	-1.04503300	2.63060300	0.74657800

RC

Rotational constants (GHZ): 3.00398 1.30581 0.96875

Zero-point correction= 0.181399 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

43.4733	82.7100	85.4434
107.2101	159.6571	163.9919
189.4734	257.8620	268.2431
317.7529	413.4517	436.9759
464.4259	498.7538	807.8818
808.0514	889.6504	937.8264
939.4877	1046.0985	1067.0399
1083.2340	1136.7324	1143.3144
1152.6497	1230.6077	1311.5769
1335.6790	1364.7543	1379.4046
1404.0876	1441.6197	1471.3852
1472.4357	1535.0647	1536.4047
1554.1192	1554.3923	1559.9463
1563.8576	1798.2483	3095.5678
3095.6945	3111.6461	3111.9593
3138.9491	3140.3401	3176.7972
3177.0877	3189.9342	3190.6697
3192.1655	3198.2898	3791.0295

Cartesian Coordinates (Å):

C	-0.58938000	-0.85113100	0.32121200
C	0.58862300	-0.85232900	-0.32010600
C	1.94788300	-0.87592700	0.33466400
C	-1.94869600	-0.87628900	-0.33341900
C	2.88035500	0.25294100	-0.14997500
C	-2.88058000	0.25465200	0.14760000
H	-0.59176900	-0.85679200	1.41093600
H	0.59104700	-0.86143500	-1.40980900
H	1.83287600	-0.82296900	1.42121900
H	2.42563400	-1.84015600	0.12319300
H	-1.83372000	-0.82700000	-1.42015300
H	-2.42699000	-1.83952500	-0.11869900
H	3.85568400	0.18665100	0.33510900
H	3.04110100	0.19240000	-1.22924900
H	2.45783700	1.23460100	0.06835600
H	-3.85577300	0.18757900	-0.33764200
H	-3.04168400	0.19738000	1.22698900
H	-2.45731000	1.23543200	-0.07336800
O	0.00179000	2.49996100	0.00070600
H	-0.00047800	1.50264400	-0.00238600

RC_A

Rotational constants (GHZ):	2.76225	1.24817	0.99651
Zero-point correction=		0.181383 (Hartree/Particle)	
Harmonic Vibrational Frequencies (cm^{-1}):			
37.7432	63.8223	79.5294	
111.9888	132.7853	186.7396	
210.6736	257.3867	298.7888	
311.2476	379.6690	422.0208	
442.7291	594.7887	765.4908	
812.3874	899.3925	911.3552	
942.6579	1047.9551	1068.4002	
1089.4392	1126.0850	1145.0640	
1157.3207	1206.5996	1319.8242	
1341.8441	1367.8115	1391.0104	
1418.1241	1437.3538	1464.6862	
1475.0497	1521.4263	1538.1978	
1550.0788	1553.9578	1558.8299	
1561.5730	1798.4192	3089.7330	
3097.1324	3108.2551	3110.4041	
3117.7059	3140.8754	3177.7780	
3182.6541	3183.6245	3192.2425	
3200.8924	3217.5990	3798.5839	
Cartesian Coordinates (Å):			
C	0.24597400	-0.46182900	0.84744400
C	-0.61265600	-0.03616600	-0.06771700
C	-1.98134600	0.49723700	0.22324000
C	1.61187400	-1.03400900	0.60964300
C	-3.08362600	-0.35277100	-0.40328200
C	2.06788600	-1.09479600	-0.83844900
H	-0.05214400	-0.40863300	1.88674200
H	-0.34461300	-0.09345700	-1.11387600
H	-2.12743100	0.55806200	1.29864000
H	-2.06156200	1.51387200	-0.16040300
H	2.33133900	-0.45488500	1.18900200
H	1.63628600	-2.03225700	1.04659800
H	-4.06318000	0.07025000	-0.20222400
H	-2.96430200	-0.41538600	-1.48156100
H	-3.06370300	-1.36407100	-0.00853500
H	3.05517800	-1.54011100	-0.90388300
H	1.39394600	-1.69336300	-1.44429200
H	2.12572000	-0.10008900	-1.26837900
H	1.04388700	1.74656700	0.15114900
O	1.70024400	2.38843800	-0.15178200
TS_1			
Rotational constants (GHZ):	7.99992	0.73349	0.70238

Zero-point correction=		0.176009 (Hartree/Particle)	
Harmonic Vibrational Frequencies (cm^{-1}):			
-1738.1537	47.6335	64.4134	
82.7347	106.1237	120.8442	
169.0511	219.1610	249.0120	
351.3242	412.3073	440.6356	
582.4548	693.4275	763.8932	
810.4869	875.4305	923.1454	
943.3933	953.9784	1033.9541	
1054.2245	1075.8755	1123.5075	
1142.5341	1153.6603	1196.0292	
1302.8284	1316.9945	1342.6237	
1366.5753	1387.5149	1408.9838	
1436.6495	1463.9690	1476.5719	
1523.0474	1535.5476	1537.6756	
1549.8603	1558.6384	1811.0030	
3095.4876	3098.7739	3108.7618	
3123.2414	3138.7036	3153.3035	
3174.9331	3181.8163	3204.7606	
3214.9721	3226.2892	3930.1264	
Cartesian Coordinates (Å):			
C	0.31249400	0.92708500	-0.11152900
C	1.17988100	0.03116500	0.32544400
C	2.65641800	0.25059900	0.43071100
C	-1.17369600	0.75592200	-0.24621700
C	3.45900400	-0.71858700	-0.43326000
C	-1.70953200	-0.59211700	0.15873900
H	0.68266600	1.89879300	-0.41077900
H	0.83047200	-0.94731100	0.62551400
H	2.89204500	1.27488100	0.15312300
H	2.96272800	0.13176500	1.46973000
H	-1.66564200	1.53136900	0.34022800
H	-1.45521300	0.95668800	-1.27879200
H	4.52624800	-0.55670700	-0.31426300
H	3.24836300	-1.75010200	-0.16331300
H	3.21272900	-0.59501000	-1.48356500
H	-2.92396300	-0.57543300	-0.05244400
H	-1.37544800	-1.41602100	-0.46089000
H	-1.59737800	-0.82539200	1.21082000
O	-4.16982900	-0.37503400	-0.14076400
H	-4.32638700	-0.05164800	0.74741900
TS_3			
Rotational constants (GHZ):	2.59567	1.44386	0.98852
Zero-point correction=		0.176321 (Hartree/Particle)	

Harmonic Vibrational Frequencies (cm^{-1}):

-1799.3740	69.1978	74.3900
111.3569	129.6225	176.1097
207.3965	236.7878	252.9196
302.8211	362.7172	417.7393
470.8269	622.5878	772.9853
809.6932	830.6476	901.6513
941.5036	944.8146	1044.8347
1083.3042	1118.0154	1133.1157
1148.6901	1181.9987	1223.0473
1325.2231	1330.7042	1349.0653
1366.8049	1415.4471	1433.3919
1463.5774	1464.2688	1533.1468
1542.5320	1549.4486	1549.8043
1558.9588	1559.5605	1809.2318
3098.0383	3105.7636	3109.1550
3116.7162	3128.4726	3163.1762
3174.4606	3183.1470	3186.4365
3187.1047	3190.4924	3932.9720

Cartesian Coordinates (Å):

C	-0.57002300	0.27784200	0.00176600
C	0.37443700	-0.57431400	0.33059100
C	1.82858200	-0.25029100	0.49204100
C	-2.03736800	0.12269500	-0.19846600
C	2.71174200	-1.04028500	-0.46913500
C	-2.55396900	-1.29508500	0.01267900
H	-0.19655800	1.44564600	-0.20789100
H	0.09870600	-1.61200100	0.48315200
H	1.97343100	0.81377600	0.34102700
H	2.12898500	-0.47552700	1.51492800
H	-2.55366200	0.80657500	0.47338700
H	-2.28624300	0.45978900	-1.20309900
H	3.76044100	-0.80735700	-0.31120100
H	2.58501500	-2.11104100	-0.33150600
H	2.46557300	-0.80550000	-1.50003200
H	-3.62621100	-1.33205000	-0.15039800
H	-2.08647800	-1.99029500	-0.67769700
H	-2.35635500	-1.63961700	1.02310700
O	0.17517500	2.63190800	-0.15793600
H	0.17154900	2.74896700	0.79286000

TS_A

Rotational constants (GHZ): 3.49284 1.42196 1.19653

Zero-point correction= 0.182043 (Hartree/Particle)

Harmonic Vibrational Frequencies (cm^{-1}):

-293.6717	75.8834	86.1349
134.9843	155.1476	198.8533
206.4236	262.8687	264.4811
317.3112	388.9781	428.7116
592.3426	750.7148	756.5216
813.6837	865.8798	911.6169
942.3134	1036.6947	1045.6910
1089.1460	1117.1139	1140.3036
1147.7756	1210.6174	1315.1568
1335.4634	1349.5413	1372.8540
1413.8910	1433.2788	1463.6096
1472.4216	1527.1096	1544.3629
1549.4665	1552.6820	1560.9450
1569.7976	1674.0246	3082.7144
3099.3662	3109.5966	3116.8513
3120.2651	3162.5567	3177.9419
3178.7385	3186.5200	3199.1842
3203.2454	3271.0509	3924.8392

Cartesian Coordinates (Å):

C	0.46277200	-0.33179400	0.82595900
C	-0.41971800	0.06568100	-0.11888200
C	-1.88064700	0.25850900	0.14508900
C	1.90578100	-0.65668300	0.60906300
C	-2.71282100	-0.93626100	-0.31406700
C	2.39664300	-0.54994500	-0.82490500
H	0.12077700	-0.36878300	1.85204300
H	-0.13585500	0.00470400	-1.15544600
H	-2.03862200	0.43135900	1.20716900
H	-2.20630900	1.15420400	-0.37315400
H	2.49954100	0.00366500	1.24218000
H	2.09267300	-1.65984800	0.99493900
H	-3.77021300	-0.75847400	-0.14252600
H	-2.57670100	-1.12203000	-1.37605300
H	-2.43172300	-1.83960000	0.21911200
H	3.45871000	-0.76661300	-0.87861000
H	1.88411400	-1.25401100	-1.47444100
H	2.23043400	0.45080900	-1.20817500
H	0.34961700	2.21662400	0.74098600
O	0.25143700	2.05136900	-0.19769600