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ARTICLE

Mechanism of Gas-Phase Ozonolysis of Sabinene in the Atmosphere

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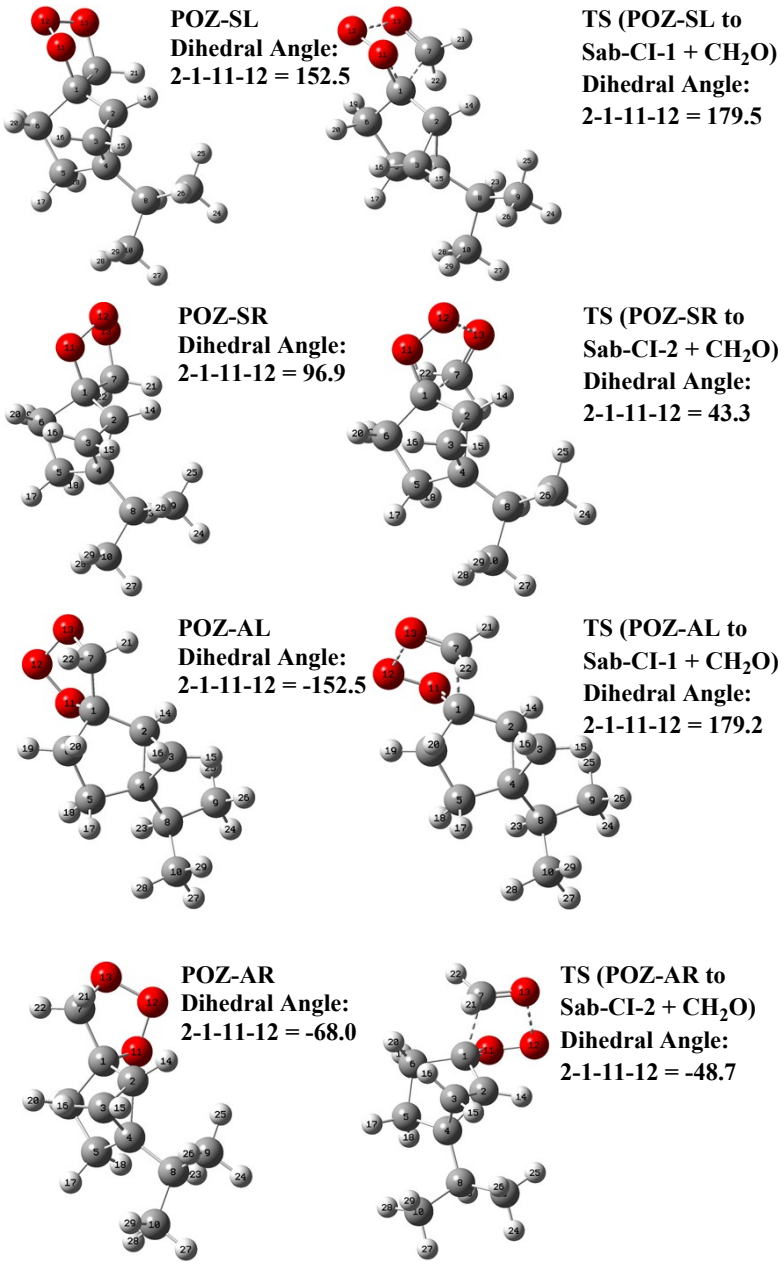

Figure S1. Structures of POZs and Their Transition States to CH_2O + Sab-CI-1 or Sab-CI-2.

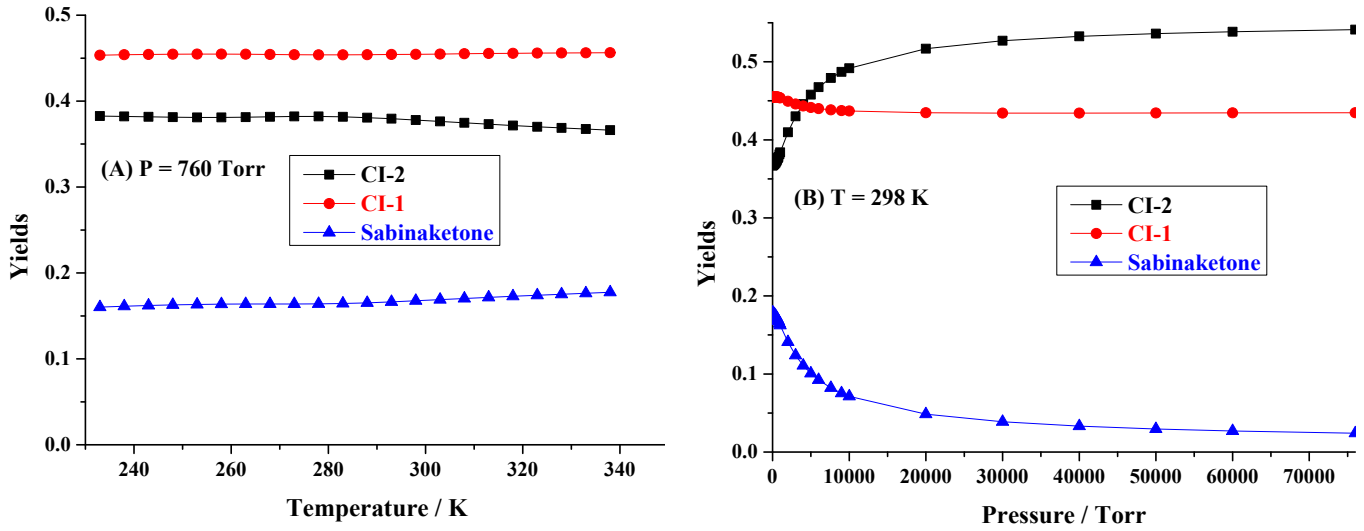

Figure S2. The dependence of product yields from RRKM-ME calculations using Mesmer. (A) Temperature dependence at 760 Torr; and (B) Pressure dependence at 298 K.

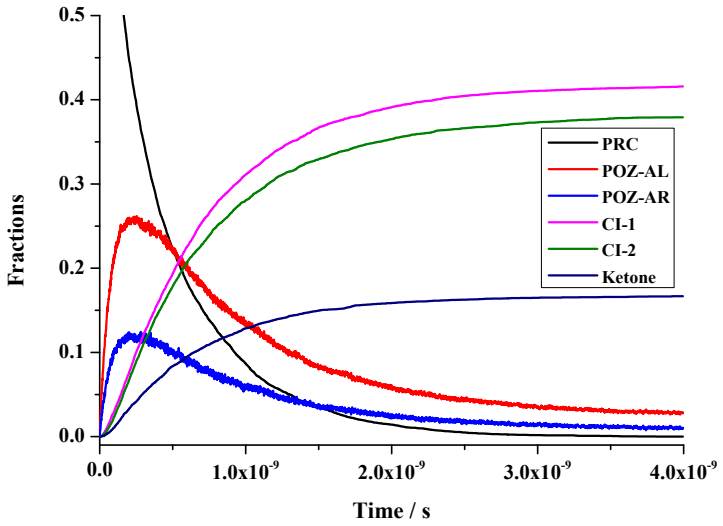

Figure S3. Time profiles for the unimolecular processes of Sabinene-O_3-PRC-anti at 298 K and 760 Torr using MultiWell-2017.

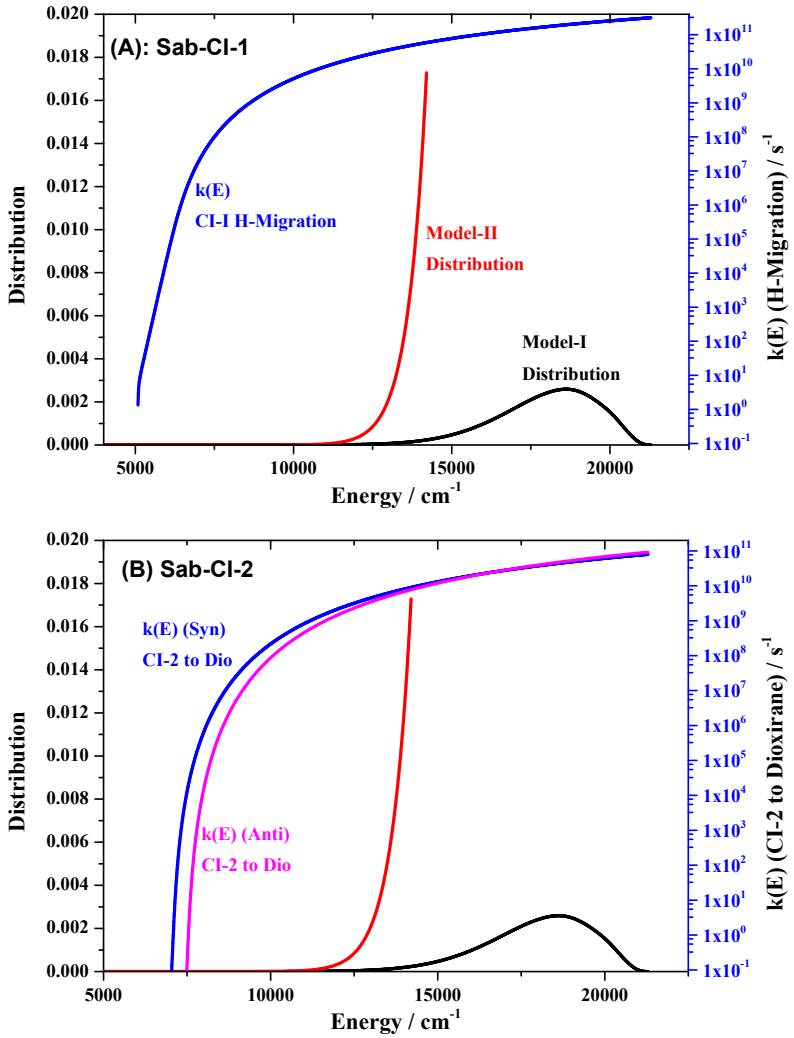

Figure S4. Normalized nascent distributions of Sab-CI-1 and Sab-CI-2 from POZ decomposition and k(E) of the CIs. Available energies are 260 kJ/mol (21300 cm^{-1}) for Model I and 170 kJ/mol (14200 cm^{-1}) for Model II. The distribution is per grain with grain size of 10 cm^{-1}.

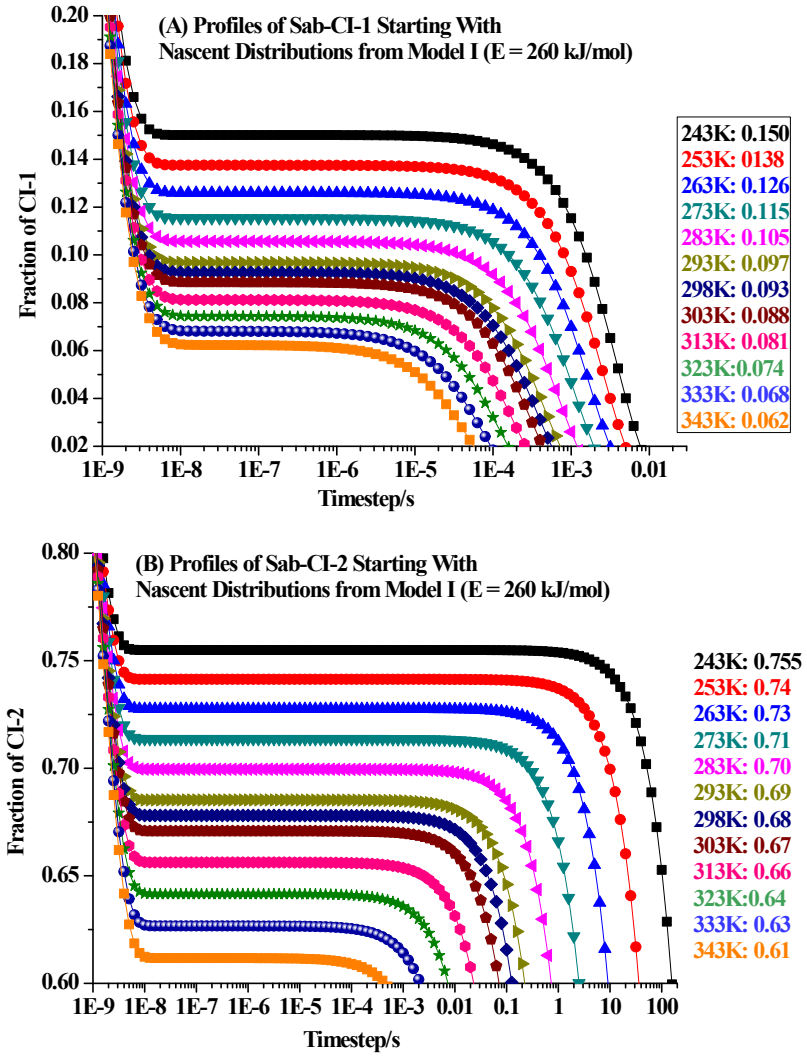

Figure S5. Decays of Sab-CI-1 and Sab-CI-2 starting from the energy distributions with Model I (using Mesmer), all at 760 Torr. Initial fractions are 1.

Table S1. Detailed energies (in kJ/mol) of species from pre-complexes to decomposition products of POZs at MO6-2X and F12a levels, respectively.

Species	M06-2X		F12a	
	ΔE_{0K}	ΔG_{298K}	ΔE_{0K}	ΔG_{298K}
PRC-Anti	−19.7	21.6	-11.5	29.8
PRC-Syn	−15.9	24.7	-8.7	31.9
TS-AL	-5.6	42.1	0.1	47.8
TS-AR	-4.6	43.0	0.8	48.4
TS-SL	3.8	51.1	7.9	55.3
TS-SR	2.3	51.1	7.2	55.9
POZ-AL	−299.9	-248.2	-243.1	-191.4
POZ-AR	−293.8	-242.3	-236.6	-185.1
TS (AL–AR)	−282.8	−228.9	-224.6	-170.7
POZ-SL	−290.2	-239.6	-233.4	-182.8
POZ-SR	−291.6	-240.4	-234.8	-183.6
TS (SL–SR)	-282.6	-230.5	-224.4	-172.3
Sab-CI-1 + CH_2O	-315.8	-259.1	-263.3	-261.7
Sab-CI-2 + CH_2O	-311.7	-257.4	-259.6	-260.4
Sabinaketone + CH_2OO	-299.3	-301.6	-254.8	257.0

Table S2. Fraction of stabilized Sab-CIs with two types of initial nascent distributions. (A) Model I: Non-Separable translational motion; and (B) Model II: Separable translational motion [(a)]

Temperature / K	Model-I Sab-CI-1 (Mesmer)	Model-I Sab-CI-2 (Mesmer)	Model-I Sab-CI-1 (MultiWell)	Model-I Sab-CI-2 (MultiWell)	Model-II Sab-CI-1 (MultiWell)	Model-II Sab-CI-2 (MultiWell)
243	0.150	0.755	0.080	0.663	0.709	0.980
253	0.138	0.74	0.074	0.651	0.692	0.978
263	0.126	0.73	0.066	0.632	0.680	0.976
273	0.115	0.71	0.057	0.610	0.653	0.977
283	0.105	0.70	0.050	0.598	0.638	0.972
293	0.097	0.69	0.047	0.582	0.625	0.971
303	0.088	0.67	0.043	0.573	0.604	0.968
313	0.081	0.66	0.037	0.539	0.596	0.966
323	0.074	0.64	0.035	0.525	0.568	0.965
333	0.068	0.63	0.032	0.516	0.553	0.960
343	0.062	0.61	0.032	0.504	0.539	0.958
298.15 [(a)]	0.093	0.68	0.045	0.582	0.608	0.970
Yields of SCIs (%) [(a)]	4.7	25.8	2.3	22.1	27.4	36.9
Total Yields of SCIs (%) [(a)]	30.5		24.4		64.3	
298.15 [(b)]	0.424	0.924	0.255	0.856	0.111	0.783
Yields of SCIs (%) [(b)]	19.1	35.1	11.4	31.7	5.0	29.0
Total Yields of SCIs (%) [(b)]	54.2		45.1		34.0	

(a) The available energy E_{Total} is set as 260 kJ/mol In Model I, and the total excess energy E_{exc} is set as 170 kJ/mol in Model II; (b) The available energy E_{Total} is set as 215 kJ/mol In Model I, and the total excess energy E_{exc} is set as 215 kJ/mol in Model II.

Table S3. Geometries & Vibrational Frequencies at M06-2X/6-311++G(2df,2p) level.

O_3			
O,0,-1.0370035806,2.3522674055,-0.02985346	796.6021		
O,0,0.1893212393,2.2570652672,-0.02985346	1376.8923		
O,0,-1.5361006987,3.4764729374,-0.02985346	1384.4189		
Sabinene			
0,1			
C,0,-1.0690728688,1.2818459124,-0.321375449	50.8681	109.8351	172.7606
C,0,0.1108544306,0.7077569469,-1.0073196202	207.5062	235.9436	261.4454
C,0,1.3985904935,1.5033503876,-0.9293054019	310.6325	328.1576	360.3722
C,0,1.156055231,0.3956501001,0.0430483163	393.1819	438.4078	459.0029
C,0,0.5739344991,0.8361479449,1.3835114229	518.1184	594.4458	650.951
C,0,-0.6180502978,1.7480756634,1.04481044	672.8725	756.6755	805.171
C,0,-2.3113498372,1.3007175493,-0.7854669071	833.1631	882.1961	909.9508
C,0,1.994694964,-0.8690985653,0.0488106339	927.8097	927.9823	943.2798
C,0,2.4789890329,-1.3024063311,-1.3317356119	952.8049	969.9439	988.1683
C,0,3.1886366561,-0.708923248,0.9912327059	998.85	1028.867	1054.909
H,0,-0.0411210033,0.0754557438,-1.8699030833	1070.3396	1074.2493	1126.3489
H,0,2.1033971213,1.3272733544,-1.7284328116	1142.2017	1163.8917	1191.4407
H,0,1.3530658398,2.5298183437,-0.5918415779	1229.4685	1243.9773	1263.4506
H,0,1.3102514894,1.3321918659,2.0168474447	1310.4255	1316.0278	1340.4342
H,0,0.2261162016,-0.0539592692,1.9148140616	1349.704	1379.7514	1402.4938
H,0,-1.4176265439,1.6987066383,1.7811120033	1409.1661	1421.5926	1459.9538
H,0,-0.2968550707,2.7904091915,0.9887909706	1489.6358	1491.1205	1495.3193
H,0,-2.5473074288,0.9364365288,-1.776672622	1501.2367	1511.9479	1516.642
H,0,-3.1289804638,1.6792428097,-0.1862974876	1522.2311	1747.1127	3024.702
H,0,1.3527691262,-1.6642901706,0.4446882109	3041.9326	3042.3577	3046.6452
H,0,2.9572582094,-2.2797352978,-1.268136011	3070.2111	3091.6703	3107.4794
H,0,1.6635615461,-1.3776709954,-2.0507635343	3117.4905	3121.1842	3128.65
H,0,3.2198105116,-0.6041525491,-1.7244684982	3134.5855	3148.2445	3154.0661
H,0,3.8026599213,-1.610109071,0.9960021827	3191.6682	3237.2716	3237.9443
H,0,2.8719677144,-0.5126898556,2.0151201421			
H,0,3.813973526,0.1249663724,0.664487081			
Sabinene--O_3 Syn-vdW			
0,1			
C,0,0.9355002236,0.1888259223,-0.7797164459	33.595	47.5303	56.5644
C,0,-0.1801112717,-0.7094670774,-0.4099759587	75.2484	84.0042	111.5964
C,0,-0.6497985607,-0.6699716782,1.0288658575	152.129	187.4136	213.7449
C,0,-1.3526033553,0.1589324975,0.0057585519	243.2592	247.145	276.7997
C,0,-0.8776591973,1.6075256124,-0.0770891623	313.4047	332.5594	362.3736
C,0,0.657540168,1.5417011618,-0.1676703841	398.0555	440.2988	457.7436
C,0,1.9423254588,-0.1027470787,-1.5990158705	520.9373	596.2389	655.7563
C,0,-2.7891322634,-0.1136513741,-0.399679995	675.3246	754.2105	792.9238
C,0,-3.1684109457,-1.5916174417,-0.3841169406	807.2877	835.6204	880.7995
C,0,-3.7476683837,0.6788548052,0.4905834011	908.3396	925.608	927.7392
O,0,2.5404804649,-0.7586745922,1.4344815677	942.8709	952.4175	972.5199
O,0,3.393910636,0.0990584828,1.1940925205	988.4764	1000.4251	1030.9341
O,0,4.1657197512,-0.1076992806,0.2558857262	1052.9402	1067.1901	1076.0879
H,0,-0.3136605018,-1.6280679565,-0.9622344132	1126.627	1142.6047	1165.6845
H,0,-1.1452470293,-1.5636593927,1.3782773867	1192.9515	1234.1974	1243.2246
H,0,-0.0167809986,-0.1920771957,1.7640474324	1266.4154	1313.2606	1316.9736
H,0,-1.2186206599,2.2074191601,0.7672019373	1339.6228	1347.9402	1350.5162
H,0,-1.2858841526,2.05380221,-0.9877102812	1377.0544	1379.4334	1403.1587
H,0,1.08943966,2.3542284572,-0.7484042016	1409.3318	1422.4021	1460.8209
H,0,1.0983481872,1.590823283,0.8322774101	1490.6389	1492.7217	1495.9414
H,0,2.0706837213,-1.0997253127,-1.999024051	1501.8157	1512.8586	1518.6572
H,0,2.6578464848,0.6503287416,-1.9012513471	1522.1794	1728.3694	3016.364
H,0,-2.8982881084,0.2497822592,-1.4278121279	3040.5036	3042.5965	3045.9327
H,0,-4.1625155495,-1.7249432755,-0.8104032448	3052.5692	3094.4569	3108.594
H,0,-2.4742951385,-2.2006469612,-0.962716213	3121.0296	3125.0495	3127.2758
H,0,-3.1978169394,-1.9789118444,0.6355333464	3129.906	3145.5185	3146.7376
H,0,-4.7844238769,0.4842414462,0.2145378886	3200.1337	3231.9834	3233.7819
H,0,-3.5753501514,1.7522298002,0.4160916768			
H,0,-3.6148114717,0.386491842,1.5346729538			
Sabinene--O_3 Anti-vdW			
0,1			
C,0,1.149950906,1.0499434482,0.3953834071	33.9859	51.9635	62.1294
C,0,-0.08250121,0.5474824529,1.0394888161	70.3824	94.3819	114.3239
C,0,-1.2825730448,1.4720251616,1.0290031695	153.8122	185.8952	210.9429
C,0,-1.1500028278,0.4212537568,-0.0248924195	239.3212	245.1742	276.8365
C,0,-0.5340481435,0.9087821486,-1.3338656017	317.2413	332.2833	355.2889
C,0,0.7637363615,1.6378492373,-0.9437538484	386.612	437.3076	458.8799
C,0,2.3844746909,0.9564339198,0.8852586838	520.8462	600.4068	646.3209

C,0,-2.1039863344,-0.7545376948,-0.1197709602	674.3804	752.9617	798.3402
C,0,-2.6098649268,-1.2566760752,1.2291260096	802.5356	828.1552	880.9549
C,0,-3.2878042584,-0.4042000925,-1.0226692314	908.4623	925.6101	930.1179
O,0,1.2316004626,-1.6193344086,-0.637052295	941.1478	948.796	974.2322
O,0,2.4585364326,-1.7222010636,-0.7398662728	983.7021	999.9888	1029.6355
O,0,3.1201656193,-1.7165060002,0.2989470212	1054.7655	1066.2197	1071.9602
H,0,0.0060979676,-0.1657763927,1.8457058807	1129.0866	1142.2877	1163.4645
H,0,-2.0011541603,1.3104138964,1.8189105962	1192.7435	1230.7522	1244.0687
H,0,-1.1341200128,2.5104885294,0.7649344745	1261.6755	1306.7876	1317.4021
H,0,-1.212993057,1.5496672503,-1.8973997494	1340.4935	1343.6072	1349.508
H,0,-0.3060203335,0.0389581944,-1.9543186788	1371.9726	1381.5976	1406.7655
H,0,1.5546527113,1.5277132395,-1.6840672802	1408.2162	1425.9304	1454.3548
H,0,0.5832482414,2.7089567787,-0.8283095723	1486.4252	1489.358	1495.5402
H,0,2.5710131366,0.5396538458,1.865561137	1503.4923	1511.9906	1519.6128
H,0,3.2399218259,1.3107542132,0.3244622732	1520.5761	1717.9271	3019.3743
H,0,-1.5413307923,-1.5678829472,-0.5916328766	3042.8172	3055.6186	3055.9013
H,0,-3.18685063,-2.1710715281,1.0914488925	3062.6963	3097.9125	3112.9541
H,0,-1.7954619493,-1.4792646982,1.9180450705	3118.6436	3122.0524	3129.3922
H,0,-3.2686785123,-0.5244883611,1.6990256361	3129.8283	3142.1454	3144.1008
H,0,-3.9805006926,-1.2430705704,-1.0982975478	3181.3395	3229.3603	3229.6584
H,0,-2.964971911,-0.1437656198,-2.0304646102			
H,0,-3.833100829,0.4487386593,-0.6119296337			
TS: Sabinene + O_3 → POZ-AL			
0,1			
C,0,1.0180081465,0.2727604585,0.8971284903	-313.3067	43.9867	55.7846
C,0,-0.2170550544,-0.5265624389,0.9898790248	78.01	111.2965	167.1342
C,0,-1.2803959658,0.0067993493,1.9323876255	182.8111	210.4066	215.2922
C,0,-1.3582951221,0.3178471646,0.4735585047	240.7956	255.688	307.2399
C,0,-0.7701517946,1.6693083717,0.0754720609	325.344	351.7787	390.8383
C,0,0.6386223001,1.7184004459,0.6883017994	438.2199	456.1857	473.7251
C,0,2.2815960061,-0.1764159455,1.1413814145	549.4177	604.9537	626.5122
C,0,-2.4656554621,-0.2255127062,-0.4104362761	693.9669	789.7331	802.0346
C,0,-2.9283962688,-1.6301842489,-0.0373189107	819.3222	822.9392	880.0815
C,0,-3.6565945782,0.7340145632,-0.4108086521	904.6542	926.9539	940.4437
O,0,1.0966435495,-0.1503625503,-1.4246964304	945.201	956.4352	971.5912
O,0,2.3418597695,0.0410564813,-1.5416472854	989.3045	1001.3254	1028.0649
O,0,3.0272367158,-0.7414773972,-0.8348604333	1047.2669	1066.343	1070.5535
H,0,-0.1613849221,-1.5918137393,0.8232652814	1126.8066	1141.9836	1158.7712
H,0,-1.9584823031,-0.7334655489,2.3306978588	1183.609	1193.1803	1242.5067
H,0,-1.0095202441,0.7875296359,2.6307317366	1243.5667	1259.9872	1282.0455
H,0,-1.3920595022,2.5036267135,0.4008607047	1301.1138	1320.4416	1348.0153
H,0,-0.6979477578,1.7053312124,-1.0131716434	1361.6384	1384.4628	1404.6597
H,0,1.3608019543,2.2359786911,0.0565862091	1408.0711	1422.8298	1456.9931
H,0,0.6363829253,2.2328593071,1.6524895061	1476.3209	1486.6876	1492.2843
H,0,2.4512578282,-1.1889615567,1.4761799151	1499.6975	1508.4991	1516.4139
H,0,3.1053215536,0.5180872729,1.2291536684	1517.8311	1623.7749	3040.2355
H,0,-2.0530150716,-0.265138493,-1.4243110367	3046.3607	3049.6518	3054.9496
H,0,-3.6428177627,-1.9933261132,-0.7759366534	3056.2484	3098.0521	3109.3267
H,0,-2.1019662803,-2.3392637874,-0.0008274697	3110.3304	3115.1757	3124.1908
H,0,-3.4325223709,-1.6356986157,0.9305411069	3126.3295	3146.8512	3168.6009
H,0,-4.4547967887,0.3621899306,-1.0536881052	3199.5173	3234.4374	3260.8325
H,0,-3.3760656282,1.7261019184,-0.7634911335			
H,0,-4.0560204314,0.8346025946,0.6009925728			
TS: Sabinene + O_3 → POZ-AR			
0,1			
C,0,1.0433954835,0.2796425979,0.9109619131	-323.4443	33.4764	52.9535
C,0,-0.1911000725,-0.5223701517,0.9992750068	87.8435	121.1754	162.1414
C,0,-1.2563968913,0.0016281659,1.9483478706	191.6538	212.0029	230.4538
C,0,-1.3355023511,0.3212757969,0.4920482813	238.9609	254.4401	314.6665
C,0,-0.7461319508,1.6745194857,0.1002646711	326.9351	356.7841	400.6092
C,0,0.659665141,1.7263843348,0.7228466973	438.5299	455.5766	483.7079
C,0,2.3006870694,-0.1925942497,1.1489393679	547.0062	603.8551	628.5501
C,0,-2.4392411049,-0.2218223519,-0.3955746155	690.536	792.5815	802.9922
C,0,-2.9072145832,-1.6252620851,-0.0220033477	818.9217	826.5594	876.2515
C,0,-3.6298161181,0.7383145807,-0.402851809	910.3108	923.7294	938.4023
O,0,1.2260800797,0.080335507,-1.4247344881	941.2228	948.6314	975.6409
O,0,1.8636277687,-1.0120153421,-1.3804059266	990.8888	998.8146	1025.5201
O,0,2.9735759766,-0.9057379874,-0.7956651156	1047.4362	1059.5655	1070.396
H,0,-0.1373790054,-1.5895585702,0.8367842968	1125.2805	1142.8088	1162.1922
H,0,-1.930033431,-0.7446291388,2.3428442765	1183.6197	1194.9553	1239.5524
H,0,-0.9836283196,0.7773203788,2.6509448241	1245.7715	1262.604	1279.3422
H,0,-1.3704194404,2.5072984377,0.4246816101	1307.0053	1320.3572	1343.7738
H,0,-0.6709196102,1.7138869169,-0.98804131	1353.2618	1381.4951	1404.7219
H,0,1.3821852428,2.2524046745,0.1018113586	1408.8988	1424.619	1455.89

H,0,0.6420134359,2.2219169195,1.6960922977	1479.3398	1486.675	1492.556
H,0,2.4492008936,-1.1908825458,1.535279266	1497.9557	1509.7272	1517.1941
H,0,3.1426761685,0.4828261957,1.1821762469	1519.1598	1617.275	3031.3108
H,0,-2.0220906391,-0.2635185331,-1.4076084103	3040.5725	3048.6614	3056.7809
H,0,-3.6138402126,-1.9903216345,-0.7669767747	3060.5553	3102.3766	3109.3522
H,0,-2.0834052862,-2.337068531,0.0262484404	3116.9937	3118.4245	3122.0435
H,0,-3.4218574408,-1.6263965868,0.9402748724	3123.2242	3145.6126	3162.2126
H,0,-4.4298770087,0.3586603206,-1.0389986102	3170.1687	3230.7853	3254.6733
H,0,-3.3518079768,1.7267519315,-0.7674857467			
H,0,-4.0264385871,0.8496671439,0.6090134866			
POZ-AL			
0,1			
C,0,1.1502418935,0.2091333575,0.1157714514	47.5978	77.157	85.7467
C,0,-0.0450957447,-0.6908253599,0.2686194109	157.0599	165.0407	222.8883
C,0,-0.8521921459,-0.5486880914,1.533159949	256.7372	261.8884	277.6481
C,0,-1.2815936467,0.1659130051,0.2880253829	300.5692	358.6443	367.2526
C,0,-0.8228703666,1.6174654813,0.1934968983	399.4488	459.539	473.9873
C,0,0.6670159568,1.59054566,0.564570382	497.1379	537.2411	585.6194
C,0,2.493417803,-0.2411499024,0.7391009208	694.803	739.487	759.0737
C,0,-2.54937654,-0.2720320782,-0.413722029	826.5208	829.8435	875.252
C,0,-3.7699772874,0.4293361169,0.1781013079	890.4496	914.5308	932.0099
C,0,-2.4661188189,-0.0586043146,-1.9240607403	939.0257	954.0536	976.7478
O,0,1.4653281788,0.2109244051,-1.2838274742	987.7828	999.5279	1005.6188
O,0,2.8391666291,0.5005279416,-1.3006424021	1019.1757	1043.0497	1049.43
O,0,3.3410471869,-0.4415306106,-0.3756543376	1069.0292	1075.5355	1086.2362
H,0,-0.0192099076,-1.6464625204,-0.2375992144	1118.5248	1141.7754	1157.2324
H,0,-1.4316124181,-1.4153061211,1.8193441793	1190.5741	1210.347	1217.6035
H,0,-0.4451782397,0.0089745132,2.3655669956	1235.7926	1265.3519	1287.5865
H,0,-1.3978661965,2.28223854,0.8389671084	1309.8216	1334.8067	1347.6753
H,0,-0.9406818798,1.9633595736,-0.8342446631	1358.1028	1368.7549	1391.1752
H,0,1.2531968186,2.3681416379,0.0771388196	1402.772	1424.5537	1435.6757
H,0,0.8090486524,1.6986520978,1.6407211806	1487.7547	1491.05	1494.7481
H,0,2.416343639,-1.1919709826,1.2620749812	1500.5978	1507.8428	1512.1594
H,0,2.8990277811,0.5299733553,1.3971452575	1517.3152	1522.5134	3026.8739
H,0,-2.6528011018,-1.347042965,-0.2325664326	3039.5925	3053.0595	3062.0647
H,0,-4.6901990752,0.0664792347,-0.2801821977	3069.3621	3073.5184	3108.6921
H,0,-3.8344055848,0.2647499481,1.2544017456	3114.0892	3118.389	3123.8655
H,0,-3.7142201944,1.5056227082,0.0033392544	3131.3807	3132.102	3138.8627
H,0,-3.3194440577,-0.5182010663,-2.4231340535	3142.7955	3172.4653	3226.3392
H,0,-1.5523272606,-0.4917618243,-2.3329516685			
H,0,-2.4757306426,1.0035632103,-2.1735477025			
POZ-AR			
0,1			
C,0,1.2203217436,0.1252403644,0.1591367693	42.931	67.7557	90.166
C,0,-0.0326044343,-0.6758769641,0.4136672493	159.3474	178.1464	225.8352
C,0,-0.9105267966,-0.2328003543,1.5545285688	254.5776	276.0276	291.5449
C,0,-1.2259096151,0.1986127869,0.1504320665	317.0805	342.3737	386.2508
C,0,-0.6890162142,1.5744444154,-0.230484094	405.2256	439.8954	457.4357
C,0,0.776987709,1.5860493569,0.2239152474	503.3789	521.0851	606.123
C,0,2.4459644297,-0.2783499304,1.0138106249	696.7732	735.2405	761.1056
C,0,-2.4787649634,-0.2666647185,-0.5676516472	820.1633	839.0655	875.906
C,0,-2.8921085506,-1.6963071369,-0.2309694911	895.7926	913.3171	925.9849
C,0,-3.6379700263,0.6905038285,-0.288121887	938.5154	944.6316	969.8938
O,0,1.7010290907,-0.1328483985,-1.1641774169	982.3535	993.857	1012.9181
O,0,2.5253359377,-1.2517672836,-0.9739238358	1021.3002	1039.2375	1062.5713
O,0,3.3642533023,-0.8174555191,0.0785616508	1067.5841	1076.7653	1112.074
H,0,-0.0047554687,-1.7237613666,0.1490508875	1130.716	1140.7707	1143.6889
H,0,-1.532750789,-0.9967629321,1.9959966241	1183.1197	1206.0651	1220.0485
H,0,-0.5371481687,0.4957885087,2.2622689204	1245.2403	1252.6184	1286.2179
H,0,-1.2601822585,2.3901059508,0.2135810398	1317.1274	1339.5062	1349.0699
H,0,-0.7480212458,1.6785545427,-1.3167777046	1355.3068	1369.8016	1383.3469
H,0,1.4222137947,2.2075116792,-0.3937975599	1404.7534	1421.4671	1427.7879
H,0,0.8638988405,1.9399444744,1.2507944362	1489.2462	1492.2577	1496.1742
H,0,2.1662265664,-1.0204604434,1.7635196465	1502.8759	1512.9621	1517.5212
H,0,2.935917529,0.5740652972,1.4807641691	1518.5888	1519.8948	3026.4268
H,0,-2.2512210148,-0.2273134134,-1.6385464252	3045.4837	3049.0375	3058.5519
H,0,-3.7140682614,-2.006951076,-0.8755863228	3073.8498	3079.9651	3105.248
H,0,-2.076466518,-2.4053347678,-0.3701835139	3112.9153	3117.4697	3125.0864
H,0,-3.2430762172,-1.7724626172,0.7995615072	3129.6782	3130.7493	3139.3439
H,0,-4.5439718942,0.3617688265,-0.7977123764	3141.3289	3188.3252	3226.317
H,0,-3.4161313453,1.7044871282,-0.6199148638			
H,0,-3.8462083015,0.7232695522,0.7837555509			
TS: Sabinene + O_3 → POZ-SL			
0,1			

C,0,0.8491525643,0.1011028416,-0.5059402252	-342.6250	37.2048	58.335
C,0,-0.3184477335,-0.6673824108,-0.0334553728	83.5414	113.0892	147.8891
C,0,-0.9727416453,-0.1935709064,1.2445118343	193.8568	200.2401	212.0351
C,0,-1.5173047234,0.2687753721,-0.0638973276	232.4014	254.4832	304.9246
C,0,-1.0065972182,1.6288690048,-0.5311832532	340.65	375.2548	400.0916
C,0,0.5268509474,1.5766419958,-0.3984891046	442.7875	459.6224	484.0656
C,0,1.8507617399,-0.4087056792,-1.2814827362	516.8043	596.8575	662.1824
C,0,-2.8918739961,-0.1470663479,-0.5542827451	685.8261	793.166	796.6529
C,0,-3.3003354456,-1.5579153029,-0.141396468	809.7312	822.9628	877.9739
C,0,-3.9437066874,0.8590374569,-0.0833283506	909.7542	925.8564	934.1624
O,0,2.0391817385,-0.1470734534,1.4586233588	941.0348	963.0971	974.3711
O,0,3.1692453334,0.1567301637,0.9811101542	981.8062	998.2178	1033.2543
O,0,3.5458612223,-0.6407462751,0.0806359425	1049.0003	1059.533	1077.2976
H,0,-0.3969516941,-1.7118400495,-0.2955275219	1128.4767	1139.7992	1163.5745
H,0,-1.5313027146,-0.9433118131,1.7841633269	1186.1389	1194.8798	1231.8116
H,0,-0.4160226467,0.4928122863,1.8677376763	1242.3098	1267.7768	1280.092
H,0,-1.4408058111,2.4536515503,0.0342425834	1316.0106	1319.2727	1342.5095
H,0,-1.2875371963,1.7607480497,-1.5793755231	1350.8335	1383.0336	1402.5427
H,0,1.0363520215,2.1594163307,-1.1632824962	1405.426	1423.6239	1456.4899
H,0,0.8456223653,1.9629154166,0.5697374303	1488.5916	1489.5663	1494.0696
H,0,1.8968501643,-1.4669299345,-1.4921590508	1498.5568	1511.1599	1516.4928
H,0,2.4676794404,0.2427885035,-1.8833728956	1519.0684	1608.4827	3026.0733
H,0,-2.855206595,-0.1151275519,-1.649107555	3040.0404	3050.3567	3057.7854
H,0,-4.2358583026,-1.8304702057,-0.6295214086	3080.6741	3099.6976	3110.0872
H,0,-2.5532389658,-2.3014607202,-0.4177254205	3118.9717	3123.2854	3124.5358
H,0,-3.4660134656,-1.6212009125,0.9350853357	3128.7509	3146.3858	3156.6028
H,0,-4.9382532483,0.5655071274,-0.4202057958	3197.8706	3235.0596	3249.0426
H,0,-3.7435091697,1.8612242097,-0.4613389185			
H,0,-3.955443898,0.9046927438,1.0079365769			
TS: Sabinene + O_3 → POZ-SR			
0,1			
C,0,0.8300231012,0.0863079717,-0.457958237	-339.4907	52.972	63.0839
C,0,-0.3302856618,-0.6979725431,0.0050561463	85.94	116.504	155.1586
C,0,-0.9851905859,-0.2539564495,1.2937782482	191.1743	214.9059	218.2435
C,0,-1.5352727471,0.2361266985,-0.0001143042	238.8191	266.386	309.1807
C,0,-1.0288459585,1.6041947326,-0.4484614332	344.4406	378.1506	398.5397
C,0,0.504247962,1.557178071,-0.3155229149	436.7686	458.6322	474.7435
C,0,1.82054169,-0.4311902415,-1.2422098283	530.2624	597.1055	663.8704
C,0,-2.90725492,-0.179189966,-0.498015945	684.8086	797.1803	801.0821
C,0,-3.3180039625,-1.5908194445,-0.0895842192	815.2892	820.6578	879.5568
C,0,-3.9611815221,0.8253312674,-0.0277835252	907.1006	926.0171	936.961
O,0,2.1524340252,0.0912100602,1.4477287182	950.5378	964.5345	975.121
O,0,2.7097342799,-1.0187399531,1.2153925205	984.2246	996.9409	1031.8752
O,0,3.3930121156,-1.0050601088,0.1562605286	1049.3441	1057.1814	1076.1582
H,0,-0.4108622576,-1.7348784979,-0.2866491899	1127.5891	1139.9278	1164.8883
H,0,-1.5406369296,-1.0168234543,1.8185460839	1189.8583	1192.235	1232.728
H,0,-0.4208538194,0.4146146654,1.9293305041	1242.7158	1266.8694	1280.7238
H,0,-1.4672837809,2.4185162821,0.1290477764	1311.2875	1319.399	1340.9087
H,0,-1.3122074416,1.7489743391,-1.4943322412	1350.4974	1382.624	1401.964
H,0,1.0137871971,2.1602828561,-1.0637355457	1405.478	1425.0681	1457.2904
H,0,0.8211208944,1.9206907247,0.6617053505	1490.2569	1491.7977	1495.304
H,0,1.7943971575,-1.4664554287,-1.5515989286	1500.3952	1511.5066	1517.9415
H,0,2.5095275169,0.2217061171,-1.7569279863	1520.1918	1606.1602	3022.1296
H,0,-2.8659211628,-0.1436168508,-1.5924440473	3041.4496	3054.0592	3060.3196
H,0,-4.2443704714,-1.8671696396,-0.5925790584	3078.7654	3104.1948	3110.7866
H,0,-2.5643032084,-2.3332580652,-0.3515330681	3118.7717	3123.8376	3127.1144
H,0,-3.501156499,-1.6517326218,0.9842143608	3135.018	3149.188	3170.6131
H,0,-4.9545896741,0.5298838595,-0.366112547	3207.3608	3236.1709	3261.7815
H,0,-3.762650139,1.8283736484,-0.4043584818			
H,0,-3.9743921281,0.869597821,1.0634918038			
POZ-SL			
0,1			
C,0,-3.2245481684,0.4860185339,-0.7661230863	39.0137	57.8637	74.7594
C,0,-2.1562881574,-0.5704575398,-0.6884509951	166.5275	174.1116	214.6873
C,0,-0.8794462343,-0.3255848852,-1.4487949283	247.5067	284.9517	289.322
C,0,-0.9559346249,0.0236509603,0.0056454882	310.7048	353.6944	382.4435
C,0,-1.293404387,1.4843465668,0.2959093217	417.2162	445.1459	456.8818
C,0,-2.4783644791,1.8188982144,-0.6170066957	505.3018	534.9295	600.6945
C,0,-4.3539412999,0.2948860107,0.2834836683	688.2064	721.0618	756.1263
C,0,-0.1347244842,-0.7107477526,1.050402979	829.4049	845.925	874.2557
C,0,0.0803785687,-2.1899856377,0.7449211171	893.173	917.8821	932.5591
C,0,1.21465828,-0.0171611974,1.2430212585	936.601	959.2568	970.4997
O,0,-3.9525087369,0.3908475272,-1.9861858998	977.0906	1004.8024	1009.3984
O,0,-5.1824928732,0.9797258218,-1.6530086456	1022.0758	1045.2754	1058.7814

O,0,-5.54178613,0.2625597953,-0.4874161717	1067.6495	1075.8491	1112.2443
H,0,-2.4700514091,-1.5915956654,-0.5254297201	1130.58	1139.2005	1141.4269
H,0,-0.3264411963,-1.2122465198,-1.7196644688	1181.1731	1206.9941	1219.2881
H,0,-0.8506763852,0.4592590851,-2.1909879652	1234.487	1253.7882	1280.2741
H,0,-0.4484631414,2.1547982091,0.1364363381	1318.0542	1338.2969	1341.6848
H,0,-1.5828755911,1.5682618538,1.3481635865	1350.2029	1366.0893	1379.879
H,0,-3.1142731094,2.6111251589,-0.2282686962	1405.4561	1422.156	1430.1366
H,0,-2.138492482,2.1297158709,-1.6037133938	1491.2893	1493.4862	1499.6625
H,0,-4.2873404088,-0.6580099385,0.8047878185	1501.9466	1512.1115	1518.6782
H,0,-4.3716452582,1.1202262745,0.9982989518	1520.1373	1529.0419	3015.2769
H,0,-0.6915563719,-0.6400356507,1.9920246963	3037.0855	3041.6615	3053.1929
H,0,0.5709276974,-2.6744188865,1.588901022	3062.4291	3089.0829	3099.5735
H,0,-0.8562698532,-2.7154048761,0.5595439771	3113.7161	3121.0233	3122.4878
H,0,0.7260164792,-2.3215806913,-0.1245497332	3127.8553	3134.5039	3146.7884
H,0,1.81789755,-0.5428949939,1.9834244592	3154.3083	3190.8542	3235.5285
H,0,1.0972578129,1.0133540137,1.5768243131			
H,0,1.7676043939,-0.0070906617,0.3011784041			
POZ-SR			
0,1			
C,0,1.1974202308,0.0417240934,0.1134505413	48.0787	58.1419	75.0141
C,0,-0.0720054625,-0.7005446809,0.4522217832	164.1815	181.9994	209.313
C,0,-0.9276564036,-0.1377525564,1.5528321918	242.1362	280.5276	296.4958
C,0,-1.2399172245,0.198703669,0.1269714746	318.3661	374.0905	411.1746
C,0,-0.6551498517,1.5252687761,-0.3538992128	426.1616	430.6703	452.0218
C,0,0.8057423246,1.5206785262,0.1065465652	467.9786	553.4084	604.8543
C,0,1.8211954469,-0.4725063798,-1.2106730262	688.592	720.564	760.9761
C,0,-2.5121775007,-0.2757084169,-0.5521958244	821.1433	842.0356	876.8777
C,0,-3.0007820586,-1.6377370681,-0.0680362669	892.9789	916.7334	932.0892
C,0,-3.621003127,0.7642312985,-0.3863840237	942.1094	962.0674	975.6972
O,0,2.2756329558,-0.1345914072,1.0339598782	985.6861	996.8807	1009.9083
O,0,3.0636755375,-1.1456583286,0.4512011959	1025.6954	1045.7539	1062.353
O,0,3.1753539766,-0.6926156685,-0.8793224089	1069.8585	1083.1738	1108.8611
H,0,-0.103092343,-1.7657718328,0.2723635498	1125.8308	1138.4103	1142.1172
H,0,-1.5713319441,-0.8469534534,2.0509606888	1181.432	1218.8652	1225.7312
H,0,-0.512513754,0.618477628,2.2047370142	1242.2575	1251.0032	1298.5446
H,0,-1.2024508416,2.3890912993,0.0242684791	1308.5373	1335.3994	1345.5434
H,0,-0.7127098236,1.5540703989,-1.4465759577	1355.8999	1375.9866	1381.8115
H,0,1.4692307568,2.108567201,-0.5246794682	1406.1734	1422.5944	1432.228
H,0,0.899983211,1.9072881913,1.1208921389	1492.1321	1493.8682	1499.2149
H,0,1.3488735486,-1.4023116039,-1.5332558295	1503.056	1509.4994	1516.5033
H,0,1.7957348823,0.2667008497,-2.0090554046	1516.9587	1529.1916	3021.3057
H,0,-2.2827428977,-0.3612324692,-1.6208360632	3038.6874	3041.5483	3049.3256
H,0,-3.8316501388,-1.9753976977,-0.6870776736	3082.4429	3083.9649	3097.3826
H,0,-2.2217780119,-2.398433939,-0.1148012148	3108.9743	3117.9152	3122.0037
H,0,-3.363301201,-1.5810355734,0.9594136265	3123.9302	3134.2939	3147.1646
H,0,-4.5432287898,0.4251714306,-0.8586919205	3157.427	3190.3668	3238.5165
H,0,-3.3493422433,1.7214871463,-0.8303533119			
H,0,-3.8242505136,0.9281225374,0.6741158496			
TS POZ-SL → CH_2OO + Sabinaketone			
0,1			
C,0,1.2939141298,0.1908443271,0.294523987	-555.5048	62.6617	74.35
C,0,0.0404767951,-0.6201438508,0.5555965842	108.2717	168.3287	189.6989
C,0,-0.8941176221,-0.0636011331,1.5973658318	223.5936	261.1404	265.4516
C,0,-1.1481625737,0.1997807524,0.1433898324	299.8727	323.87	326.9854
C,0,-0.6246590873,1.5494269058,-0.3569396957	357.3163	394.7067	432.892
C,0,0.8280716566,1.6588942575,0.1173724475	454.8992	474.4636	522.3724
C,0,1.6929631845,-0.2444607332,-1.4823665707	587.2496	615.0367	638.1312
C,0,-2.3591886985,-0.3659243906,-0.5771105633	647.2258	696.7381	777.0718
C,0,-2.8012134236,-1.7317341962,-0.0600214748	843.2974	877.935	909.3003
C,0,-3.5282958635,0.6174786733,-0.5147674151	922.444	936.9332	938.6274
O,0,2.3967225469,-0.0723133753,0.858269648	958.3994	972.4706	997.3131
O,0,3.3794732496,-1.157189026,-0.5238908073	1017.1623	1035.6424	1042.3138
O,0,2.3114438879,-1.3790022226,-1.2274510185	1068.2075	1094.2436	1124.8507
H,0,0.0960766251,-1.6914753764,0.4251087195	1139.0559	1144.3875	1168.4083
H,0,-1.5259099745,-0.7829514413,2.0968796755	1173.3653	1195.3358	1228.1536
H,0,-0.5491811199,0.742501985,2.2309074833	1251.0776	1271.3476	1283.315
H,0,-1.2337589239,2.3799362046,0.0008499315	1309.2975	1316.395	1326.256
H,0,-0.6759183882,1.5624133975,-1.4502291923	1345.645	1381.27	1406.4628
H,0,1.4705275858,2.2297386494,-0.5484947886	1414.3581	1427.0518	1483.766
H,0,0.892127909,2.1265241705,1.0992062535	1494.6473	1495.2487	1499.2594
H,0,0.7761203041,-0.3871512694,-2.0413168983	1506.7604	1509.643	1512.0401
H,0,2.3434690628,0.5897913558,-1.7172200461	1520.1806	1527.4076	3015.4838
H,0,-2.0703469135,-0.4835510412,-1.6291621993	3042.5898	3047.9229	3051.4239
H,0,-3.5697591432,-2.1455318428,-0.7123428363	3080.4423	3093.8938	3112.5994

H,0,-1.9786517003,-2.4456103237,-0.0199740498	3118.3328	3118.6766	3121.6834
H,0,-3.2320053807,-1.6493833477,0.9388478358	3131.8728	3134.7989	3143.5974
H,0,-4.4041165771,0.210580807,-1.0207230083	3191.1615	3240.9446	3246.2033
H,0,-3.2843655819,1.5707369167,-0.9829631208			
H,0,-3.7982027954,0.8104420776,0.5258936451			
TS POZ-SL → CH_2O + Sab-CI-1			
0,1			
C,0,1.2019425389,-0.0248025924,0.192382773	-541.3428	44.8923	71.276
C,0,-0.0535935697,-0.7512482616,0.4843476487	147.2394	155.6956	196.6467
C,0,-0.9254498319,-0.1406820554,1.561264576	218.3892	247.8683	263.6893
C,0,-1.191154598,0.1808673578,0.1283815183	285.5252	289.3982	316.9442
C,0,-0.5699177028,1.4911480989,-0.3554381817	344.3849	383.8985	416.7435
C,0,0.9091542245,1.4538049108,0.0536355744	452.4873	508.5661	539.4995
C,0,1.8861446293,-0.5140721045,-1.4769618266	566.605	600.9004	608.8772
C,0,-2.4538628615,-0.2798073829,-0.5769166579	697.1127	712.5242	798.4593
C,0,-2.9757656527,-1.6297366012,-0.0945264799	837.5055	877.0098	911.8982
C,0,-3.545741909,0.7819086533,-0.4412804719	918.8434	933.12	941.4946
O,0,2.2964337284,-0.4088406258,0.8438766387	955.807	973.9305	1004.7651
O,0,3.3207201616,0.3105876585,0.4782154801	1024.8367	1041.2432	1056.6842
O,0,3.0629841671,-0.046723943,-1.4614187309	1067.9915	1117.5022	1130.0901
H,0,-0.0936820917,-1.8177963122,0.3215243931	1140.5785	1165.9937	1190.1733
H,0,-1.590282358,-0.8311485269,2.0580606576	1209.3344	1226.6827	1238.1309
H,0,-0.4933570623,0.6114908829,2.2067105213	1242.2304	1268.1995	1296.833
H,0,-1.0823606503,2.3621868674,0.0528529086	1316.4221	1343.0453	1347.8464
H,0,-0.6620983995,1.5425774406,-1.4432385365	1380.638	1387.8287	1403.6631
H,0,1.5791673993,1.9417060816,-0.6479402391	1424.1782	1427.5395	1440.4824
H,0,1.0826508822,1.9106101047,1.0313063399	1489.9342	1492.0255	1494.5483
H,0,1.7478948658,-1.6025366219,-1.4638239293	1499.1885	1510.5812	1516.3022
H,0,1.1186696629,0.0409569146,-2.0345535623	1518.5905	1561.7075	2992.3583
H,0,-2.1989574377,-0.375432549,-1.638489342	3021.8242	3038.8207	3051.84
H,0,-3.7952186663,-1.9587688925,-0.7327246766	3052.5381	3066.7534	3067.3423
H,0,-2.2090430434,-2.4040334241,-0.1171347258	3100.0882	3109.4883	3121.7333
H,0,-3.364425711,-1.5594358222,0.9225545943	3122.8964	3126.3597	3145.8487
H,0,-4.4604714701,0.4609959966,-0.9394611218	3147.9564	3210.0066	3233.1329
H,0,-3.2424494211,1.7336545719,-0.8762414319			
H,0,-3.7758778731,0.9487855461,0.61327149			
TS POZ-SR → CH_2OO + Sabinaketone			
0,1			
C,0,1.260170162,-0.0316382966,0.3478245742	-562.1574	51.2467	73.8413
C,0,-0.0630073047,-0.7556597261,0.5579528089	100.1487	170.6074	189.5122
C,0,-0.9637819331,-0.13400233,1.5937884584	224.2635	264.5943	272.6987
C,0,-1.1736117539,0.165069598,0.1404386843	282.1087	314.5767	325.3201
C,0,-0.5361856474,1.4768161827,-0.3278022708	360.2852	380.2084	424.167
C,0,0.9155908033,1.458517781,0.1634119491	454.25	470.1501	521.4779
C,0,1.6219069365,-0.6357486565,-1.388595585	587.1853	610.044	636.548
C,0,-2.419633583,-0.2866624962,-0.6007050263	645.7699	701.1658	778.2723
C,0,-2.9760938308,-1.6225200018,-0.116875036	836.1877	873.526	901.6707
C,0,-3.5044985518,0.7879381433,-0.5204875491	916.018	933.8421	934.8658
O,0,2.3202099306,-0.3781907173,0.9486278664	958.6811	974.3354	1003.8014
O,0,3.5750042332,-0.8733082794,-0.5397522689	1026.2134	1036.2269	1041.9568
O,0,2.8791567679,-0.2488945966,-1.4400134461	1064.6319	1086.19	1125.4991
H,0,-0.0969246205,-1.8273039839,0.4260715518	1138.9571	1141.2414	1163.2323
H,0,-1.654972326,-0.8088335663,2.0765382947	1177.0734	1195.0056	1237.2461
H,0,-0.5625996071,0.6342737404,2.2405352518	1254.2719	1273.8331	1278.9752
H,0,-1.084068085,2.3455348719,0.0377982609	1308.679	1318.8368	1328.4834
H,0,-0.5770201964,1.5123516339,-1.4208414147	1345.6506	1372.354	1403.8911
H,0,1.6149622648,1.9492774298,-0.5109490971	1410.5448	1425.8076	1481.074
H,0,1.018675929,1.9406811493,1.1352549608	1489.6657	1494.7166	1495.8922
H,0,1.4719701962,-1.6955574695,-1.2214297753	1501.888	1508.1129	1512.3908
H,0,0.9948113026,-0.1149095939,-2.1020798327	1518.808	1520.8614	3007.7849
H,0,-2.1332511818,-0.4031914986,-1.6532925745	3040.7654	3041.5968	3058.8367
H,0,-3.7796619714,-1.9504377761,-0.7758512877	3087.799	3110.1696	3111.448
H,0,-2.2193906696,-2.4068688412,-0.1007120495	3122.9262	3123.1591	3126.0529
H,0,-3.3953647007,-1.5308581198,0.8861097532	3134.5142	3134.9868	3145.6923
H,0,-4.411242627,0.4618797925,-1.0303422387	3191.2102	3229.347	3247.9193
H,0,-3.1833254565,1.7249308317,-0.9743558898			
H,0,-3.7559161693,0.9863728953,0.5236726276			
TS POZ-SR → CH_2O + Sab-CI-2			
0,1			
C,0,1.1582788734,0.3632488676,0.3399634338	-551.4431	57.8634	73.607
C,0,0.0066502782,-0.551452315,0.550972194	134.7275	140.6907	178.0394
C,0,-0.8993751546,-0.1592097811,1.6970803362	232.4661	250.6422	262.4706
C,0,-1.2424111169,0.2520112768,0.2997583713	274.11	308.1155	319.9261
C,0,-0.8086417731,1.6696272613,-0.0725169376	343.3369	395.878	435.338

C,0,0.6688814533,1.7932715393,0.336162697	443.5974	460.2081	513.9358
C,0,1.8222289997,-0.1722956979,-1.3336250967	580.4211	597.0371	614.8318
C,0,-2.4541264947,-0.300569641,-0.428119118	705.1407	715.1814	794.7319
C,0,-2.7922389832,-1.7416780562,-0.0580500831	836.4794	882.108	891.8593
C,0,-3.6685085869,0.5981609159,-0.1923754622	921.9047	936.1341	943.0303
O,0,2.3177251105,0.1432025351,0.9514789277	971.3768	978.6604	1002.0254
O,0,2.6344737549,-1.1200105861,0.906921455	1028.9308	1039.4102	1057.7294
O,0,2.4344828606,-1.2483241913,-1.0713870984	1070.3706	1114.9924	1133.3874
H,0,0.1178604531,-1.5905573164,0.2856546688	1141.3863	1164.2263	1189.6186
H,0,-1.4559312452,-0.971724509,2.1389818899	1210.488	1227.6507	1236.9383
H,0,-0.5584335302,0.5855948467,2.4032920805	1246.0637	1258.377	1297.3804
H,0,-1.4250577822,2.4312163434,0.4042741478	1316.6379	1346.9354	1352.0748
H,0,-0.9135536654,1.7941414977,-1.1531340473	1376.941	1387.4799	1406.1085
H,0,1.2488557897,2.4239521028,-0.3342079778	1421.244	1428.4345	1437.2079
H,0,0.7755987704,2.2037934065,1.3408743559	1492.8787	1493.3401	1497.3834
H,0,0.8232581306,-0.2452458145,-1.7857309102	1502.132	1512.9007	1517.5133
H,0,2.4048101843,0.7081844568,-1.634991426	1520.9577	1555.3831	2981.0646
H,0,-2.2118667888,-0.2756635627,-1.4969981416	3017.2436	3048.6706	3054.7481
H,0,-3.5744783824,-2.1193018108,-0.7157099568	3055.0113	3056.5483	3077.5667
H,0,-1.9330281183,-2.4057036294,-0.1487416312	3103.6328	3117.8562	3121.965
H,0,-3.1697590455,-1.8051710136,0.9636828722	3128.4042	3131.6516	3138.4032
H,0,-4.5457604822,0.203883734,-0.7051386132	3155.6626	3223.6936	3244.1571
H,0,-3.5000693562,1.6136006349,-0.5504132492			
H,0,-3.8946315629,0.6486028858,0.8750213091			
TS POZ-AL → CH_2OO + Sabinaketone			
0,1			
C,0,1.1366442905,0.2222204653,-0.1926991568	-532.2289	43.7795	87.2694
C,0,-0.0497035772,-0.6604194682,0.1282671032	97.8398	142.2675	179.0674
C,0,-0.8474838169,-0.3512511273,1.36627109	229.3039	244.9537	268.2633
C,0,-1.2778942504,0.2101178953,0.0455542884	276.7965	309.3608	327.2443
C,0,-0.80698096,1.6388853744,-0.2296188783	371.9075	405.1969	435.675
C,0,0.6927313895,1.6792216142,0.1017935583	458.4232	483.8674	499.1525
C,0,2.4313877167,-0.0430284402,1.1185956049	533.1471	596.753	634.775
C,0,-2.5716393919,-0.215436768,-0.6245167104	694.4912	710.7656	776.5544
C,0,-2.9386102009,-1.6771383883,-0.387336161	830.2208	875.6108	905.5875
C,0,-3.7214447706,0.689804633,-0.1802476321	920.1689	926.0991	937.2984
O,0,1.8007895847,-0.020488711,-1.2448025551	954.7944	977.2029	992.6417
O,0,3.4847160745,-0.9199717729,-0.5314796279	1036.02	1038.8666	1054.1908
O,0,2.9456374439,-1.148434694,0.6254504947	1070.2489	1100.7284	1126.7719
H,0,-0.0247455511,-1.6674131117,-0.2603645327	1140.2957	1146.0431	1158.9227
H,0,-1.4224899614,-1.1664211812,1.7797998455	1188.4064	1192.3576	1229.831
H,0,-0.4335999217,0.3185767902,2.1101613758	1249.4001	1277.3506	1283.7294
H,0,-1.3705909249,2.3775019298,0.3409754777	1319.1041	1323.3111	1326.9794
H,0,-0.9543632137,1.8489936529,-1.2918196782	1347.9173	1380.5594	1404.4334
H,0,1.2621965333,2.3616836573,-0.5230304768	1407.8364	1426.3054	1482.9004
H,0,0.847760434,1.9558214015,1.145144918	1485.7091	1489.6171	1494.5963
H,0,1.9450876257,-0.1995317537,2.0731711602	1499.113	1507.32	1511.8981
H,0,3.0146311441,0.8549258127,0.948176105	1517.7604	1518.1236	3028.4885
H,0,-2.4217522511,-0.0772614208,-1.7008457838	3044.5301	3058.2395	3059.0466
H,0,-3.8036142593,-1.9446671675,-0.9938071582	3073.2257	3107.1201	3115.3492
H,0,-2.1265549574,-2.3538654596,-0.651326333	3126.3877	3126.8025	3127.7854
H,0,-3.2073381301,-1.8504603921,0.6559669998	3133.2775	3140.6456	3144.0925
H,0,-4.657250617,0.3843712126,-0.6489587097	3209.574	3227.7979	3257.414
H,0,-3.5416768294,1.7326375042,-0.4396235639			
H,0,-3.8498575621,0.6271806833,0.9028529866			
TS POZ-AL → CH_2O + Sab-CI-1			
0,1			
C,0,1.0964980175,0.0584564555,-0.0661699049	-543.3157	45.565	70.2609
C,0,-0.1242601384,-0.7283935283,0.2135331411	110.9277	132.227	166.8429
C,0,-0.9220097789,-0.2670532747,1.4087978515	222.2632	239.2236	256.6761
C,0,-1.3100449473,0.2017233869,0.0450458136	276.31	306.8125	314.1395
C,0,-0.7529986814,1.5678266625,-0.3453704405	358.2197	386.3247	425.5907
C,0,0.7558297485,1.5389633179,-0.0261642511	451.2965	466.4049	516.5424
C,0,2.4990013738,-0.2520396826,1.151832066	569.6528	600.778	635.414
C,0,-2.6110436465,-0.2221513156,-0.6108573625	681.6771	718.2807	801.5936
C,0,-3.0599058574,-1.633925288,-0.2461182721	819.6064	873.3283	891.9342
C,0,-3.7168250268,0.7803537196,-0.2760397706	914.6082	923.0324	937.979
O,0,1.8033077711,-0.3962372804,-1.1023049921	948.7184	975.8961	992.9627
O,0,2.8578609023,0.3334508744,-1.3242797684	1030.7422	1046.7311	1055.3453
O,0,3.5212765331,0.1904354383,0.5539282866	1070.5581	1126.7355	1134.3898
H,0,-0.1407952569,-1.7701820511,-0.0694448165	1141.6576	1153.9733	1179.0132
H,0,-1.5338676976,-1.0237896988,1.8753868831	1204.7978	1222.3706	1234.9409
H,0,-0.4657382148,0.4303087667,2.0988453351	1241.984	1255.8041	1309.6304
H,0,-1.2593826456,2.3843778282,0.1690490934	1316.3618	1345.6003	1350.0623

H,0,-0.9045268696,1.7072979205,-1.4181520719	1378.2085	1386.4725	1405.1295
H,0,1.3688118135,2.0679190144,-0.7507795488	1424.1936	1427.1373	1440.4803
H,0,0.9684198256,1.9652893261,0.9509218359	1487.0796	1490.1689	1494.4858
H,0,2.4014528391,-1.3339744647,1.309544464	1498.9164	1510.3501	1515.993
H,0,2.0497490737,0.3690587534,1.9364356462	1517.2264	1562.5192	2993.249
H,0,-2.4370151247,-0.1914735891,-1.6918716881	3035.7242	3044.1846	3050.517
H,0,-3.919547741,-1.9166733951,-0.8528754898	3055.3989	3067.5102	3101.0767
H,0,-2.2789558125,-2.375166636,-0.4148535027	3111.9104	3113.7607	3119.4881
H,0,-3.3692072351,-1.6904423558,0.7987411766	3132.5044	3136.3816	3139.6943
H,0,-4.6607364326,0.477162619,-0.7292088286	3156.9481	3199.5701	3232.4705
H,0,-3.4800351667,1.7820129293,-0.6336031782			
H,0,-3.8622026844,0.8310458977,0.8052989035			
TS POZ-AR → CH_2OO + Sabinaketone			
0,1			
C,0,1.2270398481,-0.006039852,-0.1221962186	-537.3231	43.1031	76.8064
C,0,-0.0244311728,-0.7724934032,0.2817455567	99.2344	136.3494	157.2118
C,0,-0.7884934898,-0.2817546303,1.4834488836	215.3072	244.2251	265.9002
C,0,-1.187606139,0.1670674663,0.1094260334	267.2429	305.4217	329.4148
C,0,-0.6249757308,1.5241008023,-0.3140879132	367.0476	395.8831	440.5165
C,0,0.880150686,1.4916311089,-0.0029896042	459.9909	490.2573	507.8969
C,0,2.3827566726,-0.4538937665,1.2571537887	524.0125	596.1993	631.252
C,0,-2.5102913766,-0.2426255474,-0.5138454774	694.78	706.0539	778.9542
C,0,-2.9651152686,-1.650357709,-0.1407576272	826.7486	867.6294	910.5878
C,0,-3.5999673261,0.7689406441,-0.1552200599	916.0418	923.3727	935.7251
O,0,1.8851123573,-0.4125845817,-1.1288874245	952.6156	972.3775	993.7473
O,0,3.7471843781,-0.6989484143,-0.3787590062	1031.3448	1033.3282	1047.8973
O,0,3.4931145145,-0.0199259406,0.6968092994	1063.3604	1098.7571	1122.7103
H,0,-0.0672078576,-1.8142556235,0.0001161997	1140.5163	1143.6944	1152.9969
H,0,-1.4164168184,-1.0070277599,1.9789040368	1185.3828	1193.4226	1230.4674
H,0,-0.3258524606,0.4338748843,2.151154445	1244.9165	1267.4225	1278.995
H,0,-1.1314531015,2.3531838436,0.1800112145	1308.6038	1321.5132	1329.4025
H,0,-0.7779326699,1.6321419615,-1.3908330013	1348.4593	1381.0746	1401.8233
H,0,1.4797247343,2.0569943604,-0.7110207306	1404.8766	1425.2983	1480.3297
H,0,1.0777063992,1.882674006,0.9946309507	1487.9726	1490.2357	1494.4993
H,0,2.243871962,-1.5286213284,1.2374883887	1497.888	1502.6116	1509.9338
H,0,2.125878046,0.0978811643,2.1520830818	1517.2679	1519.3894	3027.8445
H,0,-2.3603762811,-0.2149422636,-1.5985900385	3042.5115	3053.7988	3056.1316
H,0,-3.8531391777,-1.9167429519,-0.7134704226	3087.3503	3103.95	3108.8668
H,0,-2.201993336,-2.4001714842,-0.3475206797	3121.0982	3128.4317	3129.0617
H,0,-3.2326064125,-1.7111462314,0.9154876701	3132.4459	3135.1611	3147.89
H,0,-4.5539903017,0.4824050716,-0.5983440922	3190.059	3223.9981	3253.8703
H,0,-3.3554213488,1.7709538671,-0.5062336163			
H,0,-3.7301729287,0.8111063977,0.9286105133			
TS POZ-AR → CH_2O + Sab-CI-2			
0,1			
C,0,1.2161810213,0.1887391945,0.0305550005	-541.0955	41.1697	82.1719
C,0,0.039081536,-0.6757582602,0.3064269836	117.5419	141.425	191.0535
C,0,-0.8047937224,-0.2889731493,1.4893004421	234.8989	254.3191	262.6929
C,0,-1.1879448024,0.2036355136,0.1312593238	279.5108	296.8272	324.1632
C,0,-0.6990830117,1.6140185372,-0.1920028844	352.0643	389.111	433.6959
C,0,0.8029357364,1.6342062048,0.1519198847	452.3066	477.1164	523.4055
C,0,2.5815980243,-0.3213615275,1.2143014075	556.464	602.197	642.4496
C,0,-2.4523978464,-0.2576530993,-0.5683403485	687.9815	711.6811	801.1669
C,0,-2.80432844,-1.7195541112,-0.3125642061	826.7605	882.6376	901.5467
C,0,-3.6251184746,0.6429629197,-0.1763168131	915.2614	928.2933	938.7084
O,0,1.9466233285,-0.0807863738,-1.0515250387	959.931	975.3206	992.3145
O,0,2.2475238894,-1.3458370133,-1.1220828745	1033.8741	1044.2578	1049.1006
O,0,3.0254624983,-1.3965020487,0.7189323133	1077.7399	1125.8377	1135.3585
H,0,0.0937823744,-1.7070916482,-0.0005098114	1141.8697	1155.586	1183.3392
H,0,-1.3864931846,-1.0876844107,1.9239642688	1219.4342	1228.5952	1236.0583
H,0,-0.4054144896,0.4130433901,2.2104673306	1240.7839	1249.082	1301.8973
H,0,-1.2524687436,2.3815364192,0.3485420641	1318.1291	1344.1329	1354.3297
H,0,-0.8363445387,1.7933126798,-1.2607942082	1380.2237	1388.8833	1404.5662
H,0,1.3953493351,2.2644687606,-0.5072621242	1418.064	1424.4544	1444.1083
H,0,0.9728629956,1.9729073637,1.1742315941	1485.6111	1491.0953	1496.8821
H,0,1.900104518,-0.390944174,2.0722155038	1503.6379	1512.2628	1519.1008
H,0,3.2197552619,0.5726005012,1.1961147593	1520.309	1557.7563	2982.4844
H,0,-2.2731218797,-0.1386739156,-1.6423746288	3033.4064	3045.7675	3050.7184
H,0,-3.6580844405,-2.0066770141,-0.925589231	3055.6617	3058.4934	3084.3381
H,0,-1.9809062769,-2.3897596332,-0.5572452455	3109.3623	3113.4594	3118.351
H,0,-3.0856188118,-1.8823998081,0.7290596588	3127.418	3133.7543	3136.4519
H,0,-4.5389677239,0.3267099611,-0.6792741451	3139.5802	3235.2365	3240.9613
H,0,-3.4424817685,1.6847873965,-0.4386019698			
H,0,-3.7963815638,0.5886066752,0.9010594244			

Sab-CI-1			
0,1			
C,0,-1.6237084201,-0.3105182419,-0.1195852157	59.4096	82.3316	128.9191
C,0,-0.6247291315,0.4319552041,0.6363467186	178.0833	209.3773	240.9707
C,0,0.1250717572,-0.427966848,1.6481174169	254.6136	281.7813	296.3893
C,0,0.7141751691,-0.2091863352,0.3052334901	319.1439	392.4024	404.4432
C,0,0.45951032,-1.347449452,-0.684549232	488.5557	501.7026	565.5717
C,0,-1.069265483,-1.5247181769,-0.7697611234	583.262	672.1974	704.7719
O,0,-3.6312731934,-0.738628863,-0.9913820201	807.7489	821.4662	878.8088
C,0,1.9579909507,0.6429110205,0.1638480169	915.8256	924.8005	938.9159
C,0,3.2090960795,-0.2203607265,0.3153181202	943.3589	964.41	976.9063
C,0,1.9778328445,1.4199390727,-1.1503622772	987.8886	1011.733	1042.7175
O,0,-2.8009250856,0.0701997287,-0.2384171808	1057.5644	1069.0557	1087.4619
H,0,-0.7589192043,1.48456278,0.8333194346	1146.159	1165.9028	1190.6231
H,0,0.5460608312,0.1219440829,2.477998063	1228.8295	1243.4805	1265.8331
H,0,-0.2913610023,-1.3931384077,1.9034468342	1291.2279	1313.9599	1347.2436
H,0,0.8517205534,-1.0765341931,-1.6641891263	1369.9438	1392.0031	1405.3934
H,0,0.9646891393,-2.2605828855,-0.3713419531	1426.0714	1431.3317	1454.1051
H,0,-1.4616180798,-2.4103324908,-0.2639605599	1492.3661	1494.1877	1502.2094
H,0,-1.4705039189,-1.5745872929,-1.7825544516	1508.7076	1516.6908	1519.614
H,0,1.9398712043,1.3679897969,0.9837638939	1690.9841	3035.5574	3043.7364
H,0,4.1096765471,0.3921041717,0.2792101594	3053.7082	3065.6615	3074.2043
H,0,3.2010149204,-0.7647530306,1.2601905827	3101.9704	3113.93	3118.6998
H,0,3.2707630135,-0.9491159295,-0.4954077057	3122.4191	3124.6896	3134.4867
H,0,2.8279245341,2.101487532,-1.1755259304	3144.2951	3208.9442	3237.4422
H,0,1.0675142947,2.0065274802,-1.2785200775			
H,0,2.0721848701,0.7495439837,-2.0056038068			
Sab-CI-2			
0,1			
C,0,-1.6576050127,-0.0355653763,0.653215526	22.1668	71.8101	133.7007
C,0,-0.5738295581,-0.9410720052,0.3405205287	190.8245	209.5986	244.3432
C,0,-0.380679895,-1.1912409388,-1.1530864046	266.6286	271.1922	280.8523
C,0,0.4080720403,-0.1250981438,-0.4997097834	316.2037	367.3311	441.6384
C,0,-0.1662752303,1.2834410817,-0.6544616036	487.1285	503.8028	564.402
C,0,-1.6381371081,1.1937285387,-0.2044295909	590.4002	685.7893	698.666
O,0,-2.4165317291,-1.3449831027,2.3068095853	809.3678	815.3023	883.1584
C,0,1.8985386987,-0.3075830465,-0.3045772676	918.1082	921.8351	930.2372
C,0,2.6597016945,0.2090542592,-1.5243213658	938.2597	960.3968	978.6663
C,0,2.3971608053,0.3495295136,0.9802547924	990.1399	1008.0599	1048.7107
O,0,-2.4800132701,-0.1737077394,1.5745394839	1054.4634	1064.9045	1088.0629
H,0,-0.3027416982,-1.6982778746,1.0573167946	1146.7811	1172.233	1189.8916
H,0,0.1236735117,-2.1198270452,-1.3788173458	1230.1252	1238.1938	1269.8452
H,0,-1.1900555774,-0.9396946624,-1.8243495694	1306.0344	1314.4343	1344.1934
H,0,0.3735484143,1.9682674255,-0.0008404612	1371.3281	1384.4104	1400.3448
H,0,-0.0684492168,1.650732523,-1.6755630257	1421.8666	1431.2987	1472.197
H,0,-2.3171406719,1.0491380904,-1.0477317824	1488.7047	1496.607	1502.4523
H,0,-1.986409862,2.0636026806,0.3467173229	1510.8619	1515.8629	1517.8174
H,0,2.0734403202,-1.3846030566,-0.2215410551	1689.5198	3033.8246	3042.9227
H,0,3.7274921831,0.0156118551,-1.4246036446	3046.2065	3062.6908	3079.5053
H,0,2.3086906353,-0.2675665169,-2.4402126959	3110.7898	3114.9139	3123.2011
H,0,2.5272257883,1.2876533386,-1.6306522218	3124.3631	3132.4008	3135.1518
H,0,3.4447230524,0.1023243465,1.1503775193	3140.4435	3222.2408	3244.0603
H,0,1.8221008808,0.0139178157,1.8436773752			
H,0,2.3252918047,1.4367130398,0.9237948896			
Sabinaketone			
0,1			
C,0,0.0046776911,1.6093439576,2.2359048137	64.7887	99.6893	154.8827
C,0,-0.9561339575,1.0381357921,1.2568437388	212.9135	238.7177	268.9139
O,0,-0.224100979,2.4790505369,3.0328125221	282.9315	302.7197	372.9554
C,0,1.3233479789,0.8484052016,2.1088251278	416.1719	481.2507	505.0392
C,0,-0.4068226473,0.8658962137,-0.1492841186	536.0217	576.3269	660.5727
C,0,0.9418606791,-0.5077380637,1.4985103355	691.6308	787.9997	828.8725
C,0,-0.3938926822,-0.2861218569,0.7868092743	877.7192	918.2383	931.8053
C,0,-0.6049860842,-2.490513885,-0.3721485104	937.3777	949.0189	980.4727
C,0,-1.3022716663,-1.4686969804,0.5239486132	991.863	1017.4784	1042.5493
C,0,-1.7939205177,-2.1164367547,1.816603427	1050.8268	1062.7264	1091.3873
H,0,-2.011531288,1.2227654922,1.3917302907	1148.511	1172.9796	1191.0935
H,0,1.9867283052,1.4217121809,1.4582589344	1204.6971	1233.7662	1257.6033
H,0,1.804335618,0.7807889388,3.0808633802	1295.5884	1308.005	1330.4554
H,0,-1.15182382,0.8613603509,-0.9323614042	1345.9947	1373.9946	1403.9001
H,0,0.516260688,1.3669468684,-0.4081146793	1424.2915	1430.1891	1472.6071
H,0,0.8099761872,-1.2428924032,2.2932780105	1492.9312	1495.3346	1502.0998
H,0,1.699545485,-0.892769,0.8156763735	1512.8852	1516.3574	1518.4967
H,0,-1.275652025,-3.3138118856,-0.6179326941	1861.21	3031.0067	3043.1702

H,0,0.2662655678,-2.9117579909,0.1333895255	3053.1884	3070.5874	3083.3238
H,0,-0.2672878009,-2.032286293,-1.3023667168	3109.8386	3113.6274	3123.1259
H,0,-2.1757052138,-1.0828265191,-0.0112520668	3126.0374	3131.0183	3132.9275
H,0,-2.5303110851,-2.8904425397,1.5995094774	3143.1488	3194.3414	3218.6644
H,0,-2.2551018668,-1.3815585267,2.4772411557			
H,0,-0.9734665666,-2.5909298343,2.3569491898			
CH_2OO			
0,1			
O,0,0.0335840298,0.,-0.0192885257	547.2631	711.7234	946.291
O,0,0.0603929534,0.,1.3176810258	1019.9408	1264.4348	1434.3968
C,0,1.1555986871,0.,1.8976708237	1626.686	3142.6858	3296.4797
H,0,2.0606424528,0.,1.3010024661			
H,0,1.1151716904,0.,2.9779342101			
CH_2O			
0,1			
C,0,-0.810032424,1.0103650521,0.4985433	1221.8911	1276.3229	1541.1974
H,0,-0.2870768429,0.0390403551,0.4985433	1878.0981	2963.9393	3031.4725
H,0,-1.9126916746,0.9772473252,0.4985433			
O,0,-0.2126706436,2.0454033764,0.4985433			
TS POZ-AR ←→ POZ-AL			
0,1			
C,0,1.2410359569,0.2066696859,0.143451082	-130.1016	52.9202	77.2351
C,0,0.0178788677,-0.6501021861,0.3656203927	135.4729	152.1233	211.0768
C,0,-0.8649431376,-0.2940985068,1.531851439	236.5196	266.1238	286.2472
C,0,-1.204121373,0.2004339936,0.1553018106	309.5727	318.2449	382.9768
C,0,-0.7170335872,1.6130304734,-0.149705176	388.1626	445.7874	463.1702
C,0,0.7571034079,1.6496339317,0.2809310205	465.8531	502.8605	603.9678
C,0,2.4699131887,-0.1912755481,0.9375834021	692.7584	717.2087	740.5703
C,0,-2.4421595377,-0.2690266929,-0.5857115246	790.7672	840.3232	880.9957
C,0,-2.8377452153,-1.7099344283,-0.2769810405	915.9295	920.7201	926.1634
C,0,-3.6194296151,0.6650452039,-0.3032918056	941.2182	953.6819	958.2033
O,0,1.7376399277,0.029856916,-1.1816440127	972.5245	990.0526	1006.3937
O,0,2.6793272155,-1.0498514003,-1.1251935743	1023.1189	1042.0724	1055.5034
O,0,2.8785936406,-1.3514839413,0.2539537941	1069.8296	1096.226	1121.2489
H,0,0.0733018681,-1.6794706971,0.0418816686	1141.3389	1146.3085	1159.4614
H,0,-1.4580042529,-1.0997204175,1.9383594486	1186.6121	1223.4618	1233.4208
H,0,-0.5078478792,0.4082276949,2.2741819085	1240.1367	1258.5377	1265.6437
H,0,-1.3072079967,2.3795526564,0.3530843236	1322.1375	1338.4328	1347.3102
H,0,-0.7980577353,1.7834021189,-1.226131019	1361.3417	1372.823	1384.7604
H,0,1.3694390471,2.3179054576,-0.3202010676	1403.8699	1420.3442	1429.6394
H,0,0.8552885219,1.9590066892,1.3219437736	1488.3042	1492.4005	1495.6239
H,0,2.2425078925,-0.4884916148,1.9589932065	1496.3078	1501.1192	1512.5717
H,0,3.2393478952,0.5852293051,0.9062574402	1518.7008	1519.5794	3026.3194
H,0,-2.2031841426,-0.2067582551,-1.6530617139	3044.6139	3050.4842	3053.8714
H,0,-3.6349461028,-2.0284771733,-0.9481137254	3056.1327	3082.2167	3100.3756
H,0,-2.0054042844,-2.4027835218,-0.3986013468	3111.5993	3117.599	3126.515
H,0,-3.2157072813,-1.8016706712,0.742622415	3134.089	3135.9937	3142.2389
H,0,-4.5173340252,0.3226578834,-0.8182191821	3159.0395	3200.4637	3234.1079
H,0,-3.4155587814,1.6850599707,-0.6282722146			
H,0,-3.831737982,0.6870724637,0.7680694974			
TS POZ-SL ←→ POZ-SR			
0,1			
C,0,1.1886592982,-0.0416076432,0.1078336992	-117.8935	22.5625	78.2721
C,0,-0.0994676524,-0.7460586907,0.4294217188	153.2729	171.483	206.1525
C,0,-0.9366412747,-0.1653465194,1.5389860201	225.5204	253.7305	285.5423
C,0,-1.2399060721,0.1902252612,0.1168257246	294.7384	313.6534	381.4645
C,0,-0.6217578891,1.5019991699,-0.3602318855	408.8591	438.336	449.5504
C,0,0.8468958874,1.4531815761,0.080466685	456.3573	529.9324	601.9108
C,0,1.860952059,-0.5221092091,-1.1691656958	674.1961	721.2328	736.9979
C,0,-2.523468665,-0.2503399181,-0.5635569652	805.0967	847.127	876.1072
C,0,-3.0370678657,-1.6097473928,-0.0986687568	913.4582	921.7818	936.5698
C,0,-3.6105520849,0.808744611,-0.3771384578	938.8215	947.8348	969.3232
O,0,2.1972519238,-0.3772500322,1.0511692478	975.9477	985.4667	1003.2629
O,0,3.4533745487,-0.2168651458,0.3827302196	1031.0274	1042.3204	1052.3475
O,0,3.1645261757,-0.0254076282,-1.0025335648	1070.8681	1097.776	1118.6899
H,0,-0.156397397,-1.8092434626,0.2440569697	1136.9912	1141.9619	1159.1363
H,0,-1.5968622668,-0.8613150998,2.0340822266	1182.5292	1224.3412	1230.7028
H,0,-0.4950419598,0.5721734592,2.1942094275	1249.0401	1252.4398	1286.2721
H,0,-1.1404216521,2.3779515307,0.0303125312	1306.4421	1336.0791	1350.7678
H,0,-0.6947797014,1.542339861,-1.4513408107	1359.5042	1377.7598	1384.4954
H,0,1.5171252825,2.0093926078,-0.5725544373	1403.3586	1419.3603	1434.9349
H,0,0.9728814962,1.8497716648,1.0867505482	1490.2249	1494.1367	1496.5721
H,0,1.8495191273,-1.6129931979,-1.2388458289	1500.2723	1505.1239	1511.3694
H,0,1.45732239,-0.062487408,-2.0696607263	1515.1369	1527.0203	3031.0175

H,0,-2.2995170221,-0.3238606431,-1.6341340006	3038.5971	3041.2471	3044.1863
H,0,-3.8800258176,-1.9187545199,-0.7162303137	3066.6008	3084.2158	3093.9086
H,0,-2.2749202086,-2.3859733932,-0.1666768286	3112.0634	3114.3283	3117.5962
H,0,-3.3886697561,-1.563995612,0.9331087752	3121.3607	3131.7422	3152.9558
H,0,-4.5401474999,0.4971612104,-0.8538121881	3159.0775	3187.6746	3235.673
H,0,-3.3198121676,1.7680601501,-0.8039323796			
H,0,-3.8091313359,0.957040624,0.6865538858			
TS Sab-CI-1 → H-Shift			
0,1			
C,0,-1.5973527509,-0.3148018832,-0.0312207766	-1561.6367	60.0889	79.9955
C,0,-0.6234431772,0.4282451543,0.7465860028	189.2267	209.6921	234.4977
C,0,0.1629897816,-0.4216170686,1.7255929302	251.2829	268.257	298.0632
C,0,0.711043903,-0.2278758335,0.3618568292	336.6958	385.4761	407.9987
C,0,0.4260849959,-1.3718876041,-0.6194558406	450.0944	494.5426	534.8898
C,0,-1.0936355143,-1.4399993584,-0.7312838659	611.8367	655.1921	719.2483
O,0,-3.2620751435,-0.6370220404,-1.3931355403	732.6388	829.2654	867.9637
C,0,1.9368988203,0.6396356072,0.1665006492	887.7204	902.8671	933.3792
C,0,3.2016988672,-0.2113229645,0.2677516674	945.8386	964.5363	976.196
C,0,1.8926745476,1.4095756886,-1.1514141438	993.8342	996.69	1018.9356
O,0,-2.7409723163,0.1574270651,-0.3630579636	1046.9285	1065.4373	1069.6554
H,0,-0.7329973469,1.4903504261,0.9062475579	1092.8271	1150.0546	1182.7234
H,0,0.6300397119,0.1273930746,2.5310540154	1210.0791	1230.91	1261.3509
H,0,-0.2552235011,-1.3811049038,1.998263186	1283.3828	1306.8237	1343.9183
H,0,0.8768237024,-1.1605462767,-1.5896741973	1357.1782	1404.0667	1416.599
H,0,0.861852605,-2.3039133775,-0.2581597466	1422.2967	1425.4973	1476.9243
H,0,-1.6034833604,-2.3902034602,-0.5961839994	1488.4824	1495.1391	1500.2533
H,0,-1.9778164399,-1.1081352969,-1.6538491823	1507.6052	1514.1719	1517.269
H,0,1.9467354238,1.3680119311,0.9834406034	1593.8755	1876.4962	3029.7752
H,0,4.0935883277,0.4098700088,0.1867042767	3044.6274	3051.2985	3064.6553
H,0,3.2412989727,-0.7483713829,1.2160991212	3100.1185	3113.3134	3120.9525
H,0,3.2340866014,-0.9460372959,-0.5392339231	3129.2222	3132.402	3133.6351
H,0,2.74125661,2.0898869751,-1.2230825615	3134.4481	3200.5391	3225.2511
H,0,0.9770845903,1.9951703346,-1.2384633779			
H,0,1.9429816897,0.7329494115,-2.0053061504			
TS Sab-CI-1 → Dioxirane-Syn			
0,1			
C,0,-1.6118018562,-0.2471737559,-0.1881915671	-484.3514	46.6587	77.7316
C,0,-0.6317153792,0.4402064643,0.6247849376	171.3646	193.3012	211.2968
C,0,0.1127397882,-0.4409131528,1.6283736621	269.5372	275.2348	300.0671
C,0,0.7172994501,-0.2233796144,0.3027868201	318.5229	374.4838	407.8903
C,0,0.4482359871,-1.3354166641,-0.7105724455	470.0305	496.781	523.534
C,0,-1.0730288051,-1.5670342648,-0.671212556	575.0974	631.1911	687.1862
O,0,-3.4933078318,-0.818180199,-0.265736343	793.4587	813.0671	847.967
C,0,1.958563845,0.6331293709,0.1694614693	882.8155	908.6536	930.9429
C,0,3.2079843024,-0.239259439,0.2837119672	939.1145	954.526	982.4295
C,0,1.9682630322,1.4423178333,-1.1251076714	988.8282	1000.7381	1040.8712
O,0,-2.650925429,0.3439829176,-0.6128224479	1047.433	1064.2389	1090.0724
H,0,-0.7511852531,1.4921412803,0.8337973694	1143.8951	1164.6545	1190.5416
H,0,0.522669669,0.1113589033,2.4618431814	1218.5593	1226.0941	1255.1443
H,0,-0.3280691925,-1.3942303268,1.8829148905	1291.6224	1312.8345	1343.2355
H,0,0.7486989215,-1.0014070479,-1.7039331704	1352.8808	1377.0203	1404.2
H,0,1.0150919078,-2.2356098907,-0.4744722661	1425.4306	1430.3925	1469.6473
H,0,-1.3512927739,-2.3502603395,0.0317594138	1489.3175	1495.1277	1502.356
H,0,-1.5336941076,-1.8187904947,-1.6221830477	1510.926	1515.3045	1518.6859
H,0,1.9528606488,1.3361458726,1.0082789716	1618.6454	3035.1856	3046.0962
H,0,4.1088162356,0.3732527215,0.2551988267	3048.9688	3067.5353	3107.001
H,0,3.2096738133,-0.8103219426,1.2126983937	3113.7452	3116.3718	3119.5865
H,0,3.2592498307,-0.9440923369,-0.5482727521	3128.7494	3134.8654	3138.2833
H,0,2.824468145,2.1162819262,-1.1438127912	3165.3372	3208.6156	3227.4095
H,0,1.0620175904,2.0400050752,-1.2269161978			
H,0,2.0462844412,0.7923718339,-1.9974698272			
TS Sab-CI-1 → Dioxirane-Anti			
0,1			
C,0,-1.6170134201,-0.3549480705,0.0205627678	-432.5317	42.4678	64.9384
C,0,-0.6432155941,0.285684259,0.8704090112	144.5573	201.5256	205.1286
C,0,0.2342800465,-0.5914860396,1.757330703	260.9298	273.0497	303.8158
C,0,0.7097951937,-0.3106264189,0.3951280066	346.2173	401.8997	420.5326
C,0,0.3915157045,-1.3975107146,-0.6340633253	467.6577	498.7227	516.9284
C,0,-1.1069861939,-1.6824552262,-0.469116128	569.7383	666.8717	676.9525
O,0,-2.457621951,0.1674819443,-1.742699969	777.4603	807.2546	826.2334
C,0,1.8804495616,0.6211011219,0.1725295947	882.8263	915.2925	930.4753
C,0,3.1877338978,-0.1708050159,0.1930096214	940.8724	952.0787	979.2805
C,0,1.7379627125,1.4232644333,-1.1190739154	993.376	1008.3422	1028.0323
O,0,-2.7127859453,0.2034361673,-0.2779986455	1051.6524	1072.0624	1088.9816

H,0,-0.764470871,1.3307406228,1.1085471692	1144.4916	1161.9647	1190.9553
H,0,0.6968297354,-0.0452188465,2.5672873685	1217.8042	1238.0279	1266.8658
H,0,-0.1306253792,-1.5738525048,2.0213609016	1300.725	1313.8079	1346.9007
H,0,0.5608183563,-1.0086244861,-1.6374147976	1362.0162	1377.7932	1404.4658
H,0,1.0159004516,-2.2791702994,-0.4912368506	1425.6464	1430.6062	1471.4003
H,0,-1.2843355758,-2.4085109567,0.3319830444	1488.8033	1491.372	1500.5142
H,0,-1.6115924248,-2.0102740623,-1.366372175	1509.9355	1514.8219	1519.3501
H,0,1.8908262471,1.3231841628,1.0122116668	1618.9464	3035.8156	3044.6603
H,0,4.0416642497,0.49718419,0.0832288876	3046.137	3050.0893	3073.1804
H,0,3.3024587519,-0.7255903482,1.1248255265	3116.1985	3121.6964	3123.5242
H,0,3.2156195384,-0.8826876456,-0.6339497407	3127.848	3129.8431	3148.0044
H,0,2.5151680529,2.1849154152,-1.1765159449	3209.0572	3211.0892	3234.7741
H,0,0.7662147221,1.914056576,-1.1786592434			
H,0,1.8429065834,0.7818701327,-1.9944987739			
Sab-CI-1 Vinyl Hydroperoxide (VHP)			
0,1			
C,0,-1.0858832955,-1.2431026759,0.0828927389	52.5	75.4878	102.8533
C,0,-0.127978554,-0.6028282028,1.0630343756	173.4804	209.4494	229.3817
C,0,-0.995293333,0.2591075577,0.196505272	238.646	256.5778	271.3012
C,0,-2.3047361391,0.7388855745,0.8357811893	320.08	343.2319	374.7835
C,0,-3.0830609081,-0.5239315117,1.100271802	437.8882	453.4102	499.4788
C,0,-2.4084459674,-1.582823928,0.6659598367	626.5696	632.6467	666.6794
C,0,-0.3963851507,1.1555454431,-0.871678672	753.3659	824.5981	841.0028
C,0,-0.0175490371,2.5050984767,-0.2603410654	876.21	914.1459	921.6927
C,0,0.802643541,0.5518697642,-1.5962524521	935.8438	967.9682	975.7945
O,0,-2.8162296155,-2.8666812204,0.8929522228	989.0061	1006.3969	1024.4578
O,0,-2.4313385824,-3.6807842476,-0.2097996574	1038.1933	1066.8461	1087.9724
H,0,-0.7060776819,-1.7930049085,-0.7634953967	1129.8437	1144.5136	1163.247
H,0,0.9239933664,-0.655216153,0.822240009	1197.6149	1209.6614	1241.8195
H,0,-0.3641108956,-0.6888401273,2.1152661815	1258.4539	1315.94	1345.1438
H,0,-2.8461245611,1.4008637774,0.1521991231	1365.6551	1383.8632	1404.4807
H,0,-2.1187220204,1.3120099627,1.7475898253	1414.1397	1424.9319	1439.5966
H,0,-4.0307628414,-0.5669032715,1.6149693967	1482.4512	1493.8101	1496.3501
H,0,-1.1842261179,1.3237095594,-1.6138037896	1500.3941	1514.6297	1518.6571
H,0,0.3843746033,3.1780229886,-1.018282528	1727.0496	3026.2151	3034.6882
H,0,-0.8752627169,2.9930243009,0.2027138659	3040.281	3059.4295	3073.2712
H,0,0.7460201842,2.3650114519,0.5080666546	3109.3886	3123.7014	3128.4646
H,0,1.1068091197,1.2033315799,-2.4154304892	3133.1661	3142.3843	3209.0007
H,0,0.5767997055,-0.4274746857,-2.0174057295	3220.17	3230.3767	3849.5179
H,0,1.658839925,0.4504970546,-0.9277327658			
H,0,-1.7984240273,-4.2751765593,0.2093480523			
Sab-CI-1 Vinoxy-Type Radical			
0,2			
C,0,-0.9263020119,-1.2705646379,0.2452708217	58.1248	117.0068	196.5937
C,0,-0.060955323,-0.4752984151,1.2016576539	212.566	252.2148	282.3428
C,0,-0.9419573092,0.2403407685,0.2355739848	314.2531	332.4467	373.6913
C,0,-2.2840894027,0.6830785811,0.8319620563	410.687	456.7132	488.4429
C,0,-2.9534402345,-0.5693695733,1.2664711876	575.0577	606.2448	645.8604
C,0,-2.221949783,-1.7427101089,0.8321835093	698.4552	764.8601	819.2127
C,0,-0.3820594616,1.0945435456,-0.8862682843	881.7161	897.6271	922.5108
C,0,-0.1389567092,2.5191634039,-0.3858135074	937.4701	951.3698	971.7811
C,0,0.8911378345,0.534092257,-1.5120501679	989.9534	997.9854	1030.0832
O,0,-2.6025929202,-2.8963337711,0.9049069811	1066.8611	1075.2247	1122.7365
H,0,-0.4509535196,-1.8768180742,-0.5101639513	1143.489	1151.7404	1186.142
H,0,1.000446596,-0.5013962035,1.0038879284	1211.688	1250.9142	1293.69
H,0,-0.3263831395,-0.4786272843,2.2513942147	1313.0026	1348.2239	1362.9195
H,0,-2.8864983027,1.1891959749,0.0662643841	1384.6459	1406.7731	1415.5756
H,0,-2.160831957,1.4011817874,1.6482545444	1427.6552	1461.9717	1494.5171
H,0,-3.8979274648,-0.6283488234,1.7857115396	1500.5311	1508.2674	1519.507
H,0,-1.1508141262,1.1303867448,-1.6659693762	1521.0353	1721.9643	3005.8895
H,0,0.2447583544,3.1510918027,-1.1869449688	3024.3631	3043.5252	3048.1292
H,0,-1.0516452123,2.9781893015,-0.0053905661	3060.0916	3113.7189	3124.6073
H,0,0.5971269134,2.5108949339,0.4209774184	3127.2118	3133.9566	3138.7441
H,0,1.1733834281,1.1335443618,-2.3770886038	3224.6386	3231.1876	3231.5067
H,0,0.7657435391,-0.4949679202,-1.8472515262			
H,0,1.724076212,0.568801349,-0.808102272			
TS Sab-CI-2 → H-Shift			
0,1			
C,0,-1.5450566155,-0.297757788,-0.1392843734	-1299.0680	55.3952	90.4221
C,0,-0.6575397337,0.4225211332,0.6664332486	110.5358	198.6447	218.5767
C,0,0.12192678,-0.4367417716,1.6749848859	249.5126	260.58	281.576
C,0,0.6993036896,-0.25992407,0.3383978681	291.9968	342.5377	383.5086
C,0,0.4648398871,-1.3996980064,-0.6610489033	474.968	498.3096	555.6182
C,0,-1.0661948933,-1.5516922594,-0.7873115655	593.3073	644.3561	686.6396

O,0,-2.8247130875,1.4176191867,0.3689657328	735.3966	786.2051	861.248
C,0,1.914438271,0.627704605,0.1613312333	898.3012	908.9429	936.9017
C,0,3.194688356,-0.1970495212,0.2908841337	948.9773	955.854	969.9303
C,0,1.8815869718,1.4003663283,-1.1544020613	981.6591	1002.5458	1029.9487
O,0,-2.6861181761,0.2269407448,-0.3826400186	1072.1818	1075.2268	1109.5005
H,0,-1.6448856001,1.4124361064,0.7143113458	1148.8075	1167.6063	1176.5875
H,0,0.542780673,0.1253843279,2.497640893	1192.1105	1235.3748	1263.1594
H,0,-0.2933584841,-1.3985980312,1.9530490438	1287.6431	1307.2081	1348.3669
H,0,0.8825307789,-1.1259591698,-1.6290935396	1365.0356	1401.7545	1413.9256
H,0,0.9466022063,-2.3253745261,-0.3462985224	1422.5147	1460.6904	1470.9779
H,0,-1.4571547636,-2.3946578409,-0.2114256441	1492.4052	1494.4282	1502.6972
H,0,-1.4220520572,-1.6640302764,-1.8094405858	1510.2325	1516.5249	1518.4585
H,0,1.884288784,1.3552902119,0.9768991494	1554.1676	1971.9065	3035.5099
H,0,4.0751536589,0.4424572633,0.2275116222	3048.2406	3053.1895	3060.2441
H,0,3.2261882923,-0.7314996282,1.2410585861	3076.1509	3106.0109	3112.2913
H,0,3.2625200197,-0.9323495819,-0.51399773	3117.808	3123.0343	3128.2552
H,0,2.7017367287,2.1171243828,-1.1955163571	3128.3135	3134.4907	3214.8712
H,0,0.9436107709,1.9456881072,-1.2585386705			
H,0,1.9917451928,0.7344720134,-2.012184561			
TS Sab-CI-2 → Dioxirane-Syn			
0,1			
C,0,-1.6301936162,-0.2362442146,-0.1684830828	-508.6936	54.8351	93.2563
C,0,-0.6281278352,0.4509456894,0.6253149915	139.217	181.9173	230.4234
C,0,0.114147048,-0.4281431094,1.6172473392	264.9725	280.4802	283.3177
C,0,0.7117095951,-0.2006973515,0.2817905322	321.25	369.0438	399.1517
C,0,0.444776857,-1.3231712165,-0.7201940763	454.1721	499.9461	502.1828
C,0,-1.0811594095,-1.5065113229,-0.7417376468	564.7781	600.7337	697.3712
O,0,-3.1918649608,0.3910502071,0.8620757483	787.6001	813.0221	844.2813
C,0,1.9623084101,0.6415689446,0.1508490746	879.844	916.907	930.3821
C,0,3.2067457208,-0.2275982726,0.3243345146	936.5826	937.8101	975.5019
C,0,2.005452292,1.412135525,-1.1666395896	992.5182	1012.4684	1035.4346
O,0,-2.7557069408,0.2099509706,-0.5411309223	1044.9574	1064.7546	1085.3851
H,0,-0.7763429645,1.4930625146,0.8596152436	1145.385	1170.0023	1189.0291
H,0,0.5356258815,0.1113314607,2.4533449306	1219.9531	1246.0433	1258.5792
H,0,-0.3201313328,-1.3868508255,1.8658121652	1294.3765	1308.4436	1347.5454
H,0,0.7884958712,-1.0231452959,-1.7098761868	1361.7474	1374.5813	1403.1733
H,0,0.9721784899,-2.2369454456,-0.4478240058	1425.5547	1427.6178	1449.4038
H,0,-1.4283069835,-2.3228649403,-0.1012121431	1490.9729	1496.5005	1503.2363
H,0,-1.5056521123,-1.6809318137,-1.7285384225	1511.6655	1517.2219	1519.111
H,0,1.9356518394,1.3700767674,0.967154988	1621.5784	3031.0791	3042.4772
H,0,4.1111884418,0.3797071064,0.2969330953	3052.3455	3055.8589	3083.7364
H,0,3.1826088719,-0.7654870122,1.2726695641	3111.9301	3117.312	3122.2777
H,0,3.2766746999,-0.9621468751,-0.4806065725	3125.3066	3128.784	3133.4695
H,0,2.8513119823,2.0992144684,-1.1784901756	3138.3568	3220.2467	3227.2611
H,0,1.0938611674,1.9912637169,-1.3170291492			
H,0,2.1247699074,0.7376475647,-2.015842274			
TS Sab-CI-2 → Dioxirane- Anti			
0,1			
C,0,-1.6446698847,-0.3262648118,0.0980292316	-498.9934	50.463	77.2957
C,0,-0.588497645,0.3847730319,0.801583041	133.0636	198.5527	212.756
C,0,0.2214554434,-0.5338623377,1.7280590067	244.7424	267.8327	287.4534
C,0,0.7295014591,-0.2414370734,0.3723979198	305.5019	370.059	381.5164
C,0,0.4159660876,-1.3399202232,-0.6428876612	455.0204	485.3269	498.8987
C,0,-1.1021226861,-1.5649508403,-0.5584904667	577.8377	637.7105	690.3336
O,0,-2.6412454493,1.3226324956,-0.4411997446	797.3647	809.6619	831.0437
C,0,1.9528244724,0.6292010802,0.1838696635	882.1711	917.7555	936.4939
C,0,3.2226623405,-0.2184884958,0.2248978529	937.1724	957.0095	974.6484
C,0,1.8717107682,1.4520162405,-1.1001439502	979.5613	1009.5861	1037.1218
O,0,-2.879617574,-0.0579903953,0.0567337666	1057.9697	1065.4948	1088.6447
H,0,-0.7025650924,1.4224871623,1.057915921	1147.085	1169.2341	1189.2491
H,0,0.6673538996,-0.0094291359,2.5611597376	1204.6487	1239.8065	1260.8926
H,0,-0.1679007632,-1.5149955728,1.9629550517	1285.7341	1308.8679	1345.4078
H,0,0.6775601661,-1.0010848114,-1.6446965003	1353.834	1378.4845	1401.2831
H,0,0.9854446731,-2.24583653,-0.4371872813	1422.2568	1430.2603	1453.3301
H,0,-1.3858945413,-2.4310851165,0.0454838344	1488.2247	1493.5932	1497.8631
H,0,-1.5839828299,-1.6862818706,-1.5263646627	1508.3323	1515.264	1516.8383
H,0,1.9762627435,1.32410556,1.0291115243	1620.062	3035.2832	3039.0827
H,0,4.1099913518,0.4093697075,0.1467215651	3043.8598	3062.4383	3081.3117
H,0,3.2877661423,-0.7908924259,1.1509888914	3105.7902	3115.424	3117.8349
H,0,3.2413172922,-0.9212765982,-0.6106017653	3118.5173	3125.4529	3137.4765
H,0,2.6883763002,2.1723388702,-1.1418729518	3140.3331	3228.4347	3259.4152
H,0,0.9282250371,1.9953432032,-1.1601913372			
H,0,1.9538803087,0.8161722972,-1.9829121466			
Dioxirane			

0,1			
C,0,-0.4058592243,0.7057436715,0.9780664268	62.7999	81.4234	154.3416
C,0,0.2136141347,-0.4866625008,1.6619468862	202.0673	235.7932	291.6355
C,0,0.362452398,-0.3261413265,0.1837564163	305.5634	341.8932	366.3977
C,0,1.6877446613,0.3148676186,-0.2346947428	387.5347	417.7888	434.2733
C,0,1.8324493652,1.5854997287,0.6187745262	481.1035	510.1401	559.4573
C,0,0.4056669948,1.9491693513,0.9679303896	589.9635	698.1366	774.0499
C,0,-0.3140590183,-1.242125411,-0.8243047539	823.0495	870.5552	901.4667
C,0,-1.4056051477,-2.1166356063,-0.214358118	922.4899	935.2696	941.3329
C,0,-0.888413021,-0.4299230242,-1.9866763325	948.9816	973.378	978.1474
O,0,0.1512768708,2.99178559,1.8363343001	999.5859	1035.4032	1045.6878
O,0,-0.160257181,3.0824384411,0.4038088478	1068.9971	1082.3301	1123.1927
H,0,-1.4812531869,0.8014428951,0.9404638323	1144.0919	1181.5925	1192.5981
H,0,-0.4881706413,-1.2203299425,2.0267200429	1215.1127	1236.9051	1243.8864
H,0,1.0737350733,-0.3387984945,2.3010016458	1296.427	1315.0443	1340.1036
H,0,1.6437184832,0.5811197242,-1.2908080369	1350.5509	1379.76	1406.3168
H,0,2.5229115955,-0.3740828205,-0.103978191	1413.1151	1427.4736	1478.2508
H,0,2.3772999045,1.3928606901,1.5431663588	1491.9047	1494.6972	1504.9803
H,0,2.3213511553,2.411685775,0.1098836593	1514.2131	1515.5387	1521.7197
H,0,0.4647978642,-1.9042699737,-1.2179516546	1525.7201	3021.3951	3045.0887
H,0,-1.8953414085,-2.702290965,-0.9919193221	3048.4186	3067.6845	3095.0381
H,0,-1.0050532077,-2.8088996509,0.5247958245	3109.2027	3114.1586	3118.8536
H,0,-2.1732219937,-1.5063661085,0.268266264	3135.1411	3138.1833	3148.3402
H,0,-1.2927312319,-1.0885508276,-2.7552490217	3153.1445	3199.2951	3239.3632
H,0,-0.1404783306,0.2089046147,-2.4546905519			
H,0,-1.6974579083,0.2111885516,-1.6314616953			
Sab-CI-2-Vinyl Hydroperoxide (VHP)			
0,1			
C,0,-0.2096171285,-0.7644578441,-0.3732836388	63.6853	90.9395	116.6357
C,0,0.5352035001,-1.9143783894,0.18383281	174.06	187.3516	208.5644
C,0,0.9048137283,-0.4950015581,0.5700737212	220.7741	275.1737	291.9059
C,0,0.2398889835,0.2772938727,1.7175745199	297.8627	315.8932	342.3408
C,0,-0.9202054733,1.023539773,1.0038525915	398.9913	471.9688	498.6394
C,0,-1.2518480963,0.0067979911,-0.0805000743	526.1465	609.342	638.6617
C,0,2.2138773398,0.0308628502,0.0002462451	725.0039	796.6429	849.9813
C,0,2.1349189971,1.5192934572,-0.3344065973	859.2867	912.4494	927.4209
C,0,3.3776040801,-0.2639126117,0.9439053445	933.0476	959.6797	969.5186
O,0,-2.5233603755,-0.2351440696,-0.4825166951	999.7631	1015.1588	1018.233
O,0,-3.262141155,0.9827695378,-0.4590142353	1062.0936	1078.5392	1086.9725
H,0,1.24833217,-2.4501894259,-0.4317800847	1143.4642	1157.8345	1185.6535
H,0,-0.0172067501,-2.5433343596,0.8717166068	1205.8884	1250.5119	1290.3952
H,0,-0.1744305572,-0.4119883192,2.4558089487	1300.5142	1315.7214	1339.6194
H,0,0.9239143619,0.9456052721,2.2409738201	1350.9744	1394.4757	1399.1019
H,0,-0.6129346962,1.9877926049,0.5953125398	1418.9396	1445.1789	1473.3276
H,0,-1.7843163506,1.2032521933,1.6424893695	1480.5638	1489.9259	1495.046
H,0,2.3844777373,-0.5056300422,-0.9384677138	1498.9863	1511.7842	1514.2591
H,0,3.0513144339,1.8518831906,-0.8227665932	1745.4619	3032.7814	3037.2795
H,0,1.2987392081,1.7208850301,-1.0048469892	3041.5019	3056.8003	3077.5447
H,0,2.0083584344,2.1216874612,0.5676595992	3102.0139	3105.2331	3111.0459
H,0,4.3235565174,0.0763527568,0.5208090017	3116.0649	3121.0616	3123.3905
H,0,3.456872022,-1.3323808304,1.1469931423	3131.3915	3186.9168	3855.0977
H,0,3.2376482711,0.2493615783,1.897996009			
H,0,-4.0657176724,0.6942392511,-0.0122220377			
Sab-CI-1 ROO-Anti from Vinoxy-Type Radical + O_2			
0,2			
C,0,-0.6188947703,0.8938981544,0.7519965603	60.1886	81.0173	86.5404
C,0,-0.3765609659,-0.3003656465,1.6587168579	105.9096	215.2976	240.7523
C,0,0.0738002248,-0.3611745894,0.2451221284	257.7632	271.8875	289.3924
C,0,1.5556758068,-0.0316521762,0.059700007	325.0036	346.2826	379.993
C,0,1.7886809719,1.2829865468,0.7925302041	412.3828	456.6395	498.7271
C,0,0.3995721659,1.9652824936,0.8052740441	537.0696	570.0567	650.6538
C,0,-0.5669309248,-1.2646067329,-0.7971679606	685.0567	707.5611	812.4624
C,0,-1.9083375343,-1.8419453069,-0.3557740273	867.0529	894.1459	924.5857
C,0,-0.7291082022,-0.5254382074,-2.1265378157	934.8512	950.4425	966.6332
O,0,0.2306362763,3.1475671954,0.7652059222	980.5687	1018.8101	1036.2027
O,0,2.7262713956,2.0881777868,0.0814888899	1075.4628	1090.473	1096.3738
O,0,3.2525111704,3.0037359833,0.8361653924	1122.7586	1148.5912	1184.6016
H,0,-1.6329290383,1.1574558951,0.4918811059	1201.9963	1218.7065	1239.4506
H,0,-1.2708811469,-0.836166634,1.9369309971	1282.7442	1283.9449	1291.7302
H,0,0.3547204314,-0.2140465031,2.4513124086	1315.037	1350.5868	1373.0515
H,0,1.7755699476,0.1307253266,-0.9965312724	1386.3012	1410.8497	1417.5465
H,0,2.1966516738,-0.836432741,0.4184736322	1430.5115	1490.2085	1495.9489
H,0,2.1603433717,1.171709323,1.8110567758	1504.9241	1512.3589	1516.6788
H,0,0.1259022566,-2.0993903797,-0.9484040489	1523.3853	1887.0836	3040.8146

H,0,-2.3406987151,-2.4367132007,-1.159501009	3046.8229	3055.8861	3076.7427
H,0,-1.8089166249,-2.4826377176,0.5191814562	3102.2551	3113.8362	3123.7217
H,0,-2.6190830427,-1.0458244116,-0.1206167584	3127.4802	3133.0931	3135.4756
H,0,-1.1041807044,-1.19934674,-2.8962048052	3149.8887	3221.6228	3234.5393
H,0,0.2083366373,-0.1019127957,-2.4844999069			
H,0,-1.4443516604,0.2916980779,-2.0164827774			
Sab-CI-1 ROO-Syn from Vinoxy-Type Radical + O_2			
0,2			
C,0,3.0945990912,0.947027074,0.6845511364	68.2536	89.652	95.3384
C,0,3.376498062,-0.2043721154,1.6364544695	104.1924	194.6248	235.341
C,0,3.7896817911,-0.3180752892,0.2160182012	238.0967	253.8864	276.4771
C,0,5.2645124758,0.0226384421,-0.0166515745	339.313	355.7763	395.5115
C,0,5.5008324957,1.4054270541,0.5739540685	421.2528	460.9064	482.8466
C,0,4.0915348684,2.0404478548,0.6889504373	535.3385	551.7325	641.8511
C,0,3.1352197591,-1.2685432878,-0.7746380486	704.705	753.1764	810.1208
C,0,1.8096288751,-1.8399267897,-0.2805666877	854.4582	886.9877	921.1116
C,0,2.9338430881,-0.5839343833,-2.127473757	938.769	945.3977	964.8389
O,0,3.8903977798,3.2198881809,0.7009249794	976.0937	1003.5609	1035.1953
O,0,6.0644598553,1.262704725,1.8977881436	1048.7731	1080.949	1091.7313
O,0,6.5899027839,2.3659121523,2.3288382566	1122.3034	1145.2861	1182.1955
H,0,2.0690752351,1.1863999398,0.4470144546	1197.6578	1232.5422	1241.3315
H,0,2.4933162027,-0.7329237691,1.959707938	1255.6623	1294.2374	1296.2143
H,0,4.1301866095,-0.0738332041,2.4002879431	1333.294	1348.514	1357.2581
H,0,5.4774203897,0.0553942713,-1.0846100309	1384.5786	1412.0482	1419.2104
H,0,5.9283780248,-0.717189211,0.4326747652	1431.5987	1480.0838	1492.5865
H,0,6.1681170923,2.0520816186,0.0107506299	1501.4655	1509.4932	1514.82
H,0,3.8321402716,-2.1027643819,-0.9096362276	1520.0607	1877.0104	3039.766
H,0,1.3604544112,-2.4629609218,-1.053252662	3045.6045	3054.4125	3074.4903
H,0,1.9349764478,-2.4510541485,0.6119348807	3113.3893	3118.8376	3125.8374
H,0,1.1001495271,-1.0405809376,-0.0523180808	3130.656	3131.8487	3149.8213
H,0,2.5669618835,-1.2943280648,-2.8677627704	3159.9769	3197.9065	3237.1735
H,0,3.8545425607,-0.1481591531,-2.514261321			
H,0,2.1983674181,0.2174613446,-2.0357421433			
Sab-CI-1--H_2O vdW-Anti			
0,1			
C,0,1.6611343394,-0.6591639659,-0.0273836729	24.344	66.7453	83.9097
C,0,0.5736250086,-0.3543377948,-0.9363744839	106.1985	177.6868	209.0777
C,0,-0.4217796439,-1.4809960407,-1.1796631645	224.0058	228.4451	237.4638
C,0,-0.6960761471,-0.5123203355,-0.0958625451	258.9316	263.324	295.5386
C,0,-0.2759620001,-0.9817021093,1.2965366487	304.1901	330.3867	399.3968
C,0,1.1986276242,-1.4005910463,1.1797811491	402.1028	483.1096	490.5919
O,0,3.7368071099,-0.3944965951,0.8008388558	515.5714	575.9545	598.6865
C,0,-1.8168168996,0.4946045416,-0.2393421467	676.47	694.1767	798.8794
C,0,-3.1144710145,-0.0791637865,0.3267818289	824.6519	832.7811	879.962
C,0,-1.467231796,1.8297623153,0.4145641906	912.8189	928.8772	940.6805
O,0,2.811110429,-0.2304422099,-0.2354034141	945.8486	961.9343	978.094
H,0,0.7015097239,0.4162505944,-1.6805370703	999.3623	1016.5156	1043.4978
H,0,-0.984043345,-1.3765726726,-2.0969130207	1056.873	1078.9621	1092.4965
H,0,-0.1199842509,-2.4918280129,-0.9420483714	1148.1309	1178.5136	1192.7595
H,0,-0.3357167986,-0.1491918423,1.9957080062	1234.6295	1243.4038	1273.5496
H,0,-0.914178721,-1.7881711746,1.6563090367	1302.0462	1314.7437	1347.0754
H,0,1.3328796469,-2.4689668588,0.9847706843	1373.3514	1397.0503	1405.584
H,0,1.8047935017,-1.1493124079,2.0422595382	1429.7953	1433.4009	1469.0319
H,0,-1.9553217824,0.666385696,-1.3117451141	1484.7604	1493.3108	1500.5447
H,0,-3.942577155,0.6117201859,0.1709805309	1510.2754	1513.727	1519.0503
H,0,-3.366615043,-1.0298510531,-0.1446881675	1667.5189	1686.5522	3030.2749
H,0,-3.0195812088,-0.2470675839,1.4011545642	3044.0228	3055.7156	3069.126
H,0,-2.2401256452,2.5686169468,0.2032177704	3078.8235	3114.8727	3126.5045
H,0,-0.5131900213,2.2107019668,0.0496686996	3126.7045	3130.6109	3136.8152
H,0,-1.3895077226,1.7312014207,1.4976259108	3155.5444	3193.0446	3215.4339
O,0,1.9822597498,1.2710832333,2.0556256563	3244.0802	3429.1739	3965.1603
H,0,2.2336478992,2.1833263162,2.2022470079			
H,0,2.8011118027,0.8088163031,1.7720335128			
Sab-CI-1--H_2O vdW-Syn			
0,1			
C,0,1.455662231,-0.1463467365,-0.2539569392	40.8828	53.5953	80.3159
C,0,0.254932406,-0.1698084308,-1.0688895539	117.3456	158.0023	180.8937
C,0,-0.4934643943,-1.4951997875,-0.9208763805	195.9691	201.7534	218.8052
C,0,-0.9091149727,-0.3329173115,-0.1024566299	256.8444	265.0373	288.7089
C,0,-0.3403360248,-0.3269279161,1.3154000355	298.2316	328.689	393.4321
C,0,1.1859648764,-0.4759644036,1.1700283527	406.8309	482.9085	489.7684
O,0,3.6450903638,0.0590479694,0.1623536608	513.1163	567.5199	582.5932
C,0,-2.2338271567,0.3433069612,-0.3866992616	671.544	699.9344	813.3302
C,0,-3.3513675633,-0.3315245581,0.4062400473	820.8047	836.0007	878.1964

C,0,-2.1888808299,1.844222425,-0.1087741738	915.862	921.9291	935.306
O,0,2.5680775912,0.1562346746,-0.7240649708	943.723	958.4299	976.0719
H,0,0.2078987587,0.3673267526,-2.0034442782	989.6864	1013.7785	1044.8522
H,0,-1.1059007435,-1.7491198736,-1.7744993987	1054.2599	1081.8283	1090.6768
H,0,0.0409837988,-2.3216164358,-0.4716163846	1148.1676	1176.7141	1191.2238
H,0,-0.5761541195,0.6202864213,1.8000159836	1232.9022	1248.789	1269.2745
H,0,-0.7739749153,-1.1238925139,1.918199574	1299.8726	1314.5676	1346.2434
H,0,1.561218061,-1.4835468775,1.3641103726	1374.7821	1393.6741	1403.6386
H,0,1.7770385186,0.1917663578,1.7962328461	1424.5478	1432.3506	1458.1364
H,0,-2.4371286062,0.2038425613,-1.4533929588	1488.9406	1495.3169	1502.7455
H,0,-4.3189353226,0.1059176315,0.1611287824	1510.2172	1515.3529	1518.6574
H,0,-3.3939262676,-1.4009508437,0.1973803393	1662.8583	1688.0913	3035.9689
H,0,-3.190633843,-0.2018771047,1.4783291458	3046.2589	3048.972	3071.3472
H,0,-3.1168473324,2.3176907037,-0.4287273559	3079.6052	3114.2685	3119.1246
H,0,-1.3633029669,2.3221995258,-0.6371976547	3123.5947	3125.398	3132.3607
H,0,-2.0717453188,2.0464711923,0.9567328834	3135.2268	3149.075	3206.8818
O,0,3.1185712929,-2.5920963566,0.1249015284	3240.3918	3390.149	3961.9836
H,0,3.5410388564,-1.7061700471,0.1844467879			
H,0,3.7398668025,-3.1494817493,-0.343905059			
TS Sab-CI-1 + H_2O → HAHP-Anti			
0,1			
C,0,-1.2952213273,-0.586890668,0.3027816281	-693.5471	48.6018	85.5726
C,0,-0.027602254,-0.8583393131,0.9867650955	137.3303	161.7591	205.7583
C,0,0.8472912932,-1.9276579819,0.3403572705	237.6723	252.1896	257.1174
C,0,1.07053569,-0.49693329,-0.0012278987	292.6019	308.9606	338.7433
C,0,0.3896702146,-0.0407841551,-1.2948803579	384.5045	404.7985	437.7115
C,0,-1.0731971578,-0.5016299639,-1.1860458927	487.232	529.3525	576.0021
O,0,-3.4538110529,-0.1308087589,0.2408254037	588.9681	630.5753	662.3367
C,0,2.3279334631,0.2052039627,0.4777609338	679.2077	695.9934	806.8429
C,0,3.4435619765,0.0688192173,-0.5611540394	821.6907	878.3065	920.0423
C,0,2.0681743832,1.6717517978,0.8274948823	927.2246	938.5708	945.6214
O,0,-2.4068316803,-0.8797500431,0.882667147	973.2727	980.8159	996.1302
H,0,0.0440277914,-0.6914227992,2.0555154049	1012.8401	1019.5789	1049.7387
H,0,1.5502060126,-2.3943579648,1.0231282547	1065.1725	1075.0173	1103.0093
H,0,0.3977601082,-2.6040967228,-0.3797487155	1150.3776	1175.9558	1194.8426
H,0,0.4093899766,1.0508874858,-1.3497101005	1230.2048	1244.5737	1270.2523
H,0,0.8904627551,-0.4463901621,-2.1794639225	1305.2116	1314.1633	1346.2287
H,0,-1.2304425112,-1.5150397141,-1.5783253323	1365.7918	1383.1024	1403.6237
H,0,-1.7870066237,0.154944419,-1.676394162	1423.9698	1434.5835	1477.1922
H,0,2.6495404,-0.3088655748,1.3952622739	1484.3415	1488.4533	1498.1242
H,0,4.3773137557,0.4994367577,-0.1876297984	1506.3835	1512.7715	1519.2731
H,0,3.6253862491,-0.9813665401,-0.8114811246	1578.2396	1604.7557	1841.7579
H,0,3.1787362837,0.5980634054,-1.4834989447	3035.6128	3041.8231	3049.8519
H,0,2.9704597886,2.1304862637,1.2430856099	3065.5426	3074.4789	3112.1719
H,0,1.2648345852,1.7660039811,1.5646556911	3119.7399	3122.4848	3124.6239
H,0,1.7780818813,2.2486124969,-0.0563644926	3129.3611	3147.1996	3187.8707
O,0,-1.6235355068,1.3954179465,0.417468384	3201.1572	3233.8904	3907.8503
H,0,-1.5272618976,1.7071452354,1.3258631207			
H,0,-2.6445298866,0.955945773,0.3141653616			
TS Sab-CI-1 + H_2O → HAHP-Syn			
0,1			
C,0,-1.1338897746,-0.3174830146,-0.247576304	-550.2234	36.1454	73.0744
C,0,0.0296108986,-0.0180632842,-1.0749665688	125.6304	148.5969	203.1301
C,0,0.5176340621,1.4124030184,-0.970289269	227.2403	245.8506	264.5742
C,0,1.1409979756,0.3798237606,-0.1079668144	276.1821	297.3899	351.2396
C,0,0.577422047,0.2918626731,1.3073049789	379.5726	410.967	432.4243
C,0,-0.9554794449,0.2353543932,1.1486039655	477.1862	505.8644	567.0596
O,0,-3.0170442802,-1.3559486965,0.1992820177	586.4565	612.4573	668.3833
C,0,2.5646443379,-0.0583412562,-0.3804060805	698.9098	722.2546	799.43
C,0,3.5471471957,0.8361079386,0.3733482471	815.6188	879.912	915.1965
C,0,2.7900017135,-1.5309310751,-0.0439297372	927.3449	944.781	956.6583
O,0,-1.7716769749,-1.4070331962,-0.4968518134	962.9728	977.3734	998.0723
H,0,0.2048493519,-0.5963941977,-1.9695351332	1027.6249	1046.0523	1056.4154
H,0,1.0906346985,1.7575012968,-1.8191525265	1075.6453	1089.9434	1146.2544
H,0,-0.1665209558,2.136588758,-0.5501446803	1166.4882	1190.4459	1208.4914
H,0,0.9334241001,-0.6222443717,1.782589405	1232.2322	1241.5221	1274.5833
H,0,0.894382823,1.1335336672,1.922879947	1314.2986	1324.1051	1342.7175
H,0,-1.4112640974,1.217797395,1.2251302702	1366.734	1382.3648	1401.3744
H,0,-1.4537801806,-0.4239518904,1.8534457667	1422.4156	1431.5537	1482.4542
H,0,2.7359731718,0.072854449,-1.4535281663	1488.7991	1492.9892	1500.0453
H,0,4.5760380621,0.5637442533,0.1390192969	1509.3794	1514.1981	1516.6218
H,0,3.4021107778,1.8861295658,0.1174445178	1568.7968	1614.6268	1926.9426
H,0,3.4127463936,0.7274325719,1.4512997281	3030.1301	3041.8383	3049.3476
H,0,3.7782104896,-1.849249718,-0.3753181315	3078.0579	3110.3536	3116.537

H,0,2.0466846532,-2.167036457,-0.5258655464	3119.9268	3123.6701	3124.4309
H,0,2.7363011775,-1.7026599744,1.0317189666	3125.9777	3151.4927	3169.1287
O,0,-2.7002322179,0.834843906,-0.7033545111	3210.5055	3241.5846	3903.3717
H,0,-3.1515261522,-0.0709059751,-0.2705955779			
H,0,-2.847899191,0.7800980204,-1.651661637			
Sab-CI-1---$(H_2O)_2$ Anti-vdW			
0,1			
C,0,-1.4024202277,-0.3946392379,0.2622598009	34.6044	68.3731	86.7884
C,0,-0.1703617855,-0.574947145,1.0120887623	96.7698	108.302	163.386
C,0,0.6996463936,-1.6959386906,0.434715705	174.7084	218.1275	225.5187
C,0,0.9600999718,-0.2887997673,0.0349172082	238.6451	259.0011	271.9103
C,0,0.3333607136,0.1094173869,-1.3032109629	277.5287	296.9884	298.2918
C,0,-1.1662268133,-0.2242937516,-1.1969629952	300.7051	325.8284	347.6102
O,0,-3.6245419174,-0.2845618986,-0.0548293604	390.0103	409.3571	447.3226
C,0,2.2298830759,0.3971385545,0.5028851883	491.7302	520.548	565.5208
C,0,3.3315890523,0.2211989326,-0.5444210712	581.4834	585.2113	668.3757
C,0,2.0051118943,1.8730003893,0.831348165	705.5634	811.039	815.3542
O,0,-2.5203391397,-0.4148043199,0.8146395528	826.3245	877.8359	912.8973
H,0,-0.1371975377,-0.359635768,2.0708664542	920.6593	928.4058	939.092
H,0,1.368028625,-2.1490880918,1.1561663819	943.239	963.1619	977.8616
H,0,0.2478174943,-2.3872261788,-0.2670184707	990.9879	1013.4575	1046.7132
H,0,0.4380327012,1.1846158718,-1.4478745251	1055.9121	1076.0717	1089.903
H,0,0.8163549859,-0.4097986412,-2.1337415625	1152.2242	1180.6996	1194.226
H,0,-1.4734744321,-1.1458083414,-1.703702833	1231.6151	1254.0867	1273.0496
H,0,-1.8243694727,0.5621022863,-1.5663557416	1301.2941	1317.0036	1349.9462
H,0,2.5487649758,-0.1088798702,1.4225370787	1377.343	1398.4692	1406.9484
H,0,4.2765510126,0.6345044609,-0.185815216	1427.8493	1432.8398	1458.1255
H,0,3.4858053237,-0.8343253333,-0.7826653213	1488.6052	1492.0461	1502.4411
H,0,3.0688774408,0.743844274,-1.4688360356	1509.5875	1514.9349	1520.8411
H,0,2.9376753491,2.3310170671,1.1693512176	1664.6613	1690.3013	1711.833
H,0,1.259491406,1.9847523295,1.6218638623	3038.6697	3042.3898	3048.4718
H,0,1.6530268381,2.4248493561,-0.0436053403	3055.2747	3075.2718	3097.5155
O,0,-1.0890056029,2.3423659998,0.1752447198	3114.3312	3122.976	3128.3867
H,0,-0.76403293,2.9690502291,0.8241675775	3131.484	3139.6168	3149.0106
H,0,-2.057764521,2.4903623682,0.1342001128	3156.6861	3220.9826	3228.8554
O,0,-3.788406041,2.3199513737,0.1418742838	3461.6785	3960.3144	3968.6061
H,0,-3.8915992704,1.3288264238,0.0835383395			
H,0,-4.4438510123,2.705357112,-0.4408574049			
Sab-CI-1---$(H_2O)_2$ Syn-vdW			
0,1			
C,0,0.6881574864,0.8633676761,-0.3132432681	32.2666	43.5559	60.8748
C,0,-0.4144178877,0.407328312,-1.1344453812	76.4972	79.4215	111.3834
C,0,-0.6482008971,-1.1075425479,-1.0376243183	167.091	188.818	199.7289
C,0,-1.4320403452,-0.2029765677,-0.1667848899	218.0687	243.9376	252.8567
C,0,-0.8697088294,-0.0637677459,1.2507813862	262.9853	267.2286	284.3516
C,0,0.5896532127,0.4116860145,1.1000636251	289.1189	302.4478	349.5186
O,0,2.5660773019,2.0128301649,0.1559703966	398.6832	406.9076	460.4145
C,0,-2.915428378,-0.0052965639,-0.412775464	488.8528	507.3677	509.5222
C,0,-3.7178181458,-1.0558738082,0.3575044079	570.3405	583.9853	670.0023
C,0,-3.376293345,1.4108715099,-0.0656571811	699.5953	802.9339	814.5829
O,0,1.5751862275,1.6191167194,-0.7663426071	825.9058	878.4284	910.07
H,0,-0.6723526021,0.9306210022,-2.0447193093	921.6846	937.0096	943.1058
H,0,-1.1469245542,-1.5111002799,-1.9108640696	958.372	974.643	989.5879
H,0,0.1519652216,-1.7138461214,-0.6255809593	1012.653	1019.4684	1040.9685
H,0,-1.4448268143,0.6784442588,1.80798428	1061.5519	1090.637	1111.525
H,0,-0.9334839339,-1.0110499829,1.7891204895	1151.1813	1182.3328	1194.0532
H,0,1.326001585,-0.382528274,1.263679756	1240.106	1249.2244	1269.7259
H,0,0.8736072187,1.2445942665,1.7462271781	1307.5676	1317.5304	1344.8815
H,0,-3.0832620266,-0.1629444078,-1.4852502285	1375.8736	1399.3053	1403.347
H,0,-4.7839906027,-0.9671844307,0.1385648832	1424.4253	1432.9065	1454.9632
H,0,-3.3945817273,-2.0666574796,0.0978102738	1488.1503	1492.6966	1504.0399
H,0,-3.5868709522,-0.9234653367,1.4356035895	1509.2474	1516.7751	1527.2614
H,0,-4.420952068,1.5523105132,-0.3512157785	1651.9502	1667.6827	1672.6954
H,0,-2.7762675662,2.1620339564,-0.5851439146	3021.1793	3032.5497	3043.4567
H,0,-3.3039430006,1.6010997142,1.0084168227	3046.1531	3074.7259	3078.5233
O,0,3.8968471376,-0.2249307493,0.0590000547	3115.7919	3118.5576	3120.6364
H,0,3.4813567502,0.6821038589,0.1433658939	3125.3219	3126.6749	3129.0751
H,0,4.6135906613,-0.1294234949,-0.5704599202	3131.4802	3225.1104	3230.5654
O,0,2.1237315374,-2.2744354689,0.2215177861	3528.1033	3960.147	3967.7266
H,0,2.8472624669,-1.6224227724,0.117052394			
H,0,2.5317617991,-3.0675571949,0.5721333424			
TS Sab-CI-1 + $(H_2O)_2$ → HAHP-Anti + H_2O			
0,1			
C,0,0.7419456779,-0.5387637504,-0.2436608054	-531.4212	32.3348	48.415

C,0,-0.5367010343,-0.6450725798,-0.9769561673	68.7432	138.5396	161.5847
C,0,-1.4231341445,-1.7691554776,-0.4845037423	172.1558	190.7615	229.7339
C,0,-1.6338142693,-0.3798871203,0.0201054499	253.5592	270.0365	296.6523
C,0,-0.9726492321,-0.0893890222,1.3656880363	309.4087	336.0912	364.0701
C,0,0.4812092829,-0.5696145179,1.2359863246	380.3592	394.7968	426.2093
O,0,2.8992249288,-1.1115327161,0.1154833603	489.3315	529.0938	550.7645
C,0,-2.884414232,0.373628642,-0.3796221573	566.6134	570.6437	586.3754
C,0,-4.016821299,0.0920639474,0.6056901833	660.5719	681.5724	704.6003
C,0,-2.6333746489,1.8736185331,-0.5163151002	791.49	807.9748	836.3518
O,0,1.7960355758,-1.0215306171,-0.7861994061	876.1098	923.8254	932.5162
H,0,-0.5829845653,-0.3516712041,-2.0156260678	935.2497	948.2096	975.8679
H,0,-2.1289637168,-2.1446163641,-1.2116239685	995.5053	1002.253	1026.632
H,0,-0.9952510763,-2.5246150023,0.1596130286	1043.885	1048.866	1066.035
H,0,-0.9824908547,0.9842355732,1.5491596837	1079.747	1109.756	1150.386
H,0,-1.4937963296,-0.5807345608,2.1873459574	1172.873	1191.579	1228.837
H,0,0.6293528455,-1.6033887091,1.5538071902	1241.444	1262.161	1276.571
H,0,1.1996087072,0.0313196785,1.7824983771	1304.331	1317.073	1347.19
H,0,-3.1837539123,-0.0075215144,-1.3615729852	1366.196	1379.682	1404.188
H,0,-4.9405631451,0.5729967233,0.2841268339	1423.631	1434.598	1454.099
H,0,-4.2013423309,-0.9787832054,0.6983670411	1477.866	1483.952	1492.291
H,0,-3.7678695603,0.4798540889,1.5953581812	1500.239	1505.974	1512.375
H,0,-3.5238992316,2.3749887991,-0.8955345573	1519.411	1576.474	1675.47
H,0,-1.8091768234,2.077138124,-1.2002847492	1849.617	2090.969	3027.341
H,0,-2.3861578996,2.323810873,0.4457754276	3040.811	3047.235	3083.738
O,0,0.9627914474,1.3663322167,-0.346225737	3090.8	3111.692	3118.696
H,0,0.8364034539,1.6259807905,-1.2637093736	3120.139	3121.206	3131.357
H,0,2.0195985582,1.4484679314,-0.148437666	3142.71	3172.39	3196.291
O,0,3.3678004012,1.2545500571,0.0335309751	3230.733	3901.103	3943.393
H,0,3.2833435725,0.1401043762,0.1031431718			
H,0,3.7627737548,1.6046513174,0.8323582611			
TS Sab-CI-1 + $(H_2O)_2$ → HAHP-Syn + H_2O			
0,1			
C,0,0.8451906368,0.2053807723,-0.2200689063	-423.234	37.4927	55.7563
C,0,-0.3218183358,-0.2949721361,-0.9694483605	79.9478	123.0848	145.3025
C,0,-0.851216963,-1.6387160064,-0.5464566787	168.2317	218.7824	250.8295
C,0,-1.4419392886,-0.4092622486,0.0518564477	265.3869	278.7928	279.7773
C,0,-0.8772472846,-0.0143032121,1.4131897803	315.4514	338.8109	386.938
C,0,0.6576220862,-0.0339660894,1.2608598207	390.5779	414.6688	426.7843
O,0,2.2464885496,1.9730634623,0.188351829	476.7848	504.4961	522.5476
C,0,-2.8513393522,-0.0012296164,-0.3216029294	550.5482	577.0169	590.6333
C,0,-3.8624606409,-0.6551153404,0.6181575346	651.7363	695.2271	708.9864
C,0,-3.0212199796,1.5164485036,-0.3474837984	772.289	798.9797	820.7435
O,0,1.3590361389,1.2882768495,-0.6903794817	878.8271	919.6299	933.1581
H,0,-0.4894452308,0.0827559467,-1.967531078	945.6454	957.9387	978.7985
H,0,-1.4457240489,-2.1566455158,-1.2856249109	985.9834	1002.1455	1038.5172
H,0,-0.1973178836,-2.2697542408,0.0393656934	1049.9261	1065.6838	1076.2708
H,0,-1.2040551054,0.9952801572,1.6623662419	1091.8486	1148.4777	1182.1541
H,0,-1.2151054092,-0.6806583726,2.2068154125	1194.3169	1219.348	1232.4476
H,0,1.0799240589,-0.9965282239,1.5342254722	1246.3581	1273.8013	1286.1903
H,0,1.1630000785,0.7427022831,1.8246845056	1320.5506	1339.4842	1348.6958
H,0,-3.0302589171,-0.3780018952,-1.3338162731	1367.7094	1380.6055	1404.1101
H,0,-4.8824116252,-0.4161484187,0.3174816536	1424.9195	1431.067	1453.3239
H,0,-3.750972853,-1.7399145408,0.6255950955	1483.5219	1491.1072	1494.0885
H,0,-3.7249145893,-0.2934730028,1.6390884095	1502.7989	1509.534	1517.7515
H,0,-4.0004805538,1.7835493948,-0.7445758455	1519.8407	1550.55	1702.4651
H,0,-2.2588187321,1.9897484083,-0.9672677429	1827.239	2250.2358	3037.0833
H,0,-2.9500745424,1.9385991121,0.6556787996	3046.3215	3049.5222	3067.2919
O,0,3.8733174583,0.217657594,0.5593185417	3109.9099	3118.5648	3120.3643
H,0,3.2169006266,1.0920388449,0.4002255259	3124.3171	3125.5512	3135.2561
H,0,4.7386213872,0.3928056111,0.1884678339	3148.3543	3190.2605	3191.8381
O,0,2.1739145342,-1.1246869084,-0.5812107914	3239.041	3891.9814	3949.6786
H,0,3.0164003307,-0.6556681336,-0.1370653046			
H,0,2.3023027895,-1.0919256778,-1.5339746963			
Sab-CI-2--H_2O vdW-Anti			
0,1			
C,0,-0.6462839281,0.0736921109,0.6419891494	44.6103	63.3165	86.7088
C,0,-1.000665743,0.0158147933,2.0380549134	116.3076	146.2564	194.1476
C,0,-0.8897051542,-1.3873271298,2.6398576175	218.9957	221.2228	226.2754
C,0,0.2604139869,-0.4696921409,2.7567861129	253.5581	262.1906	274.6581
C,0,1.3482932282,-0.6735012901,1.7036244111	305.5835	324.3904	377.8413
C,0,0.6232615548,-0.6661721147,0.345068659	445.6077	456.1315	486.9138
O,0,-2.4009869858,1.3776125736,0.1095673353	504.6039	568.3908	594.4302
C,0,0.6230669998,0.1198560584,4.1031644338	685.3858	699.1558	807.2314
C,0,1.5676250432,-0.819013241,4.8520917883	820.1999	867.9271	885.4856

C,0,1.2097404197,1.5239978982,3.975455647	920.6383	931.874	937.481
O,0,-1.2371950439,0.6968157526,-0.259166436	944.249	965.3451	981.2631
H,0,-1.6953493186,0.7277784934,2.4496951221	1001.6544	1010.4621	1051.9281
H,0,-1.5107698119,-1.527082053,3.5128738108	1053.5248	1064.962	1092.2763
H,0,-0.8512731577,-2.2341370229,1.9689549656	1148.9379	1176.9911	1194.583
H,0,2.0476214995,0.1606478252,1.7446145798	1241.6683	1253.8594	1276.0176
H,0,1.9079875451,-1.5932793168,1.8697299244	1310.3147	1323.3363	1342.3033
H,0,0.3696192199,-1.671904105,0.0021853584	1379.25	1391.9755	1406.2745
H,0,1.1781343726,-0.179551757,-0.4527162959	1431.3829	1433.5577	1470.8268
H,0,-0.3094356051,0.1951892345,4.6710059701	1493.9689	1495.1291	1500.1397
H,0,1.7963220221,-0.4241695858,5.8417097012	1511.0204	1514.8171	1521.7579
H,0,1.1319802382,-1.8119089903,4.9705620992	1653.2143	1692.098	3035.4141
H,0,2.5113653167,-0.9237970549,4.3128771609	3040.8639	3044.902	3065.0136
H,0,1.3214203609,1.9731668448,4.9623907135	3083.9178	3106.7088	3111.6785
H,0,0.5690539633,2.1630165059,3.3669025789	3129.0922	3131.6201	3132.1315
H,0,2.2023942464,1.4948236421,3.5220622686	3139.3731	3148.6119	3227.9466
O,0,-0.8718410993,2.9790725611,1.6011697456	3275.4488	3299.9167	3950.5678
H,0,-1.5588589087,2.5549863001,1.034488156			
H,0,-0.769669681,3.8687267879,1.2616226791			
Sab-CI-2--H_2O vdW-Syn			
0,1			
C,0,-1.7025782601,-0.3890025746,-0.2947922315	42.7434	51.7176	86.0905
C,0,-0.3668039739,-0.7478297791,0.1070999265	113.2196	145.3671	188.195
C,0,-0.2195661078,-2.2237677345,0.4689329169	216.0175	223.4709	224.4228
C,0,0.10050488,-1.7991077058,-0.9070909027	244.6019	256.6671	278.128
C,0,-1.0260002486,-1.9984567469,-1.9200988495	303.5785	320.6344	373.8403
C,0,-2.2719391135,-1.3410779385,-1.2986887428	443.6692	449.0411	489.038
O,0,-1.7693933558,1.3624892412,1.1031997892	505.4904	566.494	589.5832
C,0,1.5396599286,-1.796286666,-1.3772538003	683.8031	699.3385	806.5832
C,0,1.9177240236,-3.1680765631,-1.9331427331	820.3387	842.0031	885.0985
C,0,1.8170302646,-0.690923743,-2.3933050134	917.4109	928.9871	933.3085
O,0,-2.3431976449,0.6148676493,0.0685606404	940.7439	956.3491	976.5315
H,0,0.2576091938,-0.0131952005,0.5876739463	991.2221	1008.4444	1049.3285
H,0,0.6026141801,-2.4148048455,1.1432953493	1054.0815	1074.105	1088.9203
H,0,-1.1251725818,-2.7670103299,0.6961302285	1146.8391	1172.7082	1190.5566
H,0,-0.773438582,-1.4915053124,-2.8511521921	1232.677	1240.4826	1273.2315
H,0,-1.1853101989,-3.0522685902,-2.1459689456	1306.132	1318.5365	1339.6707
H,0,-2.8936772662,-2.0561621133,-0.7539855915	1374.2083	1391.3455	1401.8362
H,0,-2.9125121806,-0.83019559,-2.0131605271	1422.6434	1434.6992	1470.7625
H,0,2.1551725979,-1.6034997781,-0.4931795994	1490.8569	1495.8748	1502.4565
H,0,2.9692048053,-3.1927653478,-2.2187529947	1509.6818	1516.5928	1519.6297
H,0,1.7429823813,-3.9534091918,-1.1971855328	1670.1281	1689.6621	3036.3827
H,0,1.328457948,-3.3993562098,-2.8229990445	3047.5977	3050.3793	3069.4745
H,0,2.8836722257,-0.6333562323,-2.6087656252	3078.5283	3114.439	3119.2929
H,0,1.4921647821,0.2809103863,-2.0202329175	3123.7789	3126.0593	3131.6983
H,0,1.3059258448,-0.882993018,-3.337818845	3138.2087	3148.2374	3236.458
O,0,-2.1816375639,-0.9179658188,2.5275610963	3242.8751	3424.738	3952.3665
H,0,-2.0137972557,0.0043289809,2.2344792398			
H,0,-2.8783039322,-0.8525239277,3.1814860452			
TS Sab-CI-2 + H_2O → aHAHP Anti			
0,1			
C,0,1.3680410354,-0.6587684877,0.0612586042	-641.4865	59.1924	81.4953
C,0,0.3570124658,-0.1796584421,-0.8947776978	118.4568	154.8451	205.7397
C,0,-0.5569318632,-1.2909278358,-1.3995449868	235.4513	249.5737	272.8973
C,0,-0.9887354681,-0.4304371896,-0.2582862542	277.7433	308.8128	324.5639
C,0,-0.7460001865,-1.0467574123,1.1224881063	379.6652	406.942	448.19
C,0,0.7222730657,-1.5133311064,1.1178573661	485.1413	501.1652	572.8178
O,0,3.0701187549,0.3806824959,-0.8691124711	585.4847	632.5058	650.118
C,0,-2.1173661043,0.5671291029,-0.4403026398	675.6093	701.4962	801.4936
C,0,-3.4750132557,-0.0916645877,-0.1888195821	823.3121	883.4179	927.693
C,0,-1.9205202017,1.8049475526,0.4394098655	935.8884	941.2088	954.2504
O,0,2.6275939657,-0.7934520299,-0.1643257698	974.1096	984.7513	1000.7669
H,0,0.5749291843,0.6665527985,-1.5312537093	1020.6887	1037.3435	1054.5913
H,0,-0.9966295188,-1.0943107177,-2.3722889197	1065.7778	1089.0687	1128.227
H,0,-0.280568753,-2.327950831,-1.2331629171	1154.7312	1180.6567	1197.3983
H,0,-0.8815122065,-0.2784033179,1.8892624504	1240.7311	1253.0514	1269.1166
H,0,-1.4383862519,-1.8673284114,1.3341503889	1306.4506	1319.1793	1351.5957
H,0,0.8338624996,-2.5624369795,0.820785508	1364.2183	1380.9302	1404.2525
H,0,1.2321052861,-1.3931167353,2.074916308	1425.3881	1434.1944	1469.4197
H,0,-2.080870132,0.8892777413,-1.4907744457	1488.2857	1491.3916	1502.1892
H,0,-4.2906795458,0.6124622591,-0.3785057502	1508.0664	1514.5791	1521.449
H,0,-3.6188520504,-0.9661119983,-0.8317969531	1586.0124	1614.5095	1871.0124
H,0,-3.5576182468,-0.4192869409,0.8540972465	3035.3605	3043.5728	3047.0043
H,0,-2.6242402748,2.5928239862,0.1544270324	3073.6562	3078.8697	3108.1436

H,0,-0.8999376666,2.1906146272,0.3543058248	3112.712	3119.4974	3131.5573
H,0,-2.1042389085,1.5716305968,1.494110292	3133.3434	3140.1013	3142.7138
O,0,1.5974424849,1.1868010363,0.8404522396	3227.8441	3259.2813	3900.0133
H,0,2.3798824988,1.1191345889,0.0549508296			
H,0,2.0569738135,1.1600516278,1.6894063043			
TS Sab-CI-2 + H_2O → HAHP Syn			
0,1			
C,0,1.197259047,0.4299244329,0.3741080664	-584.7456	48.4659	81.6158
C,0,0.3372264102,-0.3998762119,-0.473738017	118.4465	160.2261	198.1166
C,0,-0.2536405347,-1.6164127814,0.1864152469	223.6303	246.2025	254.2473
C,0,-1.0393356438,-0.3552772259,0.1860480499	265.1733	310.872	345.8338
C,0,-0.9335258843,0.4734650298,1.4629145556	385.2733	401.074	459.9507
C,0,0.5750102025,0.6336606565,1.7273200905	471.2979	505.9935	556.894
O,0,2.6789870767,0.8486579572,-1.1897382412	585.561	617.0098	674.5779
C,0,-2.2835077761,-0.2498621346,-0.6695282696	693.706	728.5114	800.568
C,0,-3.5062744241,-0.7383789933,0.1051670311	806.2501	881.5959	920.4818
C,0,-2.497443519,1.1640294435,-1.2057812222	929.8681	940.3183	952.0236
O,0,1.9339344282,1.3770000057,-0.0903731769	966.6557	977.9985	999.7051
H,0,0.4919004873,-0.3652222223,-1.5401079056	1032.109	1045.2114	1053.5022
H,0,-0.5706969883,-2.3963065796,-0.4908661857	1068.8326	1086.0213	1145.9998
H,0,0.2208791947,-1.9666045362,1.09265376	1166.5204	1190.8225	1199.2201
H,0,-1.3800671198,1.4544609732,1.3011198983	1235.9779	1246.861	1272.2335
H,0,-1.4509174823,0.0040744463,2.2993977449	1311.9716	1325.1378	1347.8192
H,0,0.9562456126,-0.1399027676,2.3935490999	1367.6151	1377.5565	1399.5163
H,0,0.854587095,1.6022075344,2.1338902954	1420.0915	1428.3843	1472.6542
H,0,-2.1319769732,-0.9148183086,-1.5254177427	1487.9633	1493.7468	1500.0783
H,0,-4.3954328529,-0.7238985343,-0.5250060225	1507.2978	1513.9746	1516.4854
H,0,-3.3618112518,-1.7549850815,0.4723676277	1573.7146	1614.0327	1923.1526
H,0,-3.6989408898,-0.0918740467,0.9638601549	3037.7272	3041.1806	3043.7733
H,0,-3.3195801321,1.1799765947,-1.9211223126	3075.6314	3088.1584	3108.2252
H,0,-1.6023458677,1.5368059895,-1.7048611455	3113.8411	3117.6863	3119.9654
H,0,-2.7534780343,1.8569553215,-0.402830605	3124.0329	3141.2059	3148.9325
O,0,2.7122982761,-0.8434575679,0.4982194413	3220.7389	3229.2933	3891.7883
H,0,2.9417168763,-0.2406118981,-0.3973449393			
H,0,3.3308171077,-0.5414886653,1.1702798329			
Sab-CI-2-$(H_2O)_2$ Anti vdW			
0,1			
C,0,1.3110070039,-1.0706229921,0.2066751073	46.7251	62.3090	79.8251
C,0,0.4491800357,-0.284441185,-0.628231275	98.5873	107.0206	120.7876
C,0,-0.4462248282,-1.0954137294,-1.570696296	144.5086	184.4061	202.1718
C,0,-0.9778758286,-0.7307583367,-0.2487550997	215.4250	235.0133	243.3303
C,0,-0.8565760063,-1.8290958191,0.8068954379	263.1901	273.8801	278.4804
C,0,0.6190317657,-2.2678448666,0.7851193151	300.6144	318.0322	349.1995
O,0,3.054325891,0.3429031669,-0.0170766306	374.5400	423.3159	446.0578
C,0,-2.0571655594,0.3219933998,-0.1202804896	483.2794	506.9454	548.1595
C,0,-3.4343270101,-0.3160863816,-0.2963438436	568.2788	595.1907	684.1683
C,0,-1.9550826284,1.0830227716,1.1994408026	702.3899	757.9547	800.4911
O,0,2.4812034074,-0.8034560313,0.5506607638	828.8460	886.7400	919.2558
H,0,0.6960387647,0.7281756416,-0.8967722176	933.9559	939.0619	944.8624
H,0,-0.778757852,-0.5168951101,-2.4206066292	967.1008	979.8652	1002.2151
H,0,-0.1704108151,-2.1177410985,-1.7896979511	1008.2781	1048.3448	1055.5261
H,0,-1.0952787406,-1.4153082366,1.7857686615	1064.4212	1069.6512	1094.6040
H,0,-1.539443754,-2.6558203347,0.6138805509	1149.0141	1174.0476	1193.7479
H,0,0.7915716314,-3.1214636303,0.1255518659	1240.4857	1256.9774	1275.0919
H,0,1.025115599,-2.5208609535,1.7607403516	1307.8469	1323.2032	1344.8240
H,0,-1.8896743709,1.0425284038,-0.9239544788	1381.9883	1398.6222	1405.2267
H,0,-4.2160886923,0.4414323702,-0.2462388198	1428.1954	1436.4865	1472.4368
H,0,-3.5155930576,-0.8287058257,-1.2558568168	1496.0240	1496.7384	1499.2521
H,0,-3.6290151632,-1.0435947028,0.495071036	1510.8558	1516.5093	1522.3210
H,0,-2.6005574188,1.9601015254,1.1712659284	1654.6387	1673.9429	1680.6660
H,0,-0.933338475,1.4198310534,1.3780167243	2920.9517	3042.8208	3048.7240
H,0,-2.2742401456,0.4652171513,2.0416661156	3065.2440	3079.1670	3092.0539
O,0,1.5197144407,2.0386955649,1.1752547439	3111.1148	3120.7622	3124.4827
H,0,2.207493525,1.4534900538,0.730467534	3134.6480	3134.7238	3141.4225
H,0,1.9720965696,2.5199460832,1.868725133	3144.7907	3230.9107	3262.5952
O,0,-0.187545707,2.8965480623,-0.8261061659	3608.3739	3959.4089	3962.0491
H,0,0.1810393326,3.628647226,-1.321893737			
H,0,0.4199553466,2.7541602899,-0.0777969413			
Sab-CI-2-$(H_2O)_2$ Syn vdW			
0,1			
C,0,-0.9289832174,-0.3160868013,0.7702108892	28.3696	50.0328	72.9854
C,0,-0.144509493,-0.2314324496,-0.4316535	80.7712	91.8973	131.3192
C,0,0.2473288636,1.1985480254,-0.8165526364	152.0324	188.9330	202.5165
C,0,1.1860637088,0.4071728935,-0.0028241256	223.8002	236.3808	244.1046

C,0,1.108499297,0.6745708674,1.4995528719	245.5194	262.2612	276.3207
C,0,-0.3789786512,0.5300946852,1.8736437148	308.1178	316.7835	355.4252
O,0,-2.3445950643,-1.8211934868,-0.1315873533	377.5984	440.9744	457.4168
C,0,2.4787914358,-0.0941209339,-0.6105124754	487.6353	501.8543	561.2698
C,0,3.580894686,0.9492709355,-0.4332648852	588.0631	590.9127	685.6317
C,0,2.9015406236,-1.4472330525,-0.043584486	703.6708	787.5957	806.6133
O,0,-1.9083405864,-1.0645708857,0.9672640895	827.0025	884.9577	919.3186
H,0,-0.2579157747,-0.9760286641,-1.2013375292	926.4297	933.0102	940.4504
H,0,0.4588906051,1.2977547675,-1.871472772	953.8049	973.1109	993.3047
H,0,-0.3278088435,2.0039188231,-0.382175741	1006.1777	1042.5035	1047.1820
H,0,1.696977165,-0.0697152007,2.0360029511	1057.9477	1085.9658	1094.6970
H,0,1.5017888465,1.6585048201,1.7526035635	1147.1858	1176.5731	1190.8218
H,0,-0.916167544,1.4798619452,1.8377587119	1236.8513	1241.2349	1274.2849
H,0,-0.5538796857,0.0741834639,2.844704158	1309.7881	1320.6424	1351.1863
H,0,2.2932611419,-0.2196398933,-1.6816087846	1378.1652	1393.3904	1401.0145
H,0,4.4997796156,0.6279601596,-0.9231868463	1421.9790	1437.9094	1472.1599
H,0,3.285168143,1.9112096751,-0.8529973619	1488.7568	1494.9948	1502.5595
H,0,3.8036530225,1.0948508924,0.6258509717	1507.5985	1515.1059	1519.8050
H,0,3.7646324367,-1.8333502276,-0.5854721582	1671.9917	1680.8370	1713.5215
H,0,2.0956912116,-2.1777137754,-0.1215337818	2931.0213	3038.1699	3044.3147
H,0,3.1879656888,-1.3648219659,1.0058558488	3053.6724	3077.7509	3081.3321
O,0,-2.8979403734,0.1406301384,-1.7178232623	3109.9865	3115.3981	3119.0213
H,0,-2.7516132469,-0.6834841989,-1.1572944963	3122.3881	3124.0985	3141.8852
H,0,-3.7296206506,0.0115634454,-2.1755669883	3150.0454	3235.3357	3249.6944
O,0,-2.5900850406,2.0811473621,0.1846582898	3505.3170	3946.7435	3957.9133
H,0,-3.4425278381,2.2773064506,0.5751399967			
H,0,-2.7758523216,1.4604504757,-0.549980473			
TS Sab-CI2-$(H_2O)_2$ Anti to HAHP-Anti + H_2O			
0,1			
C,0,-0.1247914909,-3.613788418,-2.6501378007	-612.8918	54.3063	64.9372
C,0,0.9661826395,-3.925344207,-1.7462780807	101.4156	111.2400	123.9603
C,0,1.3653752103,-5.3998819471,-1.8084994635	144.7799	194.9995	210.0594
C,0,2.1131776039,-4.4052718363,-2.6152330354	232.7914	242.3026	258.8704
C,0,1.6601780866,-4.3097604105,-4.0704218174	269.5155	273.0654	318.6757
C,0,0.1323958806,-4.1536976194,-4.0213140897	326.2877	379.6340	424.2450
O,0,-1.3008398859,-2.4250822559,-1.215728817	427.3478	453.4069	484.0756
C,0,3.5423446064,-4.0596114732,-2.2471273612	492.4952	543.2827	584.4908
C,0,4.4841833727,-5.2054801156,-2.6136123187	592.8781	598.4808	676.7661
C,0,3.997871874,-2.7503449571,-2.8889709519	695.7390	786.2743	799.1119
O,0,-1.3219829241,-3.266444642,-2.3571892833	815.3943	886.3335	910.3975
H,0,1.1152739038,-3.3759884362,-0.8323580438	930.2895	938.3963	953.1903
H,0,1.8246892598,-5.7500036349,-0.8948188424	975.5660	986.5451	992.7322
H,0,0.7052030963,-6.1119311841,-2.2845296339	1012.1435	1018.9190	1051.5387
H,0,2.0923749728,-3.4182256787,-4.5208867252	1053.4540	1073.0442	1090.5712
H,0,1.9683595003,-5.1753127055,-4.6565814423	1147.5928	1175.0820	1192.5856
H,0,-0.4011228963,-5.1023092966,-4.1186041004	1246.4020	1263.5006	1271.0021
H,0,-0.2703443909,-3.4780114221,-4.7711276377	1305.4759	1324.0783	1343.5364
H,0,3.5577652582,-3.9197700608,-1.1623941818	1375.6502	1383.4356	1402.6735
H,0,5.5100324003,-4.9641909164,-2.334972053	1423.8056	1427.2381	1429.3840
H,0,4.2024294279,-6.1318179301,-2.1119833147	1459.0998	1487.3060	1490.6673
H,0,4.4693455714,-5.3864997496,-3.6908323618	1496.5740	1506.5857	1510.7892
H,0,4.9206726493,-2.4078705666,-2.4225892532	1515.6356	1578.8325	1659.0794
H,0,3.2475782417,-1.9706175615,-2.7673162532	1951.1119	3037.6863	3041.2312
H,0,4.1972231298,-2.886720338,-3.9541182734	3049.9388	3076.7199	3081.5114
O,0,0.4850210441,-1.5243850741,-2.5132390057	3105.8676	3114.7663	3120.4744
H,0,-0.4991188642,-1.7704498084,-1.6763757153	3123.8032	3140.4952	3144.1963
H,0,0.1763881914,-0.9278131272,-3.1983034294	3144.2976	3231.4316	3258.6161
O,0,2.3278497499,-1.3959654359,-0.4743110168	3563.8348	3923.6073	3963.4165
H,0,2.1537172385,-0.6768028255,0.1337238528			
H,0,1.7252267028,-1.2603471156,-1.2297236094			
TS Sab-CI2-$(H_2O)_2$ Syn to HAHP-Syn + H_2O			
0,1			
C,0,-0.7503963372,0.3985406101,-0.9859978099	-890.8075	46.7470	68.0698
C,0,-1.7086230212,0.6857010489,-2.0346502491	80.6755	108.0221	118.0993
C,0,-2.3456778361,-0.4955361261,-2.7302804844	152.9496	176.6047	208.5074
C,0,-3.0171238978,0.0465861115,-1.5298762171	234.7920	245.3756	246.8700
C,0,-2.7132867868,-0.7062564384,-0.2360570591	252.0825	273.3513	299.8194
C,0,-1.1764129692,-0.7591369643,-0.1433064714	331.5674	373.1700	392.0138
O,0,0.5777245934,2.0712975383,-1.504283167	430.9512	460.5119	476.2461
C,0,-4.3164873943,0.8103152052,-1.6620303557	506.8810	538.9982	567.8224
C,0,-5.5004009592,-0.1526509337,-1.5842937314	584.9429	666.0110	685.0042
C,0,-4.44227581,1.9271233246,-0.6279530661	721.3309	787.4166	799.2467
O,0,0.0192608224,1.284071487,-0.4612776347	817.1374	880.1243	890.0861
H,0,-1.6691194696,1.6483655821,-2.5175375445	924.2060	935.4972	951.0908

H,0,-2.7811020561,-0.249425582,-3.6886241968	954.2378	978.2040	987.7761
H,0,-1.8316741436,-1.4458484962,-2.6870510865	1004.2623	1028.8197	1046.2950
H,0,-3.1109559244,-0.1538262143,0.6152070956	1058.7160	1088.1389	1112.7238
H,0,-3.1596249183,-1.6998684234,-0.2326972251	1147.2468	1181.5657	1191.9705
H,0,-0.7672931963,-1.6632709703,-0.6017414698	1233.7942	1247.0150	1271.8368
H,0,-0.7833817212,-0.6741449094,0.8663434307	1309.2693	1323.3939	1347.2778
H,0,-4.3114186853,1.26902937,-2.655566522	1376.0070	1383.8174	1401.4625
H,0,-6.4403427086,0.3770142557,-1.7380528267	1423.0162	1432.4380	1471.0737
H,0,-5.419894056,-0.9379115891,-2.3364741467	1488.4941	1494.4105	1502.4979
H,0,-5.5443064594,-0.6275382001,-0.6020227939	1508.8019	1510.0334	1516.5342
H,0,-5.3231340539,2.5359301798,-0.8309953507	1522.0985	1562.8842	1647.0388
H,0,-3.5675220708,2.5784793617,-0.6396097127	1878.0928	3040.5354	3043.7310
H,0,-4.5525178582,1.5237717012,0.3797696817	3047.6499	3067.7376	3075.2142
O,0,0.8722666047,-0.1397485446,-2.3084937107	3111.0948	3116.3331	3121.3648
H,0,0.8778314412,1.1032021029,-2.0973391072	3122.1027	3124.4592	3142.7779
H,0,1.6136653331,-0.4475128326,-1.7771796904	3145.7219	3230.5299	3238.4910
O,0,0.0208832997,-2.7063204168,-2.5967552059	3528.1804	3880.2070	3962.6591
H,0,0.4440861549,-3.2339672936,-3.2744613709			
H,0,0.3583950341,-1.7945402641,-2.7012152515			
HAHP-Syn			
0,1			
C,0,-1.0241664513,-0.0409486422,0.6300439598	56.3742	78.7749	99.2925
C,0,0.0762963127,-0.8306120482,-0.0543863578	151.5401	217.4818	223.2237
C,0,1.1785923933,-1.3529252749,0.8174260332	237.0068	256.7203	265.3042
C,0,1.368100429,-0.0661723928,0.071970299	293.9425	324.8816	374.0575
C,0,1.0571806541,1.1909265792,0.8966256061	387.1322	400.0475	424.8184
C,0,-0.4613425889,1.3821503805,0.7713321178	457.302	464.3186	481.0141
C,0,2.4015292043,0.0650503092,-1.0324053047	567.6713	624.9852	690.4215
C,0,3.7952481336,0.205971879,-0.420439843	739.3528	782.2445	835.9849
C,0,2.3730896777,-1.0793925956,-2.0396502804	878.2656	915.004	933.7199
O,0,-1.352708078,-0.6091704579,1.8606178683	941.7736	958.064	972.703
O,0,-2.1354845706,-0.0993715676,-0.2496345066	994.9063	1007.7873	1018.1794
O,0,-3.1686105495,0.6831370085,0.3300746983	1048.0805	1064.5589	1078.946
H,0,-0.2005370908,-1.3817695141,-0.9410061368	1080.6322	1118.9662	1138.8776
H,0,1.6910862367,-2.2337655729,0.4575196036	1148.4333	1183.0996	1190.1258
H,0,1.0319639633,-1.315262427,1.8873228879	1210.8865	1254.9473	1258.9003
H,0,1.5977495986,2.0556623334,0.5121349764	1288.4751	1323.3917	1340.9238
H,0,1.3511786752,1.0614947759,1.938886263	1349.1397	1380.3004	1391.4923
H,0,-0.9088127291,1.9286279801,1.6007899746	1402.5591	1405.2816	1423.6455
H,0,-0.6747510769,1.9164597979,-0.1572190665	1442.6284	1478.54	1492.8785
H,0,2.1700817207,0.9890606488,-1.5745164987	1496.4825	1504.7579	1509.8156
H,0,4.5467048789,0.3861028315,-1.1896662025	1516.499	1520.0047	3018.7773
H,0,3.8381482038,1.028700852,0.2943476302	3043.1551	3044.8482	3051.607
H,0,4.0631721114,-0.7106324576,0.1090828679	3054.8872	3097.8829	3112.4964
H,0,3.1356409249,-0.9242572103,-2.8029334199	3112.9612	3117.9581	3123.6852
H,0,1.4090308615,-1.1526412062,-2.541452322	3128.5431	3141.1303	3198.5073
H,0,2.5842490188,-2.0366217757,-1.559936549	3226.3401	3832.1852	3869.5361
H,0,-2.0885142045,-0.1077838456,2.2265094707			
H,0,-3.1526466588,1.4765906127,-0.217483769			
HAHP-Anti			
0,1			
C,0,-1.0301487705,0.0654471525,0.596385589	47.311	68.3452	98.1922
C,0,0.0542360435,-0.774048952,-0.0473863773	169.1997	190.5267	215.7515
C,0,1.1484047366,-1.3251973607,0.8268994049	228.1357	259.4158	278.4713
C,0,1.3712477892,-0.0514458837,0.0747571067	292.4117	321.6356	345.8817
C,0,1.1013014025,1.2152180535,0.900763505	376.125	422.8147	429.5029
C,0,-0.410589313,1.4558262674,0.7924591975	464.4326	472.5864	504.0896
C,0,2.4025657933,0.0522596165,-1.0339355339	556.1164	625.4028	661.3569
C,0,3.7990908302,0.1974779167,-0.4290183359	737.8792	787.0551	828.1487
C,0,2.3682495,-1.1133537256,-2.0166478775	875.5239	910.1088	919.231
O,0,-2.1629730275,0.0629722681,-0.2162861982	934.3355	961.0727	969.0222
O,0,-1.3275902831,-0.5467599371,1.849556898	989.2886	1010.2868	1025.5282
O,0,-2.3541813181,0.213886018,2.4699878561	1042.8275	1071.2777	1077.8057
H,0,-0.2391040424,-1.3262162805,-0.9272029117	1097.8047	1122.1119	1139.5699
H,0,1.6256510111,-2.2256630327,0.4665322897	1147.1817	1178.8559	1182.1472
H,0,1.0240244772,-1.2771767608,1.8989644233	1209.2701	1245.5677	1258.7259
H,0,1.6614129943,2.0632335707,0.5073528981	1303.3558	1330.0133	1347.3238
H,0,1.4065103081,1.0801451821,1.9388852218	1351.5638	1379.6766	1393.5575
H,0,-0.8434625126,1.978703275,1.6439452385	1404.1023	1410.5759	1423.4116
H,0,-0.6180384636,2.0274711429,-0.1133198457	1443.3795	1483.3232	1491.632
H,0,2.1736855395,0.9664817933,-1.5932137458	1495.8789	1503.3932	1509.3946
H,0,4.5480317825,0.3579542453,-1.2051318614	1515.8419	1520.6879	3017.0941
H,0,3.8496396616,1.0336668363,0.2690342882	3042.7032	3050.4998	3062.5812
H,0,4.0641405769,-0.7103698812,0.1168052836	3065.2904	3103.0068	3112.0098

H,0,3.1179583155,-0.9695642032,-2.7947915388	3118.8518	3124.4144	3127.6692
H,0,1.3975540548,-1.2059659045,-2.5020727888	3129.0677	3149.5081	3215.8761
H,0,2.5949081975,-2.0574382615,-1.5179839307	3236.7874	3856.0435	3884.5539
H,0,-2.7451234198,0.7680699732,0.0803265403			
H,0,-3.1062048638,-0.3823181279,2.3798972051			
TS HAHP-Anti → Sabinaketone + H_2O_2			
0,1			
C,0,-1.3841154894,-0.1469218424,-0.6173086547	-1691.2804	41.6208	62.9485
C,0,-0.2214295094,-0.7814606293,0.0292419444	96.7851	137.5034	157.3735
C,0,0.2835683722,-0.123265737,1.2888923976	187.9112	221.0307	234.8826
C,0,0.908001491,0.2412927303,-0.0103884842	257.038	278.8463	307.2476
C,0,0.3519429229,1.5102012648,-0.6541605525	318.9516	368.7185	401.7943
C,0,-1.1775894845,1.3595106838,-0.6328366759	406.0233	450.8928	494.1705
C,0,2.3398998333,-0.1271214783,-0.3508832452	513.9291	566.8134	599.7083
C,0,3.2822759535,1.0076840367,0.0544226079	695.5327	770.5674	798.2281
C,0,2.8076059674,-1.4393626595,0.2707874156	819.1573	879.7307	917.2969
O,0,-2.056531191,-0.7442514884,-1.5553525561	926.3918	939.061	947.742
O,0,-2.841504887,-0.5097506441,0.4728450441	973.8847	1000.1288	1026.2267
O,0,-2.6122426317,-1.4289229095,1.5143490611	1037.4116	1054.4945	1062.9138
H,0,-0.0741432892,-1.8391071869,-0.1220480711	1070.7736	1123.6619	1139.1182
H,0,0.8314443141,-0.7745603146,1.9528155059	1161.32	1169.3677	1188.3582
H,0,-0.3725061332,0.5784857727,1.7863901636	1228.2612	1240.4482	1251.046
H,0,0.7082048398,1.5621527522,-1.6853985016	1301.8649	1313.4325	1345.6983
H,0,0.6875228686,2.4113863935,-0.1407265315	1355.7789	1381.0278	1404.3888
H,0,-1.6128137502,1.8019243844,0.2606172249	1404.7538	1411.6472	1425.4009
H,0,-1.6727093358,1.7872728849,-1.4998900225	1486.471	1491.107	1493.5506
H,0,2.3819721908,-0.2349939674,-1.440040373	1500.1483	1511.5289	1516.8127
H,0,4.3153559699,0.7526849727,-0.1824217688	1521.3981	1529.552	1978.7492
H,0,3.0415816447,1.9387843762,-0.4578326529	3029.08	3042.9652	3050.2115
H,0,3.2149062739,1.1848404741,1.1301454979	3052.3454	3103.8835	3112.8329
H,0,3.7924154851,-1.7013537433,-0.1149638124	3113.6511	3120.5173	3124.4102
H,0,2.1334666262,-2.2659379439,0.0481854517	3125.5162	3144.6418	3164.5784
H,0,2.8971306946,-1.3499540319,1.3544714273	3202.7688	3242.9098	3859.8132
H,0,-2.8318555294,-0.9998554638,-0.6573064347			
H,0,-3.1019477273,-1.0281160759,2.2397837353			
TS HAHP-Syn → Sabinaketone + H_2O_2			
0,1			
C,0,-1.489530251,0.1914165531,0.6389268523	-1655.4063	24.45	68.5345
C,0,-0.1943321344,-0.4181317314,0.9906659567	112.5526	155.3745	171.8332
C,0,0.8080110808,0.5188381609,1.6360124227	222.9342	240.597	246.6564
C,0,0.8640725322,0.2749135739,0.1668039934	257.1633	273.3886	302.5806
C,0,0.156612401,1.3479581904,-0.6647913685	327.3668	358.4777	402.1811
C,0,-1.2331733326,1.5131821607,-0.0399242121	407.5706	461.0302	484.5308
C,0,2.0291258271,-0.4477896529,-0.4820109183	492.6822	601.4692	626.35
C,0,3.2269563103,0.4943149947,-0.6029590478	666.6166	701.3455	814.6239
C,0,2.4240827904,-1.736885254,0.2308294279	835.6656	881.0012	918.4703
O,0,-2.6220695925,-0.1128690082,1.1877190968	932.9315	935.3303	959.6022
O,0,-2.0471503639,-0.913777237,-0.7775024658	978.597	1000.3945	1024.071
O,0,-1.30380273,-2.0898027261,-0.9932410834	1048.6345	1059.2241	1066.1143
H,0,-0.1701670044,-1.4658482475,1.2432001579	1074.8352	1126.2787	1148.2711
H,0,1.538645857,0.0279255529,2.2616784846	1159.2887	1162.9831	1189.0725
H,0,0.47341706,1.4772101912,2.0082122161	1234.4575	1239.5963	1261.0487
H,0,0.0541945693,0.9846133364,-1.689405657	1296.6807	1315.8189	1348.6443
H,0,0.7184587346,2.2817730122,-0.6944122804	1357.5733	1389.1258	1405.2901
H,0,-1.2609483849,2.2864581432,0.7315765069	1408.2286	1417.269	1428.6353
H,0,-2.0235213676,1.7353853715,-0.7517792616	1463.7744	1490.0488	1495.6714
H,0,1.7000325478,-0.7185477725,-1.4907805564	1500.7847	1510.6828	1517.489
H,0,4.0537784841,0.0103364094,-1.1229911032	1523.7886	1549.3539	1967.584
H,0,2.9712661523,1.4023587867,-1.1492664194	3042.1059	3047.806	3051.2423
H,0,3.5756318736,0.7854874307,0.3901902758	3064.8715	3067.4815	3115.1671
H,0,3.2635912206,-2.2052017469,-0.2831293254	3117.0431	3121.3298	3128.5947
H,0,1.6011217164,-2.4503386452,0.2486268095	3131.6665	3133.2935	3146.8791
H,0,2.7408909462,-1.5460046728,1.257990985	3229.4825	3237.6533	3861.3819
H,0,-2.7317303187,-0.8772251887,0.2638026064			
H,0,-1.2443323737,-2.1106403048,-1.9538471525			
TS HAHP-Syn + H_2O → Sabinaketone + H_2O_2 + H_2O			
0,1			
C,0,0.978499419,0.3234566608,-0.8385997711	-1468.9489	25.979	64.5268
C,0,2.2808765384,-0.3145818599,-0.530824356	74.0905	115.0337	173.1862
C,0,2.7266420003,-0.1631848763,0.9074604412	183.7071	187.673	217.1455
C,0,3.2585991836,0.7615903013,-0.1384295428	236.2483	248.2111	259.5274
C,0,2.5237344903,2.1021416895,-0.2013800713	275.3144	313.9247	327.7301
C,0,1.0345768038,1.7722344636,-0.3766306874	362.3257	375.9002	427.9841
C,0,4.7198812932,0.7649088767,-0.5435712674	453.8718	470.4278	529.869

C,0,5.5190264171,1.6881212833,0.3763350344	543.1322	597.3342	612.622
C,0,5.3568990258,-0.6208175756,-0.5790109491	633.0643	674.2338	702.6252
O,0,-0.1078860429,-0.3441102778,-0.8472538936	720.4634	796.7487	825.89
O,0,1.16514939,0.5441579017,-2.7040961191	880.6998	915.0635	930.0386
O,0,1.8664816055,1.7012346915,-3.118080279	935.844	948.7915	972.4662
H,0,2.5420694833,-1.2135856358,-1.0668694548	1007.5656	1028.0937	1045.3794
H,0,3.3670433335,-0.9524166443,1.2721001711	1058.5206	1063.1553	1069.9792
H,0,2.0196901046,0.2132117098,1.6347247966	1126.4264	1141.3707	1159.1043
H,0,2.8862589058,2.6672399019,-1.0588663985	1192.6695	1222.4922	1240.0265
H,0,2.7042676258,2.695422986,0.6959339648	1244.0875	1272.9513	1302.2057
H,0,0.4882157466,1.808890441,0.5675823822	1309.1354	1340.5111	1344.8123
H,0,0.5235900974,2.4332147034,-1.0731998161	1350.7848	1374.7531	1405.5824
H,0,4.7570602712,1.1798998792,-1.5576857779	1406.9672	1417.5756	1427.03
H,0,6.569828362,1.711731635,0.086633281	1457.2928	1486.7432	1493.3086
H,0,5.139427803,2.7092773558,0.351765788	1498.0024	1509.4839	1517.1345
H,0,5.4603596966,1.3303853782,1.406726423	1518.4808	1558.9549	1601.9238
H,0,6.3689071086,-0.5562113626,-0.9783996166	1662.0399	1915.6891	3012.7016
H,0,4.796318164,-1.3155498391,-1.2040194053	3044.3837	3050.456	3062.1062
H,0,5.4314368276,-1.0444861753,0.4238436039	3067.6764	3112.1672	3114.5554
H,0,-0.8722999213,0.2367344181,-1.6008349506	3119.7397	3123.2422	3135.8338
H,0,2.6363163064,1.314604307,-3.547381885	3136.541	3139.0953	3214.5986
O,0,-1.1757770212,0.8658278778,-2.5701182913	3228.5644	3853.3687	3941.5813
H,0,-0.0203100295,0.784379063,-2.8562139972			
H,0,-1.7294977783,0.3533289221,-3.161891906			
TS HAHP-Anti + H_2O → Sabinaketone + H_2O_2 + H_2O			
0,1			
C,0,0.1438610967,-1.2422258653,0.4908640877	-1233.7397	42.9202	74.3468
C,0,0.4755796717,-2.2588289247,-0.548066533	95.0567	118.5221	163.6804
C,0,1.8215849022,-2.147363889,-1.2072769317	193.6669	227.3706	232.8715
C,0,0.6323475079,-1.5179762654,-1.8584495522	265.1338	287.8193	306.5319
C,0,0.443925433,-0.0318812441,-1.5668478294	316.5838	359.2246	378.9553
C,0,0.5960174532,0.1226671515,-0.0450759926	418.0864	434.4606	451.9167
C,0,0.071802655,-2.0263232078,-3.1740068648	477.3711	514.8793	524.8896
C,0,0.7193326209,-1.2827511446,-4.3434384906	531.737	592.9118	614.3111
C,0,0.2184985291,-3.532061503,-3.3702347479	673.6062	702.6215	775.4639
O,0,-1.0135192411,-1.3517143064,1.0753497792	787.2968	806.2379	834.3594
O,0,1.25952368,-1.4622337363,1.756222594	881.0458	918.889	930.5824
O,0,0.986527591,-2.7313409909,2.3102621207	939.0273	960.6791	976.7111
H,0,-0.0187519262,-3.2152732479,-0.4766652229	1003.8879	1042.8717	1046.5864
H,0,2.2061224823,-3.0601034211,-1.6363952585	1058.2326	1061.7131	1068.5194
H,0,2.5702544838,-1.5258597277,-0.7356981813	1130.6978	1141.8443	1165.6577
H,0,-0.5653438856,0.2550653465,-1.8713100543	1191.9399	1224.2179	1242.2114
H,0,1.1481438671,0.5947504021,-2.114474523	1255.3663	1298.5756	1314.708
H,0,1.6330193169,0.3172846334,0.2264791716	1326.7635	1349.836	1356.1064
H,0,-0.0250961321,0.9167777631,0.3631204722	1382.1174	1404.1322	1405.7938
H,0,-0.9977823527,-1.7897056702,-3.1667956298	1423.4266	1457.4305	1484.869
H,0,0.3340933091,-1.6495479125,-5.2950874454	1489.9096	1496.4698	1502.3906
H,0,0.5318582584,-0.2103033753,-4.297386486	1506.1153	1510.3294	1517.8642
H,0,1.8003609064,-1.438986803,-4.3331586986	1520.8872	1549.8886	1629.3875
H,0,-0.3120640483,-3.8412361706,-4.2704887852	1718.4776	1889.6881	3034.5813
H,0,-0.1888463722,-4.0992023827,-2.533712535	3045.9563	3049.4933	3055.5297
H,0,1.2657300956,-3.8105121294,-3.4975803083	3086.5738	3105.0223	3115.9333
H,0,-0.8805193555,-0.6190087909,2.1387340788	3120.2109	3127.6802	3134.388
H,0,0.0135587915,-2.7722358085,2.2477345452	3141.4547	3145.3774	3209.4298
O,0,-0.3005786125,-0.2271773228,3.0377155973	3233.4315	3637.8676	3941.5634
H,0,-0.307528189,0.7284866838,3.1067767372			
H,0,0.7188590237,-0.7594838305,2.5018272067			
TS HAHP-Syn + $(H_2O)_2$ → Sabinaketone + H_2O_2 + $2H_2O$			
0,1			
C,0,-0.7902764392,-0.3678468101,-0.7889477474	-1376.0844	28.5509	46.1096
C,0,0.2715618928,0.6354407093,-0.4597908968	70.2833	75.5482	99.2363
C,0,1.3479214247,0.7788340931,-1.511933154	141.0851	176.0786	192.7121
C,0,1.5737813351,-0.1035585335,-0.3252004463	204.5595	209.8228	218.4271
C,0,1.2873046032,-1.5848916913,-0.5776747145	257.7712	275.7368	288.4683
C,0,-0.1056275088,-1.6467726011,-1.2148287801	300.611	320.5851	343.1794
C,0,2.6126248893,0.2175180074,0.7325938734	393.5396	398.7824	417.6385
C,0,3.976171125,-0.3370640632,0.3196148247	447.2782	458.7414	521.043
C,0,2.7265584268,1.7029277357,1.0614478434	579.7271	599.8093	619.5227
O,0,-1.931235933,-0.0746750636,-1.2437116557	635.5378	650.4762	679.5865
O,0,-1.0322581588,-0.8217560924,1.0220146953	701.4307	710.7568	738.6445
O,0,-2.1424019444,-1.7006340532,1.0865754779	797.7617	841.9228	879.2869
H,0,0.0173834677,1.4925337091,0.1467403341	917.6197	934.2957	935.0785
H,0,1.8461309105,1.7366003372,-1.5372530352	956.8089	975.0081	1000.6891
H,0,1.189587916,0.3334352208,-2.4848307446	1022.2699	1032.4017	1050.072

H,0,1.2842563555,-2.1021550127,0.3832453013	1060.9256	1067.2323	1106.7504
H,0,2.0496141659,-2.0461090808,-1.2059879115	1128.8663	1143.4695	1167.1295
H,0,-0.0656450967,-1.6442776193,-2.3050824602	1192.8904	1222.5189	1241.259
H,0,-0.7021359553,-2.5052087911,-0.9165155323	1252.8731	1299.1615	1310.8713
H,0,2.2901221721,-0.3007908,1.6422581712	1331.7438	1346.2716	1351.6695
H,0,4.7266137195,-0.1303323536,1.0829269569	1384.2074	1395.1916	1402.9341
H,0,3.94344126,-1.4152702333,0.1645825405	1417.852	1427.175	1456.4704
H,0,4.3043437604,0.1285498781,-0.612353515	1481.0678	1484.3376	1492.2408
H,0,3.4326275531,1.8476430528,1.8790410204	1495.0291	1499.9476	1511.5221
H,0,1.7722652389,2.1284109985,1.3708480291	1518.8487	1520.8497	1588.9957
H,0,3.1004873998,2.2704260647,0.2075048848	1610.1476	1664.1469	1717.5856
H,0,-2.3620945579,1.0040852972,-0.8430861127	1786.5247	3025.4473	3040.7671
H,0,-1.759207894,-2.4629872336,1.5316611535	3051.5313	3061.045	3082.3642
O,0,-1.9984662199,1.2088273138,1.8598448482	3104.5698	3107.5615	3117.8449
H,0,-1.5084627817,0.1865050422,1.503939194	3129.1756	3132.2167	3141.7326
H,0,-2.7204643712,1.0244467649,2.4640898503	3150.1999	3203.2627	3233.4928
O,0,-2.7648250189,1.9480205082,-0.2777340509	3864.6318	3935.692	3937.0519
H,0,-2.4181118874,1.6683243798,0.8497470113			
H,0,-2.3724790091,2.7573399699,-0.6084812332			
TS HAHP-Anti + $(H_2O)_2$ → Sabinaketone + H_2O_2 + $2H_2O$			
0,1			
C,0,0.1973674311,-0.2258963807,-2.2149416538	-891.0378	38.8334	58.4167
C,0,1.4505406289,-0.8111664114,-1.6229606524	67.7533	82.2887	116.5317
C,0,2.1951956192,0.0342711863,-0.6214911922	145.2543	165.3662	200.6622
C,0,2.5991390875,0.0648039714,-2.0617253379	226.9155	249.7016	269.9217
C,0,2.0067685047,1.2100632304,-2.878050956	280.6585	313.0622	325.9649
C,0,0.5096324404,1.2369507061,-2.5397660784	364.4962	384.2697	401.851
C,0,3.9326700258,-0.4884831526,-2.5304831267	411.6985	434.18	451.9881
C,0,4.9915655568,0.6151212424,-2.5244130677	491.8875	498.6416	544.4681
C,0,4.4257611771,-1.6869521493,-1.7250582849	593.9524	602.4907	650.6751
O,0,-0.4062615006,-0.9090777397,-3.1598399813	684.8983	697.2561	708.4481
O,0,-0.8275348412,-0.184224462,-0.9646777356	726.9573	778.9863	811.2361
O,0,-2.1165084407,0.0361638562,-1.50236088	835.9841	869.057	902.4766
H,0,1.5332649924,-1.8880273093,-1.5850115683	921.0296	932.4076	940.6746
H,0,2.8281752536,-0.5059459297,0.0664227587	965.7927	975.656	1007.3339
H,0,1.6910241577,0.8872813564,-0.1890892908	1039.9571	1056.6076	1062.0117
H,0,2.148077951,0.984984997,-3.9378559644	1066.1194	1070.7789	1126.7252
H,0,2.4919551637,2.164551621,-2.6724194551	1137.4057	1142.2709	1164.405
H,0,0.3103992301,1.8661704034,-1.6748281433	1189.7328	1222.5903	1243.8292
H,0,-0.1113639973,1.5758796983,-3.3643024184	1250.3174	1292.6973	1314.7344
H,0,3.7845423203,-0.8167665483,-3.5651597868	1330.7168	1342.6144	1347.7715
H,0,5.9577362707,0.2263708453,-2.8473935777	1370.0717	1380.8969	1403.6726
H,0,4.7232144226,1.4383721384,-3.1856757293	1422.6155	1430.578	1482.7421
H,0,5.1087212089,1.0154550882,-1.5147514788	1489.615	1491.4747	1494.4842
H,0,5.3118255304,-2.1109638257,-2.1971697477	1499.8099	1510.1198	1512.8159
H,0,3.6761889416,-2.4749549044,-1.6582232628	1516.063	1521.8011	1587.1777
H,0,4.7064741681,-1.3911059834,-0.7130320928	1730.9632	1762.7259	1851.342
H,0,-0.3842179759,-2.2072402294,-2.9269738988	2046.0309	3034.9166	3041.1562
H,0,-1.9850673077,-0.3377846887,-2.4037530349	3051.9196	3052.4202	3097.301
O,0,-1.0207618304,-2.48828865,-0.3261231113	3106.5006	3111.6631	3120.7854
H,0,-0.9178346124,-1.3122366298,-0.57476192	3122.5853	3130.5854	3146.7442
H,0,-1.9169029451,-2.6874121911,-0.0448126718	3152.9819	3205.2812	3232.3248
O,0,-0.3912687573,-3.2469173439,-2.5333099334	3462.8283	3930.538	3955.3662
H,0,-0.8091026061,-2.9666192975,-1.2863979496			
H,0,-0.9337464677,-3.8106435739,-3.0857828956			
TS HAHP-Anti + HCOOH → Sabinaketone + H_2O_2 + HCOOH			
0,1			
C,0,0.4793854169,0.0456988853,-0.5493789849	-672.851	52.0102	60.2695
C,0,1.6301315003,-0.6054816249,0.1258206403	68.8625	88.0459	103.5357
C,0,2.3457504194,0.2160230393,1.1689288095	147.3103	159.6286	201.5891
C,0,2.8555002576,0.2204433007,-0.2310440304	233.7165	247.7521	254.4657
C,0,2.3842461821,1.3941767765,-1.0869541739	268.8911	281.4915	293.1489
C,0,0.859577094,1.4734448841,-0.9007636156	318.8251	360.5724	375.1689
C,0,4.1855665637,-0.406165844,-0.606458878	403.2261	427.44	454.7993
C,0,5.2948945957,0.6444904513,-0.5362196692	480.2119	502.7305	533.6144
C,0,4.56346292,-1.6179377017,0.2396536087	584.2518	603.5529	675.4679
O,0,-0.2637692375,-0.6129723367,-1.365505728	708.8095	744.4875	785.4424
O,0,-0.6450175552,0.2933980361,0.8660903767	815.487	821.2134	885.4019
O,0,-1.8888545936,0.6682318579,0.3252012423	922.9912	931.3338	945.0147
H,0,1.6516558057,-1.6833968845,0.1772122554	960.3186	976.8364	1005.244
H,0,2.8907781828,-0.3556387006,1.9049714969	1040.5729	1052.7608	1061.3126
H,0,1.8424007301,1.0894816526,1.5598413885	1066.5968	1074.8764	1102.6601
H,0,2.6250399465,1.1810663497,-2.1307390008	1129.0517	1141.9868	1169.6831
H,0,2.8781696693,2.3268774405,-0.8155679788	1197.2977	1227.0269	1243.0569

H,0,0.5881498333,2.1394696317,-0.0852575849	1258.3929	1298.4699	1320.9917
H,0,0.3298921822,1.7904292414,-1.7946715084	1333.5406	1345.2275	1360.4555
H,0,4.0905438802,-0.7363085452,-1.6465119798	1382.6724	1405.698	1408.0653
H,0,6.2582828253,0.2035466646,-0.792201627	1412.7078	1427.2418	1441.2159
H,0,5.114744664,1.4745028866,-1.2187628479	1447.1256	1475.3667	1487.3433
H,0,5.3660204144,1.0472676643,0.4765424521	1491.3459	1496.4665	1502.0727
H,0,5.4546129757,-2.0910855487,-0.1715254867	1513.9963	1519.2549	1521.1933
H,0,3.7741119238,-2.3687326195,0.267024808	1593.974	1627.2775	1638.9387
H,0,4.7952757272,-1.3243056726,1.264471645	1763.7413	2288.0715	3035.1312
H,0,-0.4050504519,-1.7407288055,-1.0179755904	3049.1858	3052.6414	3060.6086
H,0,-1.8736294896,0.2237400819,-0.5431573192	3102.7156	3106.6286	3109.6745
C,0,-0.9060577485,-2.9905016815,0.598221002	3118.9681	3123.1352	3127.5888
H,0,-1.1162112462,-4.0149625442,0.9302992057	3136.2803	3154.5837	3158.9795
O,0,-0.5882206273,-2.8740174458,-0.6213489592	3220.2231	3243.5493	3653.8705
O,0,-0.9938531793,-2.0838093059,1.4399904056			
H,0,-0.7968238011,-0.7123443432,1.1599087262			
TS HAHP-Syn + HCOOH → Sabinaketone + H_2O_2 + HCOOH			
0,1			
C,0,-1.1413282418,0.2978354852,-0.7796838211	-438.3917	37.9342	53.8791
C,0,0.0206060342,-0.5007019973,-0.3277771208	77.6273	82.473	112.1635
C,0,1.2714432431,0.3215154137,-0.0962531358	158.6225	171.4078	204.0548
C,0,1.083437642,-0.3976943906,-1.3907876201	213.4227	243.1145	246.2022
C,0,0.5317053388,0.4823257122,-2.5128670179	257.6499	270.3079	272.0328
C,0,-0.7237614436,1.158098016,-1.9442166314	305.8949	318.6003	344.1272
C,0,1.9792492253,-1.5512115559,-1.799206465	362.8971	390.1412	423.5297
C,0,3.3370540826,-1.0192430533,-2.2577801952	453.9117	461.4235	547.2979
C,0,2.1507510945,-2.6083097798,-0.7134591244	579.6368	610.9543	638.9063
O,0,-2.088065768,0.692850762,-0.0179962355	705.7199	779.1571	800.4286
O,0,-2.0835810761,-1.0767157297,-1.667763541	822.4199	881.6319	921.9016
O,0,-1.2592816549,-2.0035509914,-2.3545971182	933.314	935.5621	956.5482
H,0,-0.1455852819,-1.3793228035,0.2764631422	976.3235	997.2421	1008.6212
H,0,1.956515185,-0.0977772287,0.6256148494	1029.1953	1045.4455	1059.8156
H,0,1.1944301121,1.3999853461,-0.0651309723	1070.4547	1094.314	1122.2751
H,0,0.268966788,-0.1559112813,-3.3557374287	1148.7362	1150.1096	1184.1345
H,0,1.2655746656,1.2117267127,-2.8561007837	1198.9226	1230.2693	1241.3573
H,0,-0.5184706791,2.1511860681,-1.5405097561	1260.4415	1300.2716	1309.6332
H,0,-1.5403619024,1.2590612117,-2.6534661485	1335.3769	1341.7738	1351.5337
H,0,1.4865827903,-2.0316674383,-2.6497883852	1382.3379	1388.5132	1403.9853
H,0,3.970405363,-1.8291451477,-2.6200189657	1405.7986	1410.3483	1416.8937
H,0,3.2344133183,-0.2888154389,-3.0607261389	1428.8167	1440.5836	1471.8808
H,0,3.8522795158,-0.5344608343,-1.4257351105	1490.0376	1496.3987	1503.332
H,0,2.8181629862,-3.3957413956,-1.0635261634	1510.9688	1515.6029	1522.6784
H,0,1.1988467083,-3.0694770081,-0.4530837557	1593.9874	1607.372	1688.9972
H,0,2.5945236543,-2.1885405372,0.1918266149	1839.9754	2014.2857	3043.7418
H,0,-2.2369484454,0.0228783988,0.820659482	3049.0086	3055.4644	3075.3839
H,0,-1.8189299493,-2.2346620618,-3.1049239448	3078.9737	3096.8321	3113.4276
C,0,-2.7780736701,-2.0364236805,1.3912011398	3119.7572	3120.4895	3126.0949
H,0,-3.0868980671,-2.7612880165,2.1564109818	3135.3001	3140.1657	3142.373
O,0,-2.4625642923,-0.8955434901,1.7908699093	3201.5438	3233.6942	3844.6813
O,0,-2.7740282165,-2.450917297,0.2066962964			
H,0,-2.4259113489,-1.670149629,-0.794369376			
TS RO-Syn (from Vinoxy-Type-Radical) → C-C-Breakage			
0,2			
C,0,0.3062595162,0.7983469796,-0.7855138334	-177.7246	64.9617	94.7804
C,0,0.3459994149,-0.5620086887,-1.4686946586	119.2867	187.3531	221.4227
C,0,0.8284730615,-0.4411058698,-0.0754637691	248.5655	274.9481	296.6452
C,0,-0.1343820351,-0.9442159659,0.9948622429	339.8416	386.0197	405.1545
C,0,-1.5918008478,-0.5754054767,0.7086525208	423.48	443.1068	501.9556
C,0,-0.9894563466,1.222974707,-0.2766165782	532.9075	552.9651	617.3184
C,0,2.3077381163,-0.5100684644,0.2924108418	714.789	847.947	876.3374
C,0,3.2477276547,-0.4290945242,-0.9069070802	883.8697	926.4561	928.2451
C,0,2.6694941382,0.56895359,1.3140364375	930.983	968.1082	979.1504
O,0,-1.6066743687,2.2149283779,-0.2764766151	989.5605	1015.9307	1056.639
O,0,-2.2640772216,-1.2111565443,-0.1064102078	1103.437	1117.5004	1125.6093
H,0,0.9724148936,1.5775069964,-1.1339916447	1140.5938	1179.6961	1226.2782
H,0,1.0685568052,-0.6191950485,-2.2680308732	1233.3829	1269.5811	1313.3488
H,0,-0.597960872,-1.0572978477,-1.6429886379	1347.7545	1383.0756	1391.8578
H,0,0.1489420981,-0.5338477338,1.965467081	1404.7261	1414.8114	1427.3365
H,0,-0.0712805638,-2.0326937052,1.0496192628	1476.2016	1491.4699	1501.5875
H,0,-2.0974277001,0.0253308566,1.4823118474	1508.9895	1511.9456	1521.2098
H,0,2.4514799313,-1.4886105017,0.7618063249	1601.9697	2010.9745	3002.1482
H,0,4.2830238127,-0.4486036905,-0.5681034768	3040.9765	3049.1655	3055.1306
H,0,3.1043607925,-1.2625867675,-1.5927329183	3064.9943	3113.0827	3117.1115
H,0,3.1059705276,0.5015218946,-1.4618964942	3119.4671	3133.2584	3137.9508

H,0,3.6965633422,0.4429329695,1.6553476747 H,0,2.0232042648,0.5435805965,2.1900806362 H,0,2.5857686459,1.5598719811,0.8637492874	3150.8117	3163.2848	3257.0705
Radical from RO (from Vinoxy-Type-Radical) after C-C-Breakage 0,2			
C,0,0.040146206,-1.1322072749,0.4392520923	68.1979	74.3229	96.9613
C,0,-0.2713330364,-1.3288632378,-1.0329141586	103.1928	153.1209	204.2681
C,0,-0.4762038168,0.0082560595,-0.4205536367	233.0646	260.0568	269.8742
C,0,0.4531850611,1.154861985,-0.7911373334	291.6791	342.8248	367.2868
C,0,1.8991271071,0.8651949157,-1.1262716049	392.4396	434.9242	472.4957
C,0,1.4561677227,-1.1373750323,0.8309081922	474.0456	527.8197	566.6878
C,0,-1.890664867,0.5047224812,-0.0897084127	711.3775	775.5998	844.874
C,0,-2.9811616249,-0.556486057,-0.2076460905	878.3289	908.4101	934.8187
C,0,-1.9314636699,1.1432301741,1.300016349	954.0265	974.8332	997.8708
O,0,1.9739163034,-1.5651210651,1.7933883463	1030.4029	1050.2285	1068.5431
O,0,2.7926549883,1.6007281879,-0.8103602761	1080.7392	1122.6351	1137.9481
H,0,-0.6392965373,-1.570427161,1.1619645498	1151.558	1178.0769	1227.47
H,0,-1.128143962,-1.9483733249,-1.2452779276	1264.6021	1283.8772	1342.2252
H,0,0.570995045,-1.4849181159,-1.6892286245	1349.4487	1384.1581	1397.1033
H,0,0.4580342161,1.918590086,-0.0139332297	1411.4417	1433.2367	1447.0593
H,0,0.0399851612,1.6218832027,-1.6938261514	1460.2713	1491.48	1500.6902
H,0,2.1040364316,-0.0168016434,-1.7580260596	1503.3128	1513.0693	1521.3697
H,0,-2.1130246295,1.2824405574,-0.8269257729	1848.2426	1987.7401	3009.9578
H,0,-3.940219532,-0.1273120254,0.0804991298	3026.5379	3036.8988	3047.192
H,0,-3.0777342499,-0.9316048038,-1.2253966019	3060.493	3114.7437	3120.289
H,0,-2.7943808784,-1.4038930942,0.4559373592	3130.0751	3130.6684	3148.5752
H,0,-2.8977660313,1.6158794706,1.4740302663	3149.67	3157.394	3245.1132
H,0,-1.1612244812,1.9019756916,1.4299866042 H,0,-1.7875652458,0.3851591341,2.0720111015			
TS RO-Anti (from Vinoxy-Type-Radical) → C-C-Breakage 0,2			
C,0,0.4016013503,1.1237925076,0.416782228	-187.8631	66.2629	96.3753
C,0,0.8004442748,1.3296917591,-1.0368362668	101.6922	204.118	212.1041
C,0,0.9020811923,-0.0233952317,-0.4424026553	235.1914	288.7543	290.8824
C,0,-0.2074798504,-0.9930381925,-0.8182804709	339.2365	348.8866	414.4012
C,0,-1.6109873762,-0.3979479091,-0.7202737761	424.0378	458.1815	479.4284
C,0,-1.032383983,1.0423868577,0.6761598628	530.7858	554.1229	597.0723
C,0,2.24454866,-0.6652639968,-0.1050821956	717.4066	831.949	869.7743
C,0,3.4278438001,0.2949060925,-0.1777929371	890.6275	900.7611	933.1056
C,0,2.1943563551,-1.333702847,1.2696099671	959.8356	972.2685	983.4395
O,0,-1.7581056191,1.4874543427,1.4726270702	991.7263	1020.4277	1063.5246
O,0,-2.535451622,-1.0288039752,-0.2046780423	1073.7266	1119.7164	1126.0466
H,0,1.0155375421,1.5645222967,1.1919478298	1146.835	1179.141	1224.1136
H,0,1.6969943347,1.9161784489,-1.1657743912	1233.8356	1272.0421	1315.0127
H,0,0.0169421439,1.5363363779,-1.7512864942	1343.9438	1387.8418	1389.8894
H,0,-0.1948304005,-1.8635055591,-0.1630886248	1406.8536	1415.6839	1428.7346
H,0,-0.0464785593,-1.3410684143,-1.842845164	1472.284	1490.2184	1502.6063
H,0,-1.8475626026,0.3953596746,-1.4550251589	1511.4811	1514.235	1521.7868
H,0,2.3992121922,-1.443285305,-0.8594198514	1597.7399	2028.0922	2934.3949
H,0,4.3414588091,-0.2213922758,0.1150092442	3035.041	3043.3174	3046.0993
H,0,3.5742080967,0.6877756991,-1.1830895864	3047.918	3109.6723	3113.32
H,0,3.2997300374,1.1382330334,0.5055486909	3117.3103	3130.9246	3136.5216
H,0,3.1022952064,-1.9088947183,1.4485063222	3159.5439	3170.827	3251.8277
H,0,1.3451711724,-2.0078483173,1.3705667566 H,0,2.1178072055,-0.5789051182,2.0546458331			
P4 (Product P4 in Chart 1) 0,1			
C,0,0.2243092588,0.7862835942,-0.7668038949	64.7961	85.9768	99.5323
C,0,0.3265605081,-0.5772813087,-1.4352238802	209.9211	225.4308	267.5991
C,0,0.8241024346,-0.4154523144,-0.0468181819	277.6776	321.6813	351.8837
C,0,-0.1754737559,-0.9004941984,0.9978895877	355.9985	421.9091	428.8635
C,0,-1.4476080923,-0.1091666232,0.7625710321	472.6387	536.6202	572.4982
C,0,-1.0968957456,1.083641018,-0.1804382063	633.4254	658.1527	709.3171
C,0,2.2994652524,-0.4522390827,0.3222946641	756.0647	870.6356	899.0035
C,0,3.2287187577,-0.2907372978,-0.8770785357	911.5392	930.6537	951.6704
C,0,2.6160461626,0.6091312094,1.3770956878	970.6401	991.455	998.8295
O,0,-1.7829317977,2.0538542927,-0.3130149636	1043.6249	1075.3261	1103.6363
O,0,-2.5312621923,-0.3113726053,1.2179313832	1119.5941	1136.4868	1177.948
H,0,0.8248012847,1.5943738968,-1.1559865434	1183.8534	1218.2305	1232.9039
H,0,1.0341860978,-0.6252606539,-2.2482321854	1283.6632	1299.6178	1349.3409
H,0,-0.585038399,-1.1379045308,-1.6014497776	1385.5684	1407.6621	1411.3149
H,0,0.1644695813,-0.671470454,2.0106978798	1426.2508	1456.9037	1493.0378
H,0,-0.3660069936,-1.9725511302,0.9463703633	1501.4831	1511.245	1514.6916
H,0,2.4844109551,-1.4389551287,0.7595612458	1522.0068	1887.0519	1901.7833

H,0,4.265305475,-0.2646814393,-0.5431737465	3043.052	3048.6586	3053.0784
H,0,3.1265373673,-1.1117141755,-1.5850545106	3063.4252	3108.268	3114.3122
H,0,3.0334559447,0.645684348,-1.4049976749	3121.6393	3125.8816	3130.3218
H,0,3.6497932395,0.5226755552,1.7103782093	3137.7883	3204.5246	3234.1793
H,0,1.9769379722,0.5247074069,2.2555082718			
H,0,2.4791160945,1.6079667021,0.958337026			