Electronic Supplementary Information

Multicomponent Kinetic Analysis and Theoretical Studies on the Phenolic Intermediates in the Oxidation of Eugenol and Isoeugenol Catalyzed by Laccase

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INDEX

Table S1. **EUG** Hydrogen Atom Transfer Reaction Transition State…….....S3

Table S2. **EUG** Radical Coupling Reaction Transition State (at C_9 position)……..…….....S4

Table S3. **EUG** Radical Coupling Reaction Transition State (at C_8 position)…….……S5

Table S4. **ISO** Hydrogen Atom Transfer Reaction Transition State. ……..S6

Table S5. **ISO** Radical Coupling Reaction Transition State…….....S7

Figure S1. The EFA analysis results for **EUG** (a) and **ISO** (b)……S8

Figure S2. Plots of consuming rate versus concentration for **EUG** (a) and **ISO** (b)……...…….....S9

Figure S3. Mass spectra of possible intermediate and products in the oxidation of **EUG**…….S10

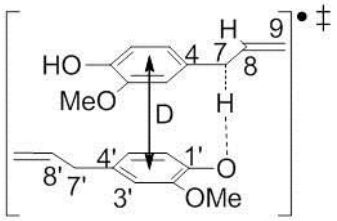
Figure S4. Mass spectra of possible intermediate and products in the oxidation of **ISO**……...S11

Figure S5. Comparison of the low-energy transition state structures for **EUG** and **ISO** HAT and RC reactions……..….....S12

Figure S6. The low-energy structures of substrates, phenoxyl radicals and *C*-center allylic radicals……S13

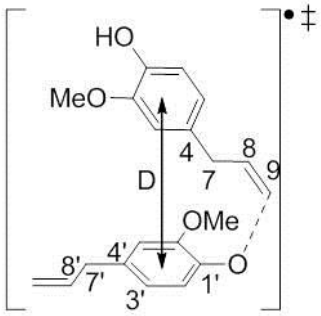
The detailed coordination, energy, frequency and spin density of the substrates, transition state and products structures……..……...S15

Table S1. **EUG** Hydrogen Atom Transfer Reaction Transition States



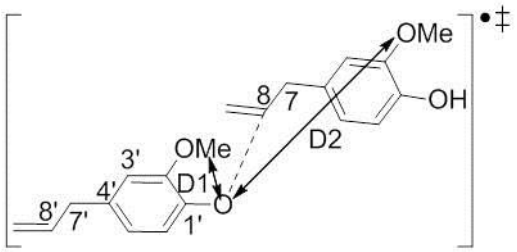
					B3lyp/6-31+G*		M06/6-31++G**	
Num.	C1'-O-C7-C4	C9-C8-C7-C4	C8'-C7'-C4'-C3'	D (Angstrom)	Enthalpy (Hartree)	ΔH(kcal/mol)	Enthalpy (Hartree)	ΔH (kcal/mol)
1	-14.46	-120.51	73.93	3.63	-1076.3746	13.77	-1075.6747	5.35
2	-15.55	126.66	140.18	3.59	-1076.3745	13.86	-1075.6734	6.18
3	-19.26	-119.45	-117.00	3.47	-1076.3744	13.88	-1075.6729	6.46
4	-121.72	-121.53	55.85	6.28	-1076.3739	14.24	-1075.6696	8.55
5	-119.30	121.24	-59.99	6.32	-1076.3739	14.21	-1075.6689	8.99
6	-122.92	-120.58	-113.53	6.29	-1076.3738	14.28	-1075.6687	9.12

Table S2. **EUG** Radical Coupling Reaction Transition States (at C_9 position).



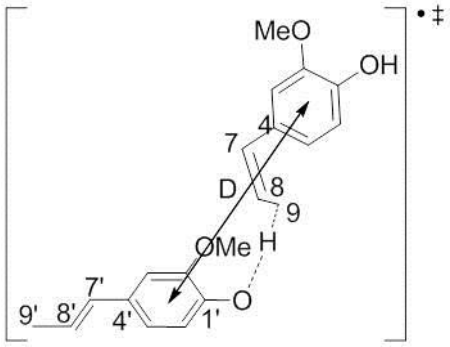
					B3lyp/6-31+G*		M06/6-31++G**	
Num.	C1'-O-C9-C8	C4-C7-C8-C9	C8'-C7'-C4'-C3'	D (Angstrom)	Enthalpy (Hatree)	ΔH (kcal/mol)	Enthalpy (Hatree)	Enthalpy (Hatree)
1	39.88	161.89	54.66	5.98	-1076.3675	18.26	-1075.6628	12.84
2	-46.34	-151.15	85.03	4.78	-1076.3649	19.86	-1075.6626	12.95
3	-57.37	-168.57	125.14	5.50	-1076.3655	19.47	-1075.6619	13.37
4	-54.08	151.08	51.09	6.29	-1076.3677	18.13	-1075.6603	14.41
5	-78.61	169.29	56.90	6.67	-1076.3660	19.19	-1075.6590	15.18
6	59.55	141.63	-119.88	7.24	-1076.3668	18.70	-1075.6580	15.80
7	68.39	138.85	51.50	7.46	-1076.3673	18.38	-1075.6574	16.18

Table S3. **EUG** Radical Coupling Reaction Transition States (at C_8 position).



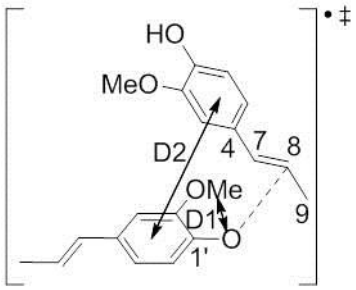
					B3lyp/6-31+G*		M06/6-31++G**	
Num.	C1'-O-C8-C7	C3'-C4'-C7'-C8'	D1 (Angstrom)	D2 (Angstrom)	Enthalpy (Hatree)	ΔH (kcal/mol)	Enthalpy (Hatree)	ΔH (kcal/mol)
1	144.75	-123.19	4.09	5.86	-1076.3647	19.99	-1075.6590	15.20
2	151.26	86.48	4.10	5.98	-1076.3646	20.03	-1075.6585	15.50
3	144.20	-88.76	4.09	5.86	-1076.3654	19.55	-1075.6581	15.78
4	173.37	-121.36	2.82	8.69	-1076.3644	20.17	-1075.6566	16.69
5	171.07	52.07	4.09	8.60	-1076.3645	20.12	-1075.6565	16.73
6	172.61	60.49	2.83	8.61	-1076.3628	21.16	-1075.6559	17.12
7	172.45	-126.63	2.84	9.29	-1076.3630	21.06	-1075.6558	17.17
8	173.15	-46.32	2.83	8.60	-1076.3628	21.19	-1075.6558	17.18
9	177.55	55.60	2.83	9.28	-1076.3629	21.10	-1075.6558	17.22
10	176.53	52.71	4.09	9.30	-1076.3629	21.09	-1075.6556	17.34

Table S4. **ISO** Hydrogen Atom Transfer Reaction Transition States



					B3lyp/6-31+G*		M06/6-31++G**	
Num.	C1'-O-C9-C8	C4-C7-C8-C9	C4'-C7'-C8'-C9'	D (Angstrom)	Enthalpy (Hatree)	ΔH (kcal/mol)	Enthalpy (Hatree)	ΔH (kcal/mol)
1	9.74	-2.23	179.69	5.08	-1076.3912	16.10	-1075.6897	8.04
2	-9.74	2.22	-179.69	5.29	-1076.3912	16.10	-1075.6897	8.05
3	-23.21	-169.85	-179.37	4.02	-1076.3926	18.17	-1075.6927	8.16
4	-22.73	5.39	-2.38	5.83	-1076.3832	17.71	-1075.6780	12.26
5	60.96	-168.59	2.75	6.43	-1076.3867	18.43	-1075.6804	12.72
6	117.68	-6.42	-2.63	7.45	-1076.3837	17.38	-1075.6750	14.12
7	-99.45	6.93	179.73	7.48	-1076.3885	17.82	-1075.6795	14.43
8	98.35	-6.83	179.89	7.39	-1076.3885	17.82	-1075.6788	14.86
9	-124.14	-176.11	2.67	7.97	-1076.3864	18.62	-1075.6761	15.44

Table S5. **ISO** Radical Coupling Reaction Transition States



					B3lyp/6-31+G*		M06/6-31++G**	
Num.	C1'-O-C8-C7	C4-C7-C8-C9	D1 (Angstrom)	D2 (Angstrom)	Enthalpy (Hatree)	ΔH (kcal/mol)	Enthalpy (Hatree)	ΔH (kcal/mol)
1	-59.02	-172.12	4.09	3.73	-1076.3985	14.46	-1075.6980	4.80
2	-55.17	-171.26	2.83	3.66	-1076.3970	15.41	-1075.6966	5.69
3	65.08	174.44	4.10	3.88	-1076.3990	14.17	-1075.6956	6.32
4	-63.25	-173.18	4.09	3.76	-1076.3973	15.24	-1075.6945	7.02
5	-68.38	25.35	4.09	6.22	-1076.3928	15.09	-1075.6840	11.64
6	68.38	-25.35	4.09	6.14	-1076.3928	15.09	-1075.6840	11.64

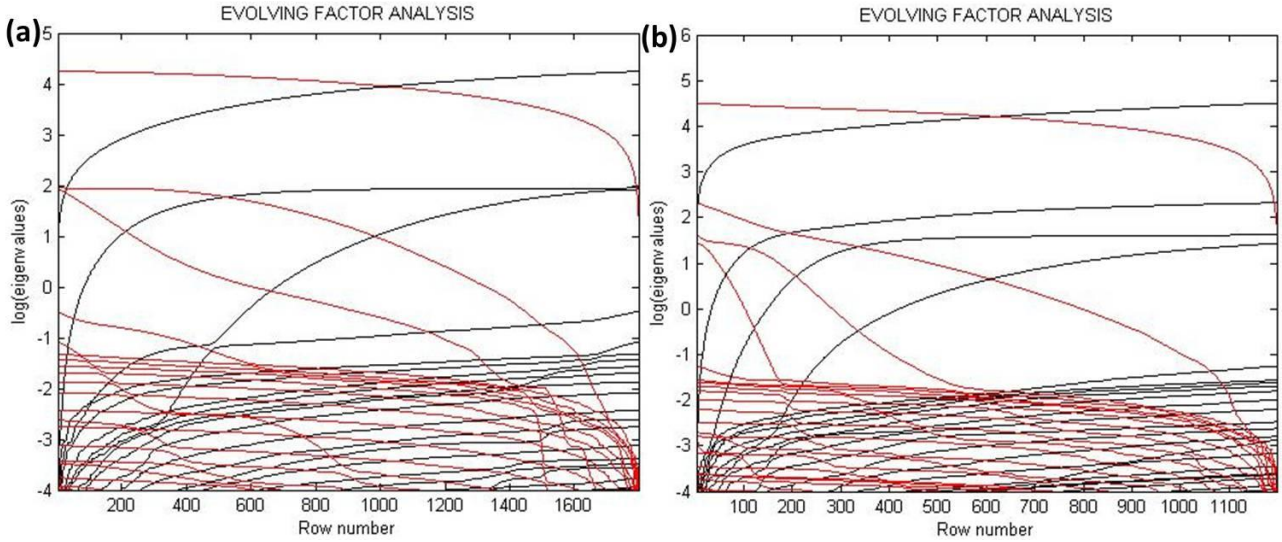


Figure S1. The EFA analysis results for **EUG** (a) and **ISO** (b).

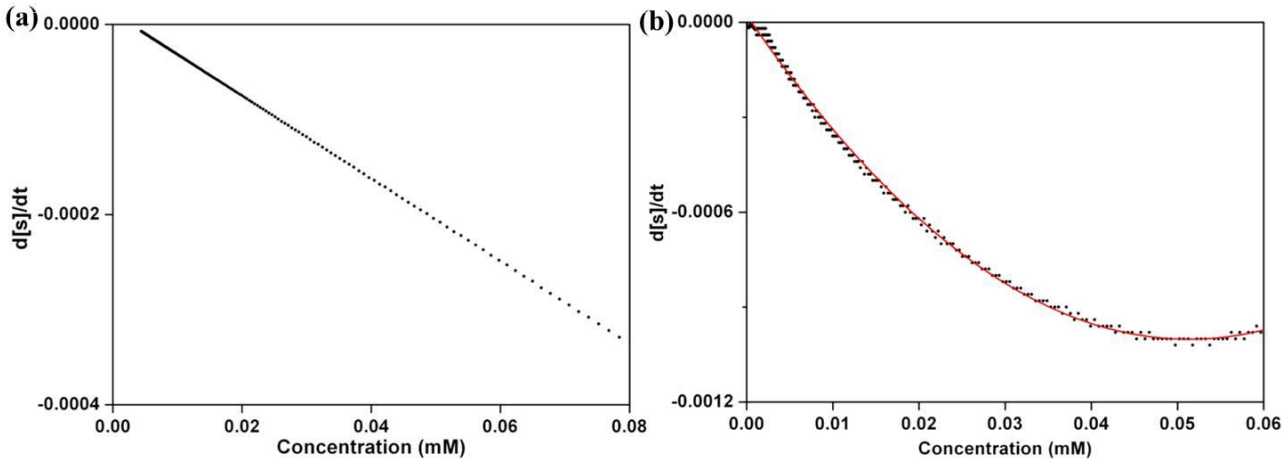


Figure S2. Plots of consuming rate versus concentration for **EUG** (a) and **ISO** (b) (the concentration profiles was obtained by the MCR-ALS resolution and the red line in (b) is the fitting result).

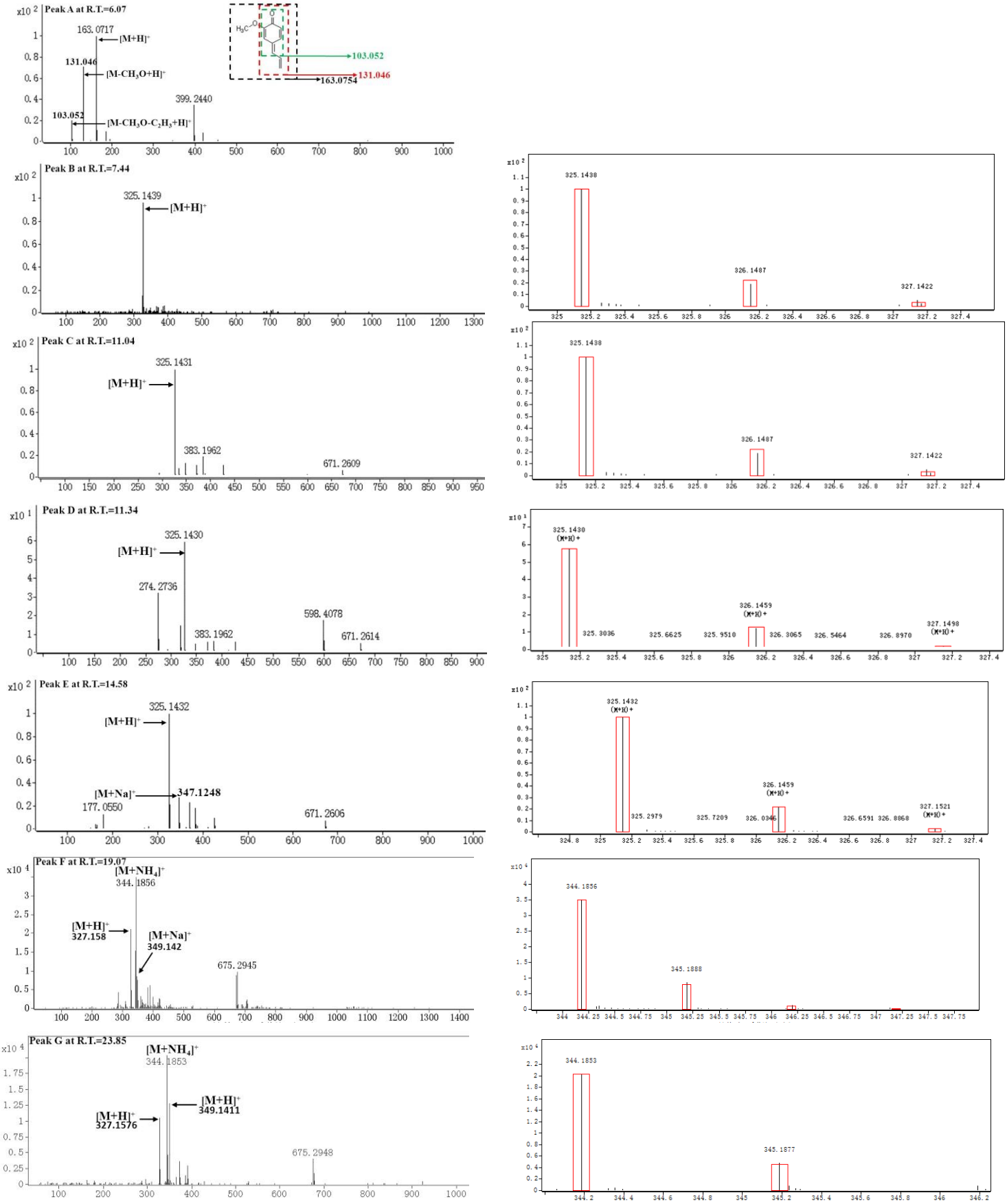


Figure S3. Mass spectra of possible intermediate and products in the oxidation of EUG (the right is the corresponding isotope figures).

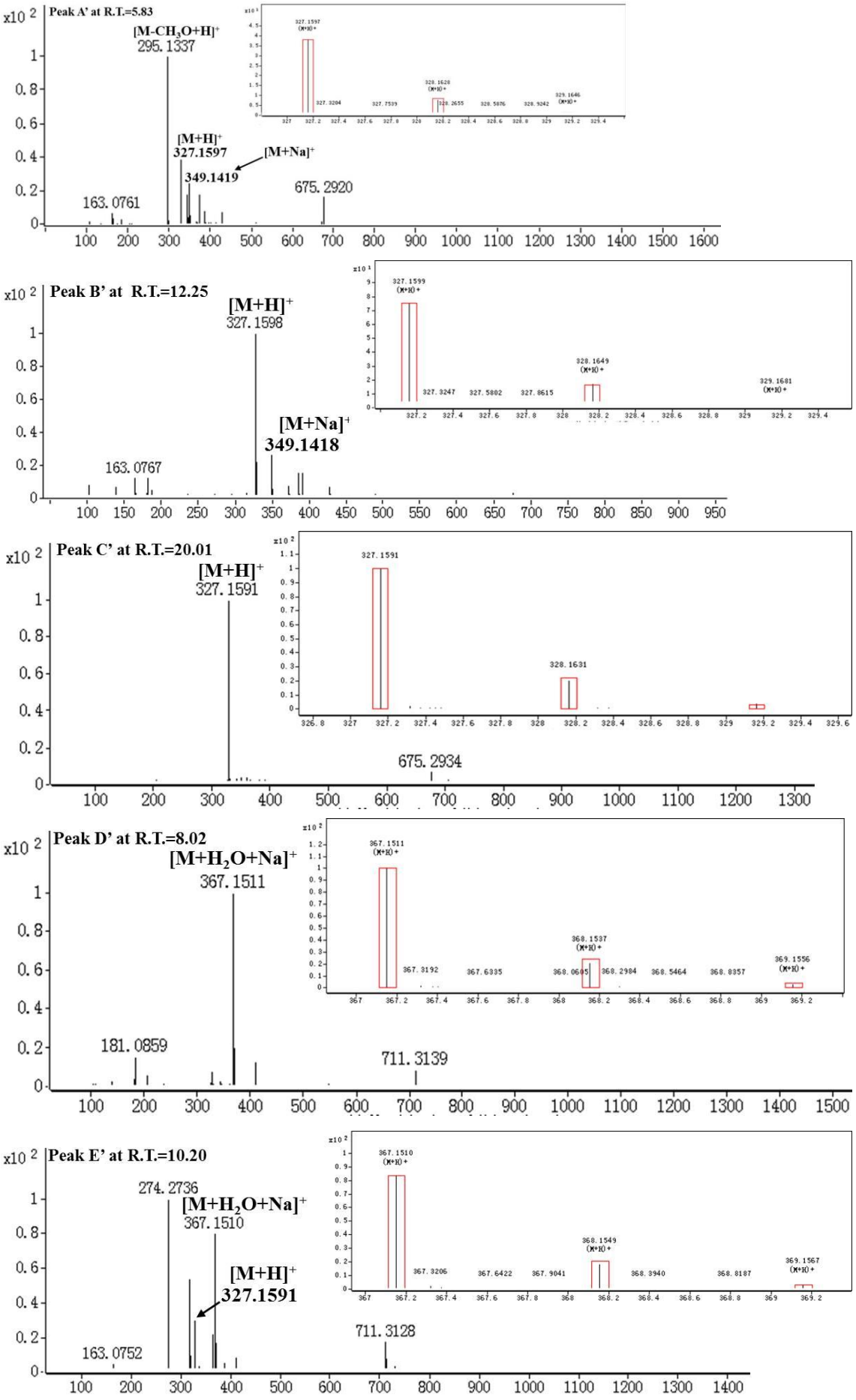


Figure S4. Mass spectra of possible intermediate and products in the oxidation of **ISO** and the insets are the corresponding isotope figures.

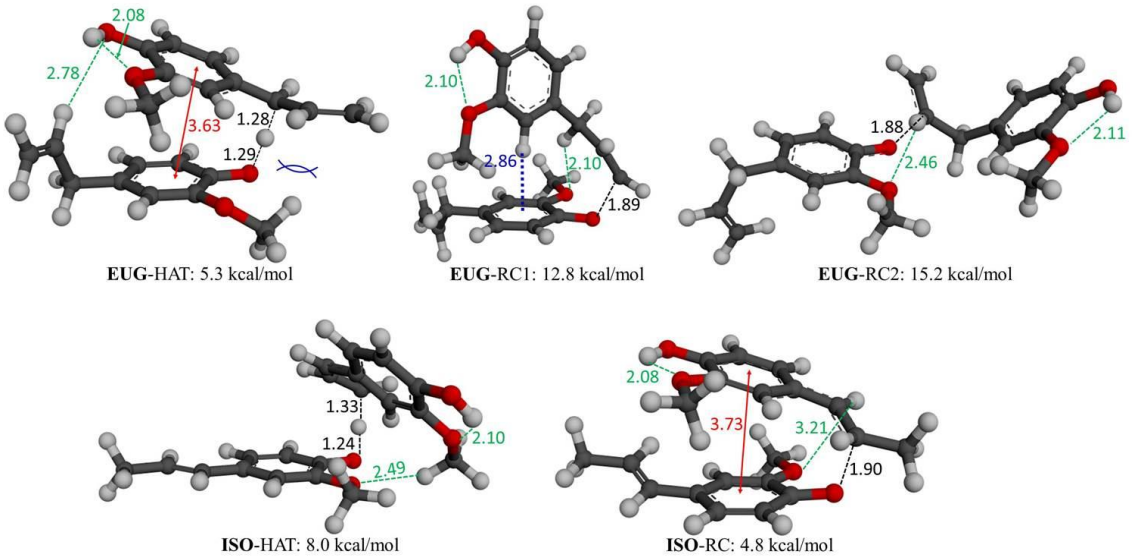


Figure S5. Comparison of the low-energy transition state structures for **EUG** and **ISO** HAT and RC reactions (the green line represents O···H distance and the red line represents the distance between the two benzene rings).

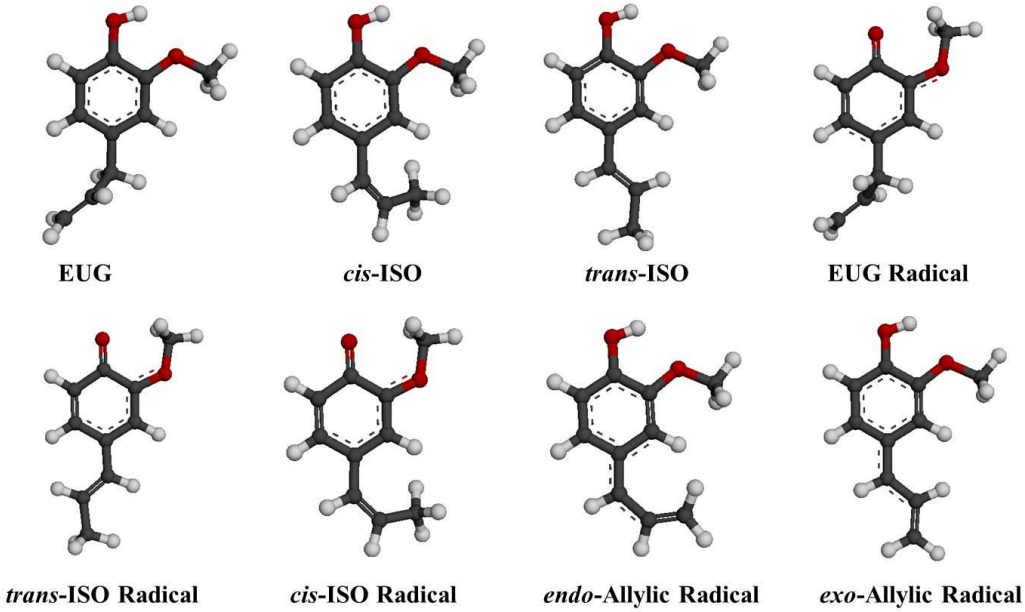


Figure S6. The low-energy structures of substrates, phenoxyl radicals and *C*-center allylic radicals optimized with CBS-QB3 method.

The detailed coordination, energy, frequency and spin density of the substrates, transition state and products structures.

EUG-Radical Coupling reaction transition state structures (coupling at C_9 position)

EUG-RC1-TS1

6	0	0.877290	-2.253519	-0.656182
6	0	0.719245	-2.860380	0.702381
6	0	-0.421632	-3.549622	1.088689
1	0	1.084926	-3.053782	-1.387386
1	0	-1.136218	-3.852162	0.326199
1	0	-0.391960	-4.164461	1.982138
1	0	1.517432	-2.696213	1.428727
1	0	-0.093629	-1.830780	-0.968769
6	0	1.955329	-1.209873	-0.748726
6	0	3.107686	-1.422283	-1.497068
6	0	1.808827	-0.000403	-0.051910
6	0	4.109724	-0.452639	-1.565566
1	0	3.230817	-2.359139	-2.038214
6	0	2.803862	0.964297	-0.118118
1	0	0.905555	0.169264	0.535573
6	0	3.963739	0.740362	-0.880475
1	0	5.013314	-0.609165	-2.149010
8	0	2.780902	2.178283	0.506786
8	0	4.932335	1.687226	-0.947330
1	0	4.652821	2.442867	-0.410947
6	0	1.651586	2.485639	1.293899
1	0	1.538020	1.770652	2.120882
1	0	1.814681	3.487212	1.696563
1	0	0.732533	2.473902	0.690589
8	0	-1.606465	-2.350276	1.959440
6	0	-1.731951	-1.137521	1.474100
6	0	-1.352797	-0.020810	2.237240
6	0	-2.290417	-0.895427	0.182993
6	0	-1.560225	1.275671	1.781361
1	0	-0.920263	-0.216662	3.216435
6	0	-2.454558	0.404487	-0.280321
6	0	-2.096668	1.502831	0.513968
1	0	-1.293063	2.124359	2.411532
1	0	-2.882779	0.595298	-1.262382
8	0	-2.615445	-2.005368	-0.522644
6	0	-2.279381	2.901209	-0.022938
6	0	-3.678398	3.175158	-0.483763
1	0	-1.586978	3.074739	-0.862370
1	0	-2.002679	3.618562	0.764363
6	0	-4.007991	3.541022	-1.721554
1	0	-4.460755	3.042188	0.267077
1	0	-5.039651	3.727760	-2.008586
1	0	-3.248875	3.673816	-2.492588
6	0	-3.110801	-1.831869	-1.831381
1	0	-3.290095	-2.832741	-2.228317
1	0	-4.053766	-1.268726	-1.832969
1	0	-2.379444	-1.312621	-2.468583

Zero correction= 0.383954 (Hartree/Particle)
Thermal correction to Energy= 0.407752
Thermal correction to Enthalpy= 0.408696
Thermal correction to Gibbs Free Energy= 0.329051
Sum of electronic and zero-point Energies= -1075.687496
Sum of electronic and thermal Energies= -1075.663698
Sum of electronic and thermal Enthalpies= -1075.662754
Sum of electronic and thermal Free Energies= -1075.742400

Freqs -- -639.9167 18.2612 33.2714

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -1076.107084

EUG-RC1-TS2

6	0	0.872448	1.819551	-1.446302
6	0	0.744429	2.811172	-0.332573
6	0	-0.278190	3.749730	-0.288130
1	0	-0.127489	1.620503	-1.865798
1	0	-0.210813	4.578482	0.409267
1	0	-0.830668	3.957433	-1.204971
1	0	1.412877	2.718837	0.524149
1	0	1.442851	2.284122	-2.272566
6	0	1.528430	0.515467	-1.071344
6	0	0.884822	-0.697948	-1.288429
6	0	2.811319	0.505062	-0.503307
6	0	1.491164	-1.907723	-0.945075
1	0	-0.115281	-0.705134	-1.719866
6	0	3.417647	-0.694768	-0.158380
1	0	3.332069	1.447167	-0.340503
6	0	2.754330	-1.914389	-0.378419
1	0	0.990535	-2.859276	-1.110480
8	0	4.658156	-0.831380	0.398447
8	0	3.345374	-3.088161	-0.043661
1	0	4.220585	-2.894108	0.321025
6	0	5.399634	0.340053	0.656429
1	0	4.876222	0.992634	1.368384
1	0	6.346836	0.017633	1.092188
1	0	5.597683	0.896485	-0.269793
8	0	-1.737405	3.023722	0.623196
6	0	-2.069476	1.802145	0.265442
6	0	-2.998767	1.565940	-0.763309
6	0	-1.489018	0.670639	0.910604
6	0	-3.371562	0.277967	-1.123785
1	0	-3.423167	2.437973	-1.258144
6	0	-1.877509	-0.614797	0.547196
6	0	-2.813401	-0.824138	-0.471095
1	0	-4.106137	0.118336	-1.912334
1	0	-1.437497	-1.483607	1.033626
8	0	-0.547677	0.946806	1.838020
6	0	-3.216469	-2.224098	-0.832553
6	0	-4.319221	-2.800776	0.012510
1	0	-2.339970	-2.890178	-0.769139
1	0	-3.531353	-2.257750	-1.887160
6	0	-4.964934	-2.171599	0.993180
1	0	-4.595216	-3.829167	-0.230186
1	0	-5.757868	-2.664261	1.549869
1	0	-4.727180	-1.145545	1.270943
6	0	0.171464	-0.134105	2.392535
1	0	0.911052	0.306192	3.064723
1	0	-0.485094	-0.800057	2.969543
1	0	0.685557	-0.711211	1.609643

Zero-point correction= 0.383932
(Hartree/Particle)
Thermal correction to Energy= 0.407588
Thermal correction to Enthalpy= 0.408532
Thermal correction to Gibbs Free Energy= 0.329331
Sum of electronic and zero-point Energies= -1075.687171
Sum of electronic and thermal Energies= -1075.663514
Sum of electronic and thermal Enthalpies= -1075.662570
Sum of electronic and thermal Free Energies= -1075.741771

Frequencies -- -682.5941 25.7220 28.8259

EUG-RC1-TS3

6	0	0.759453	1.116336	-1.853225
6	0	0.740846	2.476769	-1.235632
6	0	-0.350442	3.329750	-1.347292
1	0	-0.205715	0.619373	-1.627132
1	0	-0.245317	4.370843	-1.057212
1	0	-1.078809	3.142533	-2.136443
1	0	1.586981	2.769737	-0.611393
1	0	0.769743	1.208863	-2.952412
6	0	1.896598	0.239628	-1.408338
6	0	2.770270	-0.347665	-2.316543
6	0	2.074410	-0.006804	-0.039696
6	0	3.809565	-1.172077	-1.880393
1	0	2.644178	-0.163520	-3.382354
6	0	3.102884	-0.827236	0.396091
1	0	1.388203	0.442198	0.675278
6	0	3.981124	-1.416459	-0.528693
1	0	4.500105	-1.633612	-2.581613
8	0	3.360502	-1.143842	1.699183
8	0	4.988977	-2.218524	-0.103001
1	0	4.944372	-2.272628	0.862265
6	0	2.508737	-0.590773	2.681141
1	0	1.462603	-0.881654	2.514768
1	0	2.852573	-0.977292	3.642182
1	0	2.571342	0.506878	2.683490
8	0	-1.539316	2.970414	0.055777
6	0	-1.957567	1.718199	0.099619
6	0	-2.957230	1.255917	-0.785945
6	0	-1.408478	0.778274	1.010802
6	0	-3.365692	-0.063687	-0.803287
1	0	-3.386079	1.986576	-1.470125
6	0	-1.820981	-0.554616	0.973143
6	0	-2.784251	-0.995662	0.071062
1	0	-4.139164	-0.391654	-1.496647
1	0	-1.359908	-1.247483	1.676938
8	0	-0.434330	1.065955	1.912542
6	0	-3.204287	-2.443776	0.029691
6	0	-4.683712	-2.623772	0.185162
1	0	-2.677162	-2.988930	0.825869
1	0	-2.887388	-2.896633	-0.922182
6	0	-5.470447	-3.215893	-0.711839
1	0	-5.119543	-2.218193	1.101245
1	0	-6.540989	-3.321244	-0.555694
1	0	-5.064703	-3.621613	-1.638724
6	0	-0.315958	2.368507	2.471605
1	0	0.209537	2.234218	3.421947
1	0	0.252147	3.036096	1.816074
1	0	-1.300463	2.812295	2.653285

Zero correction= 0.384331 (Hartree/Particle)
Thermal correction to Energy= 0.407917
Thermal correction to Enthalpy= 0.408861
Thermal correction to Gibbs Free Energy= 0.330196
Sum of electronic and zero-point Energies= -1075.686429
Sum of electronic and thermal Energies= -1075.662844
Sum of electronic and thermal Enthalpies= -1075.661900
Sum of electronic and thermal Free Energies= -1075.740565

Freqs -- -673.2988 20.9658 27.7398

EUG-RC1-TS4

6	0	0.674706	-0.560954	-0.079951
6	0	0.749571	-1.902878	-0.720491
6	0	-0.041802	-2.968183	-0.311620
1	0	-0.118782	0.028174	-0.580860
1	0	0.118246	-3.948468	-0.749829
1	0	-0.447292	-2.965601	0.698869
1	0	1.312823	-1.980883	-1.652555
1	0	0.326857	-0.675101	0.960768
6	0	1.961492	0.221241	-0.126302
6	0	1.986875	1.554236	-0.522645
6	0	3.163494	-0.394137	0.253097
6	0	3.179894	2.277413	-0.537613
1	0	1.061192	2.039890	-0.827611
6	0	4.351866	0.321159	0.238113
1	0	3.147341	-1.439026	0.558231
6	0	4.363879	1.668697	-0.158399
1	0	3.208738	3.318687	-0.848072
8	0	5.581325	-0.165973	0.583176
8	0	5.525191	2.368854	-0.175677
1	0	6.238640	1.779267	0.107230
6	0	5.669511	-1.518152	0.972697
1	0	5.332938	-2.185695	0.167891
1	0	6.722266	-1.712163	1.185770
1	0	5.075562	-1.711577	1.876332
8	0	-1.686744	-2.769054	-1.178196
6	0	-2.282517	-1.608279	-1.016943
6	0	-2.405350	-0.710282	-2.090683
6	0	-2.827288	-1.213323	0.241197
6	0	-3.062729	0.505576	-1.952443
1	0	-1.966705	-1.015857	-3.038498
6	0	-3.465943	0.013481	0.375020
6	0	-3.595444	0.881758	-0.718744
1	0	-3.156572	1.175859	-2.805706
1	0	-3.875702	0.324822	1.334032
8	0	-2.649425	-2.096095	1.252915
6	0	-4.320089	2.194176	-0.547533
6	0	-3.825129	2.993529	0.618499
1	0	-5.399324	2.013945	-0.423098
1	0	-4.207692	2.778582	-1.472268
6	0	-4.582863	3.389066	1.640458
1	0	-2.761516	3.243952	0.608679
1	0	-4.176900	3.969858	2.464820
1	0	-5.645264	3.148372	1.681987
6	0	-3.190181	-1.771940	2.514173
1	0	-2.955243	-2.609610	3.173423
1	0	-2.744000	-0.852990	2.919969
1	0	-4.280619	-1.649440	2.460798

Zero-point correction= 0.383726
(Hartree/Particle)
Thermal correction to Energy= 0.407832
Thermal correction to Enthalpy= 0.408777
Thermal correction to Gibbs Free Energy= 0.326303
Sum of electronic and zero-point Energies= -1075.685302
Sum of electronic and thermal Energies= -1075.661196
Sum of electronic and thermal Enthalpies= -1075.660252
Sum of electronic and thermal Free Energies= -1075.742725

Frequencies -- -659.7060 14.7259 21.1919

EUG-RC1-TS5

6	0	1.686199	2.348325	0.072072
6	0	0.447282	2.530101	-0.740622
6	0	-0.537027	3.418538	-0.339226
1	0	2.275481	3.282441	0.052053
1	0	-0.270231	4.240222	0.322819
1	0	-1.397448	3.599354	-0.980318
1	0	0.238749	1.824799	-1.546398
1	0	1.368468	2.224047	1.120596
6	0	2.555805	1.187412	-0.324875
6	0	2.833265	0.897015	-1.658439
6	0	3.106760	0.367024	0.667898
6	0	3.633042	-0.191793	-2.005520
1	0	2.422822	1.527090	-2.445953
6	0	3.907885	-0.715552	0.327860
1	0	2.881092	0.578036	1.711460
6	0	4.172645	-1.002633	-1.020134
1	0	3.852036	-0.426149	-3.044307
8	0	4.482615	-1.587311	1.209087
8	0	4.946321	-2.063732	-1.359799
1	0	5.232399	-2.502860	-0.546102
6	0	4.221286	-1.400890	2.582940
1	0	3.144944	-1.469188	2.793743
1	0	4.744428	-2.200700	3.109841
1	0	4.598019	-0.429734	2.931318
8	0	-1.444640	2.530947	1.061569
6	0	-2.296251	1.625970	0.629348
6	0	-3.652764	1.937657	0.440351
6	0	-1.872930	0.296104	0.331237
6	0	-4.568191	0.979833	0.024991
1	0	-3.959905	2.958943	0.657561
6	0	-2.796004	-0.652062	-0.097902
6	0	-4.149168	-0.322535	-0.250987
1	0	-5.618560	1.242663	-0.092762
1	0	-2.482612	-1.671562	-0.314625
8	0	-0.550291	0.056697	0.482971
6	0	-5.123689	-1.377532	-0.713481
6	0	-5.134145	-2.585581	0.172782
1	0	-4.883089	-1.690925	-1.741122
1	0	-6.129909	-0.935143	-0.748162
6	0	-4.874288	-3.826396	-0.236578
1	0	-5.357983	-2.400155	1.225987
1	0	-4.891623	-4.671780	0.446568
1	0	-4.639176	-4.039514	-1.279607
6	0	-0.053726	-1.189743	0.041054
1	0	1.029222	-1.158858	0.188624
1	0	-0.481058	-2.020484	0.619076
1	0	-0.265194	-1.343278	-1.027151

Zero-point correction= 0.384410
(Hartree/Particle)
Thermal correction to Energy= 0.408172
Thermal correction to Enthalpy= 0.409116
Thermal correction to Gibbs Free Energy= 0.328183
Sum of electronic and zero-point Energies= -1075.683732
Sum of electronic and thermal Energies= -1075.659971
Sum of electronic and thermal Enthalpies= -1075.659026
Sum of electronic and thermal Free Energies= -1075.739960

Frequencies -- -648.7165 13.2464 20.9736

EUG-RC1-TS6

6	0	1.466985	-0.342224	1.449167
6	0	0.651383	-1.059135	0.429223
6	0	0.029792	-2.275581	0.672215
1	0	0.840573	0.426554	1.934341
1	0	-0.469445	-2.799532	-0.138640
1	0	0.406471	-2.904717	1.476099
1	0	0.400523	-0.503914	-0.478093
1	0	1.745645	-1.044849	2.249973
6	0	2.689136	0.326841	0.871670
6	0	2.919735	1.688572	1.030619
6	0	3.620523	-0.438193	0.153782
6	0	4.059332	2.291866	0.496118
1	0	2.201682	2.293402	1.581787
6	0	4.754788	0.157021	-0.377859
1	0	3.437707	-1.503519	0.021290
6	0	4.979153	1.533816	-0.207001
1	0	4.247748	3.355674	0.615996
8	0	5.731232	-0.479616	-1.091176
8	0	6.086330	2.117623	-0.729067
1	0	6.602157	1.435817	-1.182571
6	0	5.596121	-1.867346	-1.300384
1	0	4.680690	-2.097128	-1.862405
1	0	6.464982	-2.179354	-1.882557
1	0	5.582674	-2.412416	-0.346651
8	0	-1.510625	-1.868046	1.664141
6	0	-2.370830	-1.061731	1.079471
6	0	-2.579310	0.239847	1.568683
6	0	-3.134802	-1.475114	-0.048126
6	0	-3.523641	1.085832	1.009097
1	0	-1.981684	0.543966	2.425966
6	0	-4.072669	-0.613704	-0.611842
6	0	-4.282657	0.666161	-0.087224
1	0	-3.675968	2.085145	1.415246
1	0	-4.665036	-0.927912	-1.468233
8	0	-2.874427	-2.724140	-0.505000
6	0	-5.309052	1.588342	-0.697285
6	0	-4.706947	2.863801	-1.204161
1	0	-6.084023	1.830647	0.045554
1	0	-5.817300	1.065582	-1.520962
6	0	-5.056817	4.080447	-0.789846
1	0	-3.917521	2.753641	-1.951403
1	0	-4.587046	4.978219	-1.183386
1	0	-5.833301	4.218767	-0.037373
6	0	-3.642638	-3.211830	-1.581070
1	0	-3.305378	-4.234563	-1.760014
1	0	-4.713289	-3.223673	-1.334657
1	0	-3.487700	-2.616156	-2.491772

Zero-point correction= 0.383321
(Hartree/Particle)
Thermal correction to Energy= 0.406666
Thermal correction to Enthalpy= 0.407611
Thermal correction to Gibbs Free Energy= 0.327225
Sum of electronic and zero-point Energies= -1075.682329
Sum of electronic and thermal Energies= -1075.658983
Sum of electronic and thermal Enthalpies= -1075.658039
Sum of electronic and thermal Free Energies= -1075.738425

Frequencies -- -674.4349 -4.9262 13.6586

EUG-RC1-TS7

6	0	-1.767332	-0.111629	1.420588
6	0	-0.839269	0.617104	0.511731
6	0	-0.105547	1.723741	0.911597
1	0	-1.260471	-1.016228	1.798650
1	0	0.483871	2.278978	0.186172
1	0	-0.446415	2.297404	1.771013
1	0	-0.614725	0.144793	-0.447648
1	0	-1.963804	0.508623	2.309116
6	0	-3.060017	-0.521423	0.759337
6	0	-3.528172	-1.829381	0.819245
6	0	-3.821081	0.438743	0.076049
6	0	-4.736831	-2.188590	0.220778
1	0	-2.944386	-2.584813	1.342545
6	0	-5.023700	0.086449	-0.517959
1	0	-3.452517	1.461810	0.020950

6	0	-5.488453	-1.237732	-0.447281
1	0	-5.110602	-3.208440	0.262658
8	0	-5.852641	0.929988	-1.202831
8	0	-6.662862	-1.583524	-1.030848
1	0	-7.041339	-0.792344	-1.440115
6	0	-5.474571	2.284616	-1.303021
1	0	-4.525161	2.392574	-1.844868
1	0	-6.267190	2.788924	-1.858436
1	0	-5.378256	2.743318	-0.309367
8	0	1.324762	1.014335	1.901870
6	0	2.204753	0.329814	1.203344
6	0	2.296409	-1.065475	1.329824
6	0	3.113735	0.976254	0.313991
6	0	3.265033	-1.794863	0.653264
1	0	1.591137	-1.546864	2.004787
6	0	4.074695	0.237267	-0.365165
6	0	4.160768	-1.152571	-0.202981
1	0	3.327603	-2.874205	0.784311
1	0	4.784424	0.725184	-1.030352
8	0	2.959000	2.316474	0.198826
6	0	5.202490	-1.928521	-0.970975
6	0	6.582665	-1.365750	-0.822705
1	0	4.940851	-1.952550	-2.040438
1	0	5.188707	-2.972008	-0.624218
6	0	7.339142	-0.942451	-1.834415
1	0	6.961783	-1.296138	0.199585
1	0	8.336544	-0.539942	-1.676390
1	0	6.984334	-0.991759	-2.864065
6	0	3.880357	3.020746	-0.602272
1	0	3.606579	4.075000	-0.531028
1	0	4.907879	2.887466	-0.237180
1	0	3.828364	2.703127	-1.653229

Zero-point correction= 0.383457
(Hartree/Particle)
Thermal correction to Energy= 0.407763
Thermal correction to Enthalpy= 0.408708
Thermal correction to Gibbs Free Energy= 0.323527
Sum of electronic and zero-point Energies= -1075.682673
Sum of electronic and thermal Energies= -1075.658366
Sum of electronic and thermal Enthalpies= -1075.657422
Sum of electronic and thermal Free Energies= -1075.742603

Frequencies -- -669.2529 5.1458 11.0472

EUG-RC1-TS8

6	0	1.466985	-0.342223	1.449168
6	0	0.651383	-1.059134	0.429224
6	0	0.029793	-2.275580	0.672216
1	0	0.840573	0.426555	1.934341
1	0	-0.469444	-2.799531	-0.138638
1	0	0.406471	-2.904715	1.476100
1	0	0.400524	-0.503914	-0.478093
1	0	1.745645	-1.044848	2.249973
6	0	2.689137	0.326842	0.871670
6	0	2.919736	1.688573	1.030619
6	0	3.620523	-0.438192	0.153782
6	0	4.059332	2.291867	0.496117
1	0	2.201682	2.293404	1.581787
6	0	4.754788	0.157022	-0.377859
1	0	3.437707	-1.503518	0.021291
6	0	4.979154	1.533817	-0.207001
1	0	4.247748	3.355674	0.615995
8	0	5.731232	-0.479616	-1.091176
8	0	6.086330	2.117623	-0.729068
1	0	6.602157	1.435817	-1.182571
6	0	5.596121	-1.867345	-1.300383
1	0	4.680690	-2.097128	-1.862404
1	0	6.464982	-2.179353	-1.882557
1	0	5.582673	-2.412415	-0.346650
8	0	-1.510624	-1.868045	1.664141
6	0	-2.370830	-1.061731	1.079472
6	0	-2.579311	0.239848	1.568682
6	0	-3.134801	-1.475115	-0.048126
6	0	-3.523642	1.085832	1.009096
1	0	-1.981685	0.543967	2.425966
6	0	-4.072668	-0.613705	-0.611842
6	0	-4.282657	0.666160	-0.087225
1	0	-3.675969	2.085145	1.415244
1	0	-4.665035	-0.927914	-1.468233
8	0	-2.874426	-2.724141	-0.504999
6	0	-5.309053	1.588340	-0.697287
6	0	-4.706948	2.863800	-1.204162
1	0	-6.084024	1.830644	0.045552
1	0	-5.817300	1.065580	-1.520964
6	0	-5.056820	4.080445	-0.789846
1	0	-3.917522	2.753641	-1.951403
1	0	-4.587050	4.978218	-1.183386
1	0	-5.833304	4.218764	-0.037374
6	0	-3.642637	-3.211832	-1.581069
1	0	-3.305376	-4.234565	-1.760013
1	0	-4.713287	-3.223675	-1.334657
1	0	-3.487698	-2.616158	-2.491771

Zero-point correction= 0.383415
(Hartree/Particle)
Thermal correction to Energy= 0.407639
Thermal correction to Enthalpy= 0.408583
Thermal correction to Gibbs Free Energy= 0.325113
Sum of electronic and zero-point Energies= -1075.682235
Sum of electronic and thermal Energies= -1075.658011
Sum of electronic and thermal Enthalpies= -1075.657067
Sum of electronic and thermal Free Energies= -1075.740536

Frequencies -- -673.3248 12.9041 15.3168

EUG-Radical Coupling reaction transition state structure (coupling at C_8 position)

EUG-RC2-TS1

6	0	-0.461409	-2.733900	0.892010
6	0	-0.528766	-1.590706	0.106830
6	0	-1.481814	-1.490861	-1.048253
1	0	-0.858407	-3.679654	0.525868
1	0	-0.287852	-0.636621	0.580033
1	0	-1.049614	-0.811271	-1.792921
1	0	-1.579393	-2.477701	-1.520094
1	0	0.105377	-2.746748	1.819813
6	0	-2.825197	-0.989058	-0.587042
6	0	-3.015342	0.384571	-0.381605
6	0	-3.874560	-1.860569	-0.314212
6	0	-4.233264	0.862195	0.081572
1	0	-2.194559	1.067833	-0.596035
6	0	-5.100934	-1.384698	0.148388
1	0	-3.735670	-2.930003	-0.466378
6	0	-5.287009	-0.026889	0.348177
1	0	-5.929052	-2.056661	0.358460
8	0	-4.539370	2.174788	0.312865
8	0	-6.481371	0.437080	0.793711
1	0	-6.423056	1.399756	0.872115
6	0	-3.529728	3.133373	0.098090
1	0	-3.966608	4.104804	0.336458
1	0	-2.665948	2.952854	0.753212
1	0	-3.197521	3.133650	-0.949527
8	0	1.078944	-1.733451	-0.875891
6	0	2.111126	-1.142977	-0.319859
6	0	3.190786	-1.887732	0.187815
6	0	2.188532	0.279222	-0.235413
6	0	4.314271	-1.268006	0.714211
1	0	3.107843	-2.971281	0.135736
6	0	3.319076	0.889973	0.294643
6	0	4.391772	0.125456	0.771362
1	0	5.148883	-1.864330	1.081098
1	0	3.397039	1.974704	0.337460
6	0	5.626973	0.804918	1.285680
6	0	6.668065	1.086278	0.236258
1	0	6.086182	0.190598	2.075547
1	0	5.358685	1.754101	1.775270
6	0	6.580165	0.783603	-1.058062
1	0	7.568227	1.583268	0.604210
1	0	7.386714	1.022570	-1.746297
1	0	5.705491	0.284761	-1.473765
8	0	1.103646	0.948941	-0.700724
6	0	1.152522	2.356713	-0.703636
1	0	0.205260	2.697860	-1.127821
1	0	1.260939	2.760232	0.313325
1	0	1.978073	2.726892	-1.326964

Zero-point correction= 0.383414
(Hartree/Particle)
Thermal correction to Energy= 0.407367
Thermal correction to Enthalpy= 0.408311
Thermal correction to Gibbs Free Energy= 0.328300
Sum of electronic and zero-point Energies= -1075.683883
Sum of electronic and thermal Energies= -1075.659930
Sum of electronic and thermal Enthalpies= -1075.658986
Sum of electronic and thermal Free Energies= -1075.738998

Frequencies -- -612.3820 20.5590 27.5314

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -1076.106634

EUG-RC2-TS2

6	0	-0.064543	-2.619976	0.777938
6	0	-0.353351	-1.555925	-0.067181
6	0	-1.493931	-1.620136	-1.041109
1	0	-0.441735	-3.618067	0.559938
1	0	-0.113647	-0.549892	0.282238
1	0	-1.230185	-1.018801	-1.919902
1	0	-1.621076	-2.657694	-1.378600
1	0	0.656548	-2.515771	1.585140
6	0	-2.760167	-1.102584	-0.408621
6	0	-3.072288	0.260265	-0.498046
6	0	-3.602407	-1.938213	0.319418
6	0	-4.203636	0.764432	0.129380
1	0	-2.418345	0.913240	-1.073657
6	0	-4.740553	-1.437003	0.948715
1	0	-3.366814	-2.998599	0.398886
6	0	-5.045726	-0.088393	0.859869
1	0	-5.407440	-2.081464	1.515634
8	0	-4.613220	2.068940	0.107242
8	0	-6.155587	0.398735	1.469142
1	0	-6.209596	1.347510	1.286651
6	0	-3.831297	2.990380	-0.617265
1	0	-4.315084	3.962822	-0.509131
1	0	-2.810072	3.046549	-0.214786

1	0	-3.787007	2.722620	-1.681994
8	0	1.074339	-1.672815	-1.295139
6	0	2.179465	-1.078766	-0.905708
6	0	3.321902	-1.821484	-0.560569
6	0	2.269040	0.343719	-0.841320
6	0	4.511266	-1.200751	-0.207829
1	0	3.233797	-2.905297	-0.597864
6	0	3.464488	0.955654	-0.481838
6	0	4.595400	0.192560	-0.164520
1	0	5.385448	-1.796777	0.051617
1	0	3.539925	2.040215	-0.430725
6	0	5.859029	0.874144	0.272656
6	0	5.938173	1.163811	1.746999
1	0	5.983794	1.821259	-0.275233
1	0	6.728111	0.259968	-0.009151
6	0	5.016754	0.856919	2.658748
1	0	6.850258	1.672277	2.066767
1	0	5.160743	1.102878	3.707635
1	0	4.091807	0.347323	2.391168
8	0	1.132153	1.013147	-1.156219
6	0	1.173961	2.421023	-1.146255
1	0	0.181260	2.760898	-1.449619
1	0	1.399593	2.811806	-0.144028
1	0	1.916867	2.805033	-1.859042

Zero-point correction= 0.383441
(Hartree/Particle)
Thermal correction to Energy= 0.407401
Thermal correction to Enthalpy= 0.408346
Thermal correction to Gibbs Free Energy= 0.327758
Sum of electronic and zero-point Energies= -1075.683412
Sum of electronic and thermal Energies= -1075.659452
Sum of electronic and thermal Enthalpies= -1075.658508
Sum of electronic and thermal Free Energies= -1075.739095

Frequencies -- -614.7840 15.7420 23.8608

EUG-RC2-TS3

6	0	0.411802	-2.659661	-0.899074
6	0	0.550780	-1.540178	-0.089013
6	0	1.557201	-1.501771	1.024196
1	0	0.793177	-3.626256	-0.573147
1	0	0.321902	-0.566682	-0.527339
1	0	1.179629	-0.830195	1.804906
1	0	1.642642	-2.503535	1.465997
1	0	-0.193991	-2.631322	-1.801490
6	0	2.896055	-1.030503	0.519812
6	0	3.119975	0.340913	0.334439
6	0	3.908462	-1.926573	0.192004
6	0	4.334999	0.792417	-0.161125
1	0	2.328005	1.043129	0.591554
6	0	5.132174	-1.477117	-0.303154
1	0	3.742094	-2.994472	0.326419
6	0	5.352244	-0.121433	-0.481205
1	0	5.932149	-2.168454	-0.555237
8	0	4.672721	2.099874	-0.376683
8	0	6.544729	0.317115	-0.956570
1	0	6.512968	1.282646	-1.011781
6	0	3.700131	3.083520	-0.110310
1	0	4.157176	4.045837	-0.347857
1	0	2.808886	2.939860	-0.737048
1	0	3.405136	3.075175	0.948404
8	0	-1.009660	-1.661318	0.965335
6	0	-2.051914	-1.018874	0.491571
6	0	-3.189440	-1.710101	0.035230
6	0	-2.086839	0.405483	0.459034
6	0	-4.325901	-1.038547	-0.386303
1	0	-3.141875	-2.796954	0.048920
6	0	-3.230867	1.071114	0.029665
6	0	-4.358915	0.359622	-0.395325
1	0	-5.203192	-1.595897	-0.712340
1	0	-3.266040	2.158370	0.019019
6	0	-5.594549	1.090427	-0.859782
6	0	-6.818434	0.707305	-0.084203
1	0	-5.772406	0.890083	-1.927496
1	0	-5.424001	2.173351	-0.769427
6	0	-7.925854	0.200886	-0.623961
1	0	-6.761355	0.850320	0.997317
1	0	-8.788703	-0.066168	-0.019247
1	0	-8.006686	0.037421	-1.698620
8	0	-0.953192	1.024456	0.875784
6	0	-0.948976	2.431850	0.922878
1	0	0.035647	2.724837	1.294626
1	0	-1.105975	2.871154	-0.072769
1	0	-1.717480	2.812331	1.609867

Zero-point correction= 0.383704
(Hartree/Particle)
Thermal correction to Energy= 0.407686
Thermal correction to Enthalpy= 0.408630
Thermal correction to Gibbs Free Energy= 0.327986
Sum of electronic and zero-point Energies= -1075.682995
Sum of electronic and thermal Energies= -1075.659013
Sum of electronic and thermal Enthalpies= -1075.658068
Sum of electronic and thermal Free Energies= -1075.738713

Frequencies -- -614.9239 19.8311 23.2224

EUG-RC2-TS4

6	0	-0.138142	-1.616067	0.794512
6	0	-0.626897	-0.587311	-0.003277
6	0	-1.688279	-0.856520	-1.032546
1	0	-0.253554	-2.653373	0.484814
1	0	-0.643362	0.416382	0.429209
1	0	-1.555891	-0.151165	-1.861357
1	0	-1.535115	-1.864978	-1.440007
1	0	0.491159	-1.413078	1.657643
6	0	-3.070093	-0.722175	-0.445004
6	0	-3.750913	0.498687	-0.538736
6	0	-3.676972	-1.779549	0.227584
6	0	-5.010413	0.645893	0.027343
1	0	-3.281061	1.325718	-1.068052
6	0	-4.940863	-1.636494	0.796867
1	0	-3.156992	-2.733187	0.308262
6	0	-5.612440	-0.428374	0.700573
1	0	-5.426210	-2.457554	1.318365
8	0	-5.773677	1.779317	-0.006280
8	0	-6.845439	-0.291215	1.248929
1	0	-7.156621	0.608018	1.072290
6	0	-5.252519	2.906017	-0.674760
1	0	-5.068309	2.688248	-1.735718
1	0	-6.005825	3.691462	-0.592662
1	0	-4.319101	3.248792	-0.207556
8	0	0.774454	-0.217425	-1.197652
6	0	1.895209	0.210706	-0.660010
6	0	2.093854	1.568255	-0.358832
6	0	2.960938	-0.694408	-0.377360
6	0	3.299370	2.031027	0.151623
1	0	1.272237	2.250440	-0.570470
6	0	4.164168	-0.221723	0.136001
6	0	4.344899	1.141662	0.405121
1	0	3.435022	3.091982	0.356833
1	0	4.989259	-0.902984	0.335520
6	0	5.654878	1.621309	0.979932
6	0	6.844181	1.173320	0.187117
1	0	5.763403	1.265582	2.016392
1	0	5.634810	2.719739	1.028647
6	0	7.846322	0.444121	0.675846
1	0	6.854596	1.468539	-0.864691
1	0	8.690905	0.143476	0.061022
1	0	7.858259	0.128544	1.719268
8	0	2.703013	-1.993562	-0.640366
6	0	3.733622	-2.928198	-0.418598
1	0	3.335944	-3.899922	-0.717071
1	0	4.620020	-2.697152	-1.025415
1	0	4.024083	-2.964349	0.641002

Zero-point correction= 0.383324
(Hartree/Particle)
Thermal correction to Energy= 0.407502
Thermal correction to Enthalpy= 0.408447
Thermal correction to Gibbs Free Energy= 0.325963
Sum of electronic and zero-point Energies= -1075.681730
Sum of electronic and thermal Energies= -1075.657552
Sum of electronic and thermal Enthalpies= -1075.656608
Sum of electronic and thermal Free Energies= -1075.739092

Frequencies -- -641.1988 14.3473 19.3062

EUG-RC2-TS5

6	0	-0.383694	1.192189	-0.354490
6	0	-0.651902	-0.031770	0.250077
6	0	-1.676998	-0.140766	1.343184
1	0	-0.627724	2.122021	0.157391
1	0	-0.534345	-0.928712	-0.363010
1	0	-1.372434	-0.941232	2.026792
1	0	-1.673448	0.794264	1.921387
1	0	0.219044	1.256635	-1.257306
6	0	-3.051301	-0.433858	0.796232
6	0	-3.785095	0.568959	0.146421
6	0	-3.604448	-1.705822	0.903395
6	0	-5.041395	0.293410	-0.373131
1	0	-3.355299	1.564833	0.054194
6	0	-4.867091	-1.988279	0.380461
1	0	-3.046018	-2.491010	1.410433
6	0	-5.589390	-0.995184	-0.257518
1	0	-5.309484	-2.977582	0.465485
8	0	-5.851927	1.185020	-1.018433
8	0	-6.818894	-1.264664	-0.762695
1	0	-7.166477	-0.453832	-1.160611
6	0	-5.378350	2.502070	-1.187863
1	0	-6.161273	3.047556	-1.717702
1	0	-5.192870	2.984366	-0.218296
1	0	-4.456164	2.518323	-1.784618
8	0	0.860184	-0.344305	1.307475
6	0	1.995390	-0.510820	0.664932
6	0	2.358475	-1.755359	0.124345
6	0	2.910480	0.572440	0.512712
6	0	3.586112	-1.946749	-0.495080
1	0	1.648994	-2.573266	0.237429
6	0	4.139104	0.370159	-0.107598
6	0	4.488070	-0.888123	-0.616007
1	0	3.852817	-2.926800	-0.888008
1	0	4.852652	1.185783	-0.207693
6	0	5.818802	-1.074018	-1.302574

6	0	6.977616	-0.589859	-0.486218
1	0	5.819632	-0.547482	-2.269725
1	0	5.948456	-2.142122	-1.530268
6	0	7.843555	0.341714	-0.882671
1	0	7.086940	-1.042526	0.502166
1	0	7.754498	0.815146	-1.860678
1	0	8.672750	0.659222	-0.255530
8	0	2.490553	1.759089	1.002053
6	0	3.371534	2.855117	0.916762
1	0	2.858145	3.698439	1.382441
1	0	4.308029	2.658572	1.456758
1	0	3.605713	3.103864	-0.128197

Zero-point correction= 0.383470
(Hartree/Particle)
Thermal correction to Energy= 0.407571
Thermal correction to Enthalpy= 0.408515
Thermal correction to Gibbs Free Energy= 0.326477
Sum of electronic and zero-point Energies= -1075.681591
Sum of electronic and thermal Energies= -1075.657490
Sum of electronic and thermal Enthalpies= -1075.656546
Sum of electronic and thermal Free Energies= -1075.738584

Frequencies -- -653.7819 15.7682 21.6123

EUG-RC2-TS6

6	0	-0.157218	-1.346723	1.183341
6	0	-0.484814	-0.687323	0.002520
6	0	-1.609938	-1.189738	-0.858747
1	0	-0.493931	-2.368013	1.358592
1	0	-0.314680	0.391721	-0.027804
1	0	-1.462991	-0.821706	-1.881396
1	0	-1.556972	-2.286466	-0.900059
1	0	0.522716	-0.911672	1.911032
6	0	-2.946145	-0.750619	-0.317651
6	0	-3.422485	0.536894	-0.601443
6	0	-3.704336	-1.582130	0.500971
6	0	-4.629280	0.971000	-0.070843
1	0	-2.835128	1.188208	-1.246620
6	0	-4.918773	-1.151264	1.033401
1	0	-3.344901	-2.584909	0.727917
6	0	-5.385643	0.122144	0.753734
1	0	-5.521418	-1.794958	1.669062
8	0	-5.196412	2.196767	-0.275932
8	0	-6.567451	0.541291	1.269226
1	0	-6.728007	1.445774	0.964422
6	0	-4.490435	3.123882	-1.070177
1	0	-5.093185	4.033192	-1.096988
1	0	-3.508246	3.350619	-0.633336
1	0	-4.354715	2.746880	-2.093060
8	0	0.918775	-1.072516	-1.193545
6	0	2.100570	-0.614413	-0.825428
6	0	2.499559	0.699430	-1.152674
6	0	2.998443	-1.404474	-0.061796
6	0	3.719417	1.209209	-0.749531
1	0	1.803445	1.296781	-1.739487
6	0	4.217661	-0.871227	0.353609
6	0	4.596157	0.426135	0.017724
1	0	4.005253	2.226074	-1.015852
1	0	4.872737	-1.506558	0.948259
6	0	5.931446	0.978998	0.450632
6	0	5.813582	2.282071	1.180811
1	0	6.580854	1.120548	-0.426854
1	0	6.430243	0.237759	1.091628
6	0	6.393463	3.417974	0.796119
1	0	5.191518	2.271271	2.078897
1	0	7.012005	3.460157	-0.100445
1	0	6.278055	4.340952	1.358620
8	0	2.699686	-2.658111	0.363236
6	0	2.108820	-3.570142	-0.555266
1	0	2.341050	-4.569653	-0.178384
1	0	1.025602	-3.433171	-0.625901
1	0	2.541802	-3.445929	-1.555659

Zero-point correction= 0.383304
(Hartree/Particle)
Thermal correction to Energy= 0.407391
Thermal correction to Enthalpy= 0.408335
Thermal correction to Gibbs Free Energy= 0.326473
Sum of electronic and zero-point Energies= -1075.680956
Sum of electronic and thermal Energies= -1075.656870
Sum of electronic and thermal Enthalpies= -1075.655926
Sum of electronic and thermal Free Energies= -1075.737788

Frequencies -- -654.3478 17.6393 18.7308

EUG-RC2-TS7

6	0	0.259536	0.872412	0.938351
6	0	0.433023	0.250446	-0.295211
6	0	1.555026	0.657342	-1.208697
1	0	0.710011	1.844399	1.137898
1	0	0.135745	-0.798576	-0.368963
1	0	1.261884	0.438464	-2.242184
1	0	1.696029	1.745235	-1.134431
1	0	-0.421292	0.473252	1.685805
6	0	2.827333	-0.072735	-0.861332
6	0	3.716538	0.461201	0.080363
6	0	3.114326	-1.310382	-1.430166
6	0	4.862409	-0.235543	0.437020
1	0	3.499762	1.429129	0.528922
6	0	4.263477	-2.015358	-1.073160
1	0	2.431532	-1.732020	-2.166830
6	0	5.140018	-1.485231	-0.141171
1	0	4.498476	-2.980480	-1.514552
8	0	5.803745	0.184541	1.333816
8	0	6.260315	-2.167133	0.201916
1	0	6.743389	-1.645579	0.858516
6	0	5.603022	1.429311	1.964624
1	0	6.446302	1.574327	2.641935
1	0	5.582363	2.247058	1.231370
1	0	4.668843	1.434696	2.542516
8	0	-0.987244	0.879641	-1.348097
6	0	-2.188114	0.546496	-0.911149
6	0	-2.751100	-0.708603	-1.228464
6	0	-2.938594	1.413167	-0.076234
6	0	-3.986871	-1.093544	-0.744827
1	0	-2.165240	-1.365109	-1.869979
6	0	-4.178803	1.006809	0.415209
6	0	-4.718031	-0.235396	0.092310
1	0	-4.398645	-2.068898	-1.001579
1	0	-4.719789	1.698090	1.059982
6	0	-6.066162	-0.656912	0.621072
6	0	-6.000404	-1.919076	1.426564
1	0	-6.768635	-0.803142	-0.213369
1	0	-6.475676	0.155878	1.238145
6	0	-6.676004	-3.031577	1.143091
1	0	-5.333292	-1.898340	2.291465
1	0	-6.594872	-3.924843	1.757048
1	0	-7.341969	-3.083348	0.281668
8	0	-2.480803	2.618500	0.344629
6	0	-1.814913	3.468116	-0.582253
1	0	-1.943533	4.485351	-0.202513
1	0	-0.750602	3.226862	-0.664291
1	0	-2.267472	3.387345	-1.577958

Zero-point correction= 0.383271
(Hartree/Particle)
Thermal correction to Energy= 0.407429
Thermal correction to Enthalpy= 0.408373
Thermal correction to Gibbs Free Energy= 0.326016
Sum of electronic and zero-point Energies= -1075.680949
Sum of electronic and thermal Energies= -1075.656791
Sum of electronic and thermal Enthalpies= -1075.655847
Sum of electronic and thermal Free Energies= -1075.738205

Frequencies -- -661.3675 13.2195 20.4260

EUG-RC2-TS8

6	0	-0.156187	-1.302987	1.068120
6	0	-0.565719	-0.514088	-0.002375
6	0	-1.625933	-1.004244	-0.948027
1	0	-0.368057	-2.371676	1.081554
1	0	-0.522346	0.569367	0.133304
1	0	-1.498952	-0.496510	-1.912052
1	0	-1.470337	-2.077318	-1.126164
1	0	0.475434	-0.907280	1.859188
6	0	-3.005806	-0.762276	-0.393276
6	0	-3.580950	0.512183	-0.493702
6	0	-3.712638	-1.769923	0.254822
6	0	-4.835090	0.759603	0.047225
1	0	-3.033595	1.301015	-1.007198
6	0	-4.974387	-1.526895	0.796866
1	0	-3.273978	-2.763300	0.338585
6	0	-5.539652	-0.266619	0.698018
1	0	-5.536950	-2.308866	1.300280
8	0	-5.500257	1.952278	0.009174
8	0	-6.767363	-0.029950	1.222123
1	0	-6.996385	0.894904	1.052132
6	0	-4.859205	3.044769	-0.610204
1	0	-5.539365	3.893849	-0.524529
1	0	-3.912491	3.284594	-0.107071
1	0	-4.665371	2.841264	-1.672194
8	0	0.870741	-0.548940	-1.221331
6	0	1.997237	-0.031253	-0.768988
6	0	2.251523	1.350612	-0.874466
6	0	2.980934	-0.837540	-0.134426
6	0	3.417352	1.912770	-0.381523
1	0	1.493035	1.959540	-1.363736
6	0	4.139691	-0.256749	0.370423
6	0	4.373674	1.114620	0.259335
1	0	3.592503	2.983117	-0.482163
1	0	4.869845	-0.906242	0.852116
6	0	5.639405	1.712264	0.822581
6	0	6.879828	1.067188	0.283672
1	0	5.640035	1.623797	1.919753
1	0	5.652408	2.788129	0.594819
6	0	7.805121	0.468314	1.031539
1	0	6.996694	1.092176	-0.802190
1	0	8.688271	0.010119	0.593670
1	0	7.709287	0.418421	2.116167
8	0	2.815193	-2.168080	0.073458
6	0	2.320577	-2.972463	-0.990868
1	0	2.671506	-3.987987	-0.789193
1	0	1.227803	-2.951821	-1.043519
1	0	2.721838	-2.630955	-1.953084

```
 Zero-point correction=                           0.383139
(Hartree/Particle)
 Thermal correction to Energy=                    0.407272
 Thermal correction to Enthalpy=                  0.408216
 Thermal correction to Gibbs Free Energy=         0.326643
 Sum of electronic and zero-point Energies=       -1075.680908
 Sum of electronic and thermal Energies=          -1075.656776
 Sum of electronic and thermal Enthalpies=        -1075.655832
 Sum of electronic and thermal Free Energies=     -1075.737405

 Frequencies --  -644.2830             15.3409             26.3972
```

EUG-RC2-TS9

```
  6         0       0.171739    0.969522    0.429457
  6         0       0.495698   -0.153016   -0.328787
  6         0       1.590444   -0.091809   -1.356181
  1         0       0.455990    1.966467    0.093757
  1         0       0.360427   -1.129019    0.143824
  1         0       1.361361   -0.808755   -2.153123
  1         0       1.593655    0.909448   -1.811553
  1         0      -0.479316    0.902015    1.297226
  6         0       2.934641   -0.408342   -0.751273
  6         0       3.655806    0.580555   -0.067988
  6         0       3.464780   -1.692219   -0.831067
  6         0       4.880328    0.280463    0.511555
  1         0       3.242693    1.585267    0.001976
  6         0       4.693721   -1.999590   -0.246590
  1         0       2.914517   -2.466700   -1.363329
  6         0       5.405478   -1.019785    0.423926
  1         0       5.119288   -2.997890   -0.308590
  8         0       5.678327    1.157014    1.190817
  8         0       6.603080   -1.314409    0.986962
  1         0       6.949814   -0.510860    1.400198
  6         0       5.225285    2.484540    1.334780
  1         0       5.999164    3.018446    1.888912
  1         0       5.084547    2.963373    0.356050
  1         0       4.282726    2.522749    1.897684
  8         0      -0.937247   -0.368698   -1.517509
  6         0      -2.123345   -0.515765   -0.955285
  6         0      -2.577607   -1.784020   -0.542086
  6         0      -2.967398    0.599863   -0.709459
  6         0      -3.804147   -1.945861    0.079217
  1         0      -1.921393   -2.632611   -0.728305
  6         0      -4.189257    0.425538   -0.067055
  6         0      -4.625731   -0.838563    0.330453
  1         0      -4.134596   -2.937980    0.384261
  1         0      -4.801782    1.306817    0.118943
  6         0      -5.975940   -1.008384    0.982514
  6         0      -6.248651   -0.004359    2.059349
  1         0      -6.038067   -2.024890    1.398348
  1         0      -6.768188   -0.938133    0.220980
  6         0      -7.273982    0.845819    2.056057
  1         0      -5.532489    0.018497    2.884105
  1         0      -7.430824    1.559426    2.860847
  1         0      -7.997735    0.854294    1.241099
  8         0      -2.604513    1.873471   -1.007904
  6         0      -2.009860    2.138858   -2.272406
  1         0      -2.239299    3.183222   -2.501613
  1         0      -0.926485    1.985731   -2.252739
  1         0      -2.437518    1.491177   -3.047284

 Zero-point correction=                           0.383360
(Hartree/Particle)
 Thermal correction to Energy=                    0.407403
 Thermal correction to Enthalpy=                  0.408347
 Thermal correction to Gibbs Free Energy=         0.326816
 Sum of electronic and zero-point Energies=       -1075.680757
 Sum of electronic and thermal Energies=          -1075.656714
 Sum of electronic and thermal Enthalpies=        -1075.655770
 Sum of electronic and thermal Free Energies=     -1075.737301

 Frequencies --  -663.5300             18.3897             20.8545
```

EUG-RC2-TS10

```
  6         0      -0.268464    1.017290   -0.605224
  6         0      -0.544891   -0.056235    0.238560
  6         0      -1.594758    0.062763    1.306942
  1         0      -0.554288    2.030755   -0.324816
  1         0      -0.417714   -1.059831   -0.174680
  1         0      -1.314021   -0.584682    2.145804
  1         0      -1.601392    1.096416    1.683134
  1         0       0.348987    0.900293   -1.492144
  6         0      -2.955115   -0.328088    0.788000
  6         0      -3.719508    0.583598    0.046475
  6         0      -3.456929   -1.608314    1.000511
  6         0      -4.956560    0.211812   -0.458945
  1         0      -3.330613    1.585325   -0.126938
  6         0      -4.698725   -1.987894    0.490600
  1         0      -2.872619   -2.322159    1.579262
  6         0      -5.452419   -1.084452   -0.238834
  1         0      -5.101790   -2.983651    0.656456
  8         0      -5.796292    1.010844   -1.182249
  8         0      -6.662828   -1.447574   -0.729350
  1         0      -7.040229   -0.688785   -1.196931
  6         0      -5.383926    2.333468   -1.444512
  1         0      -6.194125    2.807794   -2.000962
  1         0      -5.212628    2.886674   -0.510951
  1         0      -4.468167    2.350663   -2.051048
  8         0       0.945544   -0.181439    1.369957
  6         0       2.099678   -0.375623    0.758027
  6         0       2.533840   -1.674158    0.427813
  6         0       2.925209    0.715905    0.375481
  6         0       3.723531   -1.889627   -0.248027
  1         0       1.893101   -2.503370    0.723203
  6         0       4.110677    0.485470   -0.314163
  6         0       4.523066   -0.808197   -0.638096
  1         0       4.038258   -2.904152   -0.488866
  1         0       4.716803    1.346879   -0.593313
  6         0       5.818167   -1.020379   -1.381840
  6         0       7.005506   -0.502058   -0.628281
  1         0       5.774463   -0.525250   -2.363670
  1         0       5.942371   -2.095806   -1.575370
  6         0       7.842803    0.428131   -1.084236
  1         0       7.157711   -0.924145    0.367879
  1         0       7.710061    0.873947   -2.070163
  1         0       8.688426    0.775994   -0.496486
  8         0       2.572539    2.010095    0.584051
  6         0       2.048214    2.382143    1.853354
  1         0       2.240276    3.453502    1.956097
  1         0       0.975214    2.179370    1.926759
  1         0       2.559907    1.840080    2.658263

 Zero-point correction=                           0.383503
(Hartree/Particle)
 Thermal correction to Energy=                    0.407551
 Thermal correction to Enthalpy=                  0.408496
 Thermal correction to Gibbs Free Energy=         0.326918
 Sum of electronic and zero-point Energies=       -1075.680571
 Sum of electronic and thermal Energies=          -1075.656523
 Sum of electronic and thermal Enthalpies=        -1075.655578
 Sum of electronic and thermal Free Energies=     -1075.737156

 Frequencies --  -658.0563             15.3095             25.3887
```

EUG Hydrogen Atom Transfer reaction transition state structures.

EUG-HAT-TS1

```
  6         0       2.930544    1.007813   -0.323282
  6         0       3.655022    0.676751    0.905547
  6         0       4.991717    0.647277    1.009893
  6         0       1.565247    1.538901   -0.288428
  6         0       1.088447    2.295220   -1.372717
  6         0      -0.221847    2.750605   -1.414712
  1         0       3.560820    1.492834   -1.078730
  1         0       3.062163    0.386508    1.776389
  1         0       5.485051    0.361297    1.934705
  1         0       5.630540    0.915048    0.169187
  1         0       1.768024    2.530540   -2.189917
  6         0      -1.093175    2.444289   -0.377859
  6         0      -0.642085    1.667244    0.706340
  6         0       0.666640    1.223408    0.751752
  1         0       0.999617    0.606752    1.582088
  8         0      -2.370907    2.888744   -0.407268
  1         0      -2.797581    2.625696    0.422539
  1         0      -0.590562    3.350093   -2.242895
  8         0      -1.600407    1.425760    1.643001
  6         0      -1.258869    0.615901    2.750884
  1         0      -2.174139    0.488871    3.331563
  1         0      -0.894878   -0.369093    2.426572
  1         0      -0.494332    1.103837    3.370549
  1         0       2.730922   -0.144695   -0.857926
  8         0       2.346400   -1.288983   -1.321559
  6         0       1.051383   -1.413073   -1.199793
  6         0       0.447675   -1.897674    0.004607
  6         0      -0.936260   -1.985701    0.102748
  1         0      -1.363351   -2.361713    1.033229
  6         0      -1.767989   -1.616310   -0.954915
  6         0      -1.187639   -1.134166   -2.137991
  1         0      -1.829043   -0.837875   -2.966918
  6         0       0.184635   -1.039359   -2.254427
  6         0      -3.264030   -1.717521   -0.806416
  6         0      -3.803288   -0.632657    0.075745
  1         0      -3.539519   -2.696625   -0.388582
  1         0      -3.727489   -1.649233   -1.801137
  6         0      -4.478069   -0.839231    1.205360
  1         0      -3.590464    0.387121   -0.255382
  1         0      -4.839224   -0.013726    1.814761
  1         0      -4.698207   -1.846979    1.557980
  1         0       0.654765   -0.660741   -3.159951
  8         0       1.154178   -2.207596    1.119354
  6         0       2.415405   -2.863513    1.006556
  1         0       2.418313   -3.563926    0.164648
  1         0       3.230815   -2.146349    0.870574
  1         0       2.548571   -3.411019    1.943532

 Zero-point correction=                           0.379879
(Hartree/Particle)
 Thermal correction to Energy=                    0.403644
 Thermal correction to Enthalpy=                  0.404588
 Thermal correction to Gibbs Free Energy=         0.326030
 Sum of electronic and zero-point Energies=       -1075.699402
 Sum of electronic and thermal Energies=          -1075.675637
 Sum of electronic and thermal Enthalpies=        -1075.674693
 Sum of electronic and thermal Free Energies=     -1075.753251
```

```
 Frequencies --  -2106.1363              17.4492              37.8832

Total free energy in solution:
 - with all non electrostatic terms          (a.u.) =   -1076.104643
```

EUG-HAT-TS2

```
  6          0       2.787114    1.060097   -0.834106
  6          0       3.762548    0.871584    0.241210
  6          0       5.092505    0.881603    0.067239
  6          0       1.429138    1.537938   -0.561958
  6          0       0.700097    2.181467   -1.576817
  6          0      -0.614088    2.581261   -1.380634
  1          0       3.222624    1.494234   -1.742420
  1          0       3.374818    0.658180    1.240316
  1          0       5.776117    0.701708    0.892286
  1          0       5.534418    1.074248   -0.909623
  1          0       1.184368    2.372731   -2.532871
  6          0      -1.240797    2.329446   -0.166574
  6          0      -0.536116    1.665417    0.854210
  6          0       0.778223    1.281017    0.662508
  1          0       1.306318    0.755594    1.453438
  8          0      -2.519762    2.723626    0.034132
  1          0      -2.761568    2.508948    0.947824
  1          0      -1.174467    3.095298   -2.157062
  8          0      -1.267622    1.460627    1.987732
  6          0      -0.620432    0.847458    3.085343
  1          0      -1.370554    0.753999    3.872500
  1          0      -0.242715   -0.149067    2.817698
  1          0       0.211771    1.467766    3.444677
  1          0       2.554861   -0.150390   -1.220750
  8          0       2.171223   -1.347937   -1.498975
  6          0       0.944228   -1.521427   -1.080457
  6          0      -0.156952   -1.285172   -1.939492
  6          0      -1.459204   -1.357693   -1.492729
  1          0      -2.284479   -1.135988   -2.167550
  6          0      -1.734165   -1.687527   -0.153264
  6          0      -0.668902   -1.968389    0.699258
  1          0      -0.850194   -2.241276    1.739117
  6          0       0.652544   -1.892028    0.268606
  6          0      -3.153246   -1.744526    0.351390
  6          0      -4.014074   -0.643752   -0.187769
  1          0      -3.132112   -1.692519    1.451113
  1          0      -3.607980   -2.715341    0.098465
  6          0      -5.180438   -0.829236   -0.803507
  1          0      -3.624913    0.371730   -0.068148
  1          0      -5.770376    0.005810   -1.172529
  1          0      -5.587505   -1.828591   -0.957595
  1          0       0.078392   -1.003319   -2.964068
  8          0       1.601311   -2.078111    1.217806
  6          0       2.849100   -2.678483    0.877651
  1          0       3.212913   -3.144545    1.797344
  1          0       2.718335   -3.439963    0.101590
  1          0       3.570038   -1.934908    0.522031

 Zero-point correction=                                0.380751
(Hartree/Particle)
 Thermal correction to Energy=                    0.404151
 Thermal correction to Enthalpy=                  0.405095
 Thermal correction to Gibbs Free Energy=         0.328908
 Sum of electronic and zero-point Energies=          -1075.697706
 Sum of electronic and thermal Energies=             -1075.674306
 Sum of electronic and thermal Enthalpies=           -1075.673362
 Sum of electronic and thermal Free Energies=        -1075.749549

 Frequencies --  -2101.2339              35.8061              52.2855
```

EUG-HAT-TS3

```
6          0       2.984812    0.724238   -0.758860
 6          0       3.866781    0.307292    0.331442
 6          0       5.182728    0.082973    0.198545
 6          0       1.723787    1.423986   -0.506472
 6          0       1.148317    2.195129   -1.532261
 6          0      -0.104179    2.772396   -1.387509
 1          0       3.525803    1.112433   -1.630441
 1          0       3.409667    0.119232    1.305671
 1          0       5.788873   -0.259198    1.032775
 1          0       5.690642    0.241417   -0.752039
 1          0       1.700871    2.331196   -2.460315
 6          0      -0.823510    2.578499   -0.215397
 6          0      -0.262462    1.818205    0.827992
 6          0       0.990551    1.250044    0.686681
 1          0       1.398069    0.636754    1.486260
 8          0      -2.053131    3.123972   -0.076676
 1          0      -2.379791    2.909857    0.809943
 1          0      -0.550180    3.372550   -2.176280
 8          0      -1.067710    1.715282    1.924695
 6          0      -0.575979    1.008589    3.045423
 1          0      -1.368325    1.031428    3.795691
 1          0      -0.346551   -0.034312    2.786373
 1          0       0.323727    1.491205    3.450710
 1          0       2.535420   -0.401639   -1.220586
 8          0       1.915460   -1.481279   -1.544388
 6          0       0.692693   -1.436188   -1.082355
 6          0      -0.352560   -0.865256   -1.851605
 1          0      -0.086661   -0.518387   -2.848303
 6          0      -1.623708   -0.702686   -1.348539
 1          0      -2.399783   -0.229867   -1.950008
 6          0      -1.930323   -1.126279   -0.041460
 6          0      -0.938154   -1.740101    0.715156
 1          0      -1.148219   -2.096637    1.723700
 6          0       0.361492   -1.892602    0.231510
 8          0       1.258719   -2.393139    1.111214
 6          0      -3.313431   -0.910038    0.514800
 6          0      -4.363904   -1.657933   -0.249751
 1          0      -3.552087    0.165064    0.491318
 1          0      -3.327343   -1.216857    1.571386
 6          0      -5.386543   -1.085198   -0.882362
 1          0      -4.242400   -2.742826   -0.289596
 1          0      -6.119483   -1.668793   -1.433375
 1          0      -5.524303   -0.003970   -0.869642
 6          0       2.404512   -3.113382    0.663584
 1          0       3.225773   -2.439171    0.397623
 1          0       2.696882   -3.746510    1.505436
 1          0       2.163814   -3.734675   -0.204996

 Zero-point correction=                                0.380864
(Hartree/Particle)
 Thermal correction to Energy=                    0.404374
 Thermal correction to Enthalpy=                  0.405319
 Thermal correction to Gibbs Free Energy=         0.328531
 Sum of electronic and zero-point Energies=          -1075.697368
 Sum of electronic and thermal Energies=             -1075.673857
 Sum of electronic and thermal Enthalpies=           -1075.672913
 Sum of electronic and thermal Free Energies=        -1075.749700

 Frequencies --  -2068.5534              35.1633              53.4055
```

EUG-HAT-TS4

```
 6          0       1.151703   -1.993464    0.595589
  6          0       0.159487   -1.583189    1.583173
  6          0      -0.831731   -2.379296    2.024429
  6          0       2.374747   -1.203483    0.384881
  6          0       3.560895   -1.832428   -0.013609
  6          0       4.717921   -1.100475   -0.257243
  1          0       1.325172   -3.076647    0.578926
  1          0       0.181973   -0.545715    1.923645
  1          0      -1.585709   -2.019277    2.719318
  1          0      -0.913698   -3.414237    1.692598
  1          0       3.576278   -2.915051   -0.124177
  6          0       4.707750    0.279235   -0.115442
  6          0       3.518794    0.927353    0.270208
  6          0       2.368432    0.198652    0.510412
  1          0       1.436037    0.706645    0.746291
  8          0       5.830314    0.994957   -0.354547
  1          0       5.631267    1.930364   -0.202179
  1          0       5.644737   -1.583480   -0.555499
  8          0       3.630766    2.285529    0.357700
  6          0       2.524146    3.006480    0.859649
  1          0       2.821856    4.056128    0.878882
  1          0       1.641511    2.890920    0.216127
  1          0       2.270122    2.677577    1.876306
  1          0       0.484362   -1.852992   -0.482331
  8          0      -0.367567   -1.707806   -1.472410
  6          0      -1.490911   -1.222134   -1.020592
  6          0      -1.606550    0.137905   -0.592969
  6          0      -2.796431    0.608087   -0.059114
  1          0      -2.839029    1.647458    0.265657
  6          0      -3.920255   -0.217783    0.054608
  6          0      -3.830499   -1.542313   -0.394681
  1          0      -4.702704   -2.190894   -0.322777
  6          0      -2.644415   -2.035367   -0.907276
  6          0      -5.198154    0.320980    0.646430
  6          0      -5.699344    1.544286   -0.059714
  1          0      -5.046499    0.560614    1.710223
  1          0      -5.963601   -0.467661    0.608964
  6          0      -5.902216    2.723781    0.524899
  1          0      -5.888570    1.432233   -1.129815
  1          0      -5.713953    2.867101    1.588976
  1          0      -6.264806    3.584537   -0.031100
  1          0      -2.550188   -3.068225   -1.236266
  8          0      -0.538765    0.987664   -0.622359
  6          0       0.076717    1.177961   -1.895485
  1          0       0.834029    1.956061   -1.760901
  1          0       0.549385    0.258982   -2.254884
  1          0      -0.668760    1.524393   -2.623516

 Zero-point correction=                                0.378865
(Hartree/Particle)
 Thermal correction to Energy=                    0.402303
 Thermal correction to Enthalpy=                  0.403247
 Thermal correction to Gibbs Free Energy=         0.324705
 Sum of electronic and zero-point Energies=          -1075.693972
 Sum of electronic and thermal Energies=             -1075.670534
 Sum of electronic and thermal Enthalpies=           -1075.669589
 Sum of electronic and thermal Free Energies=        -1075.748131

 Frequencies --  -1994.7963             -19.8858              21.0022
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EUG-HAT-TS5

```
6          0       0.992306   -1.884252    0.863477
 6          0      -0.063753   -1.304373    1.687770
 6          0      -1.137465   -1.990346    2.120710
```

6	0	2.248757	-1.152961	0.637063
6	0	2.256668	0.248198	0.498935
6	0	3.439547	0.919647	0.251147
1	0	1.138597	-2.957750	1.037179
1	0	-0.010936	-0.235349	1.904888
1	0	-1.931202	-1.509451	2.686450
1	0	-1.250724	-3.053563	1.908877
1	0	1.314033	0.789443	0.536425
6	0	4.649878	0.211216	0.125582
6	0	4.648229	-1.170686	0.244247
6	0	3.457289	-1.845264	0.491247
1	0	5.592071	-1.699937	0.142696
1	0	3.462583	-2.929667	0.583888
8	0	5.805419	0.870814	-0.118044
1	0	5.608650	1.817867	-0.165498
8	0	3.570179	2.269420	0.092659
6	0	2.425982	3.072599	0.297600
1	0	2.025808	2.936103	1.311129
1	0	2.747894	4.107218	0.168357
1	0	1.637457	2.843073	-0.431800
1	0	0.412429	-1.924214	-0.275048
8	0	-0.364258	-1.956653	-1.332130
6	0	-1.490645	-1.348383	-1.079924
6	0	-2.687376	-2.081595	-0.886424
1	0	-2.618288	-3.163727	-0.977468
6	0	-3.880964	-1.452515	-0.583320
1	0	-4.787027	-2.040928	-0.444400
6	0	-3.937064	-0.059932	-0.436786
6	0	-2.768608	0.685352	-0.628555
1	0	-2.781643	1.769716	-0.520811
6	0	-1.570139	0.075096	-0.964404
8	0	-0.467455	0.867379	-1.094042
6	0	-5.224032	0.639299	-0.079668
6	0	-5.122000	1.403279	1.205927
1	0	-6.024790	-0.110538	-0.003988
1	0	-5.515145	1.331318	-0.884403
6	0	-5.330677	2.713379	1.325667
1	0	-4.838042	0.819086	2.084777
1	0	-5.239011	3.223629	2.281071
1	0	-5.606384	3.322454	0.464727
6	0	0.270227	0.740578	-2.308920
1	0	-0.388886	0.922233	-3.168141
1	0	1.043936	1.513839	-2.280586
1	0	0.731880	-0.247441	-2.397866

Zero-point correction= 0.378689
(Hartree/Particle)
Thermal correction to Energy= 0.403090
Thermal correction to Enthalpy= 0.404034
Thermal correction to Gibbs Free Energy= 0.322556
Sum of electronic and zero-point Energies= -1075.694236
Sum of electronic and thermal Energies= -1075.669835
Sum of electronic and thermal Enthalpies= -1075.668891
Sum of electronic and thermal Free Energies= -1075.750370

Frequencies -- -2049.6692 15.0409 24.3173

EUG-HAT-TS6

6	0	-0.834821	1.890790	0.453579
6	0	0.180648	1.331801	1.337712
6	0	1.343265	1.947041	1.624343
6	0	-2.183812	1.308681	0.388850
6	0	-2.389093	-0.073738	0.557605
6	0	-3.659389	-0.609735	0.453211
1	0	-0.829629	2.987303	0.420860
1	0	0.022995	0.319549	1.716963
1	0	1.562582	2.944003	1.242375
1	0	2.109322	1.467441	2.228389
1	0	-1.531527	-0.722039	0.723353
6	0	-4.761893	0.215559	0.162019
6	0	-4.565144	1.576232	-0.023305
6	0	-3.287548	2.114678	0.084746
1	0	-3.140508	3.183396	-0.060026
8	0	-6.002797	-0.312785	0.056464
1	0	-5.942080	-1.264947	0.222326
1	0	-5.427411	2.198078	-0.249001
8	0	-3.976384	-1.930186	0.598167
6	0	-2.957921	-2.804849	1.037984
1	0	-3.419203	-3.787915	1.146929
1	0	-2.137098	-2.866865	0.310463
1	0	-2.553337	-2.478565	2.005566
1	0	-0.314998	1.625132	-0.683710
8	0	0.397243	1.302885	-1.736933
6	0	1.475234	0.672423	-1.358024
6	0	2.739143	1.317505	-1.369770
6	0	3.877296	0.687663	-0.911269
1	0	4.833967	1.209403	-0.915868
6	0	3.814793	-0.621969	-0.406258
6	0	2.586467	-1.283466	-0.401511
1	0	2.506066	-2.302654	-0.025018
6	0	1.432803	-0.672185	-0.879213
6	0	5.055456	-1.279535	0.140338
6	0	5.552951	-0.585588	1.373503
1	0	5.852106	-1.277410	-0.618306
1	0	4.834017	-2.332084	0.368348
6	0	6.759177	-0.034471	1.497892
1	0	4.843205	-0.526094	2.202649
1	0	7.068890	0.467653	2.410827
1	0	7.483765	-0.070714	0.684417
1	0	2.762419	2.339853	-1.741786
8	0	0.262213	-1.367489	-0.791956
6	0	-0.486244	-1.494024	-2.000876
1	0	-1.330598	-2.151395	-1.773692
1	0	-0.853192	-0.524233	-2.350073
1	0	0.134316	-1.960133	-2.777527

Zero-point correction= 0.378960
(Hartree/Particle)
Thermal correction to Energy= 0.403302
Thermal correction to Enthalpy= 0.404246
Thermal correction to Gibbs Free Energy= 0.323022
Sum of electronic and zero-point Energies= -1075.693959
Sum of electronic and thermal Energies= -1075.669618
Sum of electronic and thermal Enthalpies= -1075.668674
Sum of electronic and thermal Free Energies= -1075.749898

Frequencies -- -2063.5305 19.6472 24.9028

ISO Hydrogen Atom Transfer reaction transition state structures

ISO-HAT-TS1

6	0	-0.684166	2.998663	-1.469383
1	0	-0.390336	4.014081	-1.744005
1	0	-1.767359	2.878222	-1.382783
6	0	0.035389	1.957185	-2.133093
1	0	0.972699	2.246468	-2.612016
6	0	-0.268381	0.616224	-2.222676
6	0	-1.367151	-0.119923	-1.640579
6	0	-1.679810	-1.394217	-2.150363
6	0	-2.106672	0.350167	-0.534470
6	0	-2.707961	-2.155973	-1.612518
1	0	-1.106422	-1.781706	-2.990460
6	0	-3.113162	-0.418267	0.015470
1	0	-1.823696	1.276041	-0.050047
6	0	-3.433900	-1.674225	-0.529470
1	0	0.403869	0.013378	-2.836348
8	0	-4.418810	-2.422500	0.015837
1	0	-4.801368	-1.925315	0.754552
1	0	-2.960307	-3.135039	-2.011499
8	0	-3.837744	-0.085838	1.122163
6	0	-3.547675	1.158230	1.743795
1	0	-3.761520	1.992168	1.061551
1	0	-4.205114	1.224126	2.612065
1	0	-2.497082	1.209185	2.060490
1	0	-0.296201	2.902088	-0.199388
8	0	0.094161	2.577472	0.939684
6	0	1.055598	1.701310	0.806211
6	0	0.885042	0.344462	1.222792
6	0	1.905116	-0.577550	1.035683
1	0	1.775250	-1.609445	1.354148
6	0	3.126528	-0.212948	0.440778
6	0	3.302058	1.121546	0.036583
1	0	4.236156	1.432906	-0.425567
6	0	2.294249	2.047258	0.219488
6	0	4.152932	-1.237429	0.283939
6	0	5.387498	-1.082560	-0.218644
1	0	3.867766	-2.236507	0.626434
6	0	6.385187	-2.181151	-0.340440
1	0	5.706781	-0.097163	-0.564927
1	0	7.300609	-1.954047	0.221845
1	0	5.982837	-3.128827	0.034919
1	0	6.691584	-2.331454	-1.384136
1	0	2.419302	3.083336	-0.091076
8	0	-0.300684	0.061075	1.802344
6	0	-0.599692	-1.287062	2.091053
1	0	-0.516406	-1.915895	1.192676
1	0	0.056537	-1.683847	2.877886
1	0	-1.635248	-1.301416	2.442380

Zero-point correction= 0.380548
(Hartree/Particle)
Thermal correction to Energy= 0.404226
Thermal correction to Enthalpy= 0.405170
Thermal correction to Gibbs Free Energy= 0.327055
Sum of electronic and zero-point Energies= -1075.714305
Sum of electronic and thermal Energies= -1075.690627
Sum of electronic and thermal Enthalpies= -1075.689683
Sum of electronic and thermal Free Energies= -1075.767798

Frequencies -- -2009.1829 18.7585 32.3362

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -1076.116808

ISO-HAT-TS2

6	0	-0.684195	2.999267	1.467805
1	0	-1.767389	2.878840	1.381215
1	0	-0.390334	4.014801	1.741965
6	0	0.035269	1.958050	2.132022
1	0	0.972590	2.247475	2.610835
6	0	-0.268635	0.617160	2.222195
6	0	-1.367480	-0.119136	1.640422
6	0	-2.106948	0.350505	0.534086
6	0	-1.680279	-1.393155	2.150812

6	0	-3.113517	-0.418096	-0.015494
1	0	-1.823873	1.276115	0.049206
6	0	-2.708513	-2.155054	1.613335
1	0	-1.106938	-1.780296	2.991101
6	0	-3.434398	-1.673753	0.530051
1	0	0.403541	0.014516	2.836148
8	0	-4.419368	-2.422202	-0.014905
1	0	-4.801874	-1.925340	-0.753864
1	0	-2.960964	-3.133901	2.012789
8	0	-3.838000	-0.086156	-1.122400
6	0	-3.547609	1.157464	-1.744770
1	0	-2.496931	1.208064	-2.061233
1	0	-4.204814	1.222875	-2.613256
1	0	-3.761522	1.991889	-1.063146
1	0	-0.296170	2.902040	0.197901
8	0	0.094255	2.576850	-0.940992
6	0	1.055715	1.700788	-0.807030
6	0	2.294370	2.047135	-0.220554
1	0	2.419389	3.083406	0.089377
6	0	3.302222	1.121576	-0.037105
1	0	4.236309	1.433254	0.424854
6	0	3.126741	-0.213172	-0.440492
6	0	1.905326	-0.578177	-1.035145
1	0	1.775483	-1.610267	-1.352986
6	0	0.885204	0.343682	-1.222772
6	0	4.153195	-1.237511	-0.283052
6	0	5.387841	-1.082207	0.219199
1	0	3.868007	-2.236858	-0.624741
6	0	6.385593	-2.180662	0.341706
1	0	5.707139	-0.096524	0.564650
1	0	6.692029	-2.330237	1.385496
1	0	5.983282	-3.128614	-0.032996
1	0	7.300986	-1.953889	-0.220757
8	0	-0.300526	0.059894	-1.802108
6	0	-0.599419	-1.288402	-2.090182
1	0	-1.634969	-1.303000	-2.441512
1	0	0.056853	-1.685502	-2.876820
1	0	-0.516084	-1.916814	-1.191514

Zero-point correction= 0.380555
(Hartree/Particle)
Thermal correction to Energy= 0.404230
Thermal correction to Enthalpy= 0.405175
Thermal correction to Gibbs Free Energy= 0.327069
Sum of electronic and zero-point Energies= -1075.714299
Sum of electronic and thermal Energies= -1075.690623
Sum of electronic and thermal Enthalpies= -1075.689679
Sum of electronic and thermal Free Energies= -1075.767784

Frequencies -- -2009.3740 18.8974 32.3357

ISO-HAT-TS3

6	0	-3.577158	-2.351540	-0.013225
1	0	-4.228071	-3.027386	-0.570064
1	0	-3.850554	-2.233714	1.039508
6	0	-2.182758	-2.410697	-0.297933
1	0	-1.891637	-2.775779	-1.285808
6	0	-1.209394	-1.903562	0.525496
6	0	0.189106	-1.743712	0.218695
6	0	0.764999	-2.122206	-1.007750
6	0	1.019933	-1.122971	1.178512
6	0	2.107284	-1.892649	-1.271243
1	0	0.153824	-2.597131	-1.771404
6	0	2.351724	-0.877500	0.907880
1	0	0.578993	-0.809513	2.122614
6	0	2.908080	-1.268145	-0.323089
1	0	-1.531416	-1.537721	1.504588
8	0	4.211889	-1.028229	-0.590227
1	0	4.604476	-0.604649	0.187943
1	0	2.557456	-2.184136	-2.216841
8	0	3.235788	-0.248904	1.736819
6	0	2.754034	0.209933	2.981065
1	0	2.394464	-0.624064	3.598705
1	0	3.594584	0.693944	3.481269
1	0	1.941711	0.937927	2.846443
1	0	-3.881037	-1.158140	-0.496111
8	0	-3.950784	0.035359	-0.898064
6	0	-2.760072	0.567981	-0.825218
6	0	-1.880970	0.562696	-1.937802
6	0	-0.596415	1.054199	-1.854004
1	0	0.047799	1.017744	-2.730312
6	0	-0.105306	1.588396	-0.644604
6	0	-0.978863	1.638809	0.454195
1	0	-0.637523	2.045977	1.406247
6	0	-2.268233	1.140977	0.387778
6	0	1.258695	2.069523	-0.478412
6	0	2.266900	1.979229	-1.360595
1	0	1.472468	2.532523	0.490530
6	0	3.644314	2.485463	-1.112452
1	0	2.091483	1.503069	-2.328118
1	0	3.908353	3.288905	-1.813462
1	0	3.747952	2.876197	-0.093129
1	0	4.388337	1.691332	-1.257974
1	0	-2.264173	0.136040	-2.863126
8	0	-3.008832	1.120812	1.531519
6	0	-4.258552	1.801842	1.476023
1	0	-4.921263	1.358692	0.726206
1	0	-4.701936	1.710658	2.470243
1	0	-4.096599	2.864709	1.248612

Zero-point correction= 0.380344
(Hartree/Particle)
Thermal correction to Energy= 0.404110
Thermal correction to Enthalpy= 0.405054
Thermal correction to Gibbs Free Energy= 0.327161
Sum of electronic and zero-point Energies= -1075.717400
Sum of electronic and thermal Energies= -1075.693635
Sum of electronic and thermal Enthalpies= -1075.692690
Sum of electronic and thermal Free Energies= -1075.770583

Frequencies -- -1984.1812 27.6494 29.1872

ISO-HAT-TS4

6	0	-0.842885	2.613554	1.127300
1	0	-1.826554	2.741905	0.665324
1	0	-0.354862	3.565239	1.350879
6	0	-0.741860	1.622258	2.154737
1	0	0.034819	1.775413	2.906719
6	0	-1.504609	0.489543	2.316931
6	0	-2.525890	-0.049676	1.447716
6	0	-2.575914	0.225659	0.062521
6	0	-3.479470	-0.933179	1.982521
6	0	-3.557131	-0.340030	-0.728952
1	0	-1.799900	0.828639	-0.397322
6	0	-4.476358	-1.486201	1.190672
1	0	-3.439049	-1.175225	3.042874
6	0	-4.526876	-1.192159	-0.165975
1	0	-1.340917	-0.076331	3.235700
8	0	-5.483692	-1.740819	-0.943148
1	0	-5.342755	-1.442464	-1.854403
1	0	-5.222473	-2.160884	1.601999
8	0	-3.678918	-0.166329	-2.073690
6	0	-2.680814	0.600746	-2.725091
1	0	-2.669955	1.633938	-2.352891
1	0	-1.684901	0.162117	-2.579627
1	0	-2.934970	0.597631	-3.785836
1	0	-0.158387	2.151158	0.098054
8	0	0.436954	1.619877	-0.861831
6	0	1.303247	0.712992	-0.459943
6	0	2.692275	1.008682	-0.327322
6	0	3.599140	-0.004456	-0.043043
1	0	4.642857	0.281565	0.052166
6	0	3.188416	-1.329089	0.163452
6	0	1.807324	-1.604401	0.120233
1	0	1.463405	-2.620093	0.308997
6	0	0.896758	-0.614318	-0.182717
6	0	4.109090	-2.421622	0.467351
6	0	5.400471	-2.566897	0.120445
1	0	3.656515	-3.244137	1.025034
6	0	6.239384	-1.662474	-0.719698
1	0	5.891959	-3.476470	0.468669
1	0	6.858168	-0.993497	-0.104325
1	0	6.931135	-2.246637	-1.336913
1	0	5.636037	-1.034233	-1.383384
1	0	-0.166808	-0.837471	-0.249342
8	0	3.218463	2.239441	-0.545728
6	0	2.543248	3.375562	-0.031280
1	0	1.693351	3.661770	-0.658359
1	0	2.191661	3.183157	0.993003
1	0	3.281439	4.181193	-0.008419

Zero-point correction= 0.379899
(Hartree/Particle)
Thermal correction to Energy= 0.403900
Thermal correction to Enthalpy= 0.404844
Thermal correction to Gibbs Free Energy= 0.323947
Sum of electronic and zero-point Energies= -1075.702900
Sum of electronic and thermal Energies= -1075.678898
Sum of electronic and thermal Enthalpies= -1075.677954
Sum of electronic and thermal Free Energies= -1075.758852

Frequencies -- -2087.0660 14.8468 26.6278

ISO-HAT-TS5

6	0	-0.518002	-3.385508	-1.377133
1	0	-1.370190	-3.305402	-2.059267
1	0	-0.048081	-4.372690	-1.366782
6	0	0.359548	-2.260558	-1.313793
1	0	-0.089674	-1.277568	-1.485480
6	0	1.673729	-2.322505	-0.936393
6	0	2.532261	-1.202441	-0.636169
6	0	2.012157	0.089049	-0.399211
6	0	3.918920	-1.396049	-0.528022
6	0	2.858178	1.132273	-0.081104
1	0	0.936429	0.241689	-0.418541
6	0	4.770740	-0.343217	-0.222390
1	0	4.328402	-2.390738	-0.693960
6	0	4.250176	0.924145	0.001682
1	0	5.845373	-0.483024	-0.142309
1	0	2.129428	-3.312638	-0.848939
8	0	2.475352	2.410037	0.198278
8	0	5.072546	1.946962	0.316889
1	0	4.533742	2.740138	0.456517
6	0	1.088011	2.683039	0.227479
1	0	0.634939	2.518625	-0.760633
1	0	0.579032	2.051111	0.969091
1	0	0.984787	3.734557	0.501417
1	0	-1.163264	-3.285259	-0.243553

8	0	-1.823669	-2.933815	0.780086
6	0	-2.374770	-1.762851	0.556662
6	0	-1.758980	-0.525884	0.917893
6	0	-2.383419	0.681665	0.599258
1	0	-1.899935	1.590571	0.949358
6	0	-3.610758	0.734567	-0.067174
6	0	-4.239152	-0.487941	-0.388346
1	0	-5.207346	-0.471363	-0.886263
6	0	-3.630510	-1.686887	-0.095138
1	0	-4.095087	-2.636555	-0.353656
8	0	-0.575551	-0.387859	1.562182
6	0	-4.296258	1.981500	-0.400911
6	0	-3.774025	3.188644	-0.678832
1	0	-5.382818	1.892137	-0.460002
6	0	-2.331375	3.562392	-0.774386
1	0	-4.485960	3.986038	-0.894344
1	0	-1.941219	3.948966	0.179160
1	0	-1.709727	2.706095	-1.062941
1	0	-2.185879	4.353916	-1.517765
6	0	0.042626	-1.466027	2.253370
1	0	-0.668744	-1.976543	2.910178
1	0	0.472516	-2.195525	1.557248
1	0	0.838836	-1.004883	2.843619

Zero-point correction= 0.380073
(Hartree/Particle)
Thermal correction to Energy= 0.403816
Thermal correction to Enthalpy= 0.404760
Thermal correction to Gibbs Free Energy= 0.326750
Sum of electronic and zero-point Energies= -1075.705092
Sum of electronic and thermal Energies= -1075.681348
Sum of electronic and thermal Enthalpies= -1075.680404
Sum of electronic and thermal Free Energies= -1075.758414

Frequencies -- -2237.1531 33.5215 34.0830

ISO-HAT-TS6

6	0	-0.643972	-1.305448	-1.714205
1	0	0.195531	-1.555991	-2.367505
1	0	-1.347838	-0.599967	-2.167830
6	0	-1.223420	-2.415641	-1.016708
1	0	-0.621113	-3.325068	-0.973516
6	0	-2.436693	-2.466182	-0.377204
6	0	-3.372931	-1.391504	-0.136574
6	0	-4.726216	-1.699010	0.091708
6	0	-2.975736	-0.037675	-0.075901
6	0	-5.664588	-0.701885	0.316473
1	0	-5.041758	-2.740482	0.070823
6	0	-3.907790	0.953232	0.159896
1	0	-1.926858	0.227713	-0.149128
6	0	-5.266421	0.629055	0.346079
1	0	-2.758049	-3.444819	-0.015526
8	0	-6.173283	1.600771	0.574026
1	0	-5.712337	2.453266	0.571254
1	0	-6.714477	-0.931860	0.477234
8	0	-3.634321	2.283333	0.252953
6	0	-2.294367	2.689543	0.030530
1	0	-2.282528	3.775207	0.137417
1	0	-1.610104	2.234220	0.757682
1	0	-1.964657	2.412332	-0.980406
1	0	-0.090350	-0.552401	-0.827181
8	0	0.334498	0.346772	-0.007581
6	0	1.632296	0.524015	-0.093768
6	0	2.542051	-0.559133	0.059433
6	0	3.907854	-0.359825	-0.049594
1	0	4.546694	-1.235896	0.019853
6	0	4.444553	0.917936	-0.286924
6	0	3.541367	1.987206	-0.452343
1	0	3.938282	2.981337	-0.653687
6	0	2.176912	1.796775	-0.366339
6	0	5.873153	1.190412	-0.408516
6	0	6.921815	0.508951	0.087511
1	0	6.105071	2.100966	-0.965098
6	0	6.907317	-0.704753	0.957318
1	0	7.908510	0.907858	-0.150847
1	0	7.788690	-0.722756	1.607270
1	0	6.015947	-0.745074	1.593561
1	0	6.932245	-1.632871	0.367955
1	0	1.478206	2.620110	-0.503073
8	0	2.074779	-1.833616	0.223194
6	0	1.417009	-2.075684	1.460969
1	0	2.106922	-1.895855	2.297311
1	0	0.527864	-1.443861	1.574490
1	0	1.122332	-3.127951	1.458599

Zero-point correction= 0.380230
(Hartree/Particle)
Thermal correction to Energy= 0.404089
Thermal correction to Enthalpy= 0.405034
Thermal correction to Gibbs Free Energy= 0.324607
Sum of electronic and zero-point Energies= -1075.699779
Sum of electronic and thermal Energies= -1075.675920
Sum of electronic and thermal Enthalpies= -1075.674976
Sum of electronic and thermal Free Energies= -1075.755402

Frequencies -- -2134.7659 12.6779 22.7475

ISO-HAT-TS7

6	0	0.649012	-1.232515	-1.844266
1	0	1.348960	-0.523643	-2.299434
1	0	-0.197750	-1.471517	-2.492828
6	0	1.233663	-2.353248	-1.169286
1	0	0.641299	-3.269629	-1.146501
6	0	2.448813	-2.416591	-0.534614
6	0	3.384529	-1.347585	-0.265379
6	0	4.731316	-1.662971	-0.013593
6	0	2.992120	0.007145	-0.193308
6	0	5.668016	-0.673107	0.248774
1	0	5.043607	-2.705198	-0.043693
6	0	3.922530	0.991038	0.079332
1	0	1.946968	0.278681	-0.293684
6	0	5.274746	0.658545	0.291541
1	0	6.713068	-0.910366	0.429573
1	0	2.768393	-3.402342	-0.191443
8	0	3.651530	2.320621	0.186294
8	0	6.180078	1.623263	0.556543
1	0	5.722300	2.477345	0.556877
6	0	2.317201	2.733730	-0.054805
1	0	2.305001	3.817443	0.069367
1	0	2.005590	2.474153	-1.075725
1	0	1.618548	2.269032	0.652520
1	0	0.096942	-0.430389	-0.964031
8	0	-0.364497	0.458925	-0.208522
6	0	-1.670278	0.360082	-0.063953
6	0	-2.534928	1.295678	-0.677457
1	0	-2.066157	2.097418	-1.244280
6	0	-3.905125	1.200556	-0.573790
1	0	-4.531108	1.945924	-1.059461
6	0	-4.497626	0.138917	0.141723
6	0	-3.651969	-0.792488	0.754698
1	0	-4.069420	-1.623676	1.321026
6	0	-2.267584	-0.695114	0.678787
6	0	-5.940097	-0.026293	0.278845
6	0	-6.899047	0.769548	-0.218457
1	0	-6.252821	-0.902633	0.853687
6	0	-8.358430	0.532871	-0.041448
1	0	-6.618150	1.653534	-0.795233
1	0	-8.864547	0.415911	-1.008955
1	0	-8.547333	-0.369186	0.551227
1	0	-8.844182	1.378979	0.462453
8	0	-1.550575	-1.680296	1.275962
6	0	-0.370819	-1.344108	1.995029
1	0	-0.458065	-0.351594	2.452583
1	0	-0.268086	-2.099683	2.778652
1	0	0.516826	-1.363050	1.352284

Zero-point correction= 0.379503
(Hartree/Particle)
Thermal correction to Energy= 0.403712
Thermal correction to Enthalpy= 0.404656
Thermal correction to Gibbs Free Energy= 0.322929
Sum of electronic and zero-point Energies= -1075.704663
Sum of electronic and thermal Energies= -1075.680455
Sum of electronic and thermal Enthalpies= -1075.679511
Sum of electronic and thermal Free Energies= -1075.761238

Frequencies -- -2149.0658 8.1004 17.2899

ISO-HAT-TS8

6	0	-0.788354	-1.297860	-1.891048
1	0	0.006233	-1.594795	-2.580357
1	0	-1.502770	-0.598795	-2.338499
6	0	-1.347828	-2.368239	-1.118338
1	0	-0.759992	-3.286847	-1.073962
6	0	-2.519430	-2.373834	-0.403607
6	0	-3.418067	-1.274071	-0.135217
6	0	-2.994395	0.072681	-0.161639
6	0	-4.754486	-1.544199	0.209771
6	0	-3.889079	1.092144	0.096733
1	0	-1.948798	0.308599	-0.322981
6	0	-5.654615	-0.519256	0.464957
1	0	-5.089126	-2.578903	0.255618
6	0	-5.233199	0.803395	0.403570
1	0	-2.832570	-3.334145	0.011011
8	0	-6.102648	1.802878	0.657631
1	0	-5.629809	2.644759	0.573554
1	0	-6.692553	-0.721019	0.716025
8	0	-3.589622	2.419714	0.101637
6	0	-2.269087	2.789258	-0.258553
1	0	-1.531284	2.369956	0.436847
1	0	-2.029733	2.442493	-1.273098
1	0	-2.235862	3.879067	-0.223531
1	0	-0.171452	-0.501948	-1.079004
8	0	0.329647	0.440179	-0.362730
6	0	1.632193	0.334819	-0.237929
6	0	2.238822	-0.855300	0.245777
6	0	3.613858	-0.943028	0.374670
1	0	4.034622	-1.879854	0.738572
6	0	4.454925	0.135994	0.058252
6	0	3.855570	1.315816	-0.424060
1	0	4.478015	2.166913	-0.693087
6	0	2.487781	1.404720	-0.584000
6	0	5.892913	-0.014171	0.243786
6	0	6.833387	0.932963	0.103048
1	0	6.219713	-1.014824	0.541038
6	0	8.289782	0.704418	0.312615
1	0	6.537048	1.946378	-0.176734
1	0	8.866416	0.935136	-0.593003
1	0	8.686924	1.351732	1.105799

1	0	8.494719	-0.336053	0.588716
1	0	2.023443	2.307854	-0.974299
8	0	1.471427	-1.952700	0.524009
6	0	0.690495	-1.841306	1.706763
1	0	0.157601	-2.788204	1.824286
1	0	1.341654	-1.681416	2.577770
1	0	-0.035571	-1.021617	1.635825

Zero-point correction= 0.380161
(Hartree/Particle)
Thermal correction to Energy= 0.404095
Thermal correction to Enthalpy= 0.405039
Thermal correction to Gibbs Free Energy= 0.324986
Sum of electronic and zero-point Energies= -1075.703706
Sum of electronic and thermal Energies= -1075.679772
Sum of electronic and thermal Enthalpies= -1075.678827
Sum of electronic and thermal Free Energies= -1075.758881

Frequencies -- -2144.8231 19.5238 22.6162

ISO-HAT-TS9

6	0	-0.116477	-2.311613	1.321751
1	0	-0.156450	-3.366252	1.602136
1	0	-0.753393	-1.669957	1.941436
6	0	1.177021	-1.779365	1.011938
1	0	1.935588	-2.481992	0.659304
6	0	1.467382	-0.445195	1.047845
6	0	2.705818	0.199141	0.682299
6	0	3.839984	-0.512730	0.230910
6	0	2.792500	1.597985	0.770620
6	0	4.995248	0.160637	-0.111934
1	0	3.798682	-1.595651	0.154312
6	0	3.954320	2.275965	0.424622
1	0	1.925316	2.156835	1.118488
6	0	5.061381	1.566726	-0.016394
1	0	4.024749	3.358241	0.491236
1	0	0.663693	0.221492	1.370819
8	0	6.149911	-0.409282	-0.561087
8	0	6.194261	2.219430	-0.351797
1	0	6.852206	1.566666	-0.633500
6	0	6.190658	-1.815311	-0.681253
1	0	5.441352	-2.172496	-1.400270
1	0	7.188511	-2.066319	-1.044164
1	0	6.024491	-2.298835	0.290865
1	0	-0.785686	-2.282337	0.223531
8	0	-1.579283	-2.212505	-0.787166
6	0	-2.673284	-1.543270	-0.524736
6	0	-3.935571	-2.180744	-0.522788
6	0	-5.092312	-1.482513	-0.245227
1	0	-6.052130	-1.997392	-0.255862
6	0	-5.065184	-0.104828	0.054412
6	0	-3.812464	0.533454	0.081834
1	0	-3.717830	1.577158	0.368501
6	0	-2.645835	-0.153170	-0.208657
6	0	-6.325850	0.566416	0.351766
6	0	-6.648572	1.869271	0.253360
1	0	-7.122301	-0.108335	0.672732
6	0	-5.804861	2.995081	-0.246549
1	0	-7.664861	2.134669	0.547257
1	0	-5.260992	3.493674	0.569017
1	0	-5.061795	2.659771	-0.978728
1	0	-6.428032	3.760767	-0.721159
1	0	-3.953978	-3.244140	-0.750401
8	0	-1.458132	0.514001	-0.099569
6	0	-0.720297	0.631877	-1.312258
1	0	-1.316562	1.165551	-2.065359
1	0	0.174161	1.216683	-1.079234
1	0	-0.426871	-0.350993	-1.698521

Zero-point correction= 0.378987
(Hartree/Particle)
Thermal correction to Energy= 0.403306
Thermal correction to Enthalpy= 0.404250
Thermal correction to Gibbs Free Energy= 0.322216
Sum of electronic and zero-point Energies= -1075.701346
Sum of electronic and thermal Energies= -1075.677027
Sum of electronic and thermal Enthalpies= -1075.676083
Sum of electronic and thermal Free Energies= -1075.758117

Frequencies -- -2190.2120 14.5808 19.1024

ISO Radical Coupling reaction transition state structures

ISO-RC-TS1

6	0	-2.776373	1.159354	0.170677
6	0	-3.350823	0.416787	-0.865238
6	0	-4.827022	0.217485	-0.915823
1	0	-3.377938	1.288821	1.072845
1	0	-2.841039	0.404853	-1.830735
1	0	-5.315075	1.089658	-1.369638
1	0	-5.078590	-0.666866	-1.507415
1	0	-5.229520	0.083422	0.093990
6	0	-1.409352	1.564251	0.264933
6	0	-0.489053	1.457380	-0.808883
6	0	-0.924301	2.043002	1.501980
6	0	0.845475	1.750500	-0.619236
1	0	-0.832196	1.110331	-1.779014
6	0	0.417327	2.335455	1.691279
1	0	-1.623131	2.145129	2.330906
6	0	1.315468	2.170115	0.643257
1	0	0.796157	2.682257	2.649663
8	0	1.824062	1.679715	-1.564177
8	0	2.629990	2.418062	0.829792
1	0	3.094039	2.203458	0.005811
6	0	1.466325	1.234696	-2.856198
1	0	2.383467	1.235937	-3.447730
1	0	1.052509	0.217223	-2.818047
1	0	0.735919	1.914539	-3.316163
8	0	-2.886400	-1.398189	-0.504654
6	0	-1.597282	-1.602147	-0.455058
6	0	-0.850954	-1.904591	-1.611109
6	0	-0.880740	-1.502216	0.780873
6	0	0.527414	-2.037516	-1.573593
1	0	-1.405931	-2.022234	-2.540935
6	0	0.502550	-1.600209	0.801241
6	0	1.232850	-1.826381	-0.379281
1	0	1.082209	-2.269308	-2.483166
1	0	1.043723	-1.492102	1.737448
6	0	2.692593	-1.804559	-0.405282
6	0	3.495509	-1.250960	0.516306
1	0	3.153916	-2.241032	-1.296717
6	0	4.982217	-1.217556	0.428934
1	0	3.048528	-0.766926	1.388933
1	0	5.448635	-1.728658	1.281593
1	0	5.339413	-1.697752	-0.489304
1	0	5.359635	-0.185944	0.444526
8	0	-1.646334	-1.292995	1.874303
6	0	-0.998836	-1.138331	3.114317
1	0	-1.786860	-0.987398	3.855297
1	0	-0.420278	-2.033864	3.382788
1	0	-0.331668	-0.262795	3.107948

Zero-point correction= 0.385213
(Hartree/Particle)
Thermal correction to Energy= 0.408515
Thermal correction to Enthalpy= 0.409459
Thermal correction to Gibbs Free Energy= 0.334000
Sum of electronic and zero-point Energies= -1075.722290
Sum of electronic and thermal Energies= -1075.698988
Sum of electronic and thermal Enthalpies= -1075.698044
Sum of electronic and thermal Free Energies= -1075.773502

Frequencies -- -573.8447 31.0384 49.4689

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -1076.136598

ISO-RC-TS2

6	0	-2.521911	1.387964	0.391252
6	0	-3.156090	0.932960	-0.769697
6	0	-4.643856	0.923725	-0.860124
1	0	-3.121959	1.410237	1.304267
1	0	-2.629710	1.053383	-1.718220
1	0	-5.015145	1.915392	-1.148809
1	0	-4.982659	0.197531	-1.604064
1	0	-5.088550	0.663259	0.107342
6	0	-1.122786	1.616670	0.554644
6	0	-0.207120	1.641673	-0.528582
6	0	-0.606803	1.772261	1.861129
6	0	1.146268	1.756084	-0.295107
1	0	-0.574241	1.540611	-1.545807
6	0	0.753289	1.877230	2.094187
1	0	-1.298776	1.755764	2.700505
6	0	1.641119	1.849429	1.024074
1	0	1.155296	1.962671	3.100287
8	0	2.124845	1.794008	-1.242406
8	0	2.970826	1.913455	1.244487
1	0	3.418899	1.838973	0.387473
6	0	1.747197	1.612825	-2.591140
1	0	2.668113	1.640006	-3.176121
1	0	1.249500	0.642529	-2.728766
1	0	1.081689	2.420848	-2.924856
8	0	-2.917766	-0.962256	-0.789473
6	0	-1.659258	-1.325511	-0.707055
6	0	-0.872604	-1.501218	-1.867574
6	0	-1.011375	-1.509162	0.550318
6	0	0.486568	-1.741391	-1.793240
1	0	-1.380862	-1.411701	-2.827056
6	0	0.362186	-1.702256	0.610385
6	0	1.143332	-1.777986	-0.548736
1	0	1.071522	-1.865828	-2.705077
1	0	0.810738	-1.797947	1.597591
6	0	2.600770	-1.877213	-0.511812
6	0	3.393888	-1.522854	0.510150
1	0	3.072866	-2.234334	-1.432547
6	0	4.880090	-1.623064	0.497119
1	0	2.943039	-1.113107	1.417740
1	0	5.243029	-2.299328	1.282608
1	0	5.248105	-1.996134	-0.465641
1	0	5.349181	-0.648723	0.690598
8	0	-1.669354	-1.435543	1.736148
6	0	-2.964039	-2.011466	1.837549

1	0	-3.110836	-2.238336	2.897228
1	0	-3.741125	-1.325727	1.485049
1	0	-3.027467	-2.937670	1.252968

Zero-point correction= 0.385252
(Hartree/Particle)
Thermal correction to Energy= 0.408685
Thermal correction to Enthalpy= 0.409630
Thermal correction to Gibbs Free Energy= 0.333823
Sum of electronic and zero-point Energies= -1075.721016
Sum of electronic and thermal Energies= -1075.697582
Sum of electronic and thermal Enthalpies= -1075.696638
Sum of electronic and thermal Free Energies= -1075.772445

Frequencies -- -551.4834 31.8758 50.9980

ISO-RC-TS3

6	0	1.850367	2.265404	-0.386643
6	0	0.913416	3.262952	-0.109211
6	0	1.097685	4.644251	-0.636150
1	0	2.538876	2.447112	-1.215260
1	0	0.334126	3.190535	0.811492
1	0	0.134593	5.157546	-0.704725
1	0	1.751842	5.222414	0.029162
1	0	1.551746	4.622021	-1.633022
6	0	1.832376	0.944788	0.156754
6	0	2.664182	-0.046146	-0.424442
6	0	0.988165	0.552540	1.218914
6	0	2.622180	-1.352355	0.016484
1	0	3.319731	0.243537	-1.242351
6	0	0.943970	-0.761969	1.654826
1	0	0.349142	1.287541	1.702478
6	0	1.748096	-1.725145	1.058753
1	0	0.277125	-1.068868	2.456874
8	0	3.365449	-2.387626	-0.472638
8	0	1.702387	-3.006392	1.485706
1	0	2.323567	-3.525592	0.954200
6	0	4.281422	-2.107581	-1.508906
1	0	4.774952	-3.050405	-1.750390
1	0	3.765624	-1.727063	-2.400720
1	0	5.032926	-1.375847	-1.182991
8	0	-0.555832	2.780335	-1.223943
6	0	-1.138733	1.650636	-0.934010
6	0	-0.968194	0.505094	-1.742506
6	0	-1.971356	1.511539	0.218448
6	0	-1.599284	-0.691590	-1.462637
1	0	-0.309249	0.609913	-2.602561
6	0	-2.608383	0.310041	0.489378
6	0	-2.434232	-0.813873	-0.339749
1	0	-1.437095	-1.547356	-2.114411
1	0	-3.248770	0.210346	1.363402
6	0	-3.116869	-2.052251	0.020095
6	0	-3.053676	-3.232887	-0.613783
1	0	-3.742360	-1.993780	0.916102
6	0	-3.778454	-4.457773	-0.174153
1	0	-2.436153	-3.329266	-1.509298
1	0	-3.082696	-5.278772	0.044732
1	0	-4.370338	-4.266674	0.728301
1	0	-4.458302	-4.825740	-0.954218
8	0	-2.048847	2.613984	1.007451
6	0	-2.800828	2.522800	2.193918
1	0	-2.718866	3.493881	2.686283
1	0	-3.859607	2.313406	1.986779
1	0	-2.404499	1.742046	2.861134

Zero-point correction= 0.383396
(Hartree/Particle)
Thermal correction to Energy= 0.406887
Thermal correction to Enthalpy= 0.407832
Thermal correction to Gibbs Free Energy= 0.330442
Sum of electronic and zero-point Energies= -1075.720071
Sum of electronic and thermal Energies= -1075.696580
Sum of electronic and thermal Enthalpies= -1075.695635
Sum of electronic and thermal Free Energies= -1075.773025

Frequencies -- -562.1096 -21.1415 25.1864

ISO-RC-TS4

6	0	2.766060	-0.755816	-0.559805
6	0	3.411781	0.441186	-0.879308
6	0	4.872645	0.596894	-0.627772
1	0	3.276312	-1.413347	0.147654
1	0	3.009998	1.033050	-1.703528
1	0	5.451375	0.153458	-1.448165
1	0	5.139864	1.653898	-0.546476
1	0	5.155266	0.096337	0.304638
6	0	1.411465	-1.087451	-0.871574
6	0	0.824232	-2.203037	-0.221615
6	0	0.594418	-0.328482	-1.736395
6	0	-0.513563	-2.495741	-0.388668
1	0	1.443742	-2.800994	0.443975
6	0	-0.750365	-0.621607	-1.897599
1	0	1.011281	0.520269	-2.271468
6	0	-1.321017	-1.691389	-1.217838
1	0	-1.385930	-0.018554	-2.541511
8	0	-1.186346	-3.522922	0.212379
8	0	-2.637729	-1.964034	-1.362111
1	0	-2.842282	-2.756383	-0.844300
6	0	-0.434359	-4.442372	0.974382
1	0	-1.137786	-5.193107	1.338397
1	0	0.334662	-4.928075	0.358761
1	0	0.046476	-3.952351	1.832474
8	0	2.810379	1.672101	0.441219
6	0	1.524198	1.896783	0.397610
6	0	0.971590	2.853878	-0.478182
6	0	0.614053	1.161261	1.222850
6	0	-0.395096	3.049466	-0.576326
1	0	1.669525	3.429447	-1.084456
6	0	-0.754240	1.355345	1.107827
6	0	-1.283068	2.272818	0.182598
1	0	-0.795635	3.786434	-1.271418
1	0	-1.441349	0.789062	1.730752
6	0	-2.719394	2.416782	-0.035839
6	0	-3.670436	1.528815	0.289618
1	0	-3.023594	3.326019	-0.562945
6	0	-5.122209	1.710352	0.010801
1	0	-3.379996	0.589311	0.766470
1	0	-5.316290	2.671498	-0.478873
1	0	-5.503841	0.912471	-0.640135
1	0	-5.718353	1.673945	0.932378
8	0	1.189127	0.284919	2.079829
6	0	0.344386	-0.519027	2.864071
1	0	0.997542	-1.159560	3.462161
1	0	-0.280736	0.083907	3.538365
1	0	-0.305548	-1.147901	2.234128

Zero-point correction= 0.386097
(Hartree/Particle)
Thermal correction to Energy= 0.409276
Thermal correction to Enthalpy= 0.410220
Thermal correction to Gibbs Free Energy= 0.334944
Sum of electronic and zero-point Energies= -1075.718637
Sum of electronic and thermal Energies= -1075.695458
Sum of electronic and thermal Enthalpies= -1075.694514
Sum of electronic and thermal Free Energies= -1075.769790

Frequencies -- -591.3305 28.8434 58.1677

ISO-RC-TS5

6	0	1.114446	0.734531	-1.412180
6	0	0.675203	1.947879	-0.873567
6	0	1.542444	2.975559	-0.212105
1	0	0.440644	0.261492	-2.129230
1	0	-0.215180	2.350996	-1.354829
1	0	2.510182	3.068766	-0.721137
1	0	1.045718	3.949730	-0.220448
1	0	1.723889	2.723763	0.838778
6	0	2.269772	-0.042177	-1.074695
6	0	3.101536	0.234692	0.037692
6	0	2.584154	-1.165797	-1.867096
6	0	4.193375	-0.564383	0.311793
1	0	2.848297	1.055825	0.696543
6	0	3.686327	-1.961380	-1.595032
1	0	1.944771	-1.404934	-2.714648
6	0	4.500901	-1.667321	-0.509225
1	0	3.933192	-2.823446	-2.209034
8	0	5.055273	-0.404599	1.357591
8	0	5.572521	-2.442483	-0.234241
1	0	6.000277	-2.095402	0.562989
6	0	4.811315	0.655783	2.258515
1	0	5.592864	0.601613	3.017961
1	0	4.864689	1.627434	1.748561
1	0	3.828544	0.549484	2.736498
8	0	-0.258324	1.415487	0.734929
6	0	-1.372627	0.759638	0.564812
6	0	-1.449736	-0.628087	0.806601
6	0	-2.560618	1.413370	0.119783
6	0	-2.633443	-1.328885	0.675706
1	0	-0.529765	-1.121149	1.116847
6	0	-3.744235	0.701354	-0.016922
6	0	-3.807659	-0.676006	0.264465
1	0	-2.649733	-2.396126	0.885987
1	0	-4.653097	1.202131	-0.344302
6	0	-5.087731	-1.357868	0.104326
6	0	-5.363284	-2.645325	0.362276
1	0	-5.904647	-0.730977	-0.265849
6	0	-6.701725	-3.270038	0.169089
1	0	-6.654828	-4.108987	-0.537990
1	0	-7.094170	-3.678653	1.109887
1	0	-7.428355	-2.544683	-0.214494
8	0	-2.425656	2.735956	-0.149487
1	0	-4.574180	-3.298143	0.741527
6	0	-3.575045	3.447899	-0.542362
1	0	-3.264148	4.485802	-0.676656
1	0	-3.982344	3.066786	-1.489967
1	0	-4.356894	3.402319	0.228670

Zero-point correction= 0.383864
(Hartree/Particle)
Thermal correction to Energy= 0.408303
Thermal correction to Enthalpy= 0.409247
Thermal correction to Gibbs Free Energy= 0.326866
Sum of electronic and zero-point Energies= -1075.709338
Sum of electronic and thermal Energies= -1075.684899
Sum of electronic and thermal Enthalpies= -1075.683955
Sum of electronic and thermal Free Energies= -1075.766336

Frequencies -- -591.8589 10.2348 25.7043

ISO-RC-TS6

6	0	-1.114448	0.734530	-1.412177
6	0	-0.675203	1.947877	-0.873564
6	0	-1.542440	2.975557	-0.212100
1	0	-0.440647	0.261490	-2.129228
1	0	0.215180	2.350993	-1.354827
1	0	-1.723890	2.723756	0.838782
1	0	-1.045708	3.949725	-0.220435
1	0	-2.510175	3.068773	-0.721134
6	0	-2.269775	-0.042177	-1.074694
6	0	-3.101542	0.234693	0.037692
6	0	-2.584157	-1.165798	-1.867093
6	0	-4.193381	-0.564381	0.311792
1	0	-2.848304	1.055828	0.696542
6	0	-3.686331	-1.961380	-1.595031
1	0	-1.944772	-1.404935	-2.714645
6	0	-4.500906	-1.667319	-0.509225
1	0	-3.933195	-2.823447	-2.209033
8	0	-5.055281	-0.404596	1.357588
8	0	-5.572527	-2.442481	-0.234242
1	0	-6.000284	-2.095399	0.562987
6	0	-4.811324	0.655787	2.258512
1	0	-5.592874	0.601617	3.017957
1	0	-3.828554	0.549489	2.736496
1	0	-4.864697	1.627438	1.748558
8	0	0.258326	1.415481	0.734930
6	0	1.372629	0.759634	0.564811
6	0	1.449739	-0.628091	0.806598
6	0	2.560619	1.413367	0.119783
6	0	2.633447	-1.328888	0.675702
1	0	0.529769	-1.121155	1.116845
6	0	3.744237	0.701353	-0.016923
6	0	3.807662	-0.676007	0.264462
1	0	2.649738	-2.396129	0.885982
1	0	4.653098	1.202131	-0.344303
6	0	5.087735	-1.357868	0.104323
6	0	5.363290	-2.645324	0.362274
1	0	5.904650	-0.730976	-0.265854
6	0	6.701732	-3.270036	0.169086
1	0	7.094178	-3.678649	1.109885
1	0	6.654835	-4.108985	-0.537992
1	0	7.428361	-2.544680	-0.214497
8	0	2.425656	2.735954	-0.149485
1	0	4.574187	-3.298143	0.741527
6	0	3.575044	3.447899	-0.542360
1	0	3.264146	4.485801	-0.676653
1	0	4.356893	3.402318	0.228672
1	0	3.982343	3.066787	-1.489965

Zero-point correction= 0.383866
(Hartree/Particle)
Thermal correction to Energy= 0.408304
Thermal correction to Enthalpy= 0.409248
Thermal correction to Gibbs Free Energy= 0.326872
Sum of electronic and zero-point Energies= -1075.709336
Sum of electronic and thermal Energies= -1075.684898
Sum of electronic and thermal Enthalpies= -1075.683954
Sum of electronic and thermal Free Energies= -1075.766330

Frequencies -- -591.2722 10.2934 25.7104

The substrates and radicals structure, energy and spin density calculated with CBS-QB3 method.

Eugenol

6	0	-2.292094	-0.860624	-0.494891
6	0	-3.329494	-0.509504	0.539744
6	0	-4.534026	-0.011709	0.275363
6	0	1.476768	1.213439	0.027329
6	0	1.436814	-0.191365	-0.012883
6	0	0.225846	-0.854613	-0.173950
6	0	-0.970451	-0.133816	-0.299111
6	0	-0.918748	1.258899	-0.253729
6	0	0.293906	1.928593	-0.094009
8	0	2.671237	-0.782931	0.120573
6	0	2.750362	-2.201127	0.097996
1	0	2.177159	-2.644209	0.919557
1	0	3.804206	-2.446297	0.219784
1	0	2.391784	-2.603955	-0.855413
8	0	2.663243	1.863379	0.186210
1	0	3.350251	1.187031	0.252818
1	0	-2.692953	-0.647960	-1.492636
1	0	-2.104874	-1.940583	-0.460504
1	0	-3.038083	-0.681396	1.574329
1	0	-5.240730	0.218805	1.064668
1	0	-4.858195	0.180969	-0.743222
1	0	0.198311	-1.936821	-0.206675
1	0	-1.835561	1.831227	-0.338533
1	0	0.339540	3.010571	-0.059588

CBS-QB3 (0 K)= -537.773692 CBS-QB3 Energy= -537.761692
CBS-QB3 Enthalpy= -537.760748 CBS-QB3 Free Energy= -537.813143

Eugenol Radical

6	0	2.429429	-0.808999	-0.580510
6	0	3.374424	-0.530199	0.562762
6	0	4.540088	0.099428	0.450689
6	0	-1.517724	1.004729	0.021842
6	0	-1.341369	-0.451219	-0.051739
6	0	-0.068574	-0.997740	-0.244966
6	0	1.059007	-0.198769	-0.371163
6	0	0.918483	1.216960	-0.297722
6	0	-0.306401	1.788832	-0.114643
8	0	-2.336432	-1.341421	0.052458
6	0	-3.713180	-0.969005	0.253323
1	0	-4.242856	-1.919711	0.296611
1	0	-4.078451	-0.360139	-0.572448
1	0	-3.837402	-0.414321	1.182223
8	0	-2.635099	1.542760	0.190387
1	0	2.319176	-1.891424	-0.706632
1	0	2.864666	-0.422210	-1.509136
1	0	3.046023	-0.880276	1.539282
1	0	5.179915	0.266064	1.309772
1	0	4.900367	0.465784	-0.506116
1	0	0.008273	-2.078148	-0.296990
1	0	1.804519	1.836288	-0.385717
1	0	-0.437078	2.863270	-0.060846

CBS-QB3 (0 K)= -537.139894 CBS-QB3 Energy= -537.128100
CBS-QB3 Enthalpy= -537.127156 CBS-QB3 Free Energy= -537.179323

Mulliken atomic spin densities:

		1
1	C	-0.069362
2	C	0.047908
3	C	-0.019047
4	C	-0.409885
5	C	0.631976
6	C	-0.573777
7	C	0.613163
8	C	-0.582263
9	C	0.613121
10	O	0.045480
11	C	-0.001676
12	H	-0.001005
13	H	0.001400
14	H	0.001544
15	O	0.627957
16	H	0.006074
17	H	0.021153
18	H	-0.001946
19	H	0.001108
20	H	0.001141
21	H	0.051855
22	H	0.049267
23	H	-0.054188

trans-Isoeugenol

6	0	0.068095	0.487814	-0.000116
6	0	-1.309499	0.357059	-0.000089
6	0	-1.911495	-0.918948	0.000007
6	0	-1.104672	-2.045176	0.000073
6	0	0.283072	-1.910061	0.000049
6	0	0.897153	-0.653433	-0.000037
1	0	0.513314	1.473239	-0.000211
1	0	-1.575975	-3.020553	0.000149
1	0	0.900662	-2.801483	0.000106
8	0	-3.266525	-1.035928	0.000033
8	0	-2.218941	1.387900	-0.000185
6	0	-1.732134	2.722877	0.000174
6	0	2.363371	-0.573785	-0.000041
1	0	-3.628795	-0.139760	-0.000007
1	0	-2.611802	3.364410	0.000317
1	0	-1.133406	2.926467	-0.894073
1	0	-1.133441	2.925993	0.894552
6	0	3.133411	0.520540	-0.000029
6	0	4.632895	0.506137	0.000045
1	0	2.863326	-1.541341	-0.000057
1	0	5.023858	-0.514134	-0.000521
1	0	5.036425	1.024037	-0.878060
1	0	5.036310	1.022992	0.878828
1	0	2.672064	1.506222	-0.000028

CBS-QB3 (0 K)= -537.781859 CBS-QB3 Energy= -537.769608
CBS-QB3 Enthalpy= -537.768664 CBS-QB3 Free Energy= -537.821281

trans-Isoeugenol Radical

6	0	-0.064855	-0.919568	-0.000414
6	0	-1.383628	-0.482852	-0.000365
6	0	-1.686256	0.957379	-0.000352
6	0	-0.528854	1.836030	0.000050
6	0	0.749509	1.371544	0.000149
6	0	1.021194	-0.034327	-0.000103
1	0	0.106650	-1.989953	-0.000638
1	0	-0.751992	2.896279	0.000116
1	0	1.572635	2.075326	0.000401
8	0	-2.849478	1.406870	-0.001189
8	0	-2.314141	-1.450750	-0.000949
6	0	-3.728321	-1.186078	0.001963
6	0	2.368087	-0.577725	-0.000073
1	0	-4.022659	-0.626199	0.888473
1	0	-4.184750	-2.175127	0.003055
1	0	-4.026332	-0.626486	-0.883513
6	0	3.525985	0.107937	0.000323
6	0	4.883087	-0.522311	0.000223
1	0	2.424617	-1.664393	-0.000392
1	0	4.824152	-1.612610	0.000541
1	0	5.461036	-0.210541	-0.877500
1	0	5.461450	-0.210005	0.877468
1	0	3.508462	1.194566	0.000686

CBS-QB3 (0 K)= -537.152038 CBS-QB3 Energy= -537.139979
CBS-QB3 Enthalpy= -537.139034 CBS-QB3 Free Energy= -537.191271

Mulliken atomic spin densities:

		1
1	C	-0.620661
2	C	0.619152
3	C	-0.421829
4	C	0.591991
5	C	-0.565511
6	C	0.623426
7	H	0.054052
8	H	-0.053684
9	H	0.051021
10	O	0.600733
11	O	0.041853
12	C	-0.002008
13	C	-0.581578
14	H	0.001504
15	H	-0.001140
16	H	0.001508
17	C	0.656787
18	C	-0.043144
19	H	0.046304
20	H	0.002614
21	H	0.024278
22	H	0.024233
23	H	-0.049901

cis-Isoeugenol

6	0	-0.256927	0.354331	-0.237683
6	0	1.118512	0.358084	-0.058123
6	0	1.819387	-0.846524	0.140003
6	0	1.119320	-2.044342	0.137916
6	0	-0.260376	-2.046731	-0.050166
6	0	-0.978632	-0.856894	-0.222161
1	0	-0.776241	1.281826	-0.428244
1	0	1.670751	-2.966052	0.279340
1	0	-0.792399	-2.991623	-0.053399
8	0	3.168304	-0.834854	0.314615
8	0	1.930034	1.468362	-0.063041
6	0	1.337456	2.743650	-0.266889
6	0	-2.435914	-0.926472	-0.419882
1	0	3.452552	0.087810	0.266959
1	0	2.152428	3.464438	-0.225053
1	0	0.849927	2.803296	-1.245803
1	0	0.609073	2.972911	0.518235
6	0	-3.391969	-0.048751	-0.082228
6	0	-3.251204	1.253830	0.653388
1	0	-2.771716	-1.849390	-0.888031
1	0	-4.411712	-0.319934	-0.345262
1	0	-3.272753	2.112316	-0.030328
1	0	-4.088656	1.388127	1.344571
1	0	-2.325879	1.307138	1.229370

CBS-QB3 (0 K)= -537.778578 CBS-QB3 Energy= -537.766599
CBS-QB3 Enthalpy= -537.765655 CBS-QB3 Free Energy= -537.816879

cis-Isoeugenol Radical

6	0	0.377570	-0.449916	-0.195109
6	0	-1.006722	-0.420139	-0.075464
6	0	-1.716351	0.856079	0.114735
6	0	-0.874834	2.037591	0.130459
6	0	0.477967	1.970800	-0.003542
6	0	1.154716	0.716717	-0.148456
1	0	0.828639	-1.417119	-0.363309
1	0	-1.394165	2.980432	0.255308
1	0	1.071263	2.878981	0.012814
8	0	-2.954604	0.929029	0.245260
8	0	-1.614335	-1.614849	-0.151915
6	0	-3.042547	-1.782690	-0.090490
6	0	2.604139	0.743883	-0.270544
1	0	-3.538071	-1.237522	-0.892949
1	0	-3.189876	-2.855651	-0.207843
1	0	-3.438475	-1.441506	0.864806
6	0	3.518730	-0.227152	-0.066070
6	0	3.314238	-1.636517	0.404622
1	0	3.001307	1.719048	-0.542660
1	0	4.553879	0.053814	-0.242818
1	0	3.174428	-2.324570	-0.439009
1	0	4.195092	-1.984097	0.949866
1	0	2.446056	-1.737195	1.058191

CBS-QB3 (0 K)= -537.147304 CBS-QB3 Energy= -537.135430
CBS-QB3 Enthalpy= -537.134486 CBS-QB3 Free Energy= -537.186515

Mulliken atomic spin densities:

		1
1	C	-0.582039
2	C	0.612925
3	C	-0.432258
4	C	0.619742
5	C	-0.603147
6	C	0.609469
7	H	0.053881
8	H	-0.052995
9	H	0.048288
10	O	0.604969
11	O	0.042232
12	C	-0.001284
13	C	-0.584711
14	H	0.001223
15	H	-0.001036
16	H	0.001457
17	C	0.664510
18	C	-0.048396
19	H	0.051007
20	H	-0.055832
21	H	0.031803
22	H	0.009344
23	H	0.010847

endo-Allylic radical

6	0	-2.443497	-0.956326	0.218430
6	0	-3.448240	0.026944	0.073387
6	0	-3.375016	1.298225	-0.425006
6	0	-1.014860	-0.860991	0.112850
6	0	-0.262558	-2.054259	0.022910
6	0	1.120347	-2.041522	-0.082491
1	0	-2.808255	-1.955539	0.439091
1	0	-4.440171	-0.307870	0.371983
1	0	-4.263390	1.915969	-0.471505
1	0	-2.471609	1.716802	-0.847026
1	0	-0.785711	-3.003867	0.022652
1	0	1.688936	-2.960161	-0.161996
6	0	1.808249	-0.833304	-0.084345
6	0	1.082965	0.372424	0.034354
6	0	-0.295326	0.363995	0.130704
8	0	1.886686	1.485958	0.053606
6	0	1.274766	2.764880	0.163906
1	0	0.600776	2.953712	-0.678185
1	0	2.087216	3.489312	0.147461
1	0	0.721350	2.859744	1.103874
8	0	3.161508	-0.810475	-0.182820
1	0	3.433834	0.117035	-0.152150
1	0	-0.829502	1.290613	0.271314

CBS-QB3 (0 K)= -537.146618 CBS-QB3 Energy= -537.135001
CBS-QB3 Enthalpy= -537.134056 CBS-QB3 Free Energy= -537.184764

Mulliken atomic spin densities:

		1
1	C	0.861439
2	C	-0.687343
3	C	0.905991
4	C	-0.659833
5	C	0.602669
6	C	-0.569654
7	H	-0.077405
8	H	0.048923
9	H	-0.059334
10	H	-0.056257
11	H	-0.055939

12	H	0.048388
13	C	0.542174
14	C	-0.477336
15	C	0.661120
16	O	-0.006594
17	C	0.001696
18	H	-0.001639
19	H	0.000676
20	H	-0.002660
21	O	0.028580
22	H	-0.001519
23	H	-0.046143

endo-Allylic radical

6	0	-2.402243	-0.593660	-0.000126
6	0	-3.201865	0.564520	-0.000148
6	0	-4.567533	0.566042	-0.000187
6	0	1.844996	-0.917100	-0.000006
6	0	1.236693	0.359144	-0.000021
6	0	-0.137386	0.486800	-0.000065
6	0	-0.973085	-0.663885	-0.000084
6	0	-0.340051	-1.927594	-0.000068
6	0	1.041783	-2.051487	-0.000030
8	0	2.144545	1.389271	-0.000035
6	0	1.657415	2.725024	0.000530
1	0	1.058815	2.927611	-0.893785
1	0	2.537130	3.366235	0.000782
1	0	1.058829	2.926853	0.895024
8	0	3.198318	-1.028821	0.000033
1	0	3.558532	-0.131401	0.000093
1	0	-2.923874	-1.547579	-0.000144
1	0	-2.703737	1.531390	-0.000133
1	0	-5.131932	1.489728	-0.000204
1	0	-5.132403	-0.360135	-0.000205
1	0	-0.583687	1.471024	-0.000096
1	0	-0.953921	-2.821147	-0.000083
1	0	1.521003	-3.023013	-0.000010

CBS-QB3 (0 K)= -537.151948 CBS-QB3 Energy= -537.140189
CBS-QB3 Enthalpy= -537.139244 CBS-QB3 Free Energy= -537.190249

Mulliken atomic spin densities:

		1
1	C	0.796319
2	C	-0.640555
3	C	0.858561
4	C	0.561879
5	C	-0.451730
6	C	0.607192
7	C	-0.588938
8	C	0.621609
9	C	-0.580588
10	O	-0.006972
11	C	0.001304
12	H	-0.002023
13	H	0.000566
14	H	-0.002025
15	O	0.028803
16	H	-0.001452
17	H	-0.066512
18	H	0.045949
19	H	-0.061784
20	H	-0.057174
21	H	-0.053619
22	H	-0.057712
23	H	0.048901

The structure and energy of substrates, phenoxy radicals, allylic radicals and coupling reaction products calculated at M06/6-31++G level of theory.**

Eugenol

6	0	-2.407811	-0.851246	-0.418825
6	0	-3.131120	0.044021	0.539036
6	0	-3.935069	1.044360	0.180689
6	0	1.877076	-0.797735	0.087700
6	0	1.157983	0.402175	-0.044749
6	0	-0.219989	0.380577	-0.199005
6	0	-0.910247	-0.839965	-0.226549
6	0	-0.188777	-2.020910	-0.089222
6	0	1.198230	-2.003418	0.064965
8	0	1.937459	1.523942	0.000144
6	0	1.297564	2.774461	-0.123398
1	0	0.806513	2.873868	-1.101229
1	0	2.076779	3.533086	-0.031381
1	0	0.553160	2.918964	0.671260
8	0	3.224438	-0.776607	0.241614
1	0	3.515237	0.146414	0.232727
1	0	-2.662782	-0.553339	-1.447725
1	0	-2.765566	-1.884308	-0.298156
1	0	-2.955924	-0.153166	1.599442
1	0	-4.439795	1.666966	0.915123
1	0	-4.123361	1.268681	-0.869481
1	0	-0.782629	1.307254	-0.296051
1	0	-0.713165	-2.975067	-0.105510
1	0	1.769317	-2.921956	0.173076

Zero-point correction= 0.198055
(Hartree/Particle)
Thermal correction to Energy= 0.209807
Thermal correction to Enthalpy= 0.210751
Thermal correction to Gibbs Free Energy= 0.159875
Sum of electronic and zero-point Energies= -538.168034
Sum of electronic and thermal Energies= -538.156282
Sum of electronic and thermal Enthalpies= -538.155338
Sum of electronic and thermal Free Energies= -538.206214

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -538.382254

Eugenol Radical

6	0	-2.591162	0.690586	-0.180013
6	0	-3.239553	-0.479462	0.490536
6	0	-4.025113	-1.360930	-0.125045
6	0	1.773916	0.811381	0.027317
6	0	1.041719	-0.457348	-0.036732
6	0	-0.351726	-0.465698	-0.086177
6	0	-1.088551	0.712211	-0.081052
6	0	-0.404682	1.957806	-0.021224
6	0	0.957812	2.006443	0.028203
8	0	1.622511	-1.659032	-0.053749
6	0	3.036320	-1.849797	-0.005369
1	0	3.169601	-2.932446	-0.052158
1	0	3.456224	-1.451947	0.922044
1	0	3.531993	-1.364368	-0.849592
8	0	3.020875	0.871397	0.079623
1	0	-2.979844	1.626384	0.249444
1	0	-2.882897	0.704762	-1.242779
1	0	-3.033387	-0.594514	1.557171
1	0	-4.483354	-2.189960	0.407871
1	0	-4.241380	-1.279726	-1.190090
1	0	-0.851112	-1.432037	-0.135259
1	0	-0.988937	2.877284	-0.013984
1	0	1.502121	2.946505	0.077677

Zero-point correction= 0.184560
(Hartree/Particle)
Thermal correction to Energy= 0.196406
Thermal correction to Enthalpy= 0.197351
Thermal correction to Gibbs Free Energy= 0.144957
Sum of electronic and zero-point Energies= -537.540665
Sum of electronic and thermal Energies= -537.528818
Sum of electronic and thermal Enthalpies= -537.527874
Sum of electronic and thermal Free Energies= -537.580268

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -537.737847

trans-Isoeugenol

6	0	-0.181363	0.768760	0.000038
6	0	-1.475071	0.269051	0.000031
6	0	-1.696508	-1.115490	0.000025
6	0	-0.609238	-1.977402	-0.000056
6	0	0.686630	-1.474271	-0.000082
6	0	0.926301	-0.096247	-0.000042
1	0	-0.007258	1.842757	0.000055
1	0	-0.800152	-3.047592	-0.000066
1	0	1.521112	-2.171672	-0.000130
8	0	-2.957106	-1.613237	0.000108
8	0	-2.620632	1.015852	0.000059
6	0	-2.494218	2.419683	-0.000095
6	0	2.266299	0.494228	-0.000024
1	0	-3.575479	-0.868779	0.000010
1	0	-3.508443	2.822755	-0.000121
1	0	-1.964866	2.770573	-0.896480
1	0	-1.964862	2.770804	0.896195
6	0	3.443801	-0.143471	-0.000092
6	0	4.766096	0.544258	0.000106
1	0	2.286340	1.588373	0.000129
1	0	4.646707	1.633839	0.000059
1	0	5.363068	0.269491	0.879883
1	0	5.363368	0.269430	-0.879445
1	0	3.465997	-1.235488	-0.000280

Zero-point correction= 0.197094
(Hartree/Particle)
Thermal correction to Energy= 0.209374
Thermal correction to Enthalpy= 0.210318
Thermal correction to Gibbs Free Energy= 0.158429
Sum of electronic and zero-point Energies= -538.177582

Sum of electronic and thermal Energies= -538.165303
Sum of electronic and thermal Enthalpies= -538.164359
Sum of electronic and thermal Free Energies= -538.216247

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -538.389286

cis-Isoeugenol

6	0	-0.252752	-0.912353	-0.131690
6	0	-1.417182	-0.175623	0.010543
6	0	-1.375113	1.227992	-0.022811
6	0	-0.161113	1.866879	-0.213722
6	0	1.009596	1.124593	-0.352843
6	0	0.989704	-0.272346	-0.297512
1	0	-0.281708	-1.999617	-0.105447
1	0	-0.150719	2.952627	-0.263292
1	0	1.943945	1.644864	-0.544157
8	0	-2.511894	1.952766	0.113517
8	0	-2.671667	-0.688852	0.188010
6	0	-2.814356	-2.091371	0.199421
6	0	2.186525	-1.108009	-0.444077
1	0	-3.250578	1.338250	0.229708
1	0	-2.497700	-2.529328	-0.757052
1	0	-3.875212	-2.294499	0.355970
1	0	-2.234261	-2.543365	1.015488
6	0	3.444603	-0.847170	-0.054934
6	0	3.947057	0.353240	0.677843
1	0	2.006832	-2.080416	-0.908414
1	0	4.189235	-1.613927	-0.273567
1	0	4.715148	0.065453	1.404913
1	0	4.416189	1.079549	-0.001253
1	0	3.145507	0.874101	1.213577

Zero-point correction= 0.197723
(Hartree/Particle)
Thermal correction to Energy= 0.209667
Thermal correction to Enthalpy= 0.210611
Thermal correction to Gibbs Free Energy= 0.159475
Sum of electronic and zero-point Energies= -538.174048
Sum of electronic and thermal Energies= -538.162105
Sum of electronic and thermal Enthalpies= -538.161161
Sum of electronic and thermal Free Energies= -538.212297

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -538.385918

trans-Isoeugenol Radical

6	0	0.067349	-0.924562	0.000462
6	0	1.382286	-0.484518	0.000375
6	0	1.678694	0.953420	0.000577
6	0	0.522452	1.830228	-0.000789
6	0	-0.754474	1.363428	-0.000990
6	0	-1.019759	-0.041317	-0.000071
1	0	-0.104990	-1.999754	0.000831
1	0	0.746301	2.894403	-0.001322
1	0	-1.584449	2.066407	-0.001769
8	0	2.838379	1.407540	0.001833
8	0	2.314821	-1.443497	0.000352
6	0	3.715975	-1.175064	-0.001464
6	0	-2.360967	-0.583300	0.000276
1	0	4.010886	-0.607118	-0.887355
1	0	4.184889	-2.161364	-0.007201
1	0	4.014547	-0.615980	0.888858
6	0	-3.515730	0.111420	-0.000503
6	0	-4.864356	-0.515178	0.000310
1	0	-2.424415	-1.674630	0.001354
1	0	-4.797783	-1.608483	0.000130
1	0	-5.445852	-0.208073	0.879602
1	0	-5.447155	-0.207762	-0.877980
1	0	-3.486398	1.202669	-0.001723

Zero-point correction= 0.184219
(Hartree/Particle)
Thermal correction to Energy= 0.196408
Thermal correction to Enthalpy= 0.197352
Thermal correction to Gibbs Free Energy= 0.144495
Sum of electronic and zero-point Energies= -537.554474
Sum of electronic and thermal Energies= -537.542285
Sum of electronic and thermal Enthalpies= -537.541341
Sum of electronic and thermal Free Energies= -537.594198

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -537.748957

endo-Allylic Radical

6	0	-0.384747	-0.447976	-0.185497
6	0	0.997274	-0.420164	-0.071070
6	0	1.707952	0.853200	0.111966
6	0	0.872804	2.037495	0.119175
6	0	-0.480013	1.973531	-0.009392
6	0	-1.158276	0.721041	-0.141477
1	0	-0.841196	-1.419042	-0.350724
1	0	1.398009	2.982258	0.236744
1	0	-1.075821	2.885142	0.001926
8	0	2.944157	0.924041	0.245799
8	0	1.603608	-1.610321	-0.144216
6	0	3.020086	-1.775651	-0.096782
6	0	-2.601992	0.747978	-0.256381
1	0	3.426671	-1.443567	0.861530
1	0	3.176126	-2.848649	-0.226884
1	0	3.513279	-1.218622	-0.897553
6	0	-3.504653	-0.238751	-0.060776
6	0	-3.267043	-1.641146	0.388738
1	0	-3.009303	1.727742	-0.512933
1	0	-4.547365	0.033973	-0.227151
1	0	-2.425931	-1.715625	1.087151
1	0	-4.157149	-2.043368	0.882580
1	0	-3.047782	-2.307347	-0.458382

Zero-point correction= 0.184914
(Hartree/Particle)
Thermal correction to Energy= 0.196753
Thermal correction to Enthalpy= 0.197698
Thermal correction to Gibbs Free Energy= 0.145649
Sum of electronic and zero-point Energies= -537.549107
Sum of electronic and thermal Energies= -537.537267
Sum of electronic and thermal Enthalpies= -537.536323
Sum of electronic and thermal Free Energies= -537.588371

exo-Allylic Radical

6	0	2.290596	0.577750	0.000000
6	0	3.533988	-0.080922	-0.000034
6	0	4.738108	0.561905	-0.000031
6	0	-1.597119	-1.138173	-0.000018
6	0	-1.419100	0.258790	-0.000012
6	0	-0.149035	0.800390	0.000000
6	0	0.998606	-0.032367	0.000023
6	0	0.794603	-1.428936	0.000069
6	0	-0.482707	-1.968065	0.000050
8	0	-2.590341	0.961255	-0.000004
6	0	-2.516318	2.369736	0.000025
1	0	-2.000574	2.739284	0.896570
1	0	-3.544958	2.734002	0.000058
1	0	-2.000624	2.739319	-0.896535
8	0	-2.840176	-1.671966	-0.000089
1	0	-3.481322	-0.946335	0.000079
1	0	2.313967	1.670515	0.000011
1	0	3.539315	-1.172428	-0.000054
1	0	5.676730	0.015854	-0.000027
1	0	4.792656	1.649697	-0.000017
1	0	-0.008051	1.879036	-0.000002
1	0	1.649239	-2.100553	0.000138
1	0	-0.641981	-3.043346	0.000083

Zero-point correction= 0.184259
(Hartree/Particle)
Thermal correction to Energy= 0.196065
Thermal correction to Enthalpy= 0.197009
Thermal correction to Gibbs Free Energy= 0.145940
Sum of electronic and zero-point Energies= -537.553942
Sum of electronic and thermal Energies= -537.542137
Sum of electronic and thermal Enthalpies= -537.541193
Sum of electronic and thermal Free Energies= -537.592261

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -537.751871

cis-C-centered radical

6	0	-2.199434	-1.113610	-0.248073
6	0	-3.560429	-0.783331	-0.069967
6	0	-4.116984	0.346099	0.463480
6	0	-1.033877	-0.282077	-0.159209
6	0	-1.054412	1.126158	-0.217208
6	0	0.117680	1.866449	-0.144755
1	0	-1.997620	-2.161567	-0.478521
1	0	-4.256715	-1.571154	-0.365122
1	0	-3.524811	1.153596	0.885205
1	0	-5.196785	0.440229	0.539305
1	0	-1.995661	1.642921	-0.373912
1	0	0.103270	2.951777	-0.201717
6	0	1.344824	1.230470	-0.017062
6	0	1.394005	-0.176391	0.016371
6	0	0.230904	-0.916215	-0.059090
8	0	2.659528	-0.679288	0.124118
6	0	2.814535	-2.081001	0.120143
1	0	2.307926	-2.539367	0.980255
1	0	3.886313	-2.274881	0.188166
1	0	2.423239	-2.518293	-0.808524
8	0	2.482348	1.958414	0.054747
1	0	3.230096	1.347404	0.126162
1	0	0.264868	-2.002977	-0.029987

Zero-point correction= 0.184803
(Hartree/Particle)
Thermal correction to Energy= 0.196453
Thermal correction to Enthalpy= 0.197397
Thermal correction to Gibbs Free Energy= 0.146730
Sum of electronic and zero-point Energies= -537.548250

Sum of electronic and thermal Energies= -537.536600
Sum of electronic and thermal Enthalpies= -537.535656
Sum of electronic and thermal Free Energies= -537.586324

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -537.746307

Eugenol radical coupling product

(coupling at C9 position)

6	0	-2.716768	-1.790392	-1.489507
6	0	-2.259288	-2.844179	-0.533771
6	0	-0.941855	-2.729005	0.129697
6	0	-3.383253	1.851904	0.729684
6	0	-2.138967	1.604170	0.128550
6	0	-1.938013	0.446638	-0.612419
6	0	-2.970551	-0.488970	-0.757800
6	0	-4.197509	-0.237349	-0.149136
6	0	-4.406926	0.929650	0.585671
8	0	-1.208794	2.579116	0.344761
6	0	0.087634	2.379840	-0.182137
1	0	0.067304	2.329388	-1.279752
1	0	0.542893	1.456692	0.207086
1	0	0.686443	3.238819	0.126361
8	0	-3.583553	2.987698	1.445275
1	0	-2.760947	3.497798	1.432132
1	0	-3.632508	-2.115158	-1.998333
1	0	-1.952223	-1.631644	-2.264804
1	0	-0.905234	-1.831424	0.775459
1	0	-0.726843	-3.598011	0.761954
1	0	-0.973944	0.257651	-1.082199
1	0	-5.005070	-0.961358	-0.251547
1	0	-5.364250	1.140837	1.055724
8	0	0.084642	-2.604253	-0.874321
6	0	1.083759	-1.704233	-0.675268
6	0	1.394747	-0.835820	-1.715472
6	0	1.861027	-1.668116	0.500145
6	0	2.437678	0.079916	-1.604640
1	0	0.795488	-0.903117	-2.621955
6	0	2.891269	-0.733278	0.610389
6	0	3.189881	0.144746	-0.435754
1	0	2.658518	0.758816	-2.427991
1	0	3.498026	-0.694223	1.512912
6	0	4.280308	1.174946	-0.277279
6	0	3.733523	2.488660	0.196270
1	0	4.801080	1.322892	-1.233388
1	0	5.026872	0.805150	0.441188
6	0	3.810793	3.631456	-0.483834
1	0	3.220978	2.468080	1.162526
1	0	4.310039	3.680681	-1.451421
1	0	3.387636	4.557437	-0.101399
6	0	2.332684	-2.596790	2.631902
1	0	3.391238	-2.799404	2.417619
1	0	2.247927	-1.644872	3.174499
1	0	1.933534	-3.400203	3.253550
8	0	1.562118	-2.588913	1.452282
1	0	-2.983293	-3.546775	-0.123947

Zero-point correction= 0.386462
(Hartree/Particle)
Thermal correction to Energy= 0.410429
Thermal correction to Enthalpy= 0.411373
Thermal correction to Gibbs Free Energy= 0.330140
Sum of electronic and zero-point Energies= -1075.706921
Sum of electronic and thermal Energies= -1075.682955
Sum of electronic and thermal Enthalpies= -1075.682010
Sum of electronic and thermal Free Energies= -1075.763244

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -1076.126511

Eugenol radical coupling product

(coupling at C8 position)

6	0	1.568346	1.001903	-0.743149
6	0	0.516187	0.106506	-0.075751
6	0	0.823811	-0.176380	1.349278
6	0	2.925633	0.361378	-0.776469
6	0	3.273513	-0.522366	-1.794871
6	0	4.515045	-1.157794	-1.802459
1	0	1.594008	1.952618	-0.192606
1	0	1.216570	1.225112	-1.759107
1	0	1.426852	-1.033056	1.635977
1	0	0.549736	0.559474	2.102787
1	0	2.565972	-0.715428	-2.600585
1	0	4.798118	-1.843839	-2.596643
1	0	0.456134	-0.836972	-0.650144
8	0	-0.710039	0.820507	-0.208236
6	0	-1.872653	0.181428	0.079186
6	0	-1.985866	-1.133685	0.507991
6	0	-3.048485	0.947044	-0.101779
6	0	-3.243359	-1.696614	0.753489
1	0	-1.095363	-1.735669	0.665392
6	0	-4.288104	0.374414	0.146310
6	0	-4.400985	-0.955261	0.579956
1	0	-3.306351	-2.730162	1.090340
1	0	-5.197664	0.953411	-0.000822
6	0	-5.765200	-1.540364	0.852915
6	0	-6.696654	-1.416763	-0.313371
1	0	-6.222714	-1.051941	1.727271
1	0	-5.642957	-2.601255	1.116755
6	0	-7.877189	-0.799992	-0.277716
1	0	-6.347793	-1.858991	-1.249704
1	0	-8.247278	-0.342425	0.640065
1	0	-8.518134	-0.735470	-1.153399
8	0	-2.859528	2.221077	-0.523897
6	0	5.424328	-0.913172	-0.786627
6	0	5.085712	-0.023921	0.246264
6	0	3.848128	0.605039	0.249688
8	0	6.064727	0.138015	1.185635
6	0	5.825542	1.050744	2.233538
1	0	4.956935	0.747966	2.834183
1	0	5.661605	2.064982	1.844384
1	0	6.718018	1.044249	2.861624
8	0	6.634215	-1.525346	-0.796961
1	0	7.131059	-1.228446	-0.021420
1	0	3.577322	1.292447	1.049737
6	0	-4.000791	3.022954	-0.710216
1	0	-3.639251	3.995226	-1.050577
1	0	-4.672553	2.600946	-1.471183
1	0	-4.559027	3.152613	0.228100

Zero-point correction= 0.383651
(Hartree/Particle)
Thermal correction to Energy= 0.407696
Thermal correction to Enthalpy= 0.408640
Thermal correction to Gibbs Free Energy= 0.326643
Sum of electronic and zero-point Energies= -1075.705591
Sum of electronic and thermal Energies= -1075.681547
Sum of electronic and thermal Enthalpies= -1075.680602
Sum of electronic and thermal Free Energies= -1075.762600

Total free energy in solution:
- with all non electrostatic terms (a.u.) = -1076.127980

Isoeugenol radical coupling product

6	0	-1.087321	0.981038	-0.856777
6	0	-0.380288	2.163911	-0.799544
6	0	-0.819678	3.229955	0.014280
6	0	-1.974213	3.080856	0.776070
6	0	-2.680169	1.890701	0.739294
6	0	-2.262644	0.800954	-0.070469
1	0	-0.725281	0.165590	-1.477208
1	0	-2.295239	3.914042	1.396368
1	0	-3.576165	1.773743	1.346218
8	0	-0.119360	4.387468	0.058313
8	0	0.772597	2.436631	-1.474868
6	0	1.371929	1.386613	-2.209724
6	0	-2.990645	-0.404582	-0.034005
1	0	0.644922	4.297156	-0.530300
1	0	0.726229	1.067207	-3.039087
1	0	2.305265	1.785091	-2.611423
1	0	1.589473	0.525752	-1.562346
6	0	-2.684627	-1.658729	-0.773358
6	0	-3.932586	-2.462374	-1.057727
1	0	-3.822880	-0.460022	0.671674
1	0	-2.159551	-1.438782	-1.718925
1	0	-4.635655	-1.874626	-1.657891
1	0	-3.687147	-3.384265	-1.594294
1	0	-4.421814	-2.732798	-0.114418
8	0	-1.821754	-2.543152	0.000339
6	0	-0.497449	-2.219029	-0.004890
6	0	0.322087	-2.646348	-1.040695
6	0	0.062057	-1.475650	1.055041
6	0	1.677936	-2.327940	-1.061921
1	0	-0.129146	-3.238782	-1.834767
6	0	1.415745	-1.151742	1.024520
6	0	2.237649	-1.556679	-0.040201
1	0	2.305932	-2.667373	-1.884234
1	0	1.852301	-0.590962	1.846553
6	0	-0.330224	-0.174950	2.989205
1	0	-1.197639	0.088439	3.598177
1	0	0.454398	-0.589103	3.638324
1	0	0.047914	0.729567	2.490420
8	0	-0.781187	-1.122385	2.048572
6	0	3.651403	-1.179593	-0.121058
6	0	4.243428	-0.156508	0.509184
1	0	4.258965	-1.789749	-0.795978
6	0	5.689090	0.183820	0.386572
1	0	3.643618	0.490797	1.154575
1	0	6.203638	-0.505704	-0.292186
1	0	5.831892	1.204723	0.008949
1	0	6.194735	0.139214	1.360158

Zero-point correction= 0.386141
(Hartree/Particle)
Thermal correction to Energy= 0.410218
Thermal correction to Enthalpy= 0.411162

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Thermal correction to Gibbs Free Energy=        0.331433
Sum of electronic and zero-point Energies=         -1075.741230
Sum of electronic and thermal Energies=           -1075.717153
Sum of electronic and thermal Enthalpies=         -1075.716209
Sum of electronic and thermal Free Energies=       -1075.795938

Total free energy in solution:
 - with all non electrostatic terms         (a.u.) =   -1076.155731
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