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A Concerted Addition Mechanism in [Hmim]Br Triggered Thiol-Ene "Click" Reactions: A Typical "Ionic Liquid Effect" Revealed by DFT and Experimental Studies

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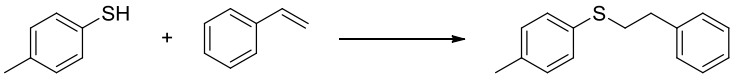
1 Experimental

1.1 Control experiments

We performed control experiments to examine the proposed mechanisms. When adding base (NaOH) into the reaction system, the reaction was severely inhibited (**Table S1**, entries 1 vs. 2), which provide strong evidence for the HBr-mediated reaction channel. The catalytic superiority of [hmim]Br over [hmmim]Br is also verified directly by the distinct reaction yields: 87% in [hmim]Br vs. 62% in [hmmim]Br (**Table S1**, entries 1 vs. 3).

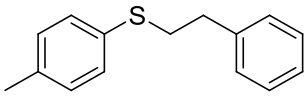
Table S1. Control experiments[a]



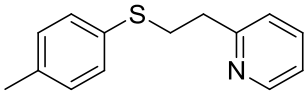
Entry	Solvent	Additive	Yield (%)[b]
1	[hmim]Br	/	87
2	[hmim]Br	NaOH (1.0 equiv)	19
3	[hmmim]Br	/	62

[a] Conditions: styrene 0.50 mmol, 0.55 mmol, 40 °C, 2 h, solvent 1.0 mL. [b] Isolated yields.

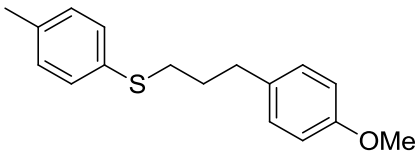
1.2 ^{1}H NMR data



Phenethyl(*p*-tolyl)sulfane,[1] light yellow oil, yield 87%, 99.2 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.17 (m, 7H), 7.13 (d, *J* = 7.8 Hz, 2H), 3.14 (dd, *J* = 9.2, 6.7 Hz, 2H), 2.91 (dd, *J* = 9.3, 6.5 Hz, 2H), 2.34 (s, 3H).



2-(2-(*p*-Tolylthio)ethyl)pyridine,[2] yellow oil, yield 93%, 106.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 – 8.49 (m, 1H), 7.58 (td, *J* = 7.7, 1.9 Hz, 1H), 7.28 (t, *J* = 8.3 Hz, 2H), 7.19 – 6.99 (m, 4H), 3.29 (t, *J* = 7.6 Hz, 2H), 3.07 (t, *J* = 7.6 Hz, 2H), 2.31 (s, 3H).



(3-(4-Methoxyphenyl)propyl)(p-tolyl)sulfane,[2] yellow oil, yield 18%, 24.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.3 Hz, 2H), 7.10 (dd, *J* = 8.4, 2.1 Hz, 4H), 6.84 (d, *J* = 8.6 Hz, 2H), 3.80 (d, *J* = 0.5 Hz, 3H), 2.88 (t, *J* = 7.2 Hz, 2H), 2.70 (t, *J* = 7.5 Hz, 2H), 2.33 (s, 3H), 1.97 – 1.87 (m, 2H).

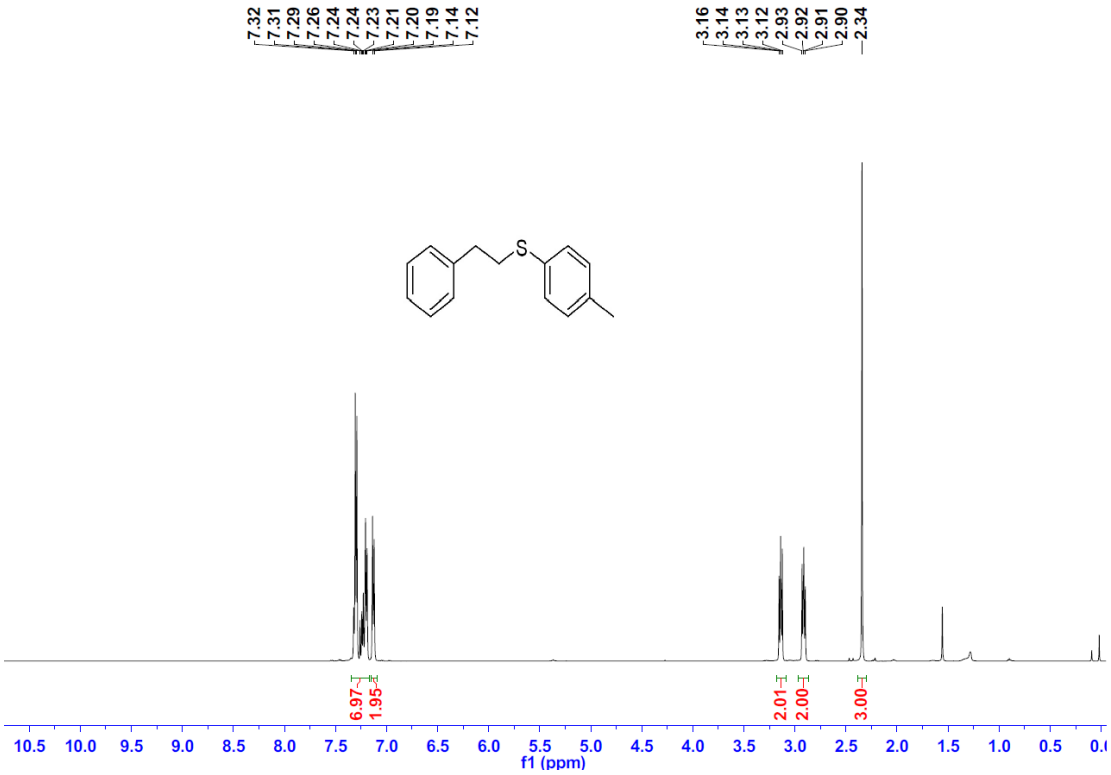
References

(1) Qureshi, Z. S.; Deshmukh, K. M.; Dhake, K. P.; Bhanage, B. M., Bronsted acidic ionic liquid: a simple, efficient and recyclable catalyst for regioselective alkylation of phenols and

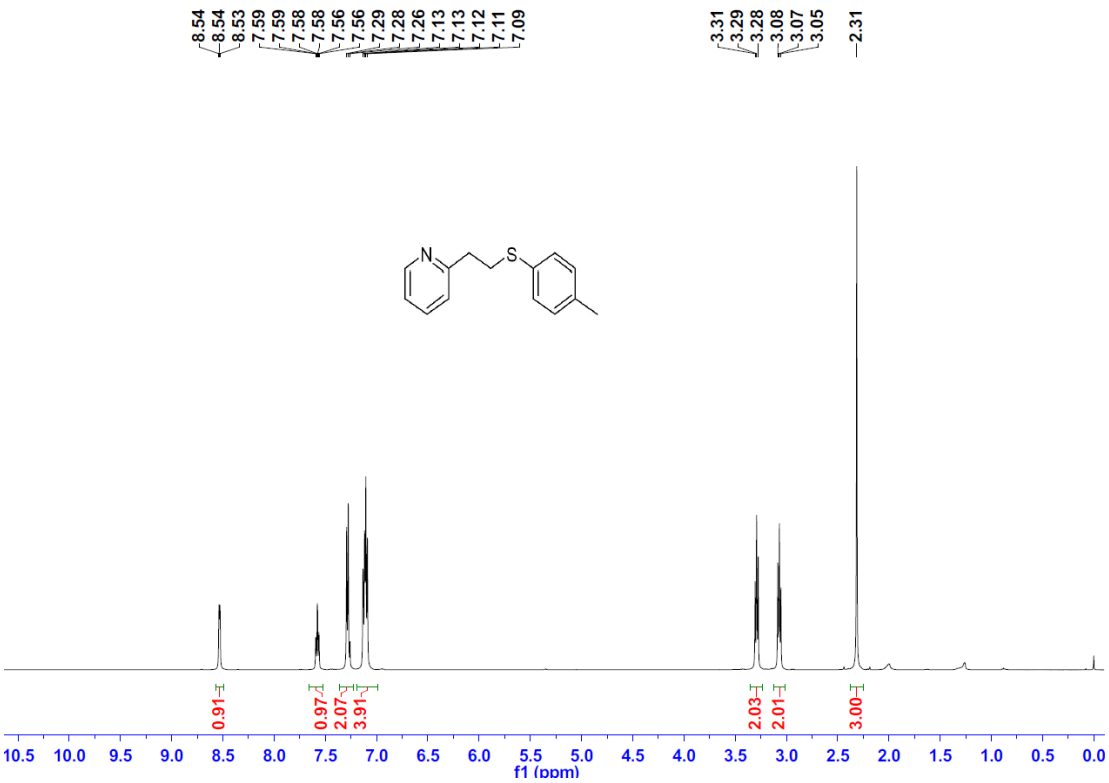
anti-Markovnikov addition of thiols to alkenes. *RSC Advances* **2011,** *1* (6), 1106-1112.

(2) Lin, Y.-m.; Lu, G.-p.; Wang, G.-x.; Yi, W.-b., Acid/Phosphide-Induced Radical Route to Alkyl and Alkenyl Sulfides and Phosphonothioates from Sodium Arylsulfinates in Water. *The Journal of Organic Chemistry* **2017**, *82* (1), 382-389.

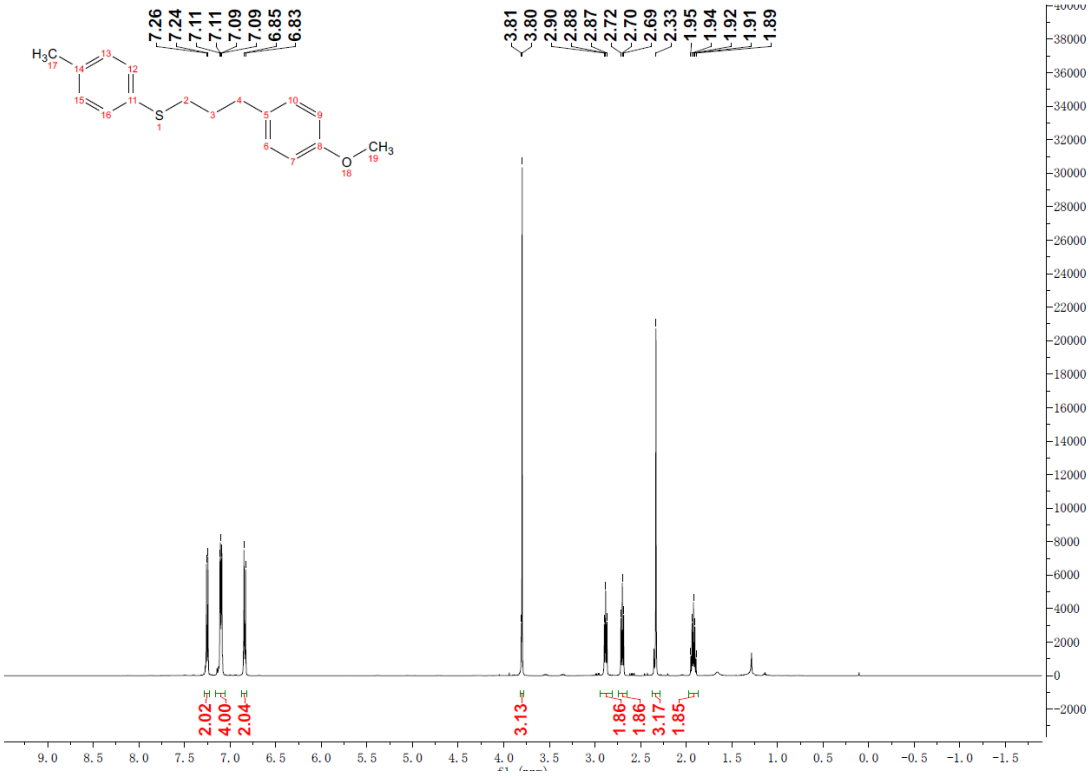
1.3 Copies of ^{1}H NMR spectra



^{1}H NMR of phenethyl(*p*-tolyl)sulfane

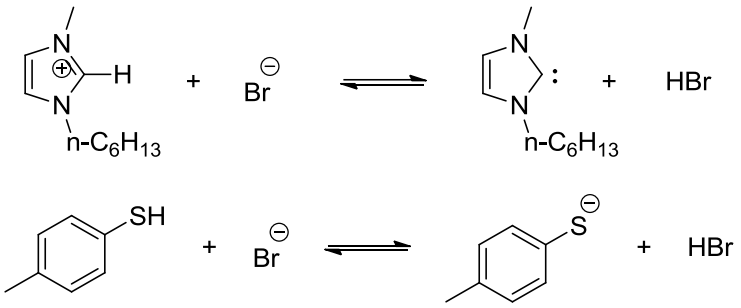


^{1}H NMR of 2-(2-(*p*-tolylthio)ethyl)pyridine



^{1}H NMR of (3-(4-methoxyphenyl)propyl)(p-tolyl)sulfane

1.4 The potential equilibrium for the formation of HBr



Scheme S1. The potential equilibrium for the formation of HBr

1.5 ESI-MS spectra

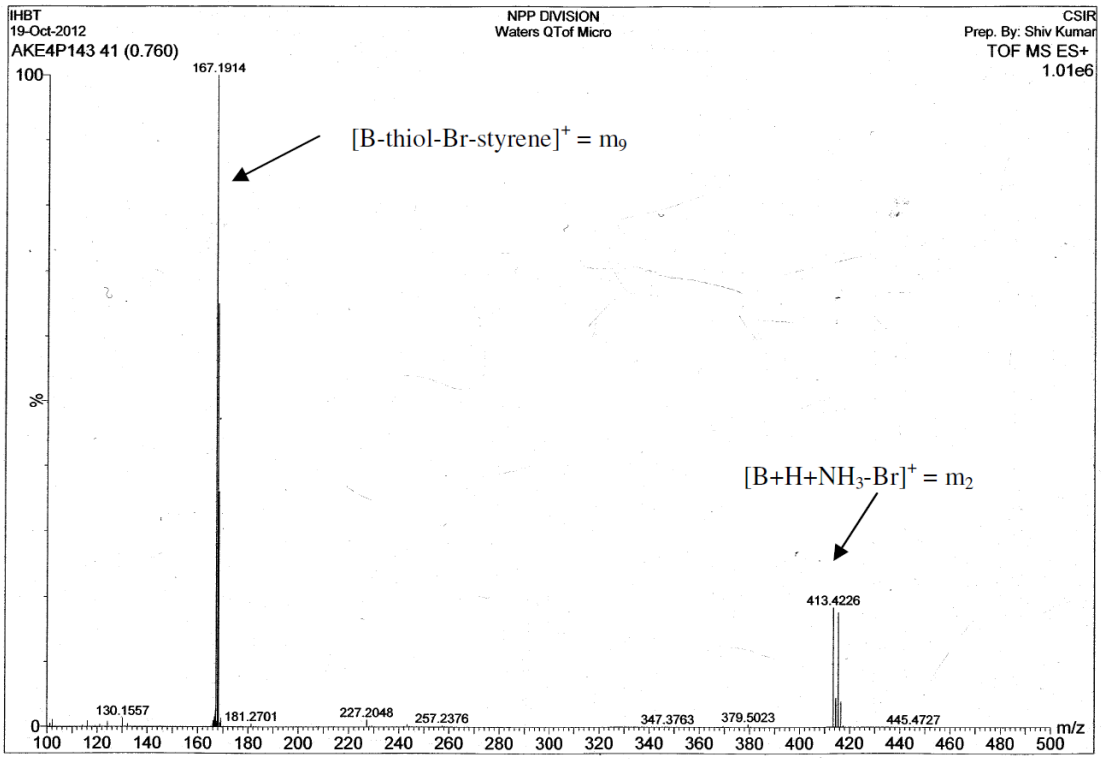


Figure S1

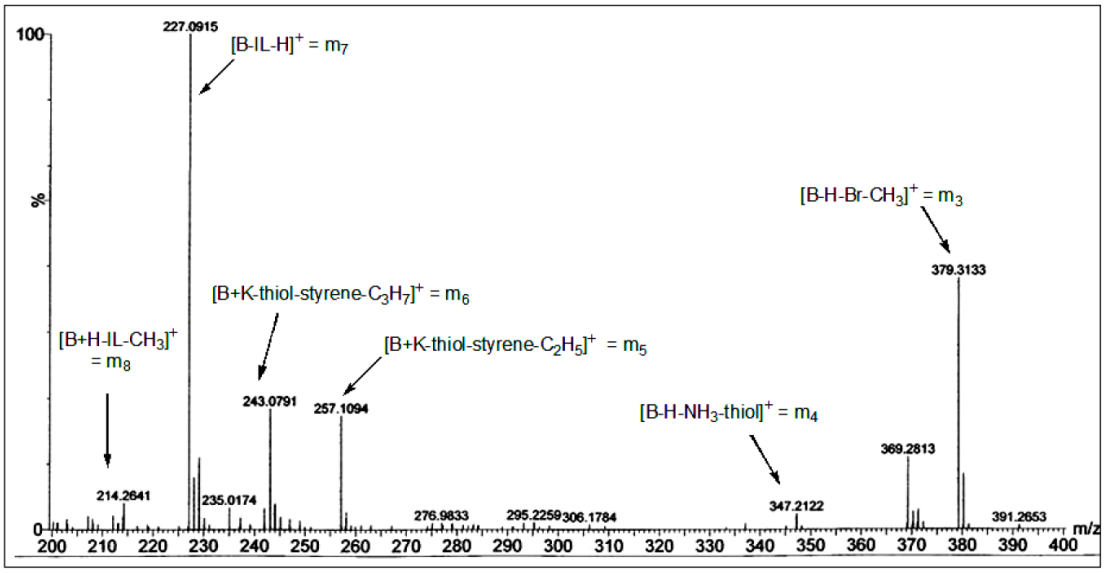


Figure S2

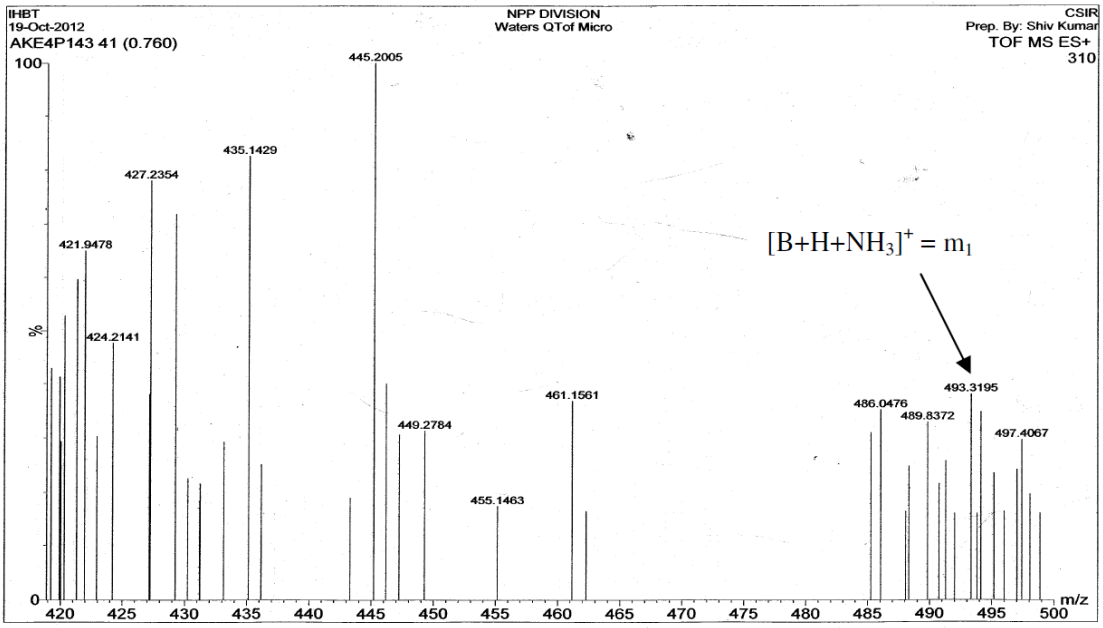


Figure S3

2 DFT calculations

2.1 The Br-mediated reaction channel

In the Br-mediated reaction channel, the Br anion mediates the proton transfer from the S atom to the α-C in concerted with the construction of the C-S bond to yield the final product. The computed free energy profile is illustrated in **Figure S1**. The reaction barrier is 34.4 kcal/mol. In the prereactive complex, the Br anion establishes the H-bond interaction with the S-H of thiol at a distance of 2.29 Å. Meanwhile, the hmim cation is situated above the styrene with its C-2 H pointing to the aromatic ring, indicating the strong π^{+}-π interactions. In the TS, the S-H bond breaks (3.18 Å), and the C-H bond is about to form (1.81 Å). The Br anion is only 1.50 Å away from the transferring proton, indicating its strong mediation effect. In the product complex, the styrene has been hydrothiolated, whereas the hmim cation and Br anion are located near the

product.

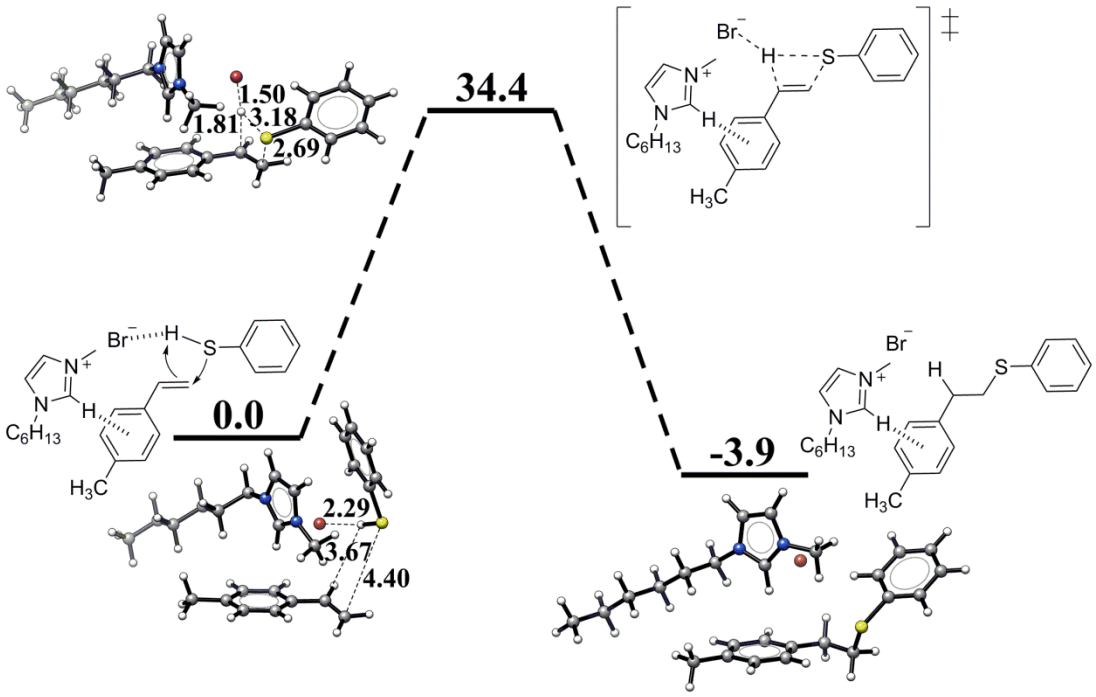


Figure S1. The free energy profile of the Br-mediated reaction channel. Energy reported in kcal/mol and distance reported in Å.

The cleavages and formations of the key bonds along the IRC pathway are shown in Figure S2. At the beginning of reaction, the styrene and thiol get closer to each other and the distance between S atom and the *β*-C of vinyl decreases by ca. 0.5 Å (red line). Afterwards, the breaking of the S-H bond is initiated (black line) by the H-bond interaction induced by the Br anion, as indicated by decrease of Br-H distance (blue line). When the S-H bond breaks almost completely near the TS, the distance between Br anion and transferring proton increases and the new C-H bond (violet line) starts to form. After the construction of C-H bond, the formation of C-S bond (red line) prompts concertedly to generate the product.

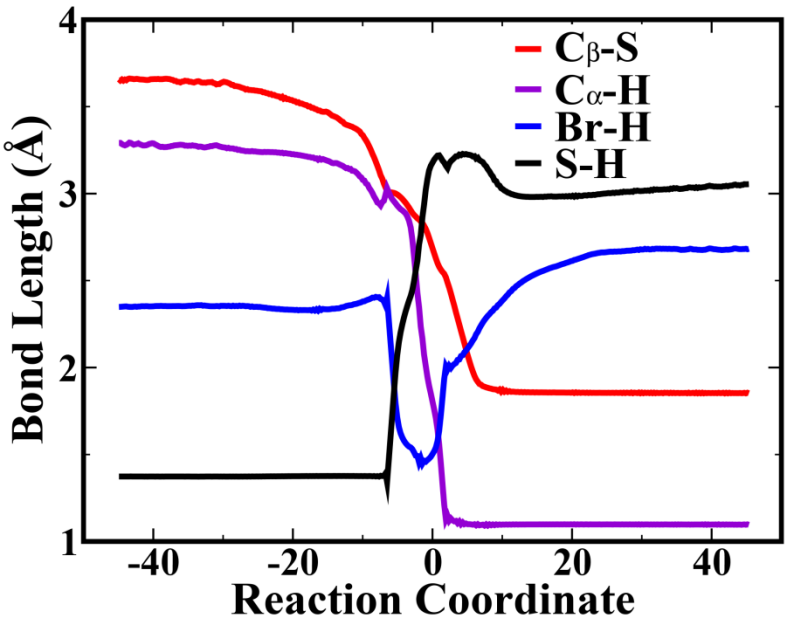


Figure S2. The bond cleavages and formations along the IRC path of the Br-mediated reaction channel.

The enthalpy, entropy and solvation free energy contributions to the reaction barriers of Br-mediated channel and HBr-mediated channel are compared in Table S2. The enthalpy change in gas phase strongly favours the HBr-mediated channel, which mainly accounts for the lower barrier of the HBr-mediated channel. This indicates that the TS of HBr-mediated channel is much more stable than the TS of Br-mediated channel, owing to the 6-membered ring formed at the reaction site of the former.

Table S2. The enthalpy, entropy and solvation free energy contributions to the reaction barriers of Br-mediated channel and HBr-mediated channel.

Reaction Channels	ΔH	-TΔS	ΔG^{vacu}	ΔG^{solv}
Br-mediated channel	41.8	0.8	42.7	-8.3
HBr-mediated channel	18.7	2.7	21.3	-0.5

2.2 Comparison of the computed reaction barriers for the four alkenes

The reactivities of the four thiol-ene systems to a great measure are reflected by the reaction barriers as well as the free energy change when the prereactive complexes are converted to the product complexes, which are compared in Figure S3. The two quantities show similar trends, which fail to follow that of the measured reactivities. For 3-(4-methoxyl-phenyl)propene and 1-octene, they are even lower than those for 2-vinylpyridine and styrene. And for

3-(4-methoxyl-phenyl)propene, the results of dihedral angle scan proved that the vinyl groups gained the rotational freedom due to the absence of the conjugated π ring (Figure S4). Further examination indicates that the solvent effect is the main cause for the lower barriers of the aliphatic alkenes (Table S3). According to the Arrenius theory, the reaction rate should also depend on the frequency factor, which measures how easy the substrates and catalytic molecules can assemble together. To rationalize the experimental kinetic data, we further examine the stabilities of the prereactive complexes.

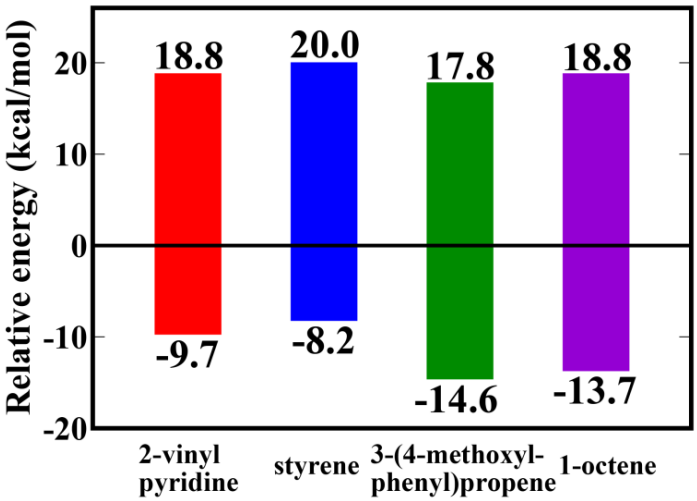


Figure S3. The free energy of the transition states (positive values) and product complex (negative values) relative to the corresponding prereactive complex (kcal/mol) for the four alkenes.

Table S3. The enthalpy, entropy and solvation free energy contributions to the reaction barriers of four alkenes with the 4-methylthiophenol.

Alkenes	ΔH	-TΔS	ΔG^{vacu}	ΔG^{solv}
styrene	17.9	2.4	20.2	-0.3
2-vinylpyridine	17.3	2.5	19.8	-1.0
1-octene	18.3	3.2	21.4	-2.7
3-(4-methoxyl-phenyl)propene	19.5	0.8	20.3	-2.6

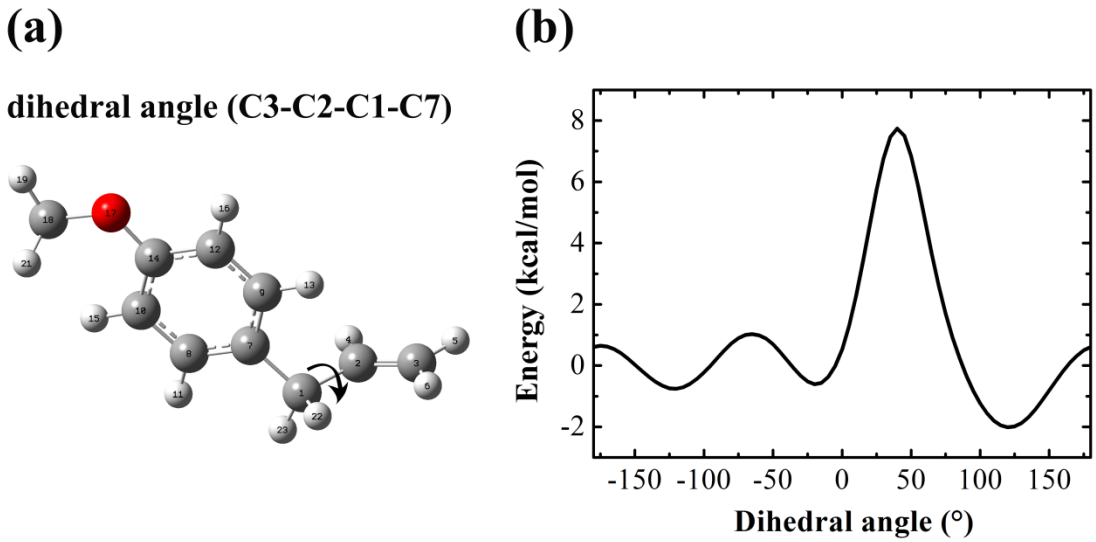


Figure S4. (a) The dihedral angle of 3-(4-methoxyl-phenyl)propene (C3-C2-C1-C7). (b) The scan analysis for C3-C2-C1-C7 dihedral angle.

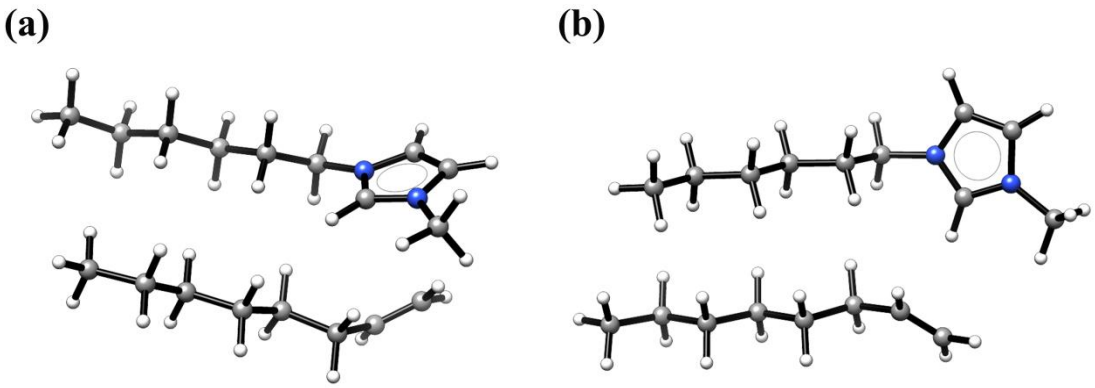


Figure S5. The two optimized conformations formed by 1-octene and IL cation

In Fig. S5a, the C-2 hydrogen of hmim cation points toward the non-functional group and in Fig S5b the C-2 hydrogen points toward the electron-rich C=C double bond. We calculated their Gibbs free energy and found that the Gibbs free energy of S5b is 0.57 kcal/mol lower than that of S5a.

2.3. Solvent descriptors of [hmim]Br and [hmmim]Br used in SMD-GIL solvation model

Table S4. Solvent descriptors of [hmim]Br and [hmmim]Br used in SMD-GIL solvation model.

Solvent	eps	Epsinf	HB Acidity	HB Basicity	Surface Tension At Interface	Carbon Aromaticity	Electronegative Halogenicity
[hmim]Br	11.50	2.0449	0.229	0.265	61.24	0.2308	0.0769
[hmmim]Br						0.2143	0.0714

2.4 The Cartesian coordinates, the number of imaginary frequencies, and computed energies of the optimized structures

2.5.1 The RC, TS and PC of the Br-mediated channel in thiol-styrene reaction

RC1

S	4.022246	-1.095024	-1.017122
C	4.291920	0.499573	-0.273358
C	3.690030	1.664899	-0.776470
C	5.152155	0.595298	0.833146
C	3.951672	2.896364	-0.176894
C	5.409328	1.834612	1.424658
C	4.808968	2.993755	0.924060
H	3.003452	1.593652	-1.613185
H	5.625924	-0.301310	1.223617
H	3.481625	3.789822	-0.579288
H	6.085522	1.892467	2.273189
H	5.015737	3.958342	1.377822
H	2.811440	-0.782808	-1.593792
C	-3.235240	-2.165166	1.067363
C	-0.834395	-3.050023	-0.179338
C	-2.962589	-1.866741	-0.275500
C	-2.284308	-2.914792	1.775966
C	-1.782124	-2.287469	-0.886175
C	-1.108003	-3.348829	1.167179
C	-4.495526	-1.673977	1.735475
C	0.406850	-3.458662	-0.857191
C	1.225572	-4.450248	-0.477135
H	-3.680388	-1.287839	-0.851318
H	-2.468456	-3.159586	2.819158
H	-1.574141	-2.012695	-1.914194
H	-0.388570	-3.917843	1.748520
H	-4.781770	-2.320366	2.570309
H	-4.364862	-0.660030	2.134509
H	-5.331494	-1.638409	1.030482
H	0.652764	-2.868036	-1.737322
H	2.132136	-4.663952	-1.033441
H	1.019710	-5.084161	0.381907
N	1.289944	-0.063541	1.565217
N	-0.091767	1.457524	0.858057
C	1.891110	-1.369107	1.835222
C	0.155201	0.139990	0.882773
C	1.806324	1.162549	1.954447
C	0.941645	2.114428	1.505978
C	-1.148267	2.070307	0.040573

H	1.496967	-1.776238	2.769783
H	1.673008	-2.037676	1.004451
H	-0.457757	-0.626513	0.441366
H	2.758291	1.250056	2.451110
H	0.992253	3.189112	1.551992
H	-0.970609	3.148490	0.055086
Br	0.717133	-0.028052	-2.136486
H	2.970335	-1.240560	1.898001
H	-0.983238	1.703918	-0.979679
C	-2.549579	1.734857	0.544435
C	-3.626048	2.282834	-0.396484
H	-2.686849	2.138298	1.556265
H	-2.654382	0.646953	0.615523
C	-5.046923	1.933475	0.054673
H	-3.526795	3.374618	-0.475919
H	-3.455467	1.884503	-1.405529
H	-5.147530	0.841547	0.116330
H	-5.211587	2.312918	1.073507
C	-6.132642	2.487234	-0.873210
C	-7.548331	2.116266	-0.422585
H	-5.960243	2.113386	-1.891344
H	-6.037924	3.580132	-0.928569
H	-8.304851	2.523736	-1.101062
H	-7.679388	1.028262	-0.391611
H	-7.756484	2.503564	0.581724

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4056.35024385
Thermal correction to enthalpy (Hartree)	0.581683
Entropy (cal/(mol*K))	225.451
Thermal correction to Gibbs free energy (Hartree)	0.474564
Solvation free energy (kcal/mol)	-20.28

TS1

S	-3.558799	0.976228	0.998053
C	-4.992973	0.345392	0.179328
C	-4.913469	-0.739125	-0.720028
C	-6.263033	0.917482	0.403363
C	-6.053651	-1.231487	-1.355728
C	-7.400902	0.421806	-0.234545
C	-7.307254	-0.657252	-1.119750
H	-3.945050	-1.186083	-0.913589
H	-6.341717	1.755178	1.089392
H	-5.960890	-2.069446	-2.042625

H	-8.366401	0.882468	-0.039978
H	-8.193291	-1.042493	-1.615951
H	-1.379904	0.036037	-1.114909
C	2.493151	2.476169	0.589105
C	0.022664	2.035543	-0.795056
C	2.467875	1.949316	-0.711038
C	1.255556	2.762097	1.190406
C	1.267359	1.729046	-1.385270
C	0.050551	2.545967	0.524268
C	3.793425	2.763940	1.299480
C	-1.227282	1.792254	-1.502884
C	-2.446279	2.266401	-1.079128
H	3.407204	1.719730	-1.208716
H	1.236883	3.162725	2.201949
H	1.284832	1.326678	-2.394994
H	-0.884799	2.755287	1.032560
H	4.025593	3.836123	1.283822
H	3.757675	2.458608	2.351270
H	4.631060	2.243579	0.824980
H	-1.156075	1.337512	-2.489014
H	-3.340022	2.086469	-1.664548
H	-2.535049	3.019456	-0.309996
N	-0.011575	-1.192218	2.187527
N	1.585889	-1.766023	0.830256
C	-1.032862	-0.375202	2.852882
C	0.906556	-0.725745	1.335046
C	0.049099	-2.571760	2.194897
C	1.057662	-2.932585	1.347095
C	2.609467	-1.658005	-0.217746
H	-1.251695	-0.813637	3.826891
H	-0.637023	0.631850	2.980908
H	1.055226	0.312412	1.081148
H	-0.623858	-3.167484	2.789328
H	1.430259	-3.902875	1.063025
H	2.700192	-2.647718	-0.671228
Br	-1.147087	-1.446608	-1.050964
H	-1.935565	-0.321911	2.225333
H	2.215196	-0.976657	-0.975613
C	3.950291	-1.170107	0.326207
C	4.993768	-1.034430	-0.785560
H	4.307231	-1.865643	1.096307
H	3.801943	-0.199759	0.812790
C	6.340242	-0.511031	-0.276946
H	5.141717	-2.007587	-1.274140

H	4.609723	-0.357735	-1.560735
H	6.186639	0.455011	0.224043
H	6.730416	-1.193807	0.490931
C	7.383806	-0.343867	-1.385806
C	8.723600	0.187166	-0.868425
H	6.988859	0.337082	-2.151789
H	7.538153	-1.309890	-1.885158
H	9.449541	0.299237	-1.680038
H	8.601407	1.166656	-0.391721
H	9.156019	-0.491955	-0.124528

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4056.27922106
Thermal correction to enthalpy (Hartree)	0.577303
Entropy (cal/(mol*K))	222.653
Thermal correction to Gibbs free energy (Hartree)	0.471513
Solvation free energy (kcal/mol)	-28.55

PC1

S	-3.351929	1.916623	0.899589
C	-4.558249	0.687945	0.397212
C	-4.199157	-0.414341	-0.390852
C	-5.875949	0.815618	0.859024
C	-5.163025	-1.366794	-0.727661
C	-6.829455	-0.151576	0.531694
C	-6.477549	-1.240450	-0.270638
H	-3.180279	-0.558445	-0.739725
H	-6.148882	1.673891	1.464851
H	-4.869337	-2.209602	-1.346337
H	-7.848422	-0.044716	0.892403
H	-7.221635	-1.986790	-0.532962
H	-1.812069	0.947864	-1.580620
C	2.319312	2.478564	0.334210
C	-0.298004	2.183597	-0.758231
C	2.111718	1.843478	-0.898257
C	1.191733	2.954579	1.013606
C	0.831192	1.683455	-1.426345
C	-0.090937	2.821058	0.472384
C	3.707414	2.671724	0.896892
C	-1.650684	2.020363	-1.416939
C	-2.848421	2.657078	-0.721557
H	2.967403	1.473166	-1.456568
H	1.314162	3.454419	1.971674
H	0.695153	1.158860	-2.367055

H	-0.929531	3.222370	1.030494
H	3.949210	3.736030	0.996993
H	3.805915	2.224533	1.893038
H	4.463755	2.219725	0.249850
H	-1.591727	2.462053	-2.421969
H	-3.727872	2.601259	-1.366575
H	-2.666817	3.714947	-0.506075
N	-0.479571	-1.719651	1.692029
N	1.419980	-1.914236	0.652398
C	-1.801890	-1.209605	2.041218
C	0.407895	-1.075958	0.920750
C	-0.079620	-3.040247	1.817715
C	1.113937	-3.158874	1.174996
C	2.532674	-1.615145	-0.251725
H	-2.015387	-1.437197	3.087403
H	-1.825886	-0.131846	1.882508
H	0.343619	-0.045021	0.612249
H	-0.680526	-3.768328	2.336837
H	1.757327	-4.010311	1.027431
H	2.722663	-2.522074	-0.831500
Br	-0.953062	-1.592778	-1.624064
H	-2.542390	-1.670517	1.384566
H	2.169996	-0.859482	-0.949770
C	3.777440	-1.153243	0.503117
C	4.947483	-0.854323	-0.437082
H	4.071346	-1.925100	1.226596
H	3.526124	-0.256270	1.081090
C	6.216011	-0.427399	0.307538
H	5.165240	-1.741337	-1.048153
H	4.655221	-0.064432	-1.141371
H	5.986802	0.433295	0.950876
H	6.530385	-1.236531	0.981973
C	7.375668	-0.065382	-0.625317
C	8.638555	0.361126	0.128381
H	7.057836	0.743872	-1.296770
H	7.603586	-0.925012	-1.269956
H	9.449233	0.617102	-0.561500
H	8.444769	1.238469	0.756480
H	8.997631	-0.441872	0.782634

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4056.36056488
Thermal correction to enthalpy (Hartree)	0.585794
Entropy (cal/(mol*K))	220.352

Thermal correction to Gibbs free energy (Hartree)	0.481098
Solvation free energy (kcal/mol)	-21.77

2.5.2 The RC, TS and PC of the HBr-mediated channel in thiol-styrene reaction

RC

S	3.640322	1.465007	0.855657
C	4.343364	0.023981	0.074468
C	4.020333	-1.280859	0.470848
C	5.245140	0.223359	-0.981379
C	4.585021	-2.371292	-0.195005
C	5.798375	-0.871974	-1.644812
C	5.466959	-2.175716	-1.260929
H	3.344469	-1.446056	1.302399
H	5.512451	1.231438	-1.284253
H	4.345271	-3.378056	0.135393
H	6.497900	-0.705166	-2.457876
H	5.909579	-3.025457	-1.769922
H	2.775833	0.799911	1.647918
C	-0.528784	2.851335	-1.908300
C	-1.274358	2.348285	0.791298
C	-1.849646	2.514229	-1.574253
C	0.416372	2.906559	-0.869187
C	-2.215140	2.264563	-0.250997
C	0.054859	2.659971	0.451321
C	-0.139405	3.173142	-3.328308
C	-1.710790	2.120356	2.175208
C	-1.006446	2.365172	3.296557
H	-2.601615	2.458141	-2.356310
H	1.451745	3.145785	-1.093812
H	-3.248291	2.020777	-0.017875
H	0.817441	2.711273	1.220078
H	-0.770407	2.646666	-4.049870
H	-0.250290	4.246783	-3.521060
H	0.905664	2.917128	-3.526236
H	-2.719355	1.722614	2.283165
H	-1.436743	2.173548	4.273648
H	-0.023325	2.827077	3.282201
N	1.020025	-1.061841	-1.473395
N	-0.778997	-1.563993	-0.364064
C	2.000033	-0.295695	-2.252917
C	-0.120578	-0.570404	-0.971621
C	1.095294	-2.409734	-1.171265
C	-0.034324	-2.723823	-0.470441

C	-2.067769	-1.413547	0.332571
H	2.151270	0.671126	-1.774272
H	2.941360	-0.841113	-2.254107
H	-0.449222	0.453105	-1.043990
H	1.943497	-3.007108	-1.461503
H	-0.361213	-3.654702	-0.036224
H	-2.032316	-0.459154	0.859814
H	-2.111406	-2.204454	1.084235
Br	0.728321	-0.645988	2.466879
H	1.637220	-0.167646	-3.274651
H	-0.112637	0.493119	2.789666
C	-3.259706	-1.469450	-0.620483
C	-4.579982	-1.264943	0.129126
H	-3.267824	-2.432092	-1.145831
H	-3.141886	-0.689964	-1.383826
C	-5.798942	-1.270819	-0.798662
H	-4.695891	-2.048823	0.889829
H	-4.543863	-0.311049	0.674822
C	-7.122882	-1.060479	-0.056447
H	-5.679807	-0.486606	-1.559802
H	-5.835391	-2.223921	-1.343999
H	-7.239981	-1.846718	0.701194
H	-7.081956	-0.109559	0.492146
C	-8.335342	-1.062371	-0.991171
H	-8.418695	-2.014198	-1.527635
H	-9.265423	-0.911078	-0.435273
H	-8.259684	-0.264344	-1.738541

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4056.73611733
Thermal correction to enthalpy (Hartree)	0.590204
Entropy (cal/(mol*K))	231.742
Thermal correction to Gibbs free energy (Hartree)	0.480096
Solvation free energy (kcal/mol)	-49.24

TS

S	4.338515	0.719767	0.937837
C	5.120183	-0.678326	0.138055
C	4.522243	-1.343232	-0.940825
C	6.333667	-1.129741	0.669422
C	5.166376	-2.447708	-1.499823
C	6.956391	-2.247571	0.110606
C	6.377540	-2.907450	-0.975384
H	3.587553	-0.984424	-1.357868

H	6.795585	-0.606205	1.500831
H	4.715068	-2.952246	-2.348566
H	7.899672	-2.593844	0.520597
H	6.868766	-3.769905	-1.413526
H	3.479033	1.037249	-0.062955
C	-2.410633	0.851896	2.787840
C	-0.012852	-0.327792	1.821313
C	-2.424165	-0.392265	2.139800
C	-1.172486	1.499260	2.929399
C	-1.247619	-0.970685	1.660608
C	0.005612	0.926731	2.446341
C	-3.676125	1.451792	3.347255
C	1.233387	-0.962635	1.295591
C	2.428199	-0.905845	2.015286
H	-3.365093	-0.922056	2.019080
H	-1.131152	2.463499	3.429401
H	-1.286149	-1.943224	1.177164
H	0.944352	1.462704	2.555324
H	-4.540928	1.227209	2.715866
H	-3.887336	1.045773	4.343426
H	-3.596648	2.537715	3.447562
H	1.084802	-1.888871	0.735797
H	3.222254	-1.613404	1.812445
H	2.529584	-0.294547	2.904404
N	-1.097995	3.068878	-0.963805
N	-1.942980	1.215652	-1.717738
C	-0.399317	3.988681	-0.065773
C	-1.534448	1.852594	-0.615417
C	-1.193488	3.198464	-2.338442
C	-1.731606	2.036211	-2.810096
C	-2.439112	-0.170101	-1.737292
H	-0.666357	5.014619	-0.320354
H	-0.703626	3.775614	0.958275
H	-1.541533	1.452531	0.384632
H	-0.875657	4.090853	-2.852551
H	-1.973767	1.725450	-3.813304
H	-1.764090	-0.754080	-1.107552
H	-2.330345	-0.528783	-2.762979
Br	1.410788	0.807092	-1.226377
H	0.677322	3.834477	-0.169724
H	1.436969	-0.215761	0.227793
C	-3.883550	-0.273566	-1.252784
C	-4.352530	-1.728438	-1.167972
H	-4.536273	0.297228	-1.924299

H	-3.957882	0.193915	-0.263313
C	-5.778067	-1.858770	-0.622099
H	-4.296679	-2.193085	-2.161563
H	-3.663951	-2.294905	-0.524809
C	-6.263996	-3.309188	-0.536395
H	-5.827598	-1.399317	0.375820
H	-6.464568	-1.282552	-1.257569
H	-6.216818	-3.763880	-1.534817
H	-5.573954	-3.884778	0.095562
C	-7.687170	-3.428307	0.015265
H	-8.401397	-2.887331	-0.615598
H	-8.008979	-4.472979	0.061889
H	-7.755759	-3.012900	1.027201

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4056.70440427
Thermal correction to enthalpy (Hartree)	0.588206
Entropy (cal/(mol*K))	222.796
Thermal correction to Gibbs free energy (Hartree)	0.482349
Solvation free energy (kcal/mol)	-49.70

PC

S	3.494309	0.017022	1.287873
C	4.616307	-0.902707	0.229684
C	4.141381	-1.594435	-0.891293
C	5.977306	-0.913409	0.551046
C	5.034182	-2.333151	-1.667218
C	6.867193	-1.631842	-0.251005
C	6.396270	-2.346698	-1.354284
H	3.090414	-1.570716	-1.153895
H	6.333934	-0.370630	1.420146
H	4.667508	-2.882148	-2.528677
H	7.924251	-1.638611	-0.005506
H	7.088273	-2.912576	-1.969517
H	2.402611	0.584440	-0.093986
C	-2.097323	1.057100	2.832882
C	0.017270	-0.613335	1.892458
C	-2.362392	-0.192646	2.249604
C	-0.757300	1.454006	2.927035
C	-1.327165	-1.009943	1.798941
C	0.280598	0.639264	2.459530
C	-3.212994	1.915199	3.375011
C	1.099289	-1.572654	1.435862
C	2.488876	-1.353925	2.035131

H	-3.388902	-0.541054	2.172565
H	-0.515311	2.407265	3.390358
H	-1.564463	-1.988600	1.388585
H	1.300302	0.992873	2.571866
H	-4.086182	1.904777	2.715011
H	-3.543661	1.547982	4.353490
H	-2.894224	2.952782	3.506584
H	0.788951	-2.585668	1.720102
H	3.100959	-2.248371	1.911766
H	2.424294	-1.133893	3.103604
N	-0.971742	3.146368	-0.882389
N	-1.810170	1.269327	-1.582648
C	-0.238710	4.085810	-0.032482
C	-1.334654	1.912379	-0.512014
C	-1.188739	3.284155	-2.242814
C	-1.722501	2.106789	-2.680546
C	-2.281858	-0.124983	-1.575390
H	-0.620722	5.094686	-0.192210
H	-0.386401	3.799351	1.008153
H	-1.240852	1.506188	0.481373
H	-0.946106	4.191095	-2.772478
H	-2.041258	1.796925	-3.662507
H	-1.673192	-0.654001	-0.840429
H	-2.055577	-0.541526	-2.559802
Br	1.561164	0.957920	-1.360757
H	0.824231	4.034467	-0.279399
H	1.159749	-1.577300	0.340715
C	-3.769743	-0.225888	-1.246548
C	-4.239110	-1.680915	-1.163318
H	-4.349749	0.314636	-2.004640
H	-3.952113	0.278066	-0.288981
C	-5.715438	-1.803520	-0.772416
H	-4.072838	-2.178445	-2.128407
H	-3.623468	-2.219564	-0.429143
C	-6.199695	-3.254051	-0.680855
H	-5.876881	-1.304933	0.194176
H	-6.330847	-1.260598	-1.502994
H	-6.037936	-3.750065	-1.647177
H	-5.582585	-3.795603	0.049008
C	-7.675515	-3.364753	-0.288643
H	-8.316686	-2.858285	-1.018818
H	-7.994604	-4.409817	-0.233579
H	-7.860428	-2.907622	0.690289

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4056.75689439
Thermal correction to enthalpy (Hartree)	0.593650
Entropy (cal/(mol*K))	223.47
Thermal correction to Gibbs free energy (Hartree)	0.487472
Solvation free energy (kcal/mol)	-48.36

2.5.3 The RC, TS and PC of the thiol-styrene reaction in [hmmim]Br

RC

S	-2.722832	1.275826	0.970322
C	-3.984775	0.065816	0.590766
C	-4.014338	-0.631431	-0.623950
C	-4.955411	-0.192816	1.567881
C	-5.001993	-1.594186	-0.845034
C	-5.935712	-1.158942	1.337609
C	-5.958820	-1.871611	0.134918
H	-3.282157	-0.415789	-1.392987
H	-4.944985	0.355425	2.505514
H	-5.027281	-2.120439	-1.794815
H	-6.685082	-1.350900	2.099067
H	-6.726403	-2.617073	-0.044409
H	-1.969645	1.064044	-0.128393
C	1.897406	2.309348	2.088908
C	0.781220	3.237416	-0.353051
C	2.618242	2.229344	0.890370
C	0.603999	2.857042	2.043401
C	2.073577	2.690792	-0.308943
C	0.055830	3.314436	0.850472
C	2.496094	1.853407	3.395705
C	0.252683	3.738438	-1.629278
C	-1.037457	3.995934	-1.920856
H	3.626534	1.824319	0.899707
H	0.027676	2.942829	2.960618
H	2.661930	2.638159	-1.221222
H	-0.931231	3.764828	0.860210
H	1.773309	1.287110	3.992784
H	3.378827	1.227682	3.237255
H	2.807137	2.711912	4.002085
H	0.997001	3.894673	-2.409066
H	-1.318852	4.386398	-2.893133
H	-1.838110	3.864043	-1.197930
N	-1.289725	-2.405615	0.695116
N	0.519993	-1.874969	-0.381274
C	-2.295956	-2.523332	1.754491

C	-0.166649	-1.660101	0.756916
C	-1.312714	-3.101877	-0.500784
C	-0.176003	-2.772506	-1.174081
C	1.796144	-1.236818	-0.753715
H	-2.009193	-3.313110	2.452928
H	-2.382793	-1.571510	2.273923
H	-2.133091	-3.749065	-0.764071
H	0.187506	-3.077620	-2.141777
H	1.721295	-0.176326	-0.505211
H	1.861698	-1.303422	-1.841314
Br	-0.783832	0.453638	-2.340637
H	-3.256299	-2.754011	1.295759
H	-0.725583	1.914300	-2.306283
C	3.006114	-1.891896	-0.091700
C	4.310636	-1.257207	-0.585425
H	3.005046	-2.966777	-0.310304
H	2.932269	-1.790113	0.998252
C	5.556351	-1.852873	0.077066
H	4.383526	-1.379241	-1.674764
H	4.281507	-0.175038	-0.399039
C	6.861539	-1.220853	-0.417856
H	5.483274	-1.729542	1.166997
H	5.583748	-2.935647	-0.107519
H	6.932275	-1.346846	-1.506472
H	6.829731	-0.137849	-0.235991
C	8.103163	-1.817196	0.250398
H	8.176410	-2.893450	0.057998
H	9.018770	-1.349148	-0.123297
H	8.074816	-1.674369	1.336658
C	0.237098	-0.790241	1.887194
H	1.077590	-0.157872	1.606988
H	-0.591364	-0.133949	2.167027
H	0.526180	-1.391572	2.755953

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4096.08442165
Thermal correction to enthalpy (Hartree)	0.619655
Entropy (cal/(mol*K))	241.299
Thermal correction to Gibbs free energy (Hartree)	0.505006
Solvation free energy (kcal/mol)	-48.54

TS

S	-4.300742	0.635064	1.375350
C	-5.092892	0.740963	-0.227227

C	-4.513300	0.194766	-1.380567
C	-6.300032	1.445390	-0.303761
C	-5.171275	0.332764	-2.603523
C	-6.934689	1.593970	-1.538466
C	-6.374923	1.037409	-2.690423
H	-3.584320	-0.360963	-1.317152
H	-6.748526	1.860400	0.593629
H	-4.734807	-0.108997	-3.494168
H	-7.872595	2.137114	-1.594715
H	-6.875997	1.145301	-3.646686
H	-3.451776	-0.381044	1.084742
C	2.531703	1.982297	2.335932
C	0.102222	1.893118	0.875411
C	2.517698	2.153684	0.945503
C	1.305675	1.749527	2.979406
C	1.322217	2.109254	0.224575
C	0.111844	1.695019	2.262733
C	3.815817	2.080640	3.120959
C	-1.166688	1.840106	0.086026
C	-2.341946	2.421580	0.558955
H	3.451209	2.337249	0.421010
H	1.288027	1.602728	4.056000
H	1.335784	2.266802	-0.850802
H	-0.816991	1.485954	2.786042
H	3.826824	1.383736	3.964479
H	4.686543	1.873315	2.492538
H	3.941847	3.088964	3.532635
H	-1.046297	1.877539	-0.999354
H	-3.157131	2.640194	-0.119410
H	-2.421181	2.809036	1.567879
N	0.922375	-3.709611	0.760333
N	1.651531	-2.342230	-0.758276
C	0.452816	-4.214355	2.050886
C	1.462904	-2.490245	0.565634
C	0.726339	-4.325829	-0.463862
C	1.185315	-3.467556	-1.414873
C	2.136522	-1.119329	-1.418345
H	1.246939	-4.136485	2.794535
H	-0.420659	-3.639244	2.369268
H	0.284867	-5.305305	-0.546887
H	1.215418	-3.553572	-2.488470
H	1.526587	-0.290313	-1.050980
H	1.920633	-1.242539	-2.481796
Br	-1.401638	-1.240685	0.175572

H	0.177787	-5.261462	1.932747
H	-1.408643	0.549219	0.131599
C	3.623595	-0.856908	-1.190327
C	4.106483	0.355090	-1.994404
H	4.199942	-1.747672	-1.467696
H	3.803332	-0.678342	-0.124053
C	5.541050	0.763138	-1.647379
H	4.035631	0.135153	-3.067968
H	3.435614	1.204869	-1.810904
C	6.030470	1.984656	-2.432076
H	5.605416	0.974683	-0.569999
H	6.216275	-0.083713	-1.832024
H	5.967453	1.771322	-3.507323
H	5.350967	2.828139	-2.247115
C	7.462071	2.389954	-2.071588
H	8.166660	1.577072	-2.279961
H	7.783819	3.264622	-2.644726
H	7.546897	2.638901	-1.007476
C	1.770388	-1.505249	1.628909
H	1.770751	-0.495678	1.221939
H	1.002197	-1.542311	2.402202
H	2.747093	-1.701956	2.084754

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4096.05190993
Thermal correction to enthalpy (Hartree)	0.617794
Entropy (cal/(mol*K))	228.064
Thermal correction to Gibbs free energy (Hartree)	0.509433
Solvation free energy (kcal/mol)	-49.27

PC

S	3.384538	-1.327698	0.924434
C	4.663552	-0.882801	-0.252791
C	4.329241	-0.411837	-1.528143
C	6.000014	-1.010564	0.137096
C	5.348172	-0.104779	-2.429186
C	7.011870	-0.673158	-0.764900
C	6.687361	-0.226187	-2.047324
H	3.292541	-0.292413	-1.819858
H	6.244949	-1.374320	1.129523
H	5.094616	0.247905	-3.423750
H	8.050486	-0.769594	-0.465926
H	7.475792	0.025602	-2.749150
H	2.336223	-0.008068	0.522442

C	-2.247258	-2.026962	2.091883
C	0.025067	-2.237143	0.385744
C	-2.391018	-2.116939	0.698288
C	-0.948568	-2.033848	2.609838
C	-1.279204	-2.221092	-0.134538
C	0.167794	-2.135986	1.772857
C	-3.456254	-1.954697	2.991343
C	1.188110	-2.423354	-0.570075
C	2.541873	-2.741946	0.058622
H	-3.387486	-2.125980	0.265462
H	-0.800992	-1.968787	3.684432
H	-1.423185	-2.313637	-1.208755
H	1.149883	-2.152662	2.234151
H	-3.187404	-1.624505	3.998366
H	-4.210850	-1.266599	2.595195
H	-3.934516	-2.936664	3.084041
H	0.951213	-3.265915	-1.232521
H	3.252427	-3.066014	-0.702787
H	2.455702	-3.536325	0.803771
N	-0.733606	3.665021	1.047982
N	-1.612391	2.423273	-0.499229
C	-0.116450	4.055331	2.316116
C	-1.284831	2.458929	0.805216
C	-0.678745	4.390689	-0.129777
C	-1.232425	3.611762	-1.098712
C	-2.174293	1.261735	-1.208681
H	-0.817413	3.899752	3.137132
H	0.789312	3.463489	2.473163
H	-0.254996	5.380519	-0.172257
H	-1.385638	3.793210	-2.149691
H	-1.546565	0.398451	-0.971753
H	-2.056897	1.473621	-2.273668
Br	1.463290	1.258765	-0.016593
H	0.141482	5.112091	2.263514
H	1.276035	-1.547195	-1.223255
C	-3.638541	0.999451	-0.862939
C	-4.243299	-0.074725	-1.773430
H	-4.209136	1.931625	-0.952728
H	-3.712652	0.677145	0.182269
C	-5.638557	-0.516346	-1.323246
H	-4.291587	0.305271	-2.802610
H	-3.577872	-0.947678	-1.801627
C	-6.254059	-1.592120	-2.223883
H	-5.583009	-0.895344	-0.292288

H	-6.304617	0.356946	-1.290338
H	-6.312205	-1.211140	-3.252060
H	-5.583290	-2.461650	-2.256832
C	-7.644602	-2.032795	-1.759373
H	-8.343487	-1.188848	-1.750545
H	-8.058974	-2.801410	-2.418611
H	-7.609921	-2.446705	-0.745016
C	-1.462920	1.376905	1.800693
H	-1.478552	0.407186	1.306912
H	-0.622823	1.370428	2.496228
H	-2.394570	1.501432	2.363785

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4096.10421707
Thermal correction to enthalpy (Hartree)	0.622423
Entropy (cal/(mol*K))	228.511
Thermal correction to Gibbs free energy (Hartree)	0.513850
Solvation free energy (kcal/mol)	-47.57

2.5.4 The RC, TS and PC for styrene

RC

S	-3.124607	2.095362	0.039805
C	-4.050314	0.569688	0.081722
C	-3.850787	-0.461882	-0.842269
C	-4.996030	0.398441	1.102355
C	-4.582418	-1.647182	-0.734680
C	-5.712969	-0.792377	1.200198
C	-5.521241	-1.841744	0.286895
H	-3.136863	-0.341589	-1.649337
H	-5.170768	1.192716	1.822251
H	-4.428033	-2.429752	-1.473688
H	-6.442658	-0.904707	1.997508
H	-2.328460	1.757316	-0.994284
C	1.265457	1.576371	3.193303
C	1.605158	2.560800	0.571357
C	2.481784	1.393841	2.528512
C	0.217009	2.242225	2.545444
C	2.646303	1.880810	1.230634
C	0.383972	2.729255	1.250930
C	1.846010	3.084316	-0.781631
C	1.006052	3.823539	-1.529835
H	3.304348	0.888501	3.024545
H	-0.730080	2.394688	3.053402

H	3.599984	1.752969	0.725843
H	-0.441883	3.245103	0.776100
H	2.821559	2.840956	-1.200687
H	1.305128	4.177753	-2.510565
H	0.034087	4.151716	-1.172822
N	-0.960431	-1.427110	0.940469
N	0.844832	-1.461723	-0.268130
C	-1.921470	-1.064047	1.989358
C	0.215067	-0.821867	0.724357
C	-1.088849	-2.480189	0.053178
C	0.045248	-2.499966	-0.707762
C	2.164184	-1.091833	-0.807668
H	-1.958179	0.021446	2.070456
H	-2.904272	-1.428942	1.698276
H	0.586972	0.035188	1.261095
H	-1.971965	-3.096984	0.031947
H	0.341802	-3.146517	-1.517757
H	2.202216	-0.001992	-0.831125
H	2.189923	-1.445693	-1.840408
Br	-0.454691	0.689626	-2.457958
H	-1.615894	-1.512182	2.937058
H	0.290816	1.871407	-2.064992
C	3.315457	-1.663758	0.016161
C	4.671467	-1.248225	-0.562978
H	3.237741	-2.757204	0.049799
H	3.225890	-1.304603	1.048970
C	5.854813	-1.758755	0.264930
H	4.759591	-1.618284	-1.593438
H	4.719581	-0.151677	-0.626276
C	7.214733	-1.338177	-0.302067
H	5.761703	-1.390285	1.296551
H	5.809258	-2.854791	0.326031
H	7.307378	-1.711090	-1.330781
H	7.254923	-0.242349	-0.368265
C	8.391067	-1.845430	0.536248
H	8.393310	-2.939802	0.591766
H	9.347877	-1.531941	0.108219
H	8.341702	-1.460021	1.561040
C	-6.339843	-3.105772	0.374344
H	-7.343200	-2.947483	-0.038105
H	-5.879448	-3.922238	-0.188840
H	-6.464307	-3.432839	1.411201
H	1.138158	1.213864	4.208392

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4056.73476011
Thermal correction to enthalpy (Hartree)	0.590428
Entropy (cal/(mol*K))	233.453
Thermal correction to Gibbs free energy (Hartree)	0.479507
Solvation free energy (kcal/mol)	-49.61

TS

S	3.899616	1.154945	1.075140
C	4.799455	-0.174820	0.284364
C	4.258198	-0.913810	-0.773617
C	6.056697	-0.507723	0.801513
C	4.997175	-1.962242	-1.322663
C	6.770806	-1.569557	0.249149
C	6.259157	-2.313071	-0.824390
H	3.288863	-0.655561	-1.186601
H	6.481873	0.065229	1.619939
H	4.579149	-2.519964	-2.156108
H	7.747619	-1.817643	0.654934
H	3.034102	1.407223	0.062846
C	-2.779158	0.893827	2.967126
C	-0.357063	-0.163170	1.992064
C	-2.757986	-0.355404	2.340327
C	-1.588561	1.618274	3.097996
C	-1.556728	-0.875388	1.851356
C	-0.390122	1.100064	2.602815
C	0.914340	-0.737690	1.461189
C	2.112459	-0.602746	2.161468
H	-3.672259	-0.932509	2.243539
H	-1.594270	2.585422	3.591928
H	-1.544106	-1.855392	1.382184
H	0.524489	1.678840	2.694185
H	0.811101	-1.672722	0.906257
H	2.947252	-1.257795	1.945704
H	2.188620	0.014583	3.048653
N	-1.633764	3.137496	-0.843500
N	-2.395128	1.236551	-1.567751
C	-0.974974	4.101988	0.037811
C	-2.011059	1.906993	-0.476641
C	-1.742555	3.243724	-2.219052
C	-2.228326	2.051284	-2.672003
C	-2.823441	-0.172232	-1.566472
H	-1.287212	5.110629	-0.233730
H	-1.268951	3.894057	1.065936

H	-1.993749	1.519973	0.528130
H	-1.470252	4.143193	-2.746774
H	-2.461249	1.716137	-3.669529
H	-2.111578	-0.716890	-0.941852
H	-2.712892	-0.535404	-2.590343
Br	0.974376	0.987591	-1.095111
H	0.107309	3.993708	-0.065805
H	1.064318	0.011277	0.364735
C	-4.253325	-0.343601	-1.058707
C	-4.643591	-1.820414	-0.952290
H	-4.944593	0.184712	-1.726397
H	-4.337748	0.130583	-0.073292
C	-6.054853	-2.020865	-0.391015
H	-4.572476	-2.293621	-1.940971
H	-3.919617	-2.341800	-0.309722
C	-6.458584	-3.494723	-0.280337
H	-6.120932	-1.550002	0.600578
H	-6.777714	-1.492909	-1.028078
H	-6.397465	-3.960243	-1.273049
H	-5.730667	-4.022358	0.351034
C	-7.866594	-3.684769	0.289905
H	-8.616859	-3.192917	-0.339359
H	-8.129355	-4.744921	0.354154
H	-7.946535	-3.259723	1.296973
H	-3.708428	1.294142	3.359130
C	7.057431	-3.437820	-1.433731
H	6.452067	-4.026895	-2.127257
H	7.918130	-3.048423	-1.989745
H	7.446440	-4.111798	-0.663806

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4056.7039688
Thermal correction to enthalpy (Hartree)	0.588081
Entropy (cal/(mol*K))	225.267
Thermal correction to Gibbs free energy (Hartree)	0.481050
Solvation free energy (kcal/mol)	-49.90

PC

S	-3.049096	-0.644466	1.569366
C	-3.984698	0.505418	0.560321
C	-3.404542	1.158235	-0.532503
C	-5.322512	0.748348	0.891843
C	-4.160221	2.068862	-1.269112
C	-6.068532	1.650370	0.135065

C	-5.501358	2.328030	-0.954391
H	-2.376363	0.964699	-0.813016
H	-5.773320	0.237918	1.736671
H	-3.701441	2.579952	-2.110757
H	-7.105734	1.834819	0.399907
H	-1.989301	-1.257972	0.212884
C	2.629557	-2.002405	2.751010
C	0.534628	-0.213292	2.117390
C	2.908111	-0.659391	2.478048
C	1.306472	-2.450382	2.697174
C	1.868698	0.221383	2.169028
C	0.272884	-1.566993	2.373532
C	-0.560932	0.796844	1.832451
C	-1.916673	0.504266	2.485427
H	3.928563	-0.292710	2.531422
H	1.071063	-3.486541	2.921385
H	2.093359	1.269806	1.990415
H	-0.742527	-1.945356	2.345207
H	-0.224461	1.770324	2.207397
H	-2.492711	1.423794	2.601249
H	-1.785613	0.062326	3.476420
N	1.923405	-3.163769	-1.323241
N	2.083527	-1.039543	-1.746308
C	1.653839	-4.397985	-0.582605
C	2.024926	-1.949957	-0.768646
C	1.883052	-3.022301	-2.700069
C	1.986009	-1.687163	-2.964261
C	2.118710	0.415726	-1.524721
H	2.181429	-5.225620	-1.057227
H	2.008704	-4.276292	0.439863
H	2.030203	-1.741329	0.287795
H	1.784303	-3.869014	-3.359718
H	1.998014	-1.150914	-3.899168
H	1.360194	0.636346	-0.769863
H	1.801626	0.880646	-2.460713
Br	-1.128586	-1.665388	-1.043179
H	0.576920	-4.581847	-0.578746
H	-0.690753	0.926801	0.751044
C	3.497402	0.910419	-1.094192
C	3.502917	2.424283	-0.862365
H	4.236162	0.643678	-1.859574
H	3.789222	0.392614	-0.172969
C	4.850659	2.941201	-0.349499
H	3.244720	2.939847	-1.797215

H	2.715534	2.685575	-0.140806
C	4.871464	4.456681	-0.124675
H	5.100137	2.430589	0.591599
H	5.639797	2.668803	-1.063797
H	4.627551	4.963831	-1.067595
H	4.076915	4.727633	0.583965
C	6.219338	4.961831	0.396988
H	7.026242	4.732974	-0.308194
H	6.206412	6.045377	0.547996
H	6.472336	4.494207	1.355363
H	3.430335	-2.683949	3.020304
C	-6.319733	3.292269	-1.774494
H	-5.682606	3.949314	-2.371828
H	-6.979201	2.751447	-2.463583
H	-6.954987	3.915639	-1.138328

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4056.75616298
Thermal correction to enthalpy (Hartree)	0.59332
Entropy (cal/(mol*K))	224.965
Thermal correction to Gibbs free energy (Hartree)	0.486432
Solvation free energy (kcal/mol)	-48.69

2.5.5 The RC, TS and PC for 2-vinylpyridine

RC

S	3.383887	2.225650	-0.279386
C	4.352763	0.726689	-0.224330
C	4.130049	-0.284729	0.716306
C	5.343136	0.547849	-1.200098
C	4.897409	-1.451484	0.679924
C	6.087031	-0.629974	-1.234063
C	5.881699	-1.654474	-0.296065
H	3.371069	-0.160950	1.480721
H	5.535096	1.327948	-1.930968
H	4.727220	-2.216758	1.433382
H	6.851556	-0.749239	-1.996962
H	2.702184	2.001631	0.860426
C	-4.306081	1.071380	-1.965261
C	-2.403353	2.493384	-0.573031
C	-4.725671	1.992459	-1.007058
C	-2.932732	0.898862	-2.154491
C	-3.762622	2.711203	-0.300920
C	-1.384294	3.300634	0.117963

C	-0.091449	3.380556	-0.238514
H	-5.781719	2.152953	-0.815823
H	-2.568360	0.175439	-2.881127
H	-4.052540	3.445836	0.443098
H	-1.748472	3.905793	0.945567
H	0.589210	4.046943	0.281664
H	0.298676	2.832115	-1.089073
N	1.309259	-1.202654	-1.133764
N	-0.422927	-1.340406	0.168901
C	2.199762	-0.782595	-2.222191
C	0.129659	-0.640669	-0.831501
C	1.517757	-2.283580	-0.296827
C	0.429254	-2.368755	0.522755
C	-1.731670	-1.057650	0.781992
H	1.882275	-1.248615	-3.157285
H	2.169981	0.303639	-2.302636
H	-0.318544	0.240515	-1.284145
H	2.420239	-2.870009	-0.345527
H	0.198218	-3.053035	1.323096
H	-1.918766	0.007865	0.651434
H	-1.628452	-1.247450	1.852626
Br	0.722374	0.966122	2.326595
H	3.214952	-1.086016	-1.974340
H	0.129826	1.907602	1.406308
C	-2.855232	-1.885717	0.162239
C	-4.214141	-1.510434	0.761342
H	-2.656811	-2.954595	0.307790
H	-2.867179	-1.709034	-0.919850
C	-5.384940	-2.190480	0.046132
H	-4.232425	-1.767927	1.828647
H	-4.343174	-0.421474	0.701865
C	-6.752174	-1.778019	0.600338
H	-5.340863	-1.948735	-1.025615
H	-5.276212	-3.281467	0.117338
H	-6.795284	-2.016571	1.671190
H	-6.854984	-0.686296	0.526579
C	-7.917789	-2.455513	-0.124991
H	-7.859021	-3.545739	-0.033137
H	-8.881031	-2.138622	0.285899
H	-7.914076	-2.212158	-1.193864
C	6.732085	-2.900315	-0.309885
H	6.271533	-3.707055	0.267031
H	6.899123	-3.260908	-1.329542
H	7.716979	-2.703071	0.129450

H	-5.016138	0.494068	-2.546678
N	-1.997775	1.575481	-1.478963

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4072.78069104
Thermal correction to enthalpy (Hartree)	0.578777
Entropy (cal/(mol*K))	231.587
Thermal correction to Gibbs free energy (Hartree)	0.468743
Solvation free energy (kcal/mol)	-48.76

TS

S	2.974094	0.804968	1.138050
C	4.443194	0.128144	0.373931
C	4.428025	-0.363321	-0.936595
C	5.610760	0.054483	1.140554
C	5.596467	-0.899255	-1.476434
C	6.764802	-0.497204	0.585137
C	6.781639	-0.979739	-0.731106
H	3.522490	-0.312038	-1.532187
H	5.625999	0.432393	2.158491
H	5.581836	-1.267805	-2.498283
H	7.667996	-0.549737	1.186349
H	2.221743	0.913635	0.005438
C	-3.179124	-2.140994	1.632837
C	-0.542195	-2.020546	0.867614
C	-2.719885	-3.023805	0.653012
C	-2.277164	-1.217171	2.156061
C	-1.384083	-2.964413	0.263978
C	0.904899	-1.960590	0.502573
C	1.841370	-1.620088	1.481348
H	-3.388903	-3.752007	0.205712
H	-2.598772	-0.498440	2.906724
H	-0.990175	-3.644875	-0.483465
H	1.235108	-2.706282	-0.222772
H	2.881358	-1.898863	1.367498
H	1.513954	-1.256507	2.447863
N	-0.351817	3.050425	0.935535
N	-1.823113	1.976997	-0.247487
C	0.633526	3.365534	1.973317
C	-1.005095	1.886609	0.806993
C	-0.747664	3.899808	-0.084140
C	-1.669782	3.221379	-0.826310
C	-2.673676	0.891602	-0.767535
H	0.303423	4.240271	2.536342

H	0.719146	2.512340	2.645188
H	-0.851616	0.993657	1.403657
H	-0.344403	4.893957	-0.190224
H	-2.216232	3.511946	-1.708886
H	-2.226414	-0.046898	-0.442066
H	-2.588262	0.926389	-1.856043
Br	0.692046	0.298502	-1.583974
H	1.603532	3.556676	1.512080
H	0.893839	-0.962925	-0.363015
C	-4.123443	1.012077	-0.304939
C	-4.992625	-0.086810	-0.924762
H	-4.520334	1.999354	-0.571738
H	-4.155098	0.942680	0.789750
C	-6.419994	-0.102151	-0.370772
H	-5.022788	0.044694	-2.014722
H	-4.523606	-1.063096	-0.745434
C	-7.299962	-1.186541	-1.000912
H	-6.383789	-0.250711	0.718200
H	-6.885457	0.880672	-0.528538
H	-7.346705	-1.026623	-2.086184
H	-6.823549	-2.166322	-0.856807
C	-8.717426	-1.215384	-0.423205
H	-9.227892	-0.258842	-0.582072
H	-9.322408	-1.997167	-0.892225
H	-8.701009	-1.407856	0.655715
C	8.044128	-1.539417	-1.336125
H	8.662427	-0.736402	-1.755147
H	8.648215	-2.060504	-0.588006
H	7.822167	-2.239821	-2.145736
H	-4.207332	-2.159853	1.976423
N	-0.991609	-1.136764	1.776421

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4072.75045893
Thermal correction to enthalpy (Hartree)	0.576096
Entropy (cal/(mol*K))	223.229
Thermal correction to Gibbs free energy (Hartree)	0.470033
Solvation free energy (kcal/mol)	-49.79

PC

S	2.076730	-0.698778	0.967346
C	3.752345	-0.263571	0.493414
C	4.044560	0.185767	-0.799390
C	4.771956	-0.331649	1.453222

C	5.353392	0.546247	-1.124784
C	6.074368	0.024233	1.110291
C	6.388982	0.466796	-0.184682
H	3.265955	0.249175	-1.550859
H	4.546192	-0.664743	2.461665
H	5.571400	0.890403	-2.131715
H	6.858456	-0.038354	1.859771
H	1.184861	-0.293009	-0.700174
C	-3.013996	-2.256679	0.884217
C	-0.402011	-2.738125	0.165635
C	-2.757746	-2.984865	-0.282321
C	-1.926108	-1.780541	1.608606
C	-1.437766	-3.222336	-0.647763
C	1.037622	-3.071615	-0.164574
C	2.057682	-2.549388	0.839786
H	-3.573806	-3.365846	-0.888232
H	-2.080283	-1.205551	2.519970
H	-1.202304	-3.795312	-1.538974
H	1.135501	-4.165220	-0.193740
H	3.067740	-2.844488	0.552733
H	1.843836	-2.919104	1.843335
N	0.424698	2.487016	1.153019
N	-1.317817	1.908490	-0.009788
C	1.518682	2.464824	2.130219
C	-0.503642	1.533334	0.983426
C	0.200668	3.493873	0.230047
C	-0.891155	3.126015	-0.500599
C	-2.456768	1.131320	-0.532202
H	1.491611	3.383309	2.718423
H	1.392042	1.603187	2.782812
H	-0.551071	0.596396	1.516801
H	0.832409	4.365441	0.171542
H	-1.388369	3.615673	-1.322000
H	-2.188532	0.077380	-0.464519
H	-2.529484	1.378358	-1.593494
Br	0.482432	-0.001891	-2.025805
H	2.472957	2.379271	1.606872
H	1.272809	-2.720956	-1.175161
C	-3.758576	1.430110	0.207337
C	-4.943465	0.718418	-0.454354
H	-3.935787	2.512502	0.226385
H	-3.660924	1.105737	1.251392
C	-6.254502	0.899206	0.316204
H	-5.065703	1.095626	-1.478664

H	-4.718754	-0.352194	-0.547095
C	-7.446074	0.200957	-0.347426
H	-6.131723	0.514767	1.338946
H	-6.472545	1.971412	0.417728
H	-7.566731	0.587069	-1.368300
H	-7.225689	-0.870607	-0.449510
C	-8.752397	0.384460	0.429539
H	-9.014519	1.444918	0.515791
H	-9.584415	-0.124732	-0.066035
H	-8.669660	-0.021223	1.444344
C	7.806003	0.826382	-0.552071
H	8.283031	1.418412	0.234914
H	8.410910	-0.077472	-0.690554
H	7.845545	1.397628	-1.482760
H	-4.026271	-2.065895	1.223520
N	-0.645996	-1.997559	1.258173

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4072.80370382
Thermal correction to enthalpy (Hartree)	0.582116
Entropy (cal/(mol*K))	222.283
Thermal correction to Gibbs free energy (Hartree)	0.476502
Solvation free energy (kcal/mol)	-48.84

2.5.6 The RC, TS and PC for 3-(4-methoxyl-phenyl)propene

RC

S	-4.190041	1.605278	0.305113
C	-4.488942	-0.158380	0.319145
C	-4.419996	-0.934781	-0.844848
C	-4.827139	-0.773784	1.531132
C	-4.668091	-2.305743	-0.784840
C	-5.086271	-2.145558	1.573546
C	-5.008614	-2.939508	0.419838
H	-4.176853	-0.473010	-1.795742
H	-4.894518	-0.184879	2.441296
H	-4.611396	-2.891464	-1.698579
H	-5.357250	-2.603606	2.520878
H	-3.390264	1.592957	-0.779657
C	-0.464166	3.604580	0.291729
C	-0.543694	4.270605	-1.055211
C	-1.625026	4.272324	-1.846907
H	0.347948	4.806221	-1.379202
H	-1.636364	4.808986	-2.790180
H	-2.554489	3.793073	-1.547382

N	-0.886334	-0.695691	1.364845
N	0.481696	-1.450490	-0.145044
C	-1.443050	0.131662	2.438990
C	0.315722	-0.517567	0.800166
C	-1.517492	-1.764403	0.753196
C	-0.657838	-2.235513	-0.197670
C	1.659981	-1.552871	-1.026753
H	-2.269345	0.726819	2.045177
H	-1.792492	-0.514582	3.244840
H	1.028674	0.242524	1.072228
H	-2.509017	-2.081070	1.033933
H	-0.756109	-3.053066	-0.893088
H	1.770365	-0.589119	-1.529167
H	1.414883	-2.300315	-1.784177
Br	-1.204560	0.745298	-2.048077
H	-0.655461	0.788536	2.805593
H	-1.047262	2.181359	-2.153320
C	2.927042	-1.929454	-0.261929
C	4.150553	-1.971038	-1.181885
H	2.782757	-2.903616	0.221143
H	3.104508	-1.196029	0.531975
C	5.444368	-2.279462	-0.422290
H	3.997116	-2.720811	-1.970014
H	4.254661	-1.003115	-1.691089
C	6.681436	-2.314134	-1.325191
H	5.585128	-1.520394	0.358519
H	5.342793	-3.244867	0.093137
H	6.538182	-3.071578	-2.107297
H	6.775392	-1.350542	-1.843768
C	7.970739	-2.608979	-0.554007
H	7.915858	-3.579935	-0.048688
H	8.838110	-2.629198	-1.220677
H	8.156132	-1.845514	0.210465
C	-5.333004	-4.412111	0.462545
H	-6.402932	-4.576660	0.288409
H	-4.789255	-4.966067	-0.308036
H	-5.090427	-4.848928	1.435453
C	0.849991	2.896921	0.569720
C	1.287417	2.715735	1.885856
C	1.665447	2.395826	-0.458683
C	2.477453	2.041702	2.187633
H	0.696904	3.119713	2.704598
C	2.861810	1.742054	-0.182841
H	1.377486	2.535860	-1.494904

C	3.275738	1.551291	1.144485
H	2.779686	1.933636	3.221964
H	3.500162	1.380985	-0.982165
O	4.448201	0.882200	1.312053
C	4.970373	0.736491	2.633373
H	5.918699	0.212729	2.519219
H	5.143912	1.713486	3.097065
H	4.297246	0.140586	3.261166
H	-1.301107	2.901078	0.401016
H	-0.613416	4.370171	1.065105

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4210.65707872
Thermal correction to enthalpy (Hartree)	0.655243
Entropy (cal/(mol*K))	245.098
Thermal correction to Gibbs free energy (Hartree)	0.538789
Solvation free energy (kcal/mol)	-46.76

TS

S	-4.820318	1.390655	0.467659
C	-5.315806	-0.312677	0.227757
C	-4.423906	-1.382102	0.368043
C	-6.638981	-0.556326	-0.160783
C	-4.872572	-2.684047	0.140259
C	-7.062722	-1.862703	-0.397954
C	-6.191710	-2.951652	-0.247594
H	-3.399343	-1.207017	0.677805
H	-7.338721	0.267531	-0.264898
H	-4.177186	-3.509239	0.268137
H	-8.093046	-2.038167	-0.695065
H	-3.649418	1.143666	1.099339
C	-0.944806	1.832840	-2.283527
C	-2.055363	0.834679	-1.956136
C	-3.380495	1.229441	-2.028795
H	-1.878407	-0.208249	-2.224094
H	-4.176884	0.499152	-2.102213
H	-3.665483	2.274481	-2.094130
N	1.274153	2.741688	1.701843
N	1.954517	0.719216	2.109193
C	0.737004	3.878276	0.954988
C	1.735677	1.616380	1.142367
C	1.159935	2.545565	3.067211
C	1.594344	1.277083	3.322330
C	2.394260	-0.668771	1.874806

H	-0.349027	3.775893	0.890284
H	1.004029	4.805375	1.463116
H	1.879787	1.454568	0.087799
H	0.786997	3.312031	3.726817
H	1.674289	0.730245	4.247701
H	1.743073	-1.078884	1.099146
H	2.196144	-1.215895	2.798908
Br	-1.279783	0.602941	1.028973
H	1.168971	3.872615	-0.045253
H	-1.879744	0.701070	-0.642855
C	3.865277	-0.755060	1.474524
C	4.278992	-2.194012	1.153192
H	4.487008	-0.353717	2.284286
H	4.037514	-0.128732	0.592583
C	5.729151	-2.295161	0.670854
H	4.138592	-2.827266	2.039856
H	3.613544	-2.597001	0.377246
C	6.153906	-3.727131	0.330546
H	5.851413	-1.659035	-0.215392
H	6.398858	-1.890886	1.442935
H	6.026644	-4.363539	1.216363
H	5.478671	-4.129536	-0.436682
C	7.600595	-3.816117	-0.162652
H	8.300499	-3.449886	0.597014
H	7.877911	-4.847407	-0.401120
H	7.746160	-3.214426	-1.067375
C	-6.672346	-4.362741	-0.476818
H	-7.194460	-4.454624	-1.434836
H	-5.841189	-5.072635	-0.474202
H	-7.375231	-4.669123	0.306496
C	0.480927	1.324608	-2.152870
C	1.534674	2.202416	-2.436473
C	0.816590	0.008181	-1.800213
C	2.874803	1.805160	-2.374173
H	1.311317	3.225115	-2.732021
C	2.142657	-0.413740	-1.754956
H	0.046223	-0.713879	-1.560470
C	3.185257	0.480888	-2.034436
H	3.652981	2.520807	-2.608751
H	2.391528	-1.439481	-1.505060
O	4.446007	-0.022468	-1.942033
C	5.543259	0.809709	-2.320222
H	6.433272	0.190511	-2.213847
H	5.445757	1.137759	-3.360744

H	5.624929	1.682146	-1.661146
H	-1.075120	2.710368	-1.637045
H	-1.085726	2.187352	-3.311866

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4210.62361880
Thermal correction to enthalpy (Hartree)	0.652889
Entropy (cal/(mol*K))	242.346
Thermal correction to Gibbs free energy (Hartree)	0.537743
Solvation free energy (kcal/mol)	-49.36

PC

S	4.285072	-1.219064	-0.297323
C	4.823729	0.464720	0.008247
C	3.911392	1.496241	0.253504
C	6.197865	0.734547	-0.003898
C	4.380198	2.793216	0.462583
C	6.649283	2.034624	0.211114
C	5.750025	3.086188	0.446244
H	2.847304	1.298072	0.286014
H	6.906307	-0.068213	-0.181223
H	3.665815	3.590429	0.647067
H	7.716809	2.235420	0.197268
H	2.729562	-1.094001	0.626186
C	1.302138	-1.497537	-2.094618
C	2.455811	-0.526289	-2.382034
C	3.826449	-1.134194	-2.094450
H	2.423557	-0.227536	-3.436843
H	4.630064	-0.562905	-2.564140
H	3.893700	-2.166333	-2.452462
N	-1.143041	-3.076785	1.160172
N	-2.001478	-1.209849	1.863147
C	-0.449528	-4.021131	0.284926
C	-1.612415	-1.883301	0.774954
C	-1.212468	-3.159861	2.539529
C	-1.761479	-1.990828	2.979669
C	-2.543889	0.161178	1.851307
H	0.627149	-3.916682	0.436125
H	-0.770821	-5.036893	0.517984
H	-1.652709	-1.523947	-0.239848
H	-0.865080	-4.025640	3.079293
H	-1.988126	-1.646804	3.975618
H	-1.896467	0.752626	1.201083
H	-2.438146	0.544307	2.868589

Br	1.410259	-0.863134	1.489104
H	-0.701256	-3.785955	-0.748726
H	2.344207	0.393776	-1.802747
C	-3.996126	0.207958	1.380951
C	-4.524762	1.643366	1.325100
H	-4.614968	-0.399971	2.052569
H	-4.062744	-0.239303	0.382439
C	-5.975406	1.717452	0.840048
H	-4.445432	2.106674	2.318092
H	-3.891662	2.233784	0.649930
C	-6.501906	3.151549	0.729686
H	-6.048663	1.228586	-0.140369
H	-6.618976	1.143953	1.521734
H	-6.421812	3.642472	1.708743
H	-5.855455	3.719324	0.047120
C	-7.951090	3.217557	0.240264
H	-8.622968	2.682278	0.920717
H	-8.301660	4.251785	0.171285
H	-8.054542	2.764558	-0.752739
C	6.251346	4.486348	0.691832
H	7.011070	4.769563	-0.043280
H	5.439347	5.215999	0.642762
H	6.712818	4.565244	1.683053
C	-0.075330	-0.875362	-2.144507
C	-1.137592	-1.530536	-2.774669
C	-0.352846	0.354501	-1.519259
C	-2.438402	-1.007226	-2.780968
H	-0.955735	-2.472718	-3.285896
C	-1.630146	0.901497	-1.533358
H	0.438576	0.892735	-1.010925
C	-2.688545	0.221304	-2.157553
H	-3.226812	-1.549669	-3.287821
H	-1.831665	1.864376	-1.075615
O	-3.903793	0.831942	-2.100556
C	-4.990205	0.251676	-2.822179
H	-5.831998	0.929278	-2.684442
H	-4.754249	0.170913	-3.888874
H	-5.247967	-0.736891	-2.423515
H	1.449506	-1.935406	-1.099812
H	1.349273	-2.327616	-2.809430

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4210.68442246
Thermal correction to enthalpy (Hartree)	0.658290

Entropy (cal/(mol*K))	238.985
Thermal correction to Gibbs free energy (Hartree)	0.544741
Solvation free energy (kcal/mol)	-47.94

2.5.7 The RC, TS and PC for 1-octene

RC

S	-4.772085	1.549736	0.372604
C	-4.706393	-0.227906	0.222279
C	-4.448893	-0.877260	-0.991538
C	-4.957899	-0.997615	1.366932
C	-4.438277	-2.270943	-1.049798
C	-4.948205	-2.391861	1.291786
C	-4.689972	-3.057522	0.083657
H	-4.265236	-0.301605	-1.892117
H	-5.180383	-0.512151	2.312999
H	-4.244435	-2.754563	-2.003592
H	-5.159467	-2.970171	2.187186
H	-4.375483	1.827156	-0.883463
C	0.422670	3.745439	0.699562
C	-0.596200	4.381624	-0.201981
C	-1.918431	4.163692	-0.151196
H	-0.206021	5.076281	-0.946329
H	-2.602492	4.683245	-0.815805
H	-2.361549	3.498603	0.586823
N	-0.937375	-0.473443	1.366709
N	0.569833	-1.228427	-0.005877
C	-1.658975	0.436058	2.259782
C	0.292124	-0.263758	0.878865
C	-1.475092	-1.592332	0.759965
C	-0.525122	-2.068676	-0.098236
C	1.821967	-1.336167	-0.777410
H	-2.368353	1.025646	1.674383
H	-2.192252	-0.148833	3.008911
H	0.943083	0.554767	1.138581
H	-2.475066	-1.934970	0.973851
H	-0.536028	-2.920113	-0.758945
H	1.990771	-0.371920	-1.264704
H	1.637285	-2.074323	-1.560656
Br	-1.396688	1.065929	-1.636889
H	-0.939150	1.088246	2.753952
H	-1.352687	2.467018	-1.245098
C	3.005794	-1.744508	0.097905
C	4.277067	-1.961611	-0.727902
H	2.749898	-2.663259	0.639738

H	3.184254	-0.968187	0.852644
C	5.479991	-2.348445	0.138050
H	4.097423	-2.745832	-1.475811
H	4.509849	-1.047012	-1.289685
C	6.762432	-2.564394	-0.671422
H	5.652351	-1.565236	0.888489
H	5.245099	-3.264187	0.698044
H	6.596755	-3.365026	-1.404439
H	6.980590	-1.658144	-1.251747
C	7.966124	-2.910789	0.208377
H	7.787828	-3.829230	0.778935
H	8.867695	-3.061695	-0.392743
H	8.173455	-2.108308	0.925496
C	1.618165	3.146076	-0.060610
C	2.746865	2.671175	0.859675
H	2.020366	3.905362	-0.743475
H	1.274032	2.323804	-0.702310
H	3.061776	3.505377	1.500177
H	2.379568	1.900917	1.558060
C	3.965091	2.136098	0.101427
C	5.095518	1.651915	1.015727
H	4.346277	2.928752	-0.556164
H	3.659565	1.316754	-0.566352
H	5.330786	2.438762	1.743756
H	4.746376	0.790921	1.603342
C	6.364195	1.275396	0.246020
H	7.137355	0.884627	0.914322
H	6.159459	0.510176	-0.509786
H	6.779721	2.146578	-0.271566
H	0.798816	4.510923	1.393139
H	-0.066331	2.981053	1.318228
C	-4.737360	-4.562779	-0.004133
H	-4.409614	-5.031480	0.928411
H	-5.760088	-4.906618	-0.198847
H	-4.108670	-4.937745	-0.816894

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4061.57234567
Thermal correction to enthalpy (Hartree)	0.682690
Entropy (cal/(mol*K))	247.621
Thermal correction to Gibbs free energy (Hartree)	0.565037
Solvation free energy (kcal/mol)	-48.98

TS

S	4.150527	0.963914	1.288012
C	5.257342	0.186285	0.113964
C	4.800700	-0.342767	-1.098019
C	6.607707	0.069960	0.462577
C	5.708080	-0.954891	-1.964115
C	7.494011	-0.562809	-0.407214
C	7.064204	-1.083495	-1.636703
H	3.757216	-0.249515	-1.380293
H	6.969330	0.481789	1.399942
H	5.347924	-1.345015	-2.911981
H	8.540745	-0.644736	-0.127584
H	3.119679	1.167822	0.430853
C	0.376779	-1.783527	1.832901
C	1.730294	-1.825160	1.116342
C	2.912040	-1.599550	1.803532
H	1.810283	-2.528029	0.281356
H	3.871234	-1.873418	1.379040
H	2.920299	-1.210792	2.816522
N	-0.585006	2.653966	1.425541
N	-1.897199	2.171562	-0.240161
C	0.258413	2.470016	2.606691
C	-1.419809	1.732738	0.928628
C	-0.491486	3.697201	0.522951
C	-1.321774	3.396743	-0.518398
C	-2.799039	1.407465	-1.123336
H	1.231998	2.084635	2.295022
H	0.376094	3.426107	3.116828
H	-1.640084	0.778224	1.376641
H	0.141989	4.551464	0.698411
H	-1.547568	3.941147	-1.420788
H	-2.315117	0.448193	-1.328459
H	-2.846619	1.960896	-2.063317
Br	1.087869	0.605560	-0.667653
H	-0.222813	1.761624	3.280886
H	1.636254	-0.767466	0.359552
C	-4.191442	1.231765	-0.519882
C	-5.143510	0.518195	-1.484717
H	-4.594666	2.218106	-0.259599
H	-4.118463	0.659870	0.413845
C	-6.559525	0.378720	-0.917135
H	-5.184733	1.071848	-2.432641
H	-4.744857	-0.476612	-1.724627
C	-7.526703	-0.325975	-1.873526
H	-6.517985	-0.174940	0.030228

H	-6.952667	1.375487	-0.673778
H	-7.594890	0.248817	-2.806605
H	-7.115532	-1.306545	-2.147702
C	-8.923764	-0.506878	-1.274791
H	-9.371113	0.459376	-1.015648
H	-9.596217	-1.007474	-1.977817
H	-8.884928	-1.111512	-0.361519
C	-0.784429	-2.162008	0.908351
C	-2.155185	-2.099499	1.586699
H	-0.621761	-3.182078	0.536255
H	-0.771428	-1.511099	0.025760
H	-2.152571	-2.735979	2.481630
H	-2.350407	-1.079627	1.957834
C	-3.297867	-2.531022	0.663040
C	-4.682542	-2.457396	1.313804
H	-3.110843	-3.560085	0.328052
H	-3.288754	-1.914121	-0.247801
H	-4.664834	-3.007268	2.263655
H	-4.908953	-1.413197	1.572598
C	-5.788987	-3.021448	0.418755
H	-6.774141	-2.914121	0.882596
H	-5.818277	-2.508484	-0.548130
H	-5.627104	-4.086665	0.221959
H	0.395068	-2.459921	2.695646
H	0.226163	-0.769821	2.230744
C	8.040284	-1.742309	-2.578983
H	8.755772	-1.012885	-2.975568
H	8.618991	-2.520742	-2.070785
H	7.527117	-2.201319	-3.427720

Number of imaginary frequencies	1
Gas phase SP energy (Hartree)	-4061.5404753700
Thermal correction to enthalpy (Hartree)	0.679949
Entropy (cal/(mol*K))	237.017
Thermal correction to Gibbs free energy (Hartree)	0.567335
Solvation free energy (kcal/mol)	-51.64

PC

S	3.359727	-0.597602	1.431242
C	4.751265	-0.323535	0.336678
C	4.704502	-0.707006	-1.009623
C	5.893292	0.295765	0.849072
C	5.808046	-0.478397	-1.826285
C	6.983152	0.537981	0.010357

C	6.961761	0.154796	-1.336116
H	3.819810	-1.179650	-1.421044
H	5.937445	0.575684	1.896660
H	5.768287	-0.785691	-2.867609
H	7.868005	1.018857	0.416776
H	2.144726	0.121546	0.172971
C	0.487149	-2.333291	1.021185
C	1.820757	-2.753663	0.393461
C	3.040286	-2.418396	1.248469
H	1.813673	-3.841014	0.243053
H	3.959497	-2.836156	0.833648
H	2.922898	-2.799279	2.267249
N	-0.145406	2.246932	1.754036
N	-1.693018	2.035587	0.241773
C	0.861059	1.893262	2.756418
C	-1.016321	1.395399	1.199771
C	-0.246059	3.464866	1.106931
C	-1.224171	3.333835	0.164141
C	-2.726921	1.430459	-0.618236
H	1.850048	1.916683	2.296781
H	0.810384	2.595960	3.589141
H	-1.125606	0.353851	1.452362
H	0.379688	4.303773	1.365106
H	-1.614856	4.039672	-0.550786
H	-2.421186	0.399466	-0.810917
H	-2.692107	1.967317	-1.569087
Br	1.271271	0.748264	-0.938404
H	0.658432	0.886219	3.119036
H	1.925460	-2.306965	-0.601247
C	-4.119725	1.495335	0.006776
C	-5.191957	0.987369	-0.962555
H	-4.340118	2.529245	0.299461
H	-4.128434	0.895650	0.925589
C	-6.582003	0.911973	-0.323628
H	-5.226615	1.646196	-1.840826
H	-4.909896	-0.006460	-1.332987
C	-7.676774	0.487952	-1.308057
H	-6.554230	0.203924	0.516026
H	-6.840483	1.889489	0.106861
H	-7.734818	1.223347	-2.121439
H	-7.394818	-0.464696	-1.774132
C	-9.048397	0.345358	-0.643518
H	-9.367468	1.289075	-0.186840
H	-9.812798	0.051266	-1.368993

H	-9.026621	-0.415327	0.145243
C	-0.699257	-2.526215	0.071170
C	-2.065903	-2.385006	0.748337
H	-0.637308	-3.527204	-0.376099
H	-0.610477	-1.815660	-0.760868
H	-2.127331	-3.088671	1.589224
H	-2.170412	-1.384446	1.198910
C	-3.245359	-2.630875	-0.196940
C	-4.612776	-2.490502	0.479452
H	-3.153537	-3.639183	-0.622223
H	-3.186183	-1.941424	-1.052516
H	-4.644651	-3.140119	1.363888
H	-4.729233	-1.464264	0.854368
C	-5.779162	-2.837655	-0.448752
H	-6.743620	-2.688619	0.046232
H	-5.768443	-2.217081	-1.351492
H	-5.726181	-3.883605	-0.769108
H	0.326580	-2.915938	1.938673
H	0.540510	-1.279764	1.334277
C	8.134823	0.421542	-2.244631
H	7.894785	1.209556	-2.967884
H	9.012879	0.743377	-1.679497
H	8.405327	-0.472296	-2.815602

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-4061.59958098
Thermal correction to enthalpy (Hartree)	0.686435
Entropy (cal/(mol*K))	239.902
Thermal correction to Gibbs free energy (Hartree)	0.572450
Solvation free energy (kcal/mol)	-50.27

2.5.8 The two different conformations formed by 1-octene and IL cation

S5a

C	1.908879	-2.464656	-0.768119
C	2.769597	-1.896159	-1.860293
C	3.851717	-1.133063	-1.680091
H	2.46141	-2.136801	-2.878315
H	4.436351	-0.75959	-2.514746
H	4.214732	-0.89059	-0.683893
N	3.380966	0.795616	1.312076
N	1.91787	1.603444	-0.08234
C	4.005488	-0.05177	2.334327
C	2.123298	0.679031	0.863697

C	4.004057	1.819639	0.622029
C	3.08537	2.323844	-0.253144
C	0.669561	1.782817	-0.860623
H	4.79907	-0.647218	1.878982
H	4.415856	0.577189	3.125514
H	1.40366	-0.045382	1.206068
H	5.027504	2.099986	0.813617
H	3.160948	3.124662	-0.971039
H	0.690004	1.059021	-1.680636
H	0.721653	2.78502	-1.290977
H	3.249217	-0.714337	2.75389
C	-0.581813	1.626396	-0.000814
C	-1.864165	1.7815	-0.825683
H	-0.559157	2.369319	0.805902
H	-0.59406	0.63679	0.470874
C	-3.122315	1.722688	0.047816
H	-1.843246	2.733836	-1.371819
H	-1.904877	0.988306	-1.584181
C	-4.421758	1.74077	-0.763547
H	-3.095143	0.81509	0.666478
H	-3.115805	2.570424	0.746541
H	-4.424767	2.618706	-1.422966
H	-4.445511	0.862091	-1.422112
C	-5.671991	1.758579	0.119945
H	-5.693566	2.651746	0.754264
H	-6.584282	1.756332	-0.48375
H	-5.705456	0.882958	0.777712
C	0.425374	-2.096344	-0.943653
C	-0.456596	-2.449787	0.256308
H	0.039025	-2.597395	-1.840074
H	0.338197	-1.021395	-1.150124
H	-0.30365	-3.501486	0.531358
H	-0.137204	-1.865257	1.135706
C	-1.945281	-2.199749	-0.005976
C	-2.832109	-2.381499	1.229257
H	-2.283546	-2.877816	-0.800893
H	-2.082394	-1.183176	-0.401254
H	-2.659117	-3.377895	1.656579
H	-2.527462	-1.661205	2.002005
C	-4.321724	-2.207606	0.921372
H	-4.931808	-2.319246	1.82273
H	-4.526476	-1.217334	0.499839
H	-4.661925	-2.952658	0.193888
H	1.99841	-3.559432	-0.759831

H	2.278039	-2.124466	0.209678

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-816.74521226
Thermal correction to enthalpy (Hartree)	0.534130
Entropy (cal/(mol*K))	184.404
Thermal correction to Gibbs free energy (Hartree)	0.446514
Solvation free energy (kcal/mol)	-51.08

S5b

C	-0.027956	-2.100822	-0.367201
C	1.086454	-2.430425	0.585639
C	1.967140	-3.428363	0.443040
H	1.139181	-1.812290	1.485186
H	2.714176	-3.639728	1.203770
H	1.936444	-4.097913	-0.413444
N	4.783098	-0.093065	0.161870
N	3.123978	1.080898	-0.612488
C	5.595278	-1.243253	0.578568
C	3.536497	-0.160852	-0.325740
C	5.179896	1.232915	0.188291
C	4.135973	1.968869	-0.294031
C	1.774193	1.438754	-1.097343
H	6.462143	-1.336115	-0.077852
H	5.920448	-1.100737	1.610182
H	2.953020	-1.067189	-0.426104
H	6.155984	1.532125	0.535639
H	4.030008	3.031889	-0.440784
H	1.454063	0.641045	-1.771989
H	1.883499	2.349509	-1.690472
H	4.984802	-2.143014	0.509512
C	0.778529	1.628940	0.047426
C	-0.620683	1.965660	-0.479511
H	1.133555	2.425193	0.712957
H	0.739103	0.709478	0.644004
C	-1.661716	2.089260	0.637786
H	-0.582090	2.903299	-1.049916
H	-0.939344	1.187317	-1.185383
C	-3.068315	2.397905	0.114367
H	-1.687806	1.153931	1.213445
H	-1.352275	2.875228	1.340284
H	-3.040758	3.326904	-0.470150
H	-3.374279	1.606154	-0.580692
C	-4.104165	2.526865	1.233776

H	-3.846115	3.341723	1.919185
H	-5.099866	2.732845	0.830151
H	-4.168111	1.604715	1.822165
C	-1.389280	-1.985256	0.339235
C	-2.529014	-1.601758	-0.608023
H	-1.313042	-1.236324	1.140005
H	-1.620076	-2.937324	0.832608
H	-2.260375	-0.682696	-1.148113
H	-2.645632	-2.380891	-1.373529
C	-3.863008	-1.387409	0.112306
C	-5.010286	-1.006076	-0.828511
H	-3.740506	-0.602406	0.871510
H	-4.132333	-2.300588	0.660544
H	-4.728239	-0.111481	-1.400677
H	-5.152466	-1.806338	-1.566888
C	-6.326138	-0.746472	-0.090391
H	-7.128122	-0.481203	-0.786171
H	-6.647737	-1.633991	0.466024
H	-6.220309	0.075115	0.627018
H	0.176560	-1.138503	-0.862692
H	-0.073431	-2.853454	-1.163109

Number of imaginary frequencies	0
Gas phase SP energy (Hartree)	-816.74815958
Thermal correction to enthalpy (Hartree)	0.534013
Entropy (cal/(mol*K))	183.478
Thermal correction to Gibbs free energy (Hartree)	0.446836
Solvation free energy (kcal/mol)	-50.00