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Supporting Information

Table S-1. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in the Gas Phase (ε = 1.0) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.862219	-0.635494	0.036358
C	-3.014446	-1.461945	-0.078013
C	-4.264304	-0.90486	-0.224655
C	-4.411238	0.502842	-0.263619
C	-3.312884	1.331676	-0.153903
C	-2.013226	0.792145	-0.00147
C	-0.853598	1.618527	0.120301
C	0.392318	1.07074	0.245958
C	0.572427	-0.360316	0.288305
C	-0.569535	-1.173491	0.20934
C	1.823854	-1.030694	0.348942
C	3.051305	-0.2925	0.288056
O	3.501098	0.216133	1.313683
O	3.703442	-0.326139	-0.896674
C	5.017328	0.255907	-0.886253
H	5.395033	0.135907	-1.902345
H	4.974858	1.315762	-0.619357
H	5.665327	-0.262856	-0.174527
H	1.269186	1.703502	0.342806
H	-0.983495	2.697971	0.098706
H	-3.4347	2.411396	-0.183285
H	-5.40221	0.933005	-0.380659
H	-5.140947	-1.540008	-0.31143
H	-2.887898	-2.541076	-0.046911
H	-0.426175	-2.248778	0.264847

Table S-2. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in the Gas Phase (ε = 1.0) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.891741	-0.650131	-0.000019
C	2.969658	-1.578801	-0.000095
C	4.276066	-1.141771	-0.000096
C	4.563898	0.24346	-0.000018
C	3.538461	1.169572	0.000053
C	2.187193	0.754143	0.000053
C	1.100089	1.682013	0.00011
C	-0.2013	1.267358	0.000109
C	-0.519814	-0.14457	0.000067
C	0.543617	-1.068436	-0.000001
C	-1.840262	-0.608706	0.000129
C	-3.142434	0.004286	-0.000046
O	-3.336056	1.215739	-0.000381
O	-4.13992	-0.910008	0.000251
C	-5.467477	-0.364545	-0.000033
H	-6.135502	-1.226374	-0.001348
H	-5.634522	0.248596	0.890186
H	-5.633404	0.250545	-0.889094
H	-1.022271	1.974417	0.000114
H	1.328113	2.745611	0.000154
H	3.760093	2.23417	0.000109
H	5.597712	0.577722	-0.000016
H	5.090904	-1.860398	-0.000156
H	2.743188	-2.642262	-0.000154
H	0.316872	-2.131101	-0.000033

Table S-3. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in Heptane (ε = 1.9) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.864771	-0.63567	0.029375
C	-3.017195	-1.461859	-0.08048
C	-4.267159	-0.903535	-0.214962
C	-4.41366	0.503734	-0.245901
C	-3.315105	1.332533	-0.140734
C	-2.01573	0.792199	-0.000574
C	-0.856002	1.618398	0.116243
C	0.38999	1.070574	0.231656
C	0.570695	-0.360382	0.266478
C	-0.572368	-1.174321	0.188994
C	1.820511	-1.027006	0.319998
C	3.051177	-0.293979	0.287332
O	3.50717	0.181802	1.326705
O	3.707876	-0.302004	-0.894711
C	5.028365	0.262998	-0.862935
H	5.409338	0.167062	-1.880267
H	4.998555	1.315508	-0.567957
H	5.667875	-0.283783	-0.164852
H	1.266448	1.704511	0.324707
H	-0.986486	2.697666	0.100444
H	-3.437931	2.412097	-0.164009
H	-5.405271	0.93452	-0.353473
H	-5.14472	-1.537565	-0.298376
H	-2.890715	-2.540963	-0.055745
H	-0.429951	-2.249539	0.23664

Table S-4. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in Heptane ($\varepsilon = 1.9$) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.899093	-0.612634	-0.141152
C	-2.990647	-1.484566	-0.40772
C	-4.288217	-1.069816	-0.205647
C	-4.552963	0.234499	0.272384
C	-3.513907	1.104246	0.540499
C	-2.171438	0.710118	0.343094
C	-1.071126	1.581715	0.608601
C	0.221872	1.18845	0.414458
C	0.517138	-0.141422	-0.072774
C	-0.559533	-1.009761	-0.338697
C	1.829208	-0.578516	-0.282902
C	3.136373	0.001041	-0.13183
O	3.343603	1.145594	0.259712
O	4.122952	-0.858679	-0.471148
C	5.454815	-0.34049	-0.341191
H	6.114171	-1.152617	-0.648464
H	5.596315	0.531175	-0.986262
H	5.65961	-0.053014	0.69385
H	1.052779	1.853604	0.616788
H	-1.281835	2.583808	0.975197
H	-3.718508	2.106967	0.907869
H	-5.580299	0.551304	0.428657
H	-5.114219	-1.744367	-0.412667
H	-2.782003	-2.48641	-0.774687
H	-0.35045	-2.010643	-0.704608

Table S-5. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in Benzene (ε = 2.2) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.86503	-0.635662	0.026309
C	-3.018246	-1.460197	-0.08617
C	-4.267634	-0.899732	-0.216218
C	-4.412552	0.507745	-0.239394
C	-3.313043	1.334911	-0.13149
C	-2.01431	0.792457	0.003926
C	-0.853504	1.617021	0.121423
C	0.391842	1.06728	0.232903
C	0.570832	-0.36398	0.259673
C	-0.573046	-1.1766	0.178704
C	1.819384	-1.0319	0.307673
C	3.050126	-0.298797	0.286044
O	3.511617	0.153697	1.333415
O	3.702728	-0.283332	-0.897976
C	5.025244	0.276457	-0.857796
H	5.404569	0.19781	-1.876875
H	4.998946	1.323213	-0.543715
H	5.663402	-0.284792	-0.170502
H	1.269395	1.699355	0.32658
H	-0.98311	2.696133	0.110335
H	-3.434649	2.41442	-0.149327
H	-5.403536	0.940023	-0.343468
H	-5.145789	-1.532028	-0.302069
H	-2.892625	-2.539197	-0.067678
H	-0.431736	-2.251873	0.219685

Table S-6. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in Benzene (ε = 2.2) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.890718	-0.650599	0.001243
C	2.96928	-1.577266	0.00166
C	4.274154	-1.137592	0.000387
C	4.559367	0.247456	-0.001179
C	3.533007	1.171692	-0.00151
C	2.183548	0.753682	-0.000479
C	1.095875	1.679651	-0.001415
C	-0.204161	1.262865	-0.001138
C	-0.519612	-0.14888	-0.000052
C	0.544309	-1.071526	0.001819
C	-1.838665	-0.612908	-0.000525
C	-3.137956	0.00188	0.001098
O	-3.328572	1.214032	0.006636
O	-4.137347	-0.908311	-0.004948
C	-5.463039	-0.358668	-0.001404
H	-6.134092	-1.217474	-0.008604
H	-5.628462	0.247712	0.893238
H	-5.627584	0.262125	-0.886142
H	-1.025724	1.969029	-0.001813
H	1.322456	2.743132	-0.002537
H	3.752855	2.236257	-0.002799
H	5.592154	0.583316	-0.002101
H	5.090067	-1.854247	0.000696
H	2.744707	-2.640633	0.002852
H	0.320018	-2.133699	0.002682

Table S-7. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in Freon-113 ($\varepsilon = 2.2$) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.864431	-0.636099	0.027889
C	-3.017847	-1.46074	-0.083833
C	-4.267018	-0.899604	-0.216748
C	-4.412003	0.50706	-0.244632
C	-3.312499	1.334198	-0.137098
C	-2.013842	0.792032	0.001564
C	-0.853407	1.616851	0.120424
C	0.391885	1.067443	0.235106
C	0.571178	-0.36387	0.26563
C	-0.572769	-1.176618	0.185372
C	1.820476	-1.030611	0.318022
C	3.050529	-0.296739	0.288184
O	3.510843	0.17105	1.329285
O	3.702441	-0.295018	-0.896787
C	5.022567	0.270795	-0.865465
H	5.397902	0.187941	-1.886189
H	4.993514	1.31959	-0.556962
H	5.666596	-0.284239	-0.177781
H	1.268935	1.700591	0.32998
H	-0.982804	2.696502	0.106914
H	-3.433803	2.414197	-0.157896
H	-5.403396	0.939147	-0.351108
H	-5.145543	-1.533304	-0.3015
H	-2.892644	-2.540278	-0.061639
H	-0.431949	-2.252984	0.229707

Table S-8. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in Freon-113 ($\varepsilon = 2.2$) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.890897	-0.650436	-0.000142
C	2.969146	-1.577708	0.002183
C	4.274404	-1.13879	0.002142
C	4.560215	0.246121	-0.000471
C	3.534369	1.171114	-0.00245
C	2.184586	0.75378	-0.00191
C	1.097225	1.680241	-0.002768
C	-0.203187	1.264175	-0.00118
C	-0.519649	-0.1475	0.00062
C	0.544095	-1.070695	-0.000271
C	-1.839023	-0.611096	-0.000563
C	-3.138997	0.002261	0.003374
O	-3.330848	1.214481	0.009859
O	-4.137692	-0.908474	-0.004685
C	-5.464107	-0.360566	-0.003535
H	-6.134271	-1.220685	-0.011301
H	-5.631958	0.246185	0.890831
H	-5.628199	0.259523	-0.889387
H	-1.024007	1.971375	-0.001281
H	1.324193	2.744171	-0.004502
H	3.755116	2.235963	-0.004235
H	5.593772	0.581504	-0.000676
H	5.090452	-1.856166	0.004125
H	2.744065	-2.6415	0.004228
H	0.319311	-2.133828	0.000637

Table S-9. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in CH_2Cl_2 ($\varepsilon = 8.9$) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.872704	-0.635232	-0.001875
C	-3.032234	-1.453881	-0.102179
C	-4.281713	-0.885469	-0.187974
C	-4.420396	0.523261	-0.17821
C	-3.315206	1.344918	-0.081422
C	-2.016181	0.794532	0.009487
C	-0.84937	1.612604	0.115573
C	0.39528	1.055383	0.19126
C	0.570039	-0.377667	0.183573
C	-0.580763	-1.184399	0.102451
C	1.816358	-1.046569	0.211645
C	3.051385	-0.324073	0.280993
O	3.500535	0.029792	1.371941
O	3.728437	-0.213712	-0.88553
C	5.050536	0.340937	-0.777796
H	5.445013	0.350256	-1.794524
H	5.018163	1.357446	-0.376313
H	5.680155	-0.278135	-0.132798
H	1.276152	1.685015	0.275745
H	-0.974199	2.692734	0.127302
H	-3.432875	2.425424	-0.073785
H	-5.412507	0.96123	-0.247394
H	-5.16543	-1.512116	-0.263552
H	-2.910762	-2.534041	-0.108854
H	-0.445658	-2.262533	0.109732

Table S-10. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in CH_2Cl_2 (ε = 8.9) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.890784	-0.65011	-0.000312
C	2.967583	-1.579562	0.001988
C	4.27351	-1.14192	0.002975
C	4.561212	0.242747	0.001794
C	3.53683	1.169863	-0.000868
C	2.186533	0.753914	-0.00199
C	1.100305	1.682217	-0.005017
C	-0.200607	1.267315	-0.004512
C	-0.519301	-0.143998	-0.001261
C	0.543379	-1.069264	-0.000953
C	-1.839211	-0.605877	-0.001887
C	-3.14021	0.003986	0.002753
O	-3.335458	1.216552	0.012948
O	-4.136448	-0.908598	-0.005706
C	-5.466465	-0.366283	-0.00152
H	-6.132446	-1.229481	-0.011153
H	-5.63583	0.235537	0.895699
H	-5.634078	0.25446	-0.886059
H	-1.019728	1.976567	-0.005494
H	1.328774	2.745818	-0.006964
H	3.75931	2.23431	-0.001703
H	5.5953	0.576495	0.002922
H	5.088753	-1.860178	0.004852
H	2.740803	-2.642938	0.003145
H	0.318349	-2.132389	-0.000329

Table S-11. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in Methanol (ε = 32.6) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.873021	-0.636037	-0.000244
C	-3.032068	-1.455549	-0.112679
C	-4.281295	-0.885172	-0.204518
C	-4.419526	0.524173	-0.188363
C	-3.314201	1.346849	-0.080294
C	-2.016764	0.794623	0.016565
C	-0.850591	1.614601	0.134945
C	0.393028	1.056564	0.212424
C	0.568049	-0.37874	0.20023
C	-0.584223	-1.189903	0.115562
C	1.814473	-1.037659	0.214175
C	3.052908	-0.321138	0.281447
O	3.529782	0.002995	1.372567
O	3.709406	-0.188683	-0.893328
C	5.047747	0.339438	-0.80294
H	5.417258	0.365501	-1.829198
H	5.04128	1.346855	-0.377316
H	5.678521	-0.310175	-0.189064
H	1.274265	1.686624	0.30369
H	-0.976724	2.69554	0.153119
H	-3.42973	2.428601	-0.068321
H	-5.412682	0.961851	-0.26146
H	-5.165954	-1.510714	-0.288799
H	-2.90885	-2.536469	-0.123917
H	-0.457988	-2.274418	0.129489

Table S-12. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in Methanol (ε = 32.6) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.890866	-0.650365	-0.00635
C	2.967763	-1.58072	-0.000223
C	4.274366	-1.142103	0.011048
C	4.562446	0.243474	0.016482
C	3.537542	1.171607	0.010601
C	2.18731	0.753973	-0.000739
C	1.10126	1.683498	-0.006908
C	-0.199157	1.266279	-0.014182
C	-0.518353	-0.145892	-0.017447
C	0.543793	-1.073749	-0.016958
C	-1.839671	-0.604389	-0.014857
C	-3.139974	0.005307	-0.003667
O	-3.336141	1.219634	0.000823
O	-4.136477	-0.905906	0.004252
C	-5.47212	-0.368366	0.022301
H	-6.133534	-1.235811	0.028526
H	-5.630239	0.237693	0.918903
H	-5.653066	0.243765	-0.866188
H	-1.016823	1.977663	-0.016996
H	1.329373	2.748033	-0.003273
H	3.758012	2.237444	0.016204
H	5.597524	0.577482	0.025401
H	5.089913	-1.861295	0.014804
H	2.739507	-2.64443	-0.004581
H	0.323858	-2.141694	-0.028007

Table S-13. Cartesian Coordinates of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in CH_3CN ($\varepsilon = 36.6$) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.871837	-0.636727	-0.004482
C	-3.032432	-1.453713	-0.107771
C	-4.281114	-0.883224	-0.189308
C	-4.417667	0.525674	-0.171458
C	-3.311388	1.345831	-0.071866
C	-2.013303	0.793359	0.014554
C	-0.845132	1.60959	0.121445
C	0.398512	1.050176	0.194291
C	0.571573	-0.383423	0.178906
C	-0.581027	-1.188218	0.09164
C	1.816233	-1.052273	0.207335
C	3.052457	-0.333866	0.291568
O	3.518962	-0.016094	1.386342
O	3.712803	-0.185383	-0.8813
C	5.044978	0.344802	-0.774095
H	5.425978	0.381809	-1.795263
H	5.034139	1.347797	-0.338946
H	5.673316	-0.305215	-0.158993
H	1.280594	1.678368	0.277456
H	-0.968624	2.689741	0.136984
H	-3.428108	2.426305	-0.058456
H	-5.409202	0.965394	-0.237127
H	-5.165777	-1.508051	-0.268072
H	-2.911979	-2.533868	-0.120844
H	-0.447634	-2.266591	0.088487

Table S-14. Cartesian Coordinates of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in CH_3CN ($\varepsilon = 36.6$) Obtained from B3LYP/6-31G* Calculations Using the PCM Solvation Model

Standard orientation:

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.890547	-0.650267	0.001348
C	-2.967604	-1.579228	0.003828
C	-4.273247	-1.140785	0.002511
C	-4.560316	0.244035	-0.001359
C	-3.535462	1.170716	-0.003914
C	-2.185538	0.753909	-0.002652
C	-1.099045	1.681808	-0.00484
C	0.201511	1.266095	-0.003811
C	0.519326	-0.14541	-0.000416
C	-0.543604	-1.070436	0.002392
C	1.838872	-0.607695	0.000238
C	3.138977	0.003485	0.004135
O	3.333641	1.216262	0.019132
O	4.135733	-0.90819	-0.010687
C	5.465497	-0.364622	-0.005484
H	6.132382	-1.22692	-0.017235
H	5.63194	0.258051	-0.888869
H	5.634264	0.236044	0.892569
H	1.021166	1.974575	-0.005451
H	-1.327123	2.745467	-0.007495
H	-3.757115	2.235295	-0.006792
H	-5.594185	0.578282	-0.002279
H	-5.08878	-1.858628	0.004401
H	-2.741242	-2.642639	0.006769
H	-0.319214	-2.133725	0.004959

Table S-15. Frequencies (cm^{-1}) and Intensities (given in parentheses) of the Singlet State of 2-Naphthyl(carbomethoxy)carbene in Different Solvents Obtained from B3LYP/6-31G* Calculation Using the PCM Solvation Model

Gas phase	Heptane	Benzene	Freon-113	CH_2Cl_2	Methanol	CH_3CN
30 (1)	29 (1)	26 (1)	-56 (1)	31 (3)	35 (1)	29 (1)
52 (3)	50 (4)	46 (3)	45 (2)	49 (3)	50 (4)	45 (4)
74 (2)	59 (2)	63 (2)	95 (3)	64 (3)	85 (0)	69 (3)
114 (1)	114 (3)	114 (1)	110 (2)	114 (7)	115 (7)	113 (5)
116 (4)	116 (3)	115 (5)	140 (3)	117 (1)	129 (1)	118 (1)
156 (4)	153 (8)	149 (5)	175 (2)	150 (7)	155 (8)	152 (6)
186 (1)	187 (1)	188 (2)	203 (7)	190 (2)	188 (1)	185 (1)
223 (18)	225 (20)	225 (22)	236 (2)	232 (34)	235 (14)	232 (13)
245 (1)	242 (1)	242 (1)	261 (7)	236 (2)	239 (6)	235 (12)
306 (27)	306 (35)	306 (34)	305 (32)	304 (42)	305 (47)	303 (43)
376 (3)	376 (6)	375 (4)	384 (2)	376 (6)	375 (5)	375 (7)
398 (13)	399 (14)	399 (17)	397 (13)	399 (16)	402 (9)	399 (11)
423 (107)	426 (109)	426 (113)	430 (120)	434 (114)	445 (126)	436 (104)
491 (12)	491 (14)	493 (14)	491 (15)	491 (18)	490 (14)	491 (17)
500 (8)	499 (10)	498 (13)	504 (19)	499 (19)	498 (15)	496 (24)
523 (14)	523 (20)	523 (21)	523 (18)	522 (21)	523 (36)	523 (24)
541 (22)	543 (19)	542 (23)	543 (26)	547 (17)	553 (29)	545 (23)
593 (6)	592 (7)	594 (9)	594 (9)	595 (13)	593 (16)	594 (10)
647 (0)	646 (2)	648 (1)	649 (4)	649 (3)	646 (4)	647 (2)
651 (5)	652 (4)	652 (4)	651 (2)	656 (1)	654 (3)	653 (1)
731 (7)	731 (7)	732 (7)	730 (7)	730 (10)	729 (15)	730 (10)
769 (21)	771 (23)	771 (23)	771 (24)	771 (27)	771 (32)	771 (27)
778 (2)	778 (2)	779 (2)	779 (1)	779 (2)	777 (6)	779 (3)
782 (4)	783 (5)	782 (5)	782 (5)	783 (5)	788 (8)	784 (6)
796 (14)	797 (18)	798 (20)	820 (20)	797 (23)	795 (39)	798 (28)
840 (27)	841 (31)	841 (32)	840 (38)	838 (34)	836 (51)	837 (37)
860 (37)	861 (40)	862 (40)	866 (38)	862 (49)	862 (54)	861 (48)
893 (15)	895 (15)	896 (15)	895 (15)	897 (15)	899 (19)	898 (17)
928 (19)	928 (22)	929 (24)	928 (24)	931 (27)	928 (27)	929 (25)
949 (5)	953 (7)	954 (7)	953 (7)	955 (10)	963 (15)	955 (11)
974 (8)	978 (9)	978 (9)	975 (6)	977 (2)	973 (16)	977 (7)
979 (2)	980 (3)	980 (3)	979 (6)	983 (7)	988 (14)	982 (7)
991 (0)	992 (0)	992 (0)	992 (1)	991 (1)	992 (4)	990 (1)
1004 (0)	1009 (0)	1009 (0)	1009 (0)	1015 (0)	1017 (0)	1015 (0)
1051 (0)	1053 (0)	1053 (0)	1054 (0)	1052 (0)	1049 (3)	1052 (1)
1059 (42)	1060 (41)	1060 (41)	1060 (42)	1057 (36)	1050 (21)	1056 (38)
1159 (55)	1159 (75)	1160 (77)	1160 (74)	1159 (116)	1152 (158)	1158 (142)
1181 (1)	1181 (2)	1181 (2)	1181 (1)	1179 (6)	1178 (15)	1179 (4)
1189 (41)	1189 (72)	1188 (75)	1190 (68)	1187 (160)	1180 (195)	1186 (167)
1192 (6)	1194 (6)	1194 (7)	1194 (6)	1194 (4)	1188 (67)	1194 (5)
1208 (399)	1208 (571)	1208 (612)	1207 (649)	1205 (925)	1203 (1285)	1203 (1077)
1216 (175)	1216 (173)	1216 (164)	1216 (160)	1213 (82)	1212 (38)	1213 (46)
1252 (245)	1254 (299)	1254 (307)	1254 (307)	1253 (348)	1249 (395)	1252 (337)
1281 (256)	1281 (263)	1281 (280)	1280 (251)	1280 (233)	1277 (167)	1279 (213)

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Table S-15. (cont.)

Gas phase		Heptane		Benzene		Freon-113		CH_2Cl_2		Methanol		CH_3CN	
1297	(18)	1298	(18)	1298	(19)	1298	(19)	1299	(17)	1297	(18)	1299	(19)
1374	(7)	1375	(9)	1375	(9)	1375	(9)	1374	(13)	1367	(18)	1373	(13)
1404	(27)	1407	(25)	1408	(25)	1408	(27)	1409	(32)	1406	(55)	1409	(36)
1422	(82)	1426	(77)	1427	(82)	1426	(77)	1428	(81)	1426	(99)	1429	(79)
1435	(44)	1438	(49)	1439	(49)	1443	(45)	1440	(54)	1439	(69)	1440	(58)
1477	(3)	1480	(6)	1480	(6)	1480	(10)	1480	(10)	1477	(21)	1480	(12)
1494	(45)	1494	(52)	1494	(56)	1496	(56)	1493	(69)	1490	(86)	1493	(64)
1513	(3)	1513	(4)	1513	(4)	1512	(4)	1510	(5)	1504	(10)	1510	(6)
1517	(22)	1520	(37)	1521	(34)	1520	(36)	1521	(47)	1517	(39)	1521	(54)
1528	(9)	1527	(12)	1527	(11)	1527	(11)	1525	(29)	1522	(80)	1525	(40)
1547	(10)	1549	(11)	1549	(11)	1550	(8)	1549	(13)	1545	(21)	1548	(13)
1604	(18)	1605	(25)	1605	(29)	1606	(26)	1603	(43)	1596	(58)	1602	(47)
1646	(51)	1647	(72)	1648	(79)	1653	(74)	1646	(133)	1643	(141)	1646	(132)
1674	(80)	1676	(116)	1676	(121)	1676	(133)	1674	(187)	1668	(264)	1673	(211)
1694	(163)	1692	(191)	1691	(201)	1691	(198)	1686	(243)	1677	(296)	1687	(261)
3071	(52)	3076	(50)	3080	(49)	3072	(50)	3074	(45)	3063	(6)	3074	(44)
3144	(25)	3149	(25)	3153	(25)	3145	(25)	3148	(25)	3103	(147)	3148	(25)
3176	(21)	3181	(20)	3186	(20)	3178	(20)	3180	(17)	3142	(7)	3180	(17)
3185	(4)	3192	(3)	3196	(3)	3187	(3)	3190	(2)	3172	(4)	3191	(1)
3188	(5)	3194	(4)	3199	(3)	3189	(3)	3193	(1)	3172	(3)	3194	(1)
3193	(0)	3200	(0)	3205	(0)	3195	(1)	3198	(0)	3176	(6)	3199	(0)
3204	(23)	3210	(18)	3215	(17)	3205	(17)	3208	(12)	3181	(3)	3209	(11)
3213	(3)	3219	(5)	3222	(5)	3212	(1)	3211	(0)	3190	(7)	3211	(0)
3216	(27)	3222	(20)	3227	(18)	3215	(18)	3214	(6)	3197	(16)	3214	(5)
3218	(4)	3226	(1)	3231	(1)	3216	(5)	3220	(12)	3206	(11)	3221	(10)

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Table S-16. Frequencies (cm^{-1}) and Intensities (given in parentheses) of the Triplet State of 2-Naphthyl(carbomethoxy)carbene in Different Solvents Obtained from B3LYP/6-31G* Calculation Using the PCM Solvation Model

Gas phase		Heptane		Benzene		Freon-113		CH_2Cl_2		Methanol		CH_3CN	
47	(1)	54	(0)	6	(2)	-47	(2)	-125	(2)	40	(2)	39	(0)
49	(1)	64	(1)	47	(0)	39	(1)	37	(3)	51	(1)	45	(2)
83	(2)	83	(2)	81	(2)	79	(2)	102	(2)	84	(2)	103	(3)
119	(1)	146	(1)	122	(2)	118	(1)	118	(7)	126	(6)	115	(2)
143	(0)	152	(1)	146	(0)	146	(0)	145	(0)	146	(1)	146	(0)
186	(0)	183	(0)	196	(1)	185	(1)	179	(2)	185	(1)	183	(1)
202	(3)	205	(5)	212	(4)	199	(4)	201	(5)	209	(8)	199	(4)
224	(2)	225	(2)	223	(2)	222	(2)	238	(2)	225	(9)	237	(3)
253	(2)	254	(3)	253	(3)	252	(3)	274	(4)	254	(10)	268	(3)
317	(0)	316	(0)	321	(0)	315	(0)	316	(0)	318	(1)	316	(0)
335	(30)	339	(35)	334	(35)	333	(37)	376	(25)	332	(55)	358	(38)
397	(5)	397	(7)	396	(6)	396	(6)	398	(10)	395	(9)	396	(8)
402	(0)	402	(0)	414	(0)	402	(0)	401	(3)	403	(1)	402	(0)
481	(11)	479	(12)	488	(11)	480	(12)	479	(15)	479	(19)	479	(15)
519	(0)	519	(0)	520	(0)	519	(0)	519	(1)	519	(1)	520	(0)
526	(0)	524	(0)	541	(1)	528	(0)	531	(4)	528	(0)	521	(0)
556	(1)	556	(2)	556	(2)	556	(2)	556	(4)	555	(5)	556	(3)
632	(5)	632	(6)	632	(7)	632	(7)	631	(31)	631	(9)	631	(8)
649	(0)	649	(0)	676	(1)	648	(0)	648	(3)	648	(0)	646	(0)
710	(2)	713	(2)	711	(2)	705	(17)	716	(8)	709	(5)	716	(4)
721	(16)	732	(18)	728	(18)	710	(2)	734	(13)	719	(26)	720	(22)
763	(21)	764	(21)	765	(0)	764	(23)	765	(22)	764	(3)	765	(23)
764	(0)	765	(1)	767	(28)	765	(1)	765	(4)	766	(25)	765	(2)
773	(1)	771	(1)	778	(0)	773	(2)	773	(5)	773	(7)	771	(3)
778	(0)	778	(0)	779	(0)	779	(0)	780	(8)	777	(1)	778	(0)
838	(23)	839	(27)	840	(25)	839	(29)	839	(37)	838	(48)	839	(36)
873	(32)	875	(34)	879	(5)	875	(34)	877	(37)	877	(17)	877	(38)
877	(5)	878	(5)	883	(23)	878	(5)	881	(5)	881	(42)	881	(6)
900	(3)	901	(4)	915	(12)	901	(4)	901	(7)	906	(13)	903	(6)
944	(7)	945	(8)	945	(8)	944	(9)	944	(12)	941	(37)	943	(11)
956	(4)	959	(4)	961	(5)	960	(4)	963	(4)	965	(28)	964	(4)
973	(5)	976	(6)	974	(5)	973	(5)	972	(6)	968	(6)	970	(8)
987	(0)	990	(0)	992	(0)	991	(0)	991	(0)	992	(0)	991	(0)
995	(0)	997	(0)	1000	(0)	998	(0)	1001	(2)	1004	(0)	999	(0)
1052	(0)	1053	(1)	1053	(1)	1053	(0)	1053	(0)	1048	(2)	1052	(0)
1063	(26)	1065	(29)	1065	(32)	1064	(29)	1064	(20)	1053	(30)	1057	(35)
1158	(34)	1158	(40)	1158	(46)	1158	(45)	1157	(61)	1152	(57)	1156	(64)
1183	(1)	1184	(27)	1183	(2)	1183	(1)	1181	(36)	1176	(36)	1181	(49)
1183	(22)	1184	(4)	1183	(32)	1183	(32)	1182	(1)	1179	(4)	1182	(2)
1187	(0)	1187	(0)	1188	(0)	1187	(0)	1186	(1)	1180	(6)	1186	(1)
1214	(70)	1215	(78)	1214	(95)	1214	(88)	1216	(388)	1211	(276)	1216	(381)
1229	(157)	1230	(233)	1229	(273)	1229	(281)	1237	(5)	1223	(359)	1234	(76)
1246	(455)	1247	(525)	1247	(507)	1246	(514)	1255	(591)	1239	(615)	1245	(671)
1280	(280)	1281	(302)	1281	(290)	1280	(288)	1280	(389)	1273	(249)	1279	(286)

Table S-16. (cont.)

Gas phase		Heptane		Benzene		Freon-113		CH_2Cl_2		Methanol		CH_3CN	
1299	(14)	1300	(16)	1301	(15)	1301	(15)	1300	(18)	1295	(25)	1300	(16)
1356	(24)	1357	(29)	1357	(28)	1356	(29)	1355	(30)	1349	(40)	1354	(36)
1395	(35)	1397	(34)	1398	(33)	1398	(33)	1397	(27)	1393	(26)	1397	(28)
1420	(58)	1421	(71)	1422	(64)	1422	(64)	1421	(82)	1417	(84)	1421	(82)
1439	(128)	1441	(136)	1443	(142)	1442	(144)	1442	(162)	1440	(157)	1442	(155)
1471	(8)	1473	(8)	1474	(8)	1473	(8)	1473	(13)	1470	(10)	1473	(8)
1491	(17)	1492	(23)	1492	(24)	1491	(24)	1490	(31)	1485	(32)	1490	(35)
1503	(45)	1505	(55)	1506	(54)	1505	(55)	1505	(61)	1500	(60)	1505	(62)
1513	(6)	1513	(7)	1512	(7)	1512	(7)	1510	(8)	1504	(35)	1509	(9)
1525	(7)	1523	(6)	1524	(6)	1523	(6)	1520	(4)	1510	(4)	1520	(5)
1540	(24)	1542	(30)	1542	(31)	1542	(31)	1541	(35)	1538	(47)	1541	(40)
1591	(4)	1592	(5)	1593	(5)	1593	(5)	1591	(16)	1586	(8)	1591	(7)
1637	(6)	1638	(7)	1639	(8)	1638	(8)	1637	(8)	1635	(14)	1638	(12)
1662	(16)	1663	(20)	1664	(21)	1664	(21)	1662	(16)	1658	(38)	1663	(30)
1701	(156)	1698	(196)	1700	(206)	1698	(205)	1692	(268)	1681	(376)	1691	(297)
3071	(48)	3075	(44)	3079	(44)	3072	(44)	3074	(39)	3065	(5)	3074	(37)
3143	(24)	3148	(23)	3152	(23)	3145	(23)	3148	(23)	3127	(86)	3149	(23)
3180	(23)	3185	(22)	3190	(20)	3182	(21)	3185	(1)	3145	(9)	3185	(1)
3181	(0)	3186	(0)	3191	(0)	3182	(0)	3186	(19)	3170	(1)	3187	(18)
3183	(12)	3189	(12)	3194	(13)	3185	(12)	3187	(9)	3173	(3)	3187	(7)
3186	(3)	3192	(2)	3197	(1)	3188	(1)	3191	(2)	3175	(7)	3191	(0)
3197	(0)	3205	(23)	3210	(21)	3199	(1)	3200	(2)	3179	(0)	3200	(2)
3199	(35)	3211	(5)	3216	(4)	3201	(25)	3202	(18)	3187	(5)	3203	(16)
3212	(36)	3217	(28)	3222	(26)	3213	(27)	3214	(25)	3198	(9)	3215	(18)
3244	(4)	3246	(4)	3246	(4)	3244	(4)	3243	(5)	3236	(8)	3244	(5)

Table S-17. Calculated Dipole Moments (Debye) Using the PCM Solvation Model for the Singlet and Triplet States of 2-Naphthyl(carbomethoxy)carbene

		B3LYP/6-31G*		B3LYP/6-311+G**// B3LYP/6-31G*	
	ε	Singlet	Triplet	Singlet	Triplet
Gas	1.0	5.0	1.4	5.4	1.6
Heptane	1.9	5.8	1.7	6.2	1.9
Benzene	2.2	5.9	1.8	6.3	1.9
Freon-113	2.2[a]	5.9	1.8	6.4	1.9
CH_2Cl_2	8.9	6.8	2.1	7.3	2.3
Methanol	32.6	7.7	2.6	8.1	2.8
CH_3CN	36.6	7.2	2.2	7.7	2.4

[a] The Freon-113 solvent was modeled as CCl_4.

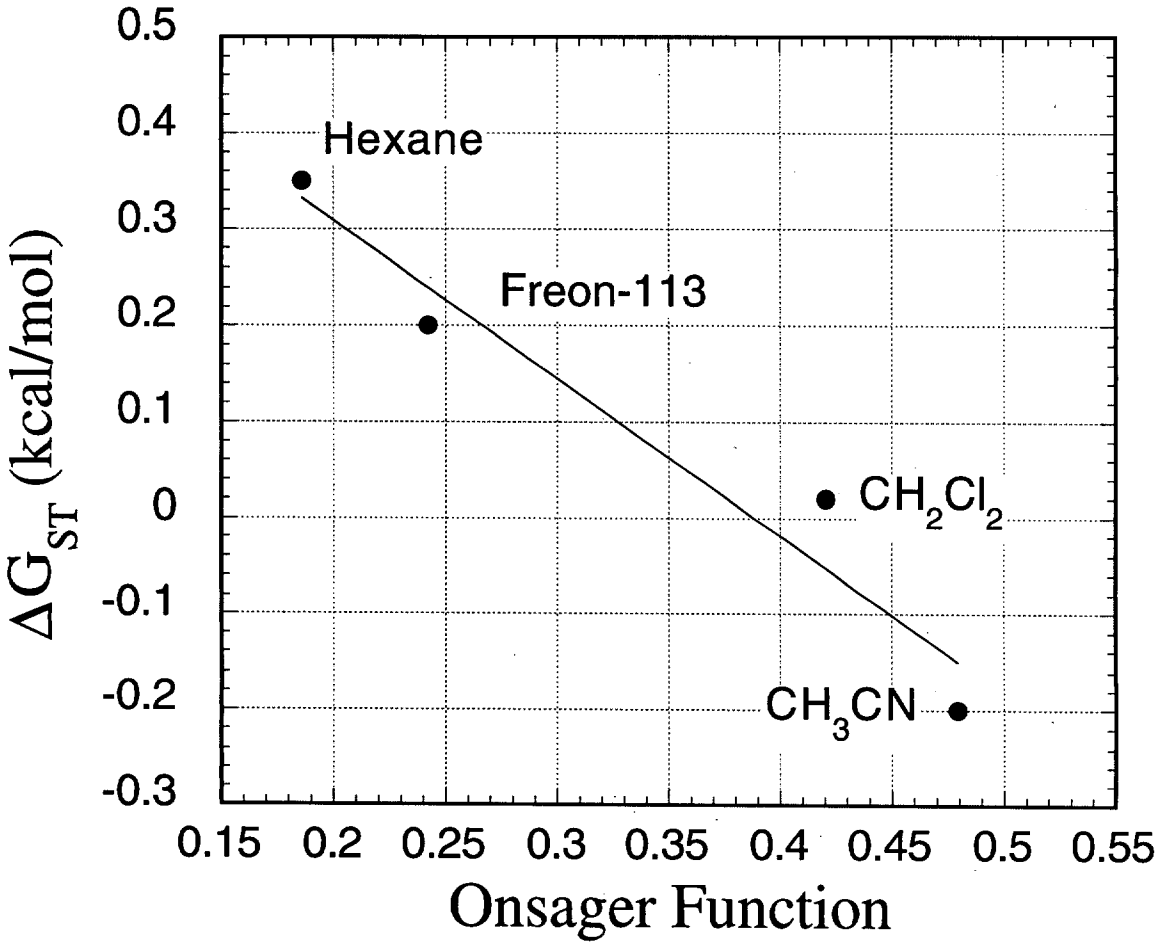


Figure S-1. Plot of experimentally-derived ΔG_{ST} at 294 K as a function of the Onsager function. When possible the average of the ΔG_{ST} values derived in the 1680 – 1540 cm^{-1} and 1260 – 1140 cm^{-1} spectral regions is used.

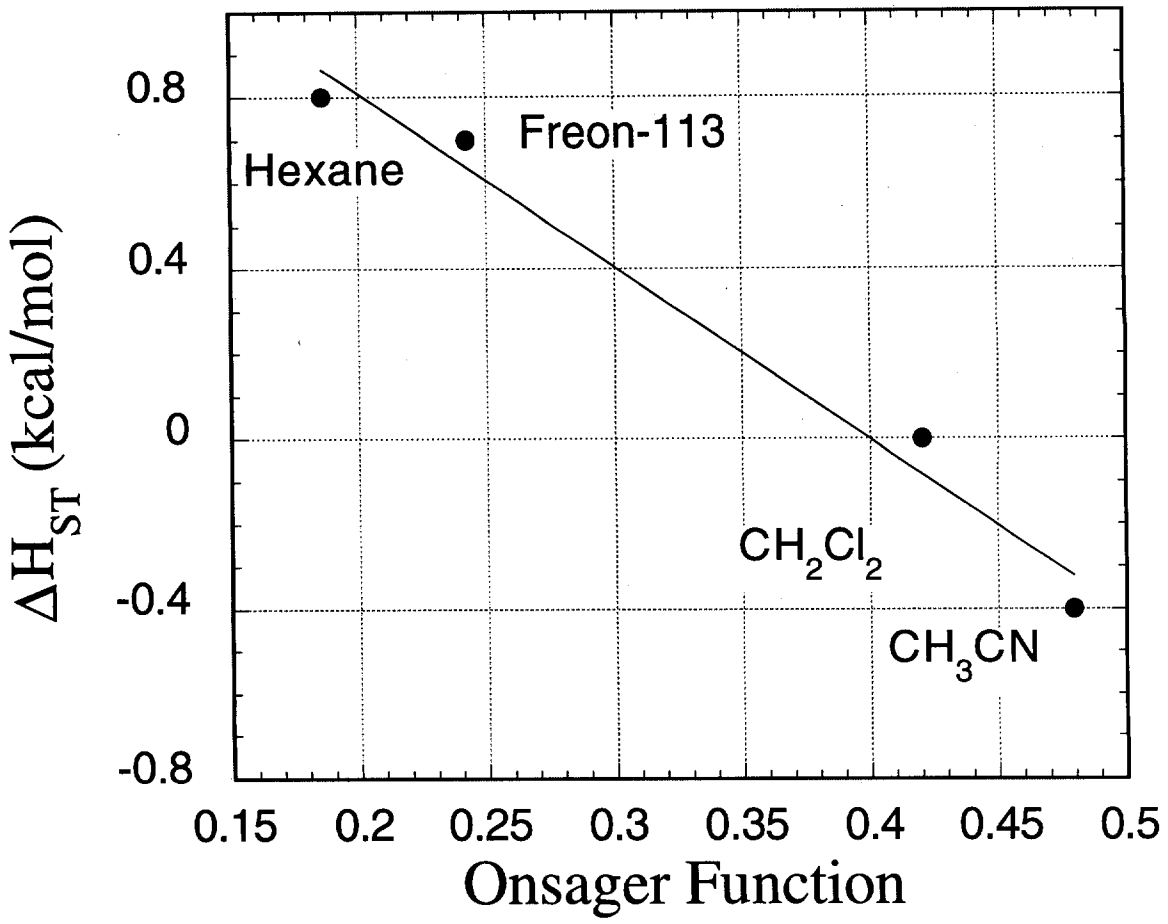


Figure S-2. Plot of experimentally-derived ΔH_{ST} as a function of the Onsager function. When possible the average of the ΔH_{ST} values derived in the 1680 – 1540 cm^{-1} and 1260 – 1140 cm^{-1} spectral regions is used.

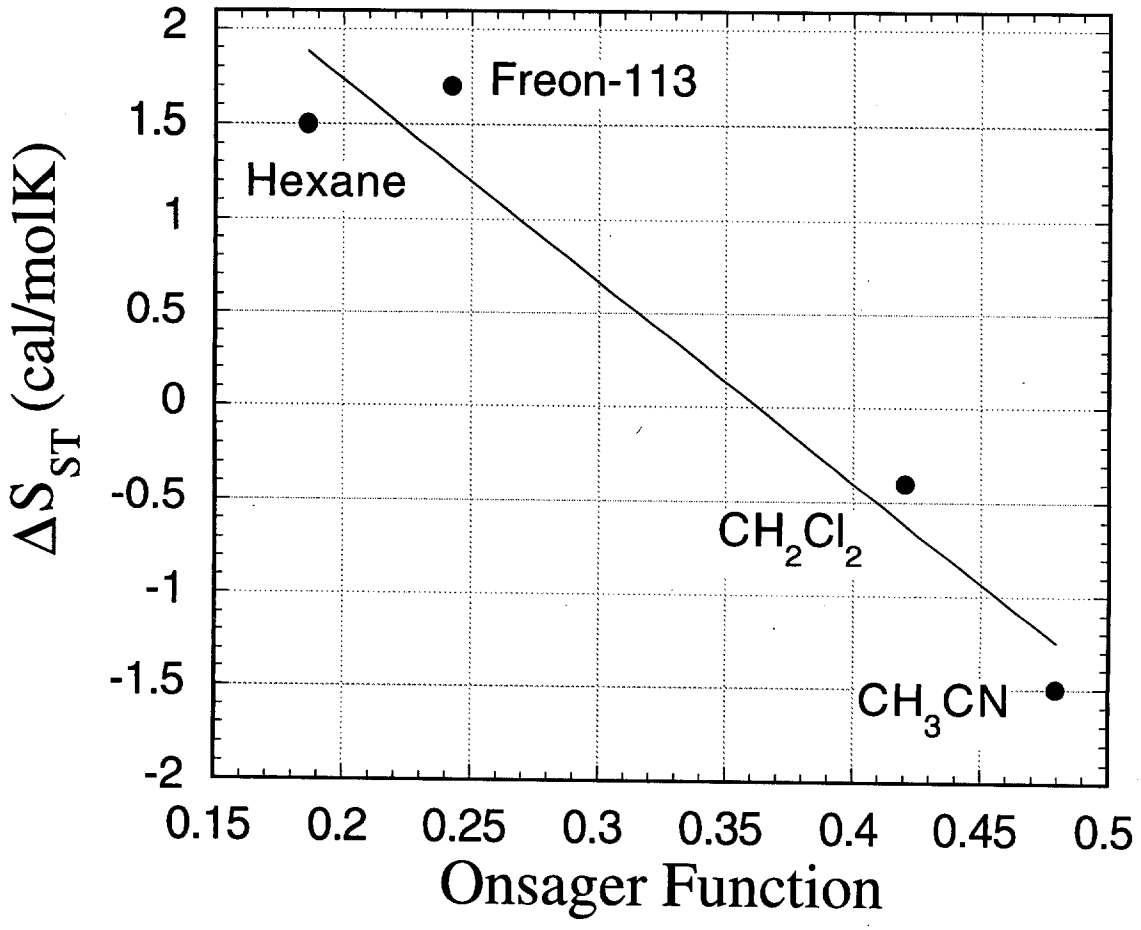


Figure S-3. Plot of experimentally-derived ΔS_{ST} as a function of the Onsager function. When possible the average of the ΔS_{ST} values derived in the 1680 – 1540 cm^{-1} and 1260 – 1140 cm^{-1} spectral regions is used.

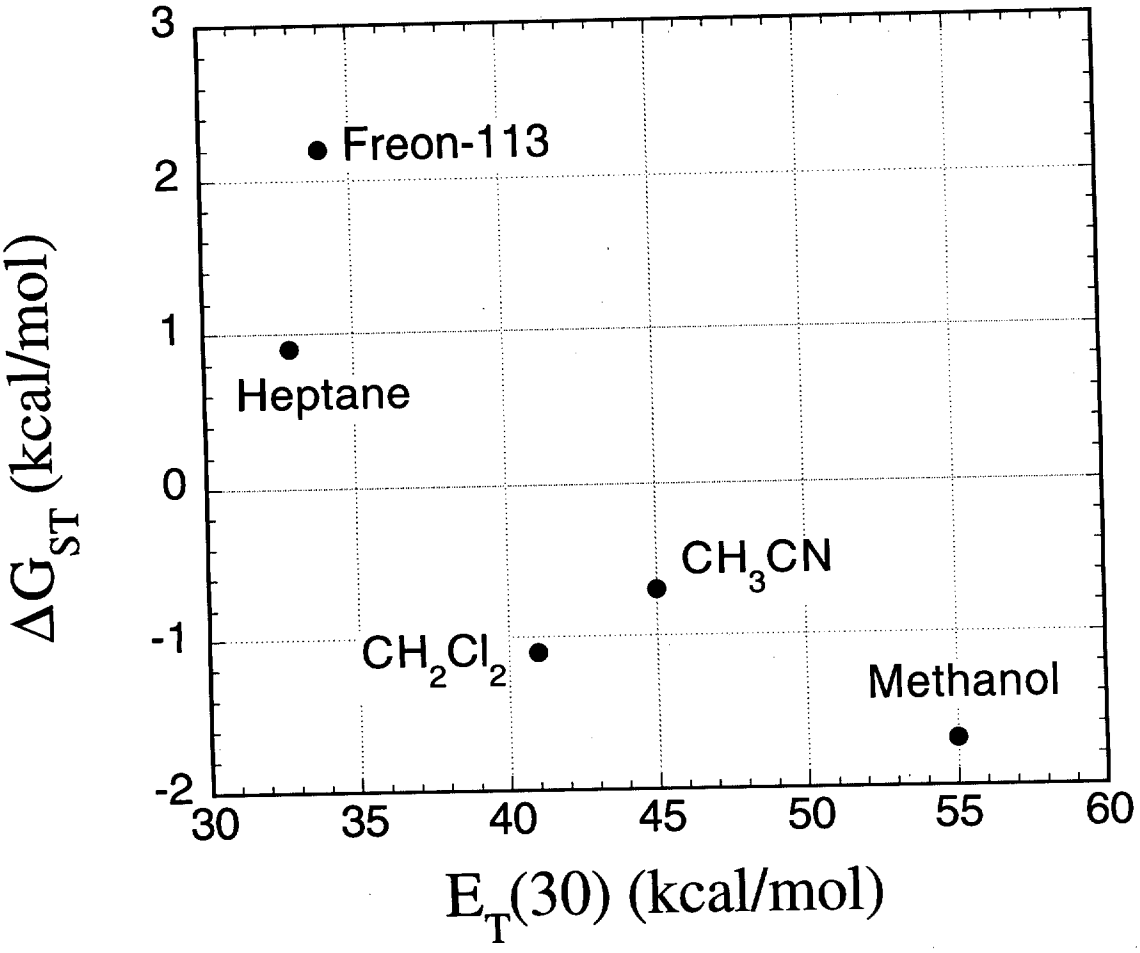


Figure S-4. Plot of computationally-derived (B3LYP/6-311+G**//B3LYP/6-31G* level using the PCM solvation model and corrected to 298 K) ΔG_{ST} as a function of the solvent polarity parameter $E_T(30)$.

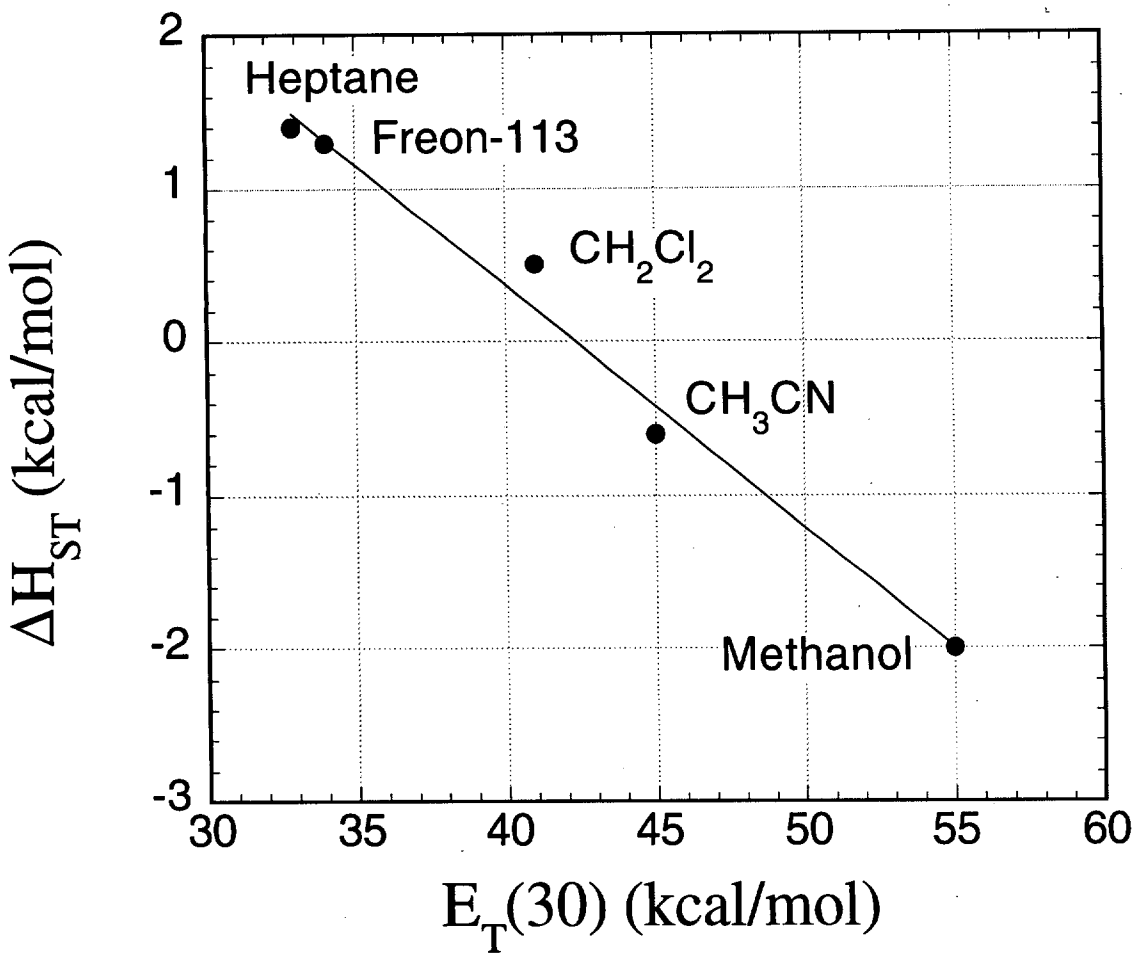


Figure S-5. Plot of computationally-derived (B3LYP/6-311+G**//B3LYP/6-31G* level using the PCM solvation model and corrected to 298 K) ΔH_{ST} as a function of the solvent polarity parameter $E_T(30)$.

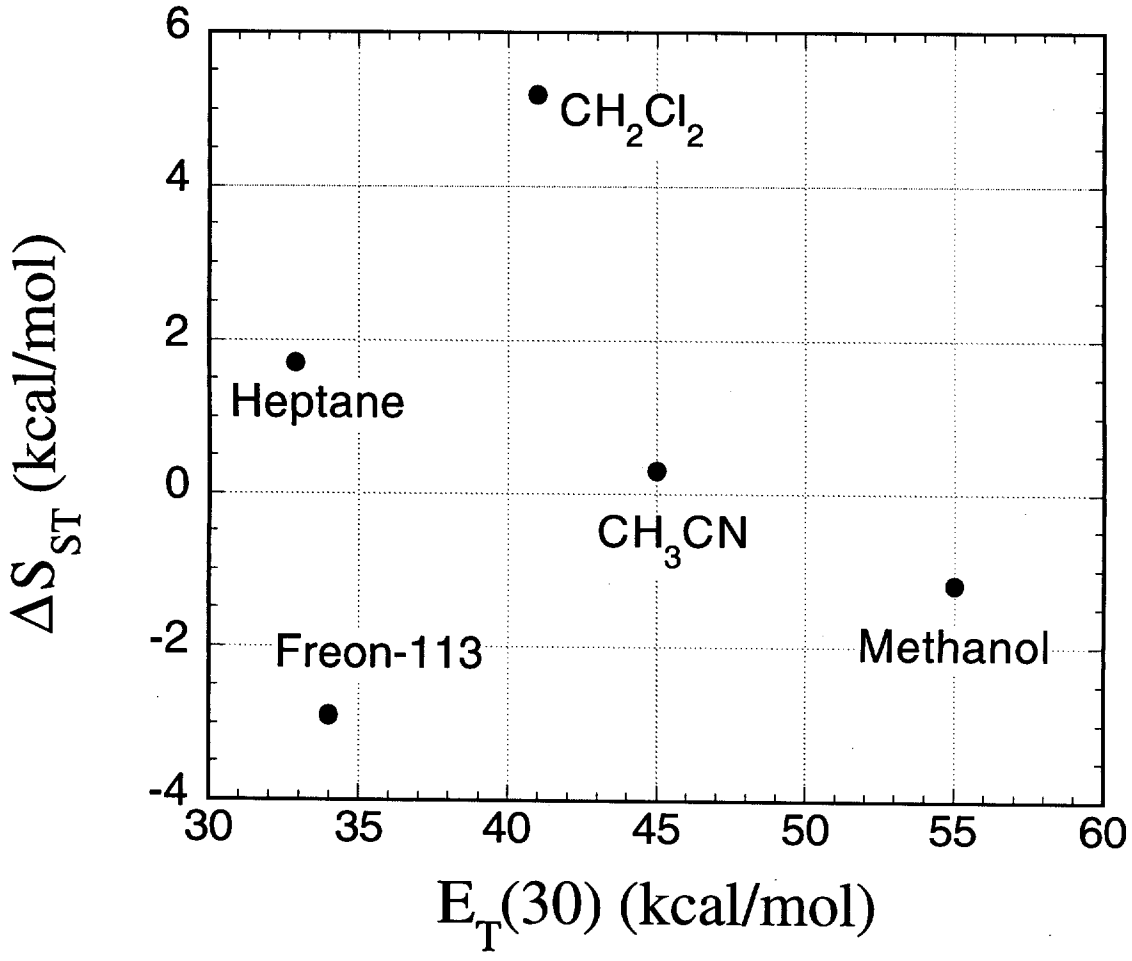


Figure S-6. Plot of computationally-derived (B3LYP/6-311+G**//B3LYP/6-31G* level using the PCM solvation model and corrected to 298 K) ΔS_{ST} as a function of the solvent polarity parameter $E_T(30)$.

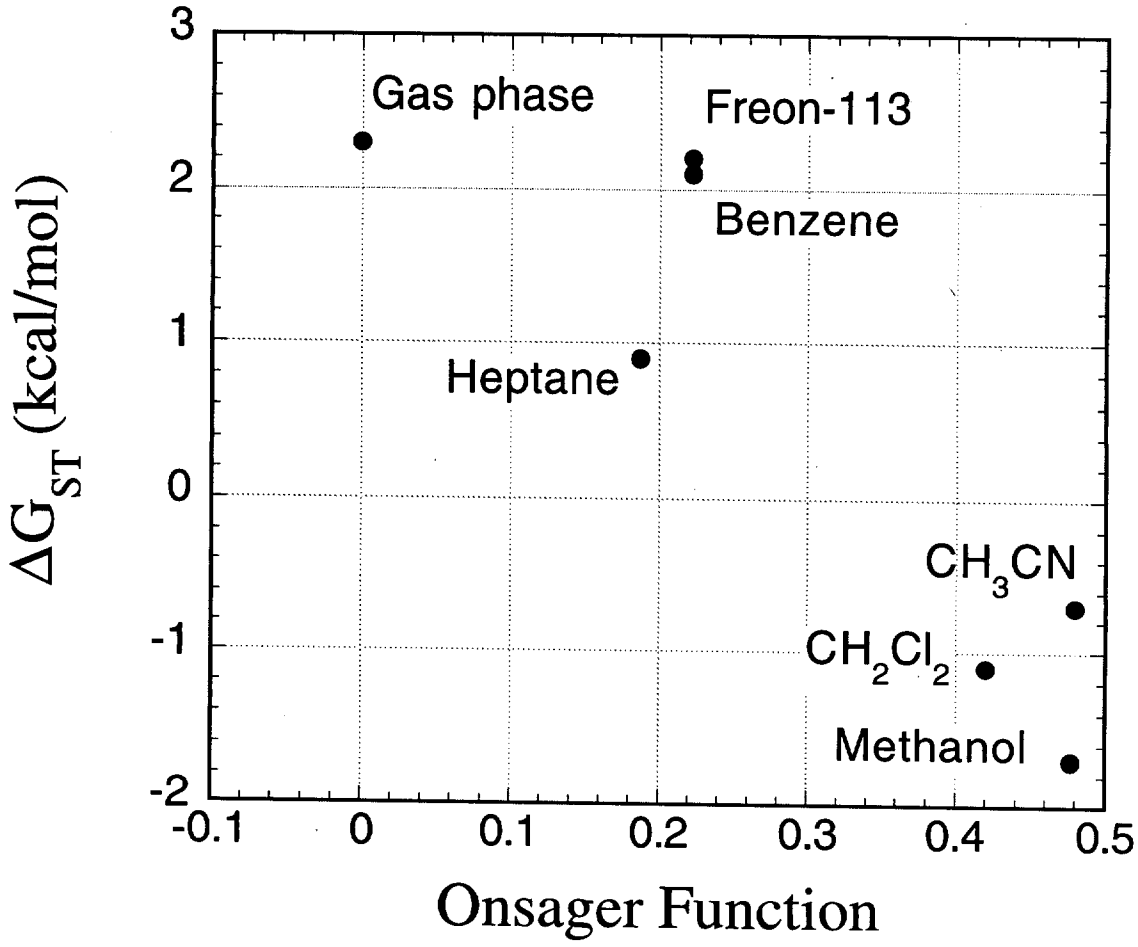


Figure S-7. Plot of computationally-derived (B3LYP/6-311+G**//B3LYP/6-31G* level using the PCM solvation model and corrected to 298 K) ΔG_{ST} as a function of the Onsager function.

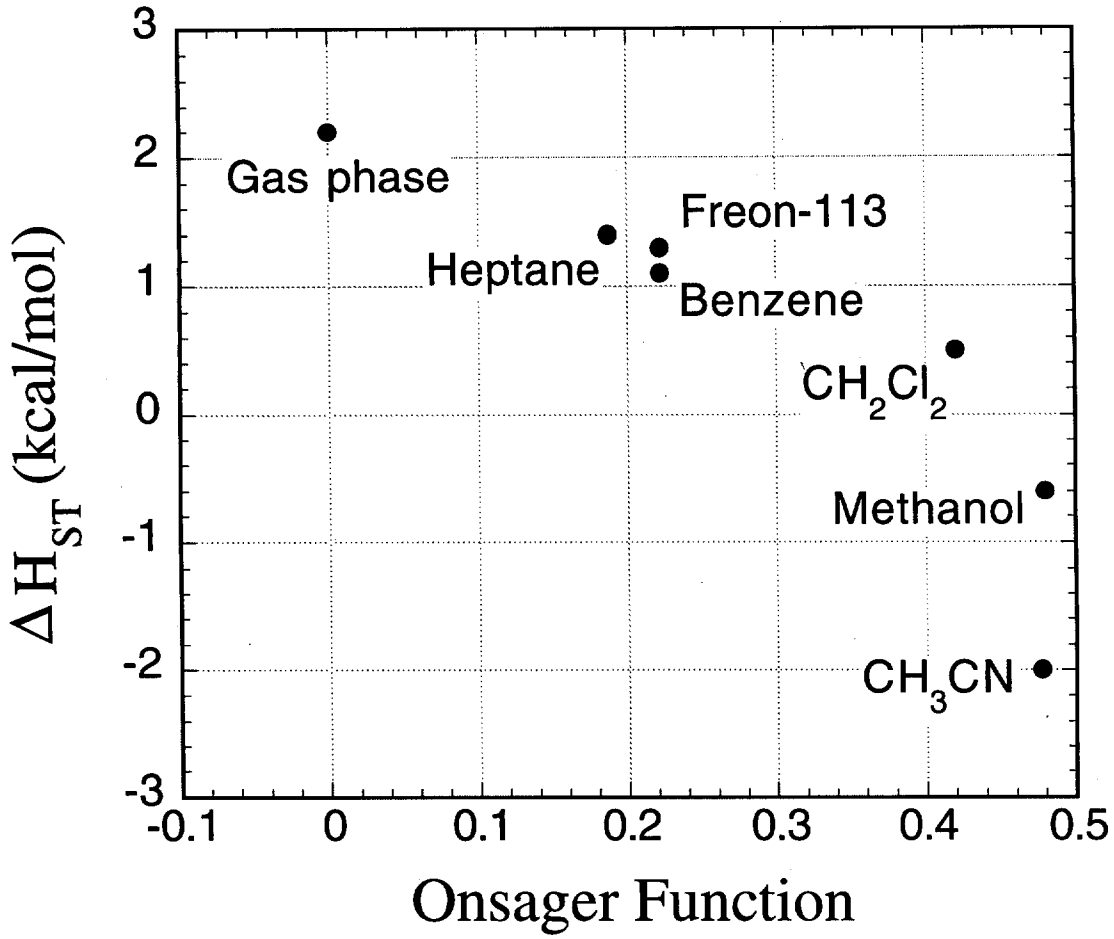


Figure S-8. Plot of computationally-derived (B3LYP/6-311+G**//B3LYP/6-31G* level using the PCM solvation model and corrected to 298 K) ΔH_{ST} as a function of the Onsager function.

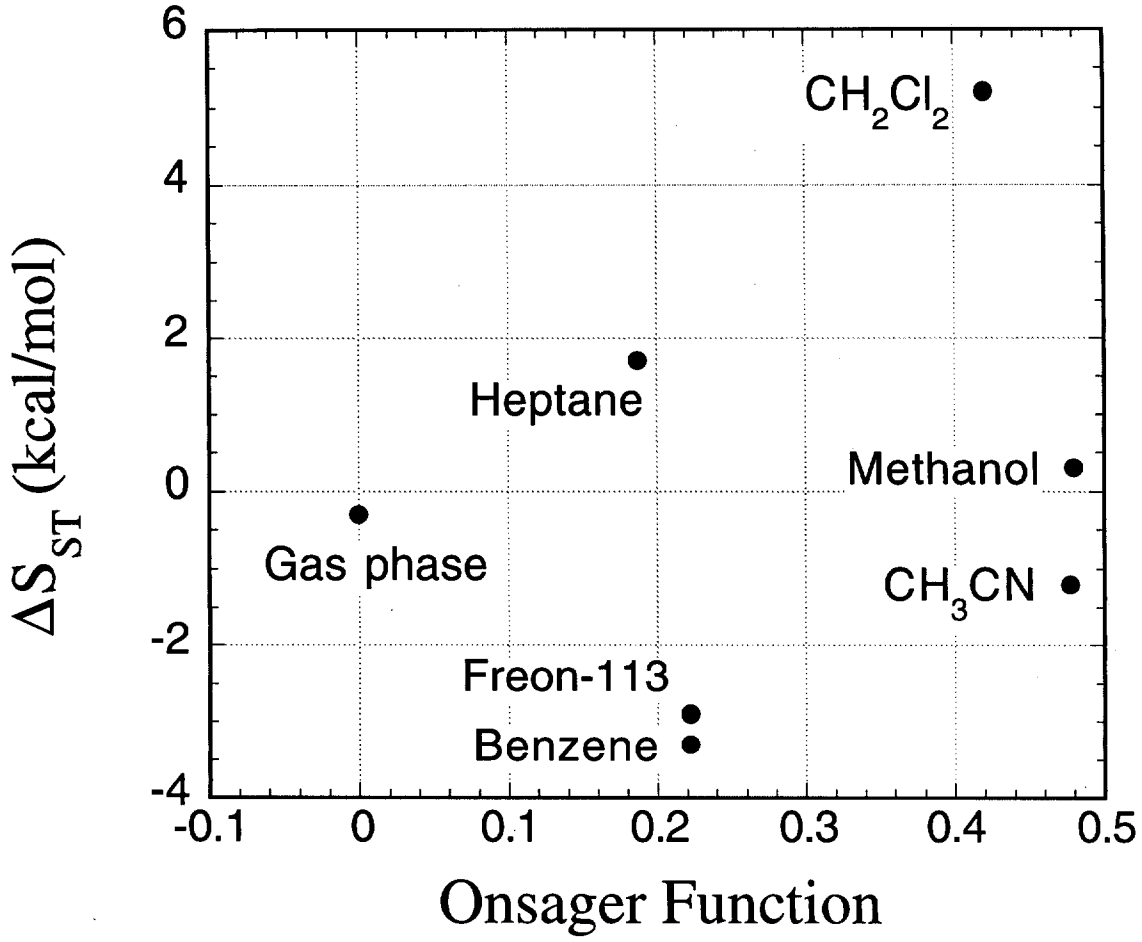


Figure S-9. Plot of computationally-derived (B3LYP/6-311+G**//B3LYP/6-31G* level using the PCM solvation model and corrected to 298 K) ΔS_{ST} as a function of the Onsager function.