

Mechanistic investigation on the formation of indolizines from 2-enynylpyridines

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1 Gaussian full reference

All the calculations were performed with the Gaussian03 package.¹

2 Nucleophile-assisted

2.1 Model A

E1

SCF Energy: -950.164545076

Num. Imaginary Frequencies: 0

C	-5.361876	1.091596	0.018424
C	-6.222888	-0.009694	0.174177
C	-5.655761	-1.282472	0.210828
N	-4.347266	-1.530011	0.108105
C	-3.503852	-0.483796	-0.043677
C	-3.988708	0.840241	-0.090611
C	-2.056320	-0.680109	-0.163080
C	-1.304552	-1.816278	-0.171943
C	0.114640	-1.687976	-0.303503
Li	4.243994	0.230201	0.014967
C	1.327762	-1.659452	-0.416130
O	4.252684	-1.383437	-0.519372
C	4.741264	-2.676507	-0.597123
O	4.018608	0.945472	1.838287
O	4.197027	1.601811	-1.356119
C	3.056107	0.224554	2.618734
C	5.112072	1.426422	2.615949
C	3.915064	2.994965	-1.344368
C	4.261893	1.036025	-2.673622
C	-5.871362	2.427874	-0.027745
H	-7.294474	0.128740	0.262829
H	-6.294564	-2.155658	0.330786
H	-3.297915	1.667690	-0.212702
H	2.422478	-1.594270	-0.508020
H	5.433830	-2.930154	0.231082
H	5.300165	-2.866603	-1.535788
H	3.933349	-3.437106	-0.564014
H	3.526199	-0.637028	3.108420
H	2.282302	-0.130136	1.936363
H	2.613353	0.885857	3.374494
H	5.652291	0.594000	3.086037
H	4.758402	2.115365	3.394314
H	5.784564	1.959682	1.940559
H	4.705448	3.557033	-1.860477
H	3.866333	3.309063	-0.299735
H	2.951833	3.201414	-1.830145
H	5.095945	1.478295	-3.234111
H	3.321160	1.217221	-3.209160
H	4.410153	-0.036397	-2.529519
H	-1.503873	0.250964	-0.264352
C	-1.806092	-3.238630	-0.060101
H	-1.475040	-3.811251	-0.934509
H	-2.889612	-3.277597	0.019475
H	-1.354257	-3.718120	0.816644
C	-6.308030	3.557558	-0.066406
H	-6.691917	4.551782	-0.101299

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E2-TS

SCF Energy: -950.143473731

Num. Imaginary Frequencies: 1

Imaginary Frequency: -256.6866

Li	-2.332537	0.291773	0.200841
O	-3.909911	-0.261901	-0.492419
C	-5.176247	0.196661	-0.861819
H	-5.328975	1.263958	-0.624451
H	-5.347647	0.083276	-1.950334
H	-5.969295	-0.379041	-0.358890
O	-1.854426	-0.524675	1.916553
C	-0.562859	-0.600794	2.522040
C	-2.734080	-1.573940	2.336548
H	-0.648545	-0.526651	3.614492
H	0.028179	0.232604	2.140103
H	-0.062797	-1.539386	2.255181
H	-2.278371	-2.553771	2.145250
H	-2.956254	-1.476679	3.407393
H	-3.644322	-1.474142	1.743827
O	-1.834557	2.195546	0.220734
C	-1.730594	3.001410	1.391329
C	-1.855413	2.958755	-0.986600
H	-1.748465	2.328075	2.249633
H	-0.791155	3.569959	1.387469
H	-2.575939	3.699325	1.458022
H	-0.926730	3.534692	-1.091931
H	-1.945669	2.250823	-1.811308
H	-2.712790	3.644467	-0.993106
C	-2.801142	-0.648922	-1.941436
C	-1.597679	-0.938345	-1.742481
C	-0.339348	-1.317620	-1.259651
H	-3.561263	-0.504984	-2.693781
C	-0.182373	-2.804693	-0.978352
C	0.673945	-0.390094	-1.089167
C	2.014316	-0.580141	-0.582231
H	0.041109	-2.981709	0.077125
H	-1.092646	-3.340575	-1.255386
H	0.665861	-3.213009	-1.534300
H	0.450691	0.629376	-1.394556
N	2.413833	-1.780671	-0.082206
C	3.665115	-1.895380	0.375431
C	4.604994	-0.868503	0.392725
C	4.207709	0.388756	-0.111762
C	2.907713	0.523827	-0.599326
H	3.936774	-2.878320	0.758836
H	5.605329	-1.025622	0.779288
C	5.115782	1.495857	-0.125196
H	2.579657	1.477016	-1.001259
C	5.890520	2.428292	-0.131879
H	6.573041	3.247183	-0.142384

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E3

SCF Energy: -950.160704464

Num. Imaginary Frequencies: 0

Li	2.627397	-0.626711	-0.041896
O	2.214340	-2.333542	-0.831070
C	0.855192	-2.613932	-1.196586
C	3.087134	-3.446990	-1.005985
H	0.468848	-3.451201	-0.602301
H	0.272469	-1.716388	-0.985497
H	0.795257	-2.862517	-2.263806
H	2.757549	-4.295744	-0.392534
H	4.082157	-3.131543	-0.686857
H	3.115834	-3.754015	-2.059952
O	4.566251	-0.425749	0.147884
C	5.224603	0.106886	-1.006070
C	4.916124	0.284778	1.346276
H	4.393862	-0.202376	2.171418
H	4.593053	1.328637	1.272993
H	5.999247	0.224246	1.512446
H	6.313517	0.043900	-0.883531
H	4.921503	1.146944	-1.170237
H	4.923524	-0.503196	-1.860881
C	2.817895	3.706914	-0.804095
O	2.772106	2.400673	-0.253546
C	1.499582	2.024555	0.226449
C	1.186997	0.749789	0.455303
C	-0.129824	0.376281	0.940818
H	2.491335	4.463290	-0.075561
H	3.857493	3.907524	-1.077191
H	2.188078	3.789656	-1.701815
H	0.863327	2.895035	0.428528
C	-0.167553	-0.263163	2.316335
C	-1.244742	0.522724	0.149269
H	0.761197	-0.045233	2.852235
H	-0.284255	-1.352303	2.249742
H	-1.023854	0.089311	2.895424
C	-2.618551	0.108003	0.381485
H	-1.086196	1.019429	-0.806368
N	-2.949286	-0.668505	1.445723
C	-4.230183	-1.018808	1.606378
C	-5.268078	-0.653903	0.753883
C	-4.944955	0.145020	-0.363315
C	-3.612863	0.521556	-0.541948
H	-4.442632	-1.638805	2.476827
H	-6.287880	-0.972309	0.937854
C	-5.956598	0.559321	-1.288388
H	-3.335951	1.140005	-1.389487
C	-6.817921	0.906231	-2.067919
H	-7.573809	1.214689	-2.753306

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E4

SCF Energy: -950.156013484

Num. Imaginary Frequencies: 0

C	1.376251	-0.922612	0.144149
N	1.369996	-0.015343	1.196200
C	2.546424	0.416665	1.687957
C	3.787890	0.082080	1.178975
C	3.817939	-0.761105	0.026803
C	2.625983	-1.245896	-0.484083
C	0.144640	-1.411019	-0.346346
H	2.476622	1.099860	2.534263
H	4.702159	0.463706	1.616478
C	5.067427	-1.110427	-0.579256
H	2.630655	-1.915316	-1.338370
C	-1.082940	-1.604331	0.423125
H	0.149274	-1.840625	-1.344667
C	-0.994137	-1.907108	1.920337
H	-1.988798	-1.944705	2.371878
H	-0.379229	-1.175154	2.447823
H	-0.514165	-2.884410	2.053580
C	-2.289202	-1.666533	-0.149845
Li	-0.176704	0.817825	0.242801
O	0.347405	2.054984	-1.221720
C	0.913940	3.310207	-0.845424
C	0.869029	1.557843	-2.457312
H	0.719867	4.065451	-1.618523
H	0.433097	3.612527	0.086557
H	1.996518	3.216893	-0.690155
H	0.650727	2.262321	-3.270477
H	1.952203	1.400588	-2.384858
H	0.376481	0.603929	-2.647775
O	-1.655154	1.850002	1.027836
C	-2.760493	2.147412	0.161511
C	-2.069677	1.580947	2.368552
H	-3.310117	3.017678	0.543729
H	-3.427197	1.282230	0.073517
H	-2.338801	2.383151	-0.816809
H	-2.565435	2.462747	2.795500
H	-1.171953	1.349710	2.943971
H	-2.753630	0.724341	2.396437
C	-3.442895	-1.857733	-0.734402
O	-4.376366	-0.831608	-0.931748
H	-3.759057	-2.817784	-1.152082
C	-5.703709	-1.290357	-1.151989
H	-6.112604	-1.784488	-0.259394
H	-6.306865	-0.410180	-1.384927
H	-5.750785	-1.989607	-1.999164
C	6.133037	-1.395073	-1.083720
H	7.067051	-1.653707	-1.527471

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E4-TS

SCF Energy: -950.138027055

Num. Imaginary Frequencies: 1

Imaginary Frequency: -41.4803

Li	-0.840744	0.831860	-0.192893
O	-0.508447	1.224359	1.697301
C	-0.857775	0.236222	2.681746
C	0.735540	1.869634	1.991903
H	-0.961218	0.715714	3.664034
H	-1.805838	-0.206418	2.374614
H	-0.092263	-0.545207	2.716195
H	0.671398	2.388146	2.957525
H	0.920002	2.599536	1.200800
H	1.554365	1.141898	2.015220
O	-1.652185	2.466905	-0.883177
C	-1.720418	2.706214	-2.290121
C	-2.401896	3.404608	-0.113163
H	-2.268041	3.135104	0.935259
H	-3.467161	3.358524	-0.376346
H	-2.032542	4.424664	-0.283148
H	-1.321490	3.700872	-2.528260
H	-2.757490	2.634783	-2.643314
H	-1.112128	1.938553	-2.769483
C	-4.649316	-1.845173	1.298385
O	-3.319417	-1.401902	1.047249
C	-3.097136	-1.016717	-0.272576
C	-1.983543	-1.263714	-0.925348
C	-0.874214	-1.423226	-1.624911
H	-4.858905	-2.784202	0.769871
H	-4.728227	-2.008831	2.374922
H	-5.386561	-1.088508	0.992162
H	-3.928304	-0.462556	-0.717820
C	-0.726773	-2.603922	-2.569959
C	0.262138	-0.448798	-1.524571
H	-1.632864	-3.215090	-2.627211
H	0.107465	-3.229906	-2.232272
H	-0.474384	-2.243644	-3.575055
C	1.364496	-0.704687	-0.643386
H	0.572319	-0.068651	-2.502028
N	1.205085	-1.521679	0.445150
C	2.248564	-1.714767	1.261798
C	3.505608	-1.138133	1.117697
C	3.694769	-0.283753	0.000265
C	2.632631	-0.074328	-0.869996
H	2.064533	-2.387877	2.100568
H	4.310232	-1.341359	1.814421
C	4.962424	0.343862	-0.230626
H	2.763768	0.565953	-1.737325
C	6.038943	0.871589	-0.415194
H	6.986123	1.330307	-0.583347

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PP-Z

SCF Energy: -950.164125351

Num. Imaginary Frequencies: 1

C	-4.106138	-0.937051	0.012164
C	-3.035488	-1.823224	-0.207156
C	-1.760640	-1.282690	-0.363299
N	-1.478188	0.022597	-0.313134
C	-2.493949	0.885430	-0.092053
C	-3.820316	0.432337	0.065830
C	-2.246791	2.325588	-0.015319
C	-1.075085	3.013914	0.035149
C	0.231436	2.448595	0.036674
Li	3.019437	-0.702451	0.012050
C	1.408169	2.133142	0.063422
O	3.969199	0.708239	0.040367
C	5.020038	1.565864	-0.227797
O	2.233991	-1.606772	-1.566603
O	2.621750	-1.545031	1.711850
C	1.453896	-0.700702	-2.363796
C	3.162172	-2.360563	-2.345639
C	1.680346	-2.539441	2.094020
C	3.161401	-0.806712	2.816538
C	-5.443690	-1.417916	0.175068
H	-3.200538	-2.893584	-0.259195
H	-0.914397	-1.943409	-0.546085
H	-4.621669	1.143986	0.234302
H	2.429773	1.725037	0.073809
H	5.584519	1.289595	-1.141950
H	5.764714	1.602167	0.593638
H	4.685533	2.613718	-0.381679
H	2.106456	0.029655	-2.857368
H	0.766318	-0.182679	-1.693010
H	0.886456	-1.261177	-3.118201
H	3.876297	-1.697573	-2.851189
H	2.632439	-2.965305	-3.093550
H	3.700772	-3.022015	-1.663269
H	2.146906	-3.282095	2.755757
H	1.338455	-3.030804	1.180872
H	0.821932	-2.086143	2.607437
H	3.735071	-1.474364	3.472909
H	2.351807	-0.334553	3.387784
H	3.804903	-0.041035	2.378368
H	-3.153183	2.925245	0.028544
C	-1.096473	4.529146	0.120114 S-13
H	-0.585799	4.867669	1.028467
H	-2.119520	4.915326	0.124261
H	-0.557664	4.965334	-0.728422
C	-6.575240	-1.828649	0.313352
H	-7.571990	-2.187715	0.435022

Z1

SCF Energy: -950.177539451

Num. Imaginary Frequencies: 0

C	-3.878060	0.039171	-0.489122
C	-3.248342	-1.195495	-0.779031
C	-1.873584	-1.263949	-0.617692
N	-1.092469	-0.245401	-0.216669
C	-1.674150	0.960899	0.059657
C	-3.083835	1.101915	-0.070979
C	-0.918166	2.095209	0.528641
C	0.451821	2.288832	0.610023
C	1.468943	1.367790	0.210626
Li	0.849179	-0.626633	0.245816
C	2.456835	1.696943	-0.619685
O	3.480322	0.797454	-0.949494
C	4.646164	1.409704	-1.478166
O	1.516943	-1.985322	-1.072605
O	1.029290	-1.622518	2.002656
C	1.441325	-1.554403	-2.434887
C	2.775400	-2.588509	-0.766216
C	0.195866	-2.714814	2.372974
C	1.443880	-0.831922	3.118898
C	-5.294828	0.189521	-0.624653
H	-3.819969	-2.052720	-1.114199
H	-1.352358	-2.197430	-0.826227
H	-3.541642	2.058716	0.155771
H	2.543230	2.628489	-1.198229
H	5.324200	0.606262	-1.776731
H	5.144851	2.039575	-0.727719
H	4.415208	2.027574	-2.358782
H	2.220291	-0.811413	-2.640459
H	0.459558	-1.099867	-2.573399
H	1.550337	-2.413915	-3.110345
H	3.589626	-1.872508	-0.928092
H	2.930041	-3.482138	-1.386515
H	2.745158	-2.871850	0.287057
H	0.718518	-3.382671	3.071765
H	-0.045735	-3.263371	1.460616
H	-0.732792	-2.359399	2.839589
H	2.061405	-1.431163	3.801947
H	0.571694	-0.443130	3.661187
H	2.019671	0.000718	2.713014
H	-1.543430	2.919993	0.862330
C	0.919550	3.580686	1.265408
H	1.523241	3.362712	2.153715
H	0.087394	4.227034	1.562458
H	1.570977	4.136178	0.578660
C	-6.495648	0.307957	-0.740793
H	-7.551195	0.417908	-0.842641

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Z2b-TS

SCF Energy: -950.152488816

Num. Imaginary Frequencies: 1

Imaginary Frequency: -214.4687

C	-3.682322	-0.530627	-0.227129
C	-2.819867	-1.621509	-0.467791
C	-1.456876	-1.368132	-0.551562
N	-0.891023	-0.152916	-0.435744
C	-1.712690	0.916937	-0.239201
C	-3.112189	0.736192	-0.111560
C	-1.192860	2.263974	-0.128911
C	0.030093	2.757281	-0.520670
C	1.027714	2.055304	-1.201461
Li	1.345197	-0.276848	-0.012173
C	2.026874	1.468602	-1.640267
O	3.073384	0.308699	-0.328856
C	4.358371	0.087200	-0.790045
O	1.532142	-2.344140	-0.511513
O	1.209896	-0.232698	2.047131
C	1.917722	-2.551908	-1.868589
C	2.349063	-3.066146	0.406778
C	0.064130	-0.431636	2.866256
C	2.233867	0.521651	2.701688
C	-5.095931	-0.717366	-0.109321
H	-3.206685	-2.628629	-0.571312
H	-0.761669	-2.190081	-0.696426
H	-3.745647	1.599202	0.063086
H	2.681383	1.168295	-2.436385
H	4.720455	-0.934605	-0.562801
H	5.094644	0.791974	-0.359780
H	4.439388	0.194835	-1.895543
H	2.944657	-2.206376	-2.037901
H	1.234418	-1.970790	-2.491105
H	1.838154	-3.615488	-2.133586
H	3.401924	-2.775054	0.302726
H	2.249765	-4.148116	0.241469
H	2.003885	-2.811030	1.409537
H	0.332011	-0.978602	3.781556
H	-0.655451	-1.014292	2.289874
H	-0.389699	0.529883	3.142911
H	2.616151	-0.029518	3.572532
H	1.838643	1.491405	3.034214
H	3.018534	0.673789	1.959204
H	-1.897288	2.987149	0.273341
C	0.348347	4.222108	-0.262634 S-17
H	-0.465708	4.715629	0.275493
H	1.265766	4.313985	0.329032
H	0.520384	4.751183	-1.206196
C	-6.292445	-0.882675	-0.010084
H	-7.345816	-1.024177	0.075714

Z2-TS

SCF Energy: -950.136562614

Num. Imaginary Frequencies: 1

Imaginary Frequency: -344.4464

C	3.566113	0.038526	-0.126697
C	2.835899	0.828889	-1.081967
C	1.515927	0.525645	-1.309042
N	0.872753	-0.468740	-0.655443
C	1.574350	-1.323314	0.175331
C	2.931935	-1.032139	0.484020
C	0.793794	-2.436581	0.508375
C	-0.414778	-2.469740	-0.232654
C	-0.677955	-1.419922	-1.096500
Li	-1.341641	0.478871	0.036947
C	-1.649724	-0.854698	-1.863111
O	-2.711905	-0.086694	-1.182280
C	-3.980759	-0.732229	-1.170363
O	-1.152582	2.430617	-0.287438
O	-1.643001	0.514130	1.994338
C	-1.655448	3.012020	-1.492040
C	-0.208563	3.260571	0.387675
C	-1.170143	-0.483452	2.905861
C	-2.697815	1.305752	2.535415
C	4.932026	0.344397	0.158819
H	3.321719	1.646221	-1.602240
H	0.908563	1.084339	-2.020784
H	3.473374	-1.671211	1.174407
H	-1.524697	-0.509502	-2.885688
H	-4.692129	-0.058756	-0.678076
H	-3.933553	-1.683069	-0.624526
H	-4.317860	-0.932020	-2.194998
H	-2.185817	3.948021	-1.270661
H	-2.340873	2.283845	-1.926972
H	-0.835600	3.219493	-2.192334
H	-0.667799	4.220466	0.660122
H	0.670954	3.441035	-0.242581
H	0.099223	2.730822	1.290367
H	-0.752667	-0.008084	3.803212
H	-0.397572	-1.055912	2.389473
H	-1.989992	-1.153021	3.197450
H	-2.360706	1.830956	3.439256
H	-3.564399	0.679163	2.785502
H	-2.979664	2.033957	1.773394
H	1.137621	-3.247310	1.138707
C	-1.353945	-3.652113	-0.161076 S-19
H	-2.016519	-3.587532	0.711947
H	-0.792418	-4.589308	-0.073574
H	-1.982221	-3.694789	-1.054530
C	6.090540	0.621322	0.392193
H	7.109867	0.854734	0.597994

Z3

SCF Energy: -950.178352562

Num. Imaginary Frequencies: 1

C	4.346663	-0.765235	-0.283039
C	3.348536	-1.768558	-0.005516
C	2.075424	-1.420209	0.332478
N	1.717154	-0.084714	0.426280
C	2.660984	0.940769	0.125150
C	3.969810	0.574354	-0.212801
C	1.973393	2.148849	0.256019
C	0.638920	1.869453	0.617666
C	0.486808	0.462486	0.729455
Li	-2.443807	-0.289617	-0.089462
C	-0.670139	-0.395578	0.947405
O	-1.789350	0.287144	1.596945
C	-1.676261	0.483482	3.004436
O	-4.018726	-1.466039	-0.056024
O	-2.581599	0.692017	-1.780399
C	-4.475213	-1.978541	1.196957
C	-4.334631	-2.318225	-1.156206
C	-1.357373	0.979259	-2.472431
C	-3.680431	1.476357	-2.235723
C	5.672868	-1.146767	-0.628581
H	3.610291	-2.818185	-0.071023
H	1.297124	-2.143852	0.530202
H	4.690613	1.356941	-0.426010
H	-0.441461	-1.312947	1.505469
H	-2.552419	1.050091	3.338945
H	-0.763984	1.042555	3.243432
H	-1.642834	-0.483512	3.527160
H	-5.569683	-2.063396	1.199427
H	-4.155515	-1.273646	1.964971
H	-4.031933	-2.962672	1.396734
H	-5.422083	-2.435805	-1.251820
H	-3.871860	-3.305443	-1.027909
H	-3.936238	-1.843773	-2.054230
H	-1.458624	0.728114	-3.536118
H	-0.582593	0.369623	-2.007640
H	-1.097651	2.038980	-2.365113
H	-3.873009	1.292432	-3.301327
H	-3.483422	2.546004	-2.085784
H	-4.555074	1.182210	-1.652004
H	2.402419	3.131369	0.108081
C	-0.419607	2.917498	0.825960
H	-0.050146	3.893190	0.492716
H	-0.711253	3.024484	1.878545
H	-1.338776	2.695683	0.271606
C	6.802366	-1.487867	-0.924240
H	7.794147	-1.780735	-1.179984

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2.2 Model B

E1

SCF Energy: -874.016173029

Num. Imaginary Frequencies: 0

C	5.593269	-2.073554	-0.050160
C	6.590325	-1.114450	0.139666
C	6.197752	0.224547	0.213897
N	4.932992	0.641356	0.114895
C	3.959916	-0.279109	-0.070151
C	4.271463	-1.655310	-0.155397
C	2.552031	0.112188	-0.187698
C	1.956170	1.336959	-0.165371
C	0.533237	1.399898	-0.308412
Li	-3.739249	-0.016994	0.021234
C	-0.672230	1.531651	-0.429935
O	-3.616440	1.581235	-0.540746
C	-3.975444	2.913989	-0.643893
O	-3.563193	-0.734147	1.850098
O	-3.841458	-1.406829	-1.330272
C	-2.547626	-0.082861	2.624752
C	-4.687505	-1.128786	2.632044
C	-3.669502	-2.817450	-1.304718
C	-3.891254	-0.854419	-2.654047
H	5.842335	-3.129096	-0.115303
H	7.636606	-1.388854	0.227529
H	6.942300	1.005239	0.361535
H	3.474239	-2.377464	-0.304178
H	-1.764572	1.602734	-0.533154
H	-4.634164	3.252055	0.181820
H	-4.519419	3.139006	-1.583805
H	-3.096440	3.592047	-0.631006
H	-2.949929	0.816777	3.106410
H	-1.748537	0.204102	1.939691
H	-2.157530	-0.769531	3.386934
H	-5.163390	-0.256666	3.099697
H	-4.384314	-1.838871	3.412749
H	-5.399473	-1.613290	1.960366
H	-4.514777	-3.322389	-1.792240
H	-3.617905	-3.120901	-0.257050
H	-2.738571	-3.105285	-1.811694
H	-4.772481	-1.232810	-3.188588
H	-2.982109	-1.120129	-3.208581
H	-3.945912	0.228366	-2.522092
H	1.881546	-0.733946	-0.319744
C	2.640151	2.676705	-0.007546
H	2.406535	3.309664	-0.871938
H	3.717545	2.567462	0.089689
H	2.239436	3.191209	0.874154

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E2-TS

SCF Energy: -873.994053913

Num. Imaginary Frequencies: 1

Imaginary Frequency: -257.7040

Li	-1.879515	0.035380	0.167630
O	-3.337182	-0.853853	-0.459224
C	-4.657520	-0.577402	-0.824454
H	-4.923309	0.487884	-0.702541
H	-4.847694	-0.836357	-1.884003
H	-5.362735	-1.173222	-0.224665
O	-1.254158	-0.545754	1.931420
C	0.026331	-0.299716	2.515481
C	-1.891515	-1.720944	2.443234
H	-0.070751	-0.153833	3.599804
H	0.427129	0.603324	2.053582
H	0.711789	-1.131655	2.315527
H	-1.239109	-2.594755	2.319873
H	-2.129935	-1.591084	3.507275
H	-2.802757	-1.861032	1.860094
O	-1.844394	2.007628	0.143912
C	-2.095477	2.806501	1.296764
C	-1.976843	2.730616	-1.080261
H	-1.989063	2.157321	2.167134
H	-1.373229	3.631371	1.360337
H	-3.113412	3.218108	1.270004
H	-1.252312	3.554682	-1.118722
H	-1.780577	2.027953	-1.891079
H	-2.993150	3.133656	-1.181661
C	-2.201666	-1.045960	-1.908910
C	-0.959286	-1.065951	-1.730671
C	0.348805	-1.147766	-1.234369
H	-2.979817	-1.101846	-2.655050
C	0.805239	-2.552002	-0.865197
C	1.150901	-0.025346	-1.127090
C	2.501138	0.094357	-0.621054
H	1.015844	-2.625498	0.205336
H	0.039810	-3.282212	-1.136676
H	1.742939	-2.797290	-1.370459
H	0.729742	0.905275	-1.500772
N	3.120902	-0.958252	-0.022897
C	4.369653	-0.795023	0.426719
C	5.095241	0.393663	0.338229
C	4.463680	1.489390	-0.265984
C	3.171188	1.343308	-0.744247
H	4.819099	-1.672614	0.891127
H	6.107182	0.457219	0.724763
H	4.979718	2.441118	-0.364284
H	2.663498	2.174592	-1.225572

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E3

SCF Energy: -874.011013652

Num. Imaginary Frequencies: 0

Li	-2.021449	0.731400	0.127340
O	-1.508028	2.512823	-0.396376
C	-0.144282	2.787690	-0.748430
C	-2.328221	3.678346	-0.361590
H	0.301442	3.481312	-0.024827
H	0.393764	1.838932	-0.726592
H	-0.096130	3.225385	-1.753666
H	-1.953482	4.392324	0.383654
H	-3.334486	3.356225	-0.087827
H	-2.350498	4.164234	-1.346131
O	-3.980306	0.640981	0.176013
C	-4.541027	0.218363	-1.073719
C	-4.468058	-0.137895	1.278652
H	-4.009445	0.264947	2.183743
H	-4.179570	-1.187159	1.155885
H	-5.559172	-0.042146	1.349960
H	-5.634673	0.306580	-1.044981
H	-4.246125	-0.814245	-1.291129
H	-4.147166	0.885026	-1.844393
C	-2.700079	-3.743945	-0.486477
O	-2.426174	-2.360219	-0.344559
C	-1.106393	-2.069514	0.055145
C	-0.714405	-0.830397	0.353760
C	0.677230	-0.562834	0.685699
H	-2.574253	-4.281506	0.464871
H	-3.740086	-3.835331	-0.811433
H	-2.050853	-4.210015	-1.241768
H	-0.479712	-2.968452	0.095949
C	0.926362	-0.022025	2.081870
C	1.674970	-0.716127	-0.246956
H	0.060536	-0.227282	2.718675
H	1.101655	1.061425	2.068923
H	1.825753	-0.457774	2.522528
C	3.091794	-0.392089	-0.167471
H	1.369547	-1.136754	-1.203685
N	3.592302	0.312464	0.880101
C	4.901288	0.586709	0.901469
C	5.806351	0.205085	-0.089382
C	5.301042	-0.514485	-1.179927
C	3.947298	-0.811923	-1.221158
H	5.248420	1.152044	1.766342
H	6.857824	0.462358	-0.010356
H	5.958367	-0.837681	-1.983288
H	3.529438	-1.372312	-2.052720

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E4

SCF Energy: -874.005728015

Num. Imaginary Frequencies: 0

C	1.707955	-1.247618	-0.298917
N	1.915161	-0.511741	0.860250
C	3.174643	-0.288318	1.278888
C	4.312765	-0.689079	0.596452
C	4.122583	-1.354392	-0.639723
C	2.849985	-1.622684	-1.088638
C	0.380480	-1.504546	-0.715429
H	3.264709	0.270759	2.210580
H	5.301756	-0.478550	0.988057
H	4.982150	-1.670079	-1.226578
H	2.688277	-2.163033	-2.017264
C	-0.788943	-1.661274	0.145529
H	0.237561	-1.771064	-1.759454
C	-0.613279	-2.210001	1.563459
H	-1.552244	-2.163637	2.121231
H	0.165942	-1.676833	2.111850
H	-0.299682	-3.259121	1.496828
C	-2.039301	-1.473686	-0.292068
Li	0.386783	0.606585	0.226732
O	0.854453	2.000484	-1.111586
C	1.579730	3.145091	-0.664814
C	1.139580	1.655662	-2.469389
H	1.333923	4.019696	-1.281926
H	1.279075	3.332349	0.367430
H	2.661315	2.961806	-0.707675
H	0.875034	2.488096	-3.134671
H	2.201685	1.408342	-2.589997
H	0.534501	0.780547	-2.707577
O	-0.797820	1.671431	1.380546
C	-1.977606	2.222204	0.777853
C	-1.011904	1.259969	2.731537
H	-2.330149	3.081547	1.363524
H	-2.764274	1.463676	0.699042
H	-1.695008	2.552291	-0.222908
H	-1.291655	2.122452	3.351011
H	-0.072792	0.836903	3.091353
H	-1.799946	0.499135	2.784226
C	-3.256071	-1.419921	-0.766802
O	-4.050557	-0.265616	-0.699816
H	-3.743441	-2.249290	-1.287509
C	-5.441124	-0.511095	-0.858131
H	-5.843847	-1.103702	-0.024378
H	-5.933486	0.463688	-0.877756
H	-5.651443	-1.035804	-1.801383

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E4-TS

SCF Energy: -873.987148726

Num. Imaginary Frequencies: 1

Imaginary Frequency: -44.7282

Li	0.523911	0.810885	0.269742
O	0.149552	1.432853	-1.551604
C	0.262681	0.491214	-2.632736
C	-0.999897	2.276505	-1.683750
H	0.367978	1.032415	-3.582338
H	1.148563	-0.115660	-2.442645
H	-0.617635	-0.158451	-2.657013
H	-0.937037	2.855502	-2.614619
H	-1.000826	2.960194	-0.832028
H	-1.920515	1.682404	-1.676361
O	1.683245	2.198759	1.010396
C	1.932765	2.251921	2.415755
C	2.542892	3.044882	0.250030
H	2.262319	2.924272	-0.797109
H	3.593392	2.755992	0.389299
H	2.414420	4.093383	0.550214
H	1.779688	3.271584	2.793016
H	2.959193	1.931111	2.637338
H	1.222985	1.571018	2.886766
C	3.726233	-2.335790	-1.714327
O	2.521082	-1.680107	-1.334144
C	2.445419	-1.395981	0.028175
C	1.344951	-1.513259	0.736637
C	0.266556	-1.549834	1.498952
H	3.780756	-3.343528	-1.282168
H	3.715604	-2.407757	-2.803757
H	4.609782	-1.761669	-1.398170
H	3.386028	-1.039014	0.457389
C	-0.031514	-2.778098	2.343013
C	-0.686504	-0.392475	1.565689
H	0.756304	-3.535546	2.281961
H	-0.978760	-3.218029	2.009778
H	-0.162929	-2.482830	3.391520
C	-1.874688	-0.390458	0.755811
H	-0.873586	-0.072246	2.595110
N	-1.915651	-1.113233	-0.406924
C	-3.024905	-1.069787	-1.156453
C	-4.164991	-0.324616	-0.861990
C	-4.138497	0.427848	0.329361
C	-3.014459	0.398812	1.130107
H	-2.998374	-1.680540	-2.060759
H	-5.031840	-0.342755	-1.514282
H	-5.001778	1.020010	0.625918
H	-2.983180	0.962770	2.059363

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PP-Z

SCF Energy: -874.019590975

Num. Imaginary Frequencies: 0

C	-4.221865	-2.103203	0.237584
C	-2.989052	-2.734617	0.064175
C	-1.867257	-1.928191	-0.144057
N	-1.895109	-0.592369	-0.181869
C	-3.083467	0.023540	-0.004344
C	-4.269773	-0.713597	0.200553
C	-3.174286	1.485783	-0.027857
C	-2.200838	2.433134	-0.045718
C	-0.794572	2.200721	-0.028653
Li	2.711589	-0.152682	-0.028339
C	0.423481	2.184903	0.000815
O	3.299011	1.455514	0.032588
C	4.101076	2.527298	-0.289221
O	2.140260	-1.308946	-1.522926
O	2.462968	-1.063312	1.664301
C	1.030961	-0.824334	-2.294810
C	3.127647	-1.957956	-2.321324
C	1.792667	-2.277426	1.990791
C	2.718278	-0.226504	2.797077
H	-5.126519	-2.682583	0.396241
H	-2.896816	-3.815656	0.081342
H	-0.891005	-2.386346	-0.295808
H	-5.212792	-0.191208	0.331397
H	1.510733	2.048285	0.026925
H	4.692134	2.372940	-1.218087
H	4.841963	2.768000	0.504435
H	3.521931	3.463716	-0.453679
H	1.370396	-0.072421	-3.018710
H	0.317412	-0.373930	-1.602417
H	0.553490	-1.656754	-2.826992
H	3.554095	-1.261884	-3.056146
H	2.693458	-2.818905	-2.845622
H	3.915904	-2.305481	-1.649878
H	2.398810	-2.880659	2.679588
H	1.646472	-2.825630	1.058644
H	0.817706	-2.070351	2.450319
H	3.396943	-0.732219	3.497222
H	1.778497	0.016848	3.309724
H	3.174288	0.683565	2.401636
H	-4.196399	1.858398	-0.010071
C	-2.583205	3.903062	-0.065166
H	-2.166059	4.419586	0.807098
H	-3.669373	4.031888	-0.065210
H	-2.170953	4.393690	-0.954622

S-33

Z1

SCF Energy: -874.029545578

Num. Imaginary Frequencies: 0

C	-4.281630	0.301816	-0.984432
C	-3.708529	-0.966014	-1.175855
C	-2.360463	-1.105984	-0.868597
N	-1.573784	-0.115244	-0.414062
C	-2.111783	1.126578	-0.229000
C	-3.491998	1.334554	-0.513500
C	-1.340127	2.230589	0.292151
C	0.021413	2.346694	0.514016
C	1.019084	1.357840	0.245878
Li	0.291649	-0.609938	0.240556
C	2.099451	1.601301	-0.492843
O	3.089469	0.629924	-0.703051
C	4.352828	1.155576	-1.072800
O	0.983528	-2.011406	-1.015997
O	0.272784	-1.608623	1.998342
C	1.059403	-1.595622	-2.381953
C	2.140479	-2.745535	-0.610563
C	-0.578885	-2.705240	2.313222
C	0.680105	-0.866438	3.148812
H	-5.332443	0.472018	-1.204487
H	-4.283276	-1.807980	-1.545995
H	-1.869218	-2.069838	-0.995726
H	-3.913394	2.323213	-0.357405
H	2.301224	2.507711	-1.084536
H	5.003533	0.305786	-1.293446
H	4.797406	1.745619	-0.258023
H	4.281157	1.791770	-1.968364
H	1.928776	-0.944880	-2.531459
H	0.146985	-1.038568	-2.598510
H	1.124955	-2.471141	-3.042069
H	3.039892	-2.127346	-0.715777
H	2.240903	-3.659776	-1.210808
H	2.001472	-3.007902	0.439052
H	-0.076495	-3.404175	2.995722
H	-0.809873	-3.217451	1.377421
H	-1.511617	-2.356294	2.776593
H	1.273500	-1.499888	3.822123
H	-0.195425	-0.481280	3.688949
H	1.279709	-0.031955	2.782468
H	-1.947760	3.096543	0.546468
C	0.496929	3.626823	1.188258
H	1.001149	3.397049	2.133804
H	-0.323303	4.323265	1.393064
H	1.239768	4.131235	0.556580

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Z2b-TS

SCF Energy: -874.005130214

Num. Imaginary Frequencies: 1

Imaginary Frequency: -238.8782

C	-3.619752	-2.050426	-0.283233
C	-2.432010	-2.741964	-0.550505
C	-1.255070	-2.002372	-0.628254
N	-1.180633	-0.667044	-0.479265
C	-2.336709	0.017889	-0.256239
C	-3.568892	-0.674132	-0.134670
C	-2.347242	1.461401	-0.110063
C	-1.404056	2.383354	-0.495692
C	-0.225072	2.125533	-1.203513
Li	0.925255	0.019766	-0.009452
C	0.933314	1.952720	-1.612197
O	2.292480	1.258842	-0.287752
C	3.580754	1.375216	-0.776060
O	1.896225	-1.809162	-0.531597
O	0.771553	-0.063445	2.042483
C	2.347078	-1.943835	-1.875777
C	2.817224	-2.341629	0.417086
C	-0.220579	-0.709712	2.833289
C	1.452668	0.975891	2.749003
H	-4.564538	-2.579742	-0.195952
H	-2.413049	-3.818984	-0.678603
H	-0.305005	-2.502389	-0.792229
H	-4.472784	-0.106561	0.064783
H	1.660880	1.918777	-2.401956
H	4.197667	0.479279	-0.569536
H	4.121318	2.243125	-0.352076
H	3.606428	1.508840	-1.882634
H	3.293047	-1.408130	-2.026820
H	1.579619	-1.509065	-2.519273
H	2.483881	-3.003141	-2.134476
H	3.787863	-1.833376	0.344891
H	2.957838	-3.419279	0.256454
H	2.392299	-2.166899	1.406055
H	0.229823	-1.160278	3.728715
H	-0.672961	-1.489867	2.220316
H	-0.997489	0.003268	3.140969
H	2.012278	0.558097	3.597732
H	0.732985	1.717350	3.123255
H	2.125664	1.441836	2.027642
H	-3.261338	1.860502	0.322269
C	-1.651167	3.854216	-0.193614 S-37
H	-2.586678	3.993868	0.355864
H	-1.694558	4.437548	-1.120252
H	-0.829525	4.262449	0.405635

Z2-TS

SCF Energy: -873.989587236

Num. Imaginary Frequencies: 1

Imaginary Frequency: -344.2087

C	-3.583498	-1.775575	0.165021
C	-2.641120	-2.209917	-0.812611
C	-1.613552	-1.353767	-1.148325
N	-1.470008	-0.142653	-0.573099
C	-2.417339	0.344914	0.305392
C	-3.479887	-0.517859	0.714076
C	-2.176428	1.694533	0.586604
C	-1.123589	2.216271	-0.210166
C	-0.467891	1.357868	-1.072536
Li	1.065311	-0.114464	0.005826
C	0.597780	1.256176	-1.917054
O	1.916732	0.942913	-1.328058
C	2.849226	2.015824	-1.387736
O	1.651636	-1.973243	-0.327512
O	1.429861	0.027462	1.933820
C	2.369041	-2.322213	-1.513840
C	1.250619	-3.108561	0.440589
C	0.622145	0.765589	2.856575
C	2.705015	-0.326672	2.472652
H	-4.392921	-2.435887	0.464598
H	-2.716569	-3.190044	-1.271922
H	-0.849961	-1.614208	-1.881351
H	-4.205203	-0.158893	1.439430
H	0.549223	0.890752	-2.940247
H	3.789538	1.666378	-0.946461
H	2.480659	2.888040	-0.832388
H	3.025406	2.311948	-2.429680
H	3.290258	-2.861962	-1.258750
H	2.609178	-1.386712	-2.020124
H	1.750287	-2.954320	-2.164599
H	2.127235	-3.688628	0.756707
H	0.579127	-3.751437	-0.141992
H	0.721104	-2.735063	1.317992
H	0.416933	0.159893	3.748703
H	-0.312401	1.011029	2.348588
H	1.134036	1.689425	3.156774
H	2.584771	-0.945509	3.370941
H	3.279514	0.573035	2.727914
H	3.234529	-0.894659	1.706575
H	-2.790833	2.294660	1.246583
C	-0.758235	3.682616	-0.171693 S-39
H	-0.124756	3.915360	0.694212
H	-1.657903	4.305367	-0.091273
H	-0.206678	3.960976	-1.073688

Z3

SCF Energy: -874.032111063

Num. Imaginary Frequencies: 0

C	4.837594	-1.025479	-1.248976
C	3.742576	-1.937334	-1.376476
C	2.527339	-1.653850	-0.816378
N	2.346504	-0.481435	-0.103321
C	3.406525	0.472297	0.016973
C	4.650434	0.160872	-0.563287
C	2.879543	1.541787	0.737464
C	1.527822	1.259753	1.042033
C	1.200890	-0.015430	0.517817
Li	-1.995099	-0.172793	-0.096713
C	-0.048156	-0.758122	0.450099
O	-0.997331	-0.397956	1.499954
C	-0.737560	-0.925888	2.797462
O	-3.673552	-1.176115	-0.257802
O	-2.338052	1.486958	-1.071937
C	-4.233734	-1.920481	0.827738
C	-4.327163	-1.437728	-1.503064
C	-1.263433	2.120361	-1.771474
C	-3.538040	2.263113	-1.058802
H	5.795942	-1.257970	-1.703649
H	3.853613	-2.862320	-1.933067
H	1.664279	-2.298319	-0.909848
H	5.456118	0.883907	-0.462533
H	0.087583	-1.848171	0.455200
H	-1.508622	-0.546730	3.476706
H	0.251733	-0.607915	3.150253
H	-0.770972	-2.025013	2.782007
H	-5.288543	-1.656141	0.970994
H	-3.664755	-1.661886	1.721505
H	-4.152273	-2.998325	0.638432
H	-5.391463	-1.179466	-1.442290
H	-4.226034	-2.495642	-1.775875
H	-3.843100	-0.817632	-2.259087
H	-1.525918	2.258729	-2.828594
H	-0.396599	1.464484	-1.679190
H	-1.036732	3.096035	-1.322389
H	-3.894208	2.442676	-2.081128
H	-3.369069	3.225640	-0.559734
H	-4.286750	1.693403	-0.506763
H	3.417475	2.441580	1.009023
C	0.605355	2.190168	1.779092 S-41
H	1.068494	3.177755	1.882356
H	0.361401	1.835858	2.788821
H	-0.350300	2.316550	1.259205

2.3 Model C

E1

SCF Energy: -834.699526406

Num. Imaginary Frequencies: 0

C	-6.204582	1.451761	0.419980
C	-6.912211	0.249355	0.424250
C	-6.199268	-0.930436	0.180030
N	-4.887535	-0.973254	-0.055034
C	-4.197893	0.188859	-0.060551
C	-4.833718	1.423252	0.175329
C	-2.755849	0.148594	-0.322346
C	-2.060211	-0.983238	-0.577415
C	-0.667235	-1.028001	-0.836810
Li	3.652413	-0.077905	-0.042387
C	0.525833	-1.120272	-1.070876
O	3.453117	-1.153912	-1.343207
C	3.761095	-2.248070	-2.133146
O	3.547582	-0.409247	1.899441
O	3.766092	1.807623	-0.491524
C	2.526974	-1.348218	2.264159
C	4.702492	-0.498263	2.729748
C	3.664690	3.007833	0.262693
C	3.740152	2.012529	-1.911929
H	-6.710732	2.395472	0.603003
H	-7.981071	0.218315	0.609384
H	-6.714204	-1.889661	0.174870
H	-4.252388	2.340644	0.162697
H	1.610415	-1.157639	-1.252232
H	4.434795	-2.971161	-1.630048
H	4.265017	-1.963327	-3.079010
H	2.859818	-2.824454	-2.429708
H	2.906515	-2.374991	2.193330
H	1.701442	-1.220754	1.562479
H	2.181306	-1.149513	3.286693
H	5.156537	-1.495811	2.662112
H	4.442064	-0.288597	3.775579
H	5.416934	0.249624	2.378929
H	4.515144	3.671515	0.054789
H	3.666597	2.731074	1.318945
H	2.730921	3.536768	0.028671
H	4.617670	2.592499	-2.226210
H	2.824217	2.544063	-2.200761
H	3.750943	1.014250	-2.355108
H	-2.236822	1.104114	-0.311124
H	-2.605555	-1.925773	-0.591264

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E2-TS

SCF Energy: -834.680087322

Num. Imaginary Frequencies: 1

Imaginary Frequency: -247.9643

Li	-1.924622	-0.132609	0.167680
O	-3.362678	-0.680634	-0.781746
C	-4.672343	-0.292645	-1.065169
H	-4.926410	0.702319	-0.656471
H	-4.856781	-0.246978	-2.156635
H	-5.393147	-1.018734	-0.657492
O	-1.171157	-1.442040	1.409342
C	0.139570	-1.406020	1.980751
C	-1.644850	-2.773567	1.177151
H	0.147676	-1.935636	2.942795
H	0.396098	-0.356918	2.136584
H	0.875369	-1.850604	1.300706
H	-0.930212	-3.331421	0.558681
H	-1.787810	-3.296400	2.132014
H	-2.592583	-2.680635	0.644495
O	-1.855855	1.664652	0.957851
C	-2.066095	1.940442	2.339586
C	-1.979724	2.818904	0.126790
H	-1.968049	0.995410	2.876441
H	-1.317558	2.653758	2.709589
H	-3.071106	2.351210	2.505276
H	-1.226088	3.569346	0.399180
H	-1.820164	2.491878	-0.901519
H	-2.982352	3.256186	0.221699
C	-2.178564	-0.350239	-2.217597
C	-0.942722	-0.330918	-2.013635
C	0.366968	-0.446389	-1.553840
H	-2.960464	-0.260506	-2.954135
H	0.768545	-1.460464	-1.513176
C	1.217436	0.555270	-1.159575
C	2.560536	0.318327	-0.663654
H	0.901087	1.592762	-1.235044
N	2.970865	-0.959466	-0.451139
C	4.215408	-1.166206	-0.013524
C	5.133838	-0.149715	0.262875
C	4.714231	1.170674	0.063470
C	3.427277	1.407863	-0.400523
H	4.497731	-2.208561	0.131592
H	6.130699	-0.385774	0.620524
H	5.386127	2.001366	0.263263
H	3.078927	2.421981	-0.575653

E3

SCF Energy: -834.695166352

Num. Imaginary Frequencies: 0

Li	-1.908242	0.753550	0.075715
O	-1.349958	2.562537	-0.281076
C	0.031812	2.877560	-0.506633
C	-2.191401	3.713359	-0.247444
H	0.407458	3.527370	0.293364
H	0.584206	1.937514	-0.503693
H	0.149665	3.380648	-1.474812
H	-1.885006	4.391930	0.559605
H	-3.208880	3.362716	-0.066432
H	-2.148652	4.250030	-1.204535
O	-3.870338	0.725316	0.179236
C	-4.481523	0.210306	-1.011022
C	-4.325656	0.044493	1.359149
H	-3.837232	0.520307	2.211993
H	-4.045274	-1.013240	1.315039
H	-5.413390	0.154331	1.456889
H	-5.572221	0.317831	-0.950908
H	-4.208142	-0.841115	-1.152572
H	-4.108485	0.806213	-1.847357
C	-2.780512	-3.784981	-0.199980
O	-2.483244	-2.402960	-0.090449
C	-1.131710	-2.121466	0.186456
C	-0.677729	-0.871926	0.297945
C	0.726140	-0.610278	0.510499
H	-2.548187	-4.324159	0.730017
H	-3.852173	-3.869213	-0.399739
H	-2.226742	-4.253923	-1.026132
H	-0.541104	-3.033647	0.331791
H	0.998851	-0.059136	1.414578
C	1.755018	-0.870755	-0.347274
C	3.142119	-0.478090	-0.127348
H	1.546480	-1.402242	-1.274802
N	3.450580	0.313561	0.931270
C	4.727572	0.650752	1.126396
C	5.784794	0.251671	0.303868
C	5.475324	-0.554876	-0.796681
C	4.153114	-0.920600	-1.014621
H	4.921527	1.283660	1.992255
H	6.802165	0.563381	0.517695
H	6.256444	-0.893768	-1.472587
H	3.883502	-1.551225	-1.857237

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E4

SCF Energy: -834.694063627

Num. Imaginary Frequencies: 0

C	-1.665007	-1.391394	0.003341
N	-1.884618	-0.426300	-0.968696
C	-3.144955	-0.175642	-1.368261
C	-4.273079	-0.776790	-0.831769
C	-4.073201	-1.697130	0.226418
C	-2.797567	-1.995634	0.647307
C	-0.329536	-1.695056	0.358766
H	-3.245936	0.574478	-2.152683
H	-5.263499	-0.530744	-1.198049
H	-4.926326	-2.180489	0.696720
H	-2.625051	-2.723750	1.434995
C	0.779511	-1.458134	-0.524488
H	-0.155100	-2.269519	1.263892
H	0.495727	-1.175669	-1.544889
C	2.091160	-1.559586	-0.288116
Li	-0.394936	0.638628	-0.196632
O	-0.854840	1.745250	1.376401
C	-1.563045	2.964124	1.154226
C	-1.183274	1.129334	2.625350
H	-1.340366	3.687480	1.949708
H	-1.224868	3.362271	0.195846
H	-2.645281	2.783481	1.118478
H	-0.922036	1.797612	3.456149
H	-2.252533	0.887252	2.666809
H	-0.601676	0.209045	2.686854
O	0.833181	1.839959	-1.151002
C	2.012667	2.265508	-0.452609
C	1.079481	1.588340	-2.536489
H	2.400688	3.188978	-0.902221
H	2.779125	1.482281	-0.471570
H	1.715101	2.458307	0.579457
H	1.393872	2.512286	-3.039356
H	0.143325	1.233164	-2.970671
H	1.855963	0.822979	-2.657468
C	3.371214	-1.697284	-0.069059
O	4.205180	-0.615851	0.261310
H	3.916155	-2.639911	-0.175850
C	5.402512	-0.991241	0.928109
H	5.971911	-1.730671	0.346103
H	6.002832	-0.084882	1.034094
H	5.195663	-1.407118	1.924410

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E4-TS

SCF Energy: -834.663941627

Num. Imaginary Frequencies: 1

Imaginary Frequency: -100.1040

Li	-0.435962	0.840894	-0.066566
O	-0.140352	0.533062	1.841876
C	-0.367668	-0.791619	2.355561
C	1.045609	1.128810	2.380327
H	-0.482939	-0.747493	3.446548
H	-1.282400	-1.167210	1.895488
H	0.464815	-1.447321	2.082052
H	0.962649	1.211958	3.471998
H	1.133245	2.128102	1.948023
H	1.930604	0.538239	2.118427
O	-1.543617	2.439602	-0.134185
C	-1.754687	3.121541	-1.371898
C	-2.374402	2.914915	0.923191
H	-2.120961	2.334763	1.811403
H	-3.434968	2.772974	0.675842
H	-2.187060	3.980726	1.109914
H	-1.534940	4.191479	-1.260791
H	-2.791952	2.995117	-1.708816
H	-1.073240	2.675297	-2.097024
C	-3.886438	-2.895882	0.241592
O	-2.683592	-2.132683	0.244695
C	-2.547615	-1.301960	-0.862181
C	-1.411518	-1.118041	-1.496618
C	-0.299941	-0.846893	-2.148668
H	-3.885008	-3.629860	-0.574485
H	-3.930647	-3.416916	1.199966
H	-4.769022	-2.247344	0.140371
H	-3.466271	-0.783835	-1.149778
H	-0.113650	-1.446378	-3.052721
C	0.692878	0.205392	-1.759971
C	1.885774	-0.173604	-1.048050
H	0.900195	0.892762	-2.585035
N	1.887180	-1.291259	-0.256825
C	3.000968	-1.603146	0.419144
C	4.182188	-0.864352	0.405245
C	4.195214	0.293127	-0.397965
C	3.068026	0.637038	-1.117278
H	2.942208	-2.515039	1.016197
H	5.049536	-1.181294	0.974922
H	5.090878	0.907219	-0.464495
H	3.066707	1.518383	-1.754190

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PP-Z

SCF Energy: -834.694473396

Num. Imaginary Frequencies: 0

C	-4.743474	-1.237548	0.184932
C	-3.630417	-2.060828	0.002867
C	-2.386275	-1.446903	-0.165655
N	-2.192150	-0.125402	-0.158155
C	-3.263882	0.675756	0.027315
C	-4.559866	0.140794	0.195198
C	-3.100200	2.130144	0.057203
C	-1.969587	2.879854	0.055883
C	-0.611412	2.480979	0.033013
Li	2.598964	-0.308477	-0.043359
C	0.592685	2.290809	0.028072
O	3.322912	1.228731	-0.042605
C	4.235740	2.229417	-0.320590
O	1.853920	-1.329363	-1.567602
O	2.338006	-1.179453	1.667548
C	0.803323	-0.627249	-2.250763
C	2.823750	-1.869186	-2.464415
C	1.581248	-2.317229	2.059018
C	2.754267	-0.355935	2.764972
H	-5.734779	-1.662098	0.315816
H	-3.718632	-3.142448	-0.013883
H	-1.496346	-2.055695	-0.320395
H	-5.403377	0.810158	0.335577
H	1.657105	2.012000	0.017892
H	4.815947	2.043303	-1.247526
H	4.983590	2.365280	0.487505
H	3.752015	3.219612	-0.457490
H	1.215049	0.214060	-2.821498
H	0.111861	-0.247641	-1.496510
H	0.277151	-1.311991	-2.928685
H	3.312551	-1.070453	-3.037187
H	2.352028	-2.579403	-3.156420
H	3.569863	-2.393306	-1.862965
H	2.171475	-2.968129	2.718640
H	1.321030	-2.861577	1.148989
H	0.662397	-2.014149	2.578783
H	3.435062	-0.915254	3.420255
H	1.881318	-0.020925	3.339829
H	3.260042	0.502774	2.318737
H	-4.035595	2.682830	0.105668
H	-2.115706	3.959730	0.091006

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Z1

SCF Energy: -834.711254864

Num. Imaginary Frequencies: 0

C	-4.476340	-0.690376	0.039830
C	-4.051525	0.624443	0.282607
C	-2.681304	0.859130	0.294448
N	-1.743722	-0.081812	0.092518
C	-2.138791	-1.367567	-0.137161
C	-3.527033	-1.675596	-0.167037
C	-1.195158	-2.449937	-0.346230
C	0.179248	-2.457758	-0.357225
C	1.102305	-1.362425	-0.184381
Li	0.210384	0.471524	0.040370
C	2.386824	-1.781460	-0.187109
O	3.444992	-0.907961	-0.032778
C	4.737276	-1.495128	-0.107713
O	0.667787	1.529569	1.716266
O	0.584075	1.865611	-1.400813
C	0.369252	0.768114	2.887270
C	2.024823	1.978851	1.696776
C	-0.103333	3.094458	-1.588720
C	1.140619	1.343553	-2.608755
H	-5.534917	-0.935194	0.016367
H	-4.753623	1.432945	0.455952
H	-2.304490	1.863315	0.483766
H	-3.830435	-2.701210	-0.353059
H	2.719161	-2.826786	-0.299880
H	5.459198	-0.689919	0.044885
H	4.912649	-1.954093	-1.090486
H	4.877645	-2.257176	0.671358
H	1.008357	-0.122094	2.942330
H	-0.673468	0.456752	2.811030
H	0.507484	1.382891	3.787511
H	2.713624	1.125622	1.673555
H	2.229467	2.608780	2.573646
H	2.153227	2.564029	0.784963
H	0.567419	3.856220	-2.010832
H	-0.450804	3.426090	-0.607933
H	-0.965160	2.965846	-2.258663
H	1.884682	2.041127	-3.017640
H	0.352486	1.172970	-3.354980
H	1.611788	0.395224	-2.348546
H	-1.682672	-3.409984	-0.505533
H	0.597277	-3.464806	-0.527538

Z2b-TS

SCF Energy: -834.683025774

Num. Imaginary Frequencies: 1

Imaginary Frequency: -213.6807

C	4.053324	1.094094	-0.161281
C	3.036094	2.052544	-0.244001
C	1.724677	1.599324	-0.369479
N	1.369337	0.304255	-0.432885
C	2.356341	-0.634175	-0.382979
C	3.711206	-0.246928	-0.226106
C	2.045793	-2.048329	-0.462385
C	0.899894	-2.645535	-0.922332
C	-0.226268	-2.077512	-1.509994
Li	-0.875997	-0.023642	-0.040096
C	-1.308345	-1.612527	-1.894893
O	-2.517485	-0.756762	-0.482766
C	-3.822320	-0.701632	-0.935750
O	-1.376083	2.052052	-0.138202
O	-0.691805	-0.495649	1.959933
C	-1.844710	2.429794	-1.431130
C	-2.275018	2.432006	0.901067
C	0.439055	-0.317435	2.803456
C	-1.553960	-1.546815	2.404340
H	5.092455	1.392465	-0.052144
H	3.246602	3.116011	-0.201509
H	0.901058	2.307036	-0.396599
H	4.475191	-1.016620	-0.173459
H	-2.010482	-1.340328	-2.659449
H	-4.345966	0.218041	-0.608624
H	-4.432401	-1.557944	-0.590861
H	-3.888726	-0.704176	-2.047378
H	-2.800385	1.942002	-1.656390
H	-1.094773	2.103572	-2.154743
H	-1.962453	3.520736	-1.494029
H	-3.254134	1.957336	0.760848
H	-2.395561	3.524179	0.924879
H	-1.841136	2.087432	1.840756
H	0.123764	-0.068873	3.827023
H	1.029224	0.503102	2.393377
H	1.054874	-1.226900	2.826746
H	-1.981848	-1.299104	3.386096
H	-0.996203	-2.490283	2.480302
H	-2.334592	-1.636405	1.647800
H	2.849217	-2.713226	-0.157242
H	0.877322	-3.735283	-0.867844

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Z2-TS

SCF Energy: -834.664457143

Num. Imaginary Frequencies: 1

Imaginary Frequency: -365.2147

C	3.804170	1.088000	0.273060
C	2.910047	1.763324	-0.611005
C	1.771601	1.103758	-1.015844
N	1.465843	-0.139478	-0.581350
C	2.357104	-0.855069	0.201033
C	3.537702	-0.202317	0.668123
C	1.944712	-2.189247	0.310454
C	0.847733	-2.441062	-0.545894
C	0.315412	-1.403742	-1.285907
Li	-1.012314	0.013470	-0.012566
C	-0.760028	-1.051785	-2.047870
O	-2.054343	-0.825001	-1.373414
C	-2.947012	-1.931723	-1.454882
O	-1.479740	1.940752	-0.135242
O	-1.354951	-0.284144	1.916405
C	-2.122780	2.429994	-1.314664
C	-0.900999	2.973059	0.659746
C	-0.607946	-1.187977	2.738071
C	-2.606332	0.084585	2.489461
H	4.709987	1.585296	0.608459
H	3.118532	2.769233	-0.960677
H	1.046792	1.547184	-1.698552
H	4.226926	-0.749751	1.305222
H	-0.726529	-0.538590	-3.003430
H	-3.876937	-1.647606	-0.947682
H	-2.518244	-2.818342	-0.969870
H	-3.159478	-2.173127	-2.503570
H	-2.944923	3.106933	-1.045925
H	-2.508108	1.557576	-1.843260
H	-1.405983	2.966680	-1.950010
H	-1.672002	3.684837	0.984870
H	-0.124506	3.507835	0.098398
H	-0.449375	2.496222	1.530918
H	-0.351841	-0.707126	3.691507
H	0.299773	-1.450049	2.191863
H	-1.192288	-2.096572	2.934300
H	-2.456516	0.576775	3.460072
H	-3.244405	-0.798391	2.628469
H	-3.087397	0.778785	1.798585
H	2.487053	-2.951037	0.855130
H	0.457476	-3.442463	-0.702951

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Z3

SCF Energy: -834.707686469

Num. Imaginary Frequencies: 0

C	4.565013	-0.062585	-1.411304
C	3.530722	-0.829328	-2.037937
C	2.332639	-1.024500	-1.411819
N	2.113021	-0.482739	-0.157528
C	3.103252	0.323484	0.485722
C	4.339339	0.501038	-0.174226
C	2.546210	0.743789	1.690862
C	1.240862	0.200152	1.772744
C	0.974719	-0.562123	0.621346
Li	-1.883690	-0.013858	-0.107770
C	-0.237941	-1.210535	0.136352
O	-1.268881	-1.270235	1.173254
C	-1.103630	-2.252509	2.195047
O	-3.679655	-0.353258	-0.804294
O	-1.691661	1.955378	-0.043454
C	-4.174487	-1.692317	-0.771208
C	-4.357238	0.477034	-1.743970
C	-0.476622	2.464013	-0.617581
C	-2.059853	2.643663	1.151263
H	5.516910	0.073771	-1.913946
H	3.684937	-1.264625	-3.019646
H	1.511407	-1.583547	-1.840152
H	5.103100	1.095898	0.318422
H	-0.087294	-2.210231	-0.291568
H	-1.916708	-2.125922	2.918425
H	-0.138938	-2.131351	2.700514
H	-1.154275	-3.262643	1.764181
H	-5.230382	-1.702639	-0.470172
H	-3.573666	-2.232398	-0.038690
H	-4.070779	-2.167348	-1.755568
H	-5.424199	0.549931	-1.494281
H	-4.250352	0.078926	-2.762025
H	-3.897824	1.464934	-1.686200
H	-0.608655	3.517746	-0.895459
H	-0.270388	1.866750	-1.506393
H	0.354413	2.355305	0.087650
H	-2.241455	3.706406	0.942010
H	-1.272953	2.550049	1.909878
H	-2.980052	2.185732	1.520880
H	3.045233	1.354118	2.431398
H	0.545514	0.331156	2.590959 S-61

3 Pseudocoarctate

3.1 Model A

carbene

SCF Energy: -517.449104911

Num. Imaginary Frequencies: 0

Imaginary Frequency: -33.3000

C	1.402890	0.819705	0.000000
C	0.000000	0.729405	0.000000
N	-0.593044	-0.517857	0.000000
C	0.138068	-1.658680	0.000000
C	1.508862	-1.607952	0.000000
C	2.169841	-0.342164	0.000000
C	-1.028857	1.711523	0.000000
C	-2.248335	1.066611	0.000000
C	-2.051862	-0.368799	0.000000
C	-3.015550	-1.339460	0.000000
C	-3.606254	1.692645	0.000000
H	-0.428596	-2.582694	0.000000
H	2.084315	-2.525061	0.000000
C	3.595742	-0.278909	0.000000
H	1.874727	1.795367	0.000000
H	-0.849573	2.778378	0.000000
H	-2.576976	-2.353592	0.000000
H	-4.368260	0.910931	0.000000
H	-3.742360	2.327506	0.883000
H	-3.742360	2.327506	-0.883000
C	4.806757	-0.234036	0.000000
H	5.872584	-0.192680	0.000000

E-enynylpyridine

SCF Energy: -517.471995430

Num. Imaginary Frequencies: 0

C	-1.149790	-0.736554	-0.000069
C	-0.014132	0.097294	0.000220
N	-0.131593	1.443724	0.000408
C	-1.357786	1.972837	0.000275
C	-2.536303	1.227701	-0.000024
C	-2.433381	-0.174351	-0.000196
C	1.302616	-0.550270	0.000358
C	2.555514	-0.019875	0.000159
C	2.934235	1.443769	-0.000297
C	3.660704	-0.930627	0.000309
C	4.632670	-1.658085	0.000191
H	-1.404950	3.060127	0.000420
H	-3.505057	1.714399	-0.000109
C	-3.599135	-1.003120	-0.000493
H	-1.033975	-1.815079	-0.000202
H	1.248064	-1.636123	0.000594
H	5.475957	-2.310319	0.000264
H	3.549398	1.664844	0.880167
H	3.551047	1.663886	-0.879826
H	2.053504	2.080967	-0.001322
C	-4.587774	-1.703405	-0.000745
H	-5.457476	-2.320664	-0.000968

indoizine

SCF Energy: -633.315437667

Num. Imaginary Frequencies: 0

C	-1.362360	0.391998	0.219167
N	-0.035062	0.012330	0.169753
C	0.765121	1.151731	-0.066931
C	-0.101237	2.244536	-0.167704
C	-1.418619	1.774371	0.005738
C	0.525251	-1.240166	0.292379
C	1.877865	-1.396373	0.223154
C	2.737452	-0.264831	0.000502
C	2.162599	0.987893	-0.147588
C	-2.447940	-0.576615	0.515158
O	-2.589443	-1.524959	-0.548944
C	-3.621183	-2.465757	-0.304241
C	-2.664018	2.616545	-0.014841
H	-0.165684	-2.063462	0.413678
H	2.304479	-2.387072	0.320775
C	4.150543	-0.445787	-0.075930
H	2.780852	1.860484	-0.326683
H	0.199890	3.267120	-0.348892
H	-2.247553	-1.124646	1.454303
H	-3.388746	-0.025610	0.657108
H	-3.643408	-3.146094	-1.158059
H	-3.432547	-3.044774	0.613606
H	-4.601158	-1.972654	-0.211690
H	-3.449612	2.167750	-0.632092
H	-3.077002	2.761313	0.991238
H	-2.447687	3.607271	-0.424218
C	5.350501	-0.615512	-0.137540
H	6.405295	-0.758458	-0.193730

TS-cheletropic

SCF Energy: -633.230276165

Num. Imaginary Frequencies: 1

Imaginary Frequency: -575.8671

C	1.053741	-0.049512	-0.285299
N	-0.362278	-0.289996	-0.175253
C	-1.013331	0.916024	0.029284
C	-0.030656	1.947267	0.069612
C	1.211604	1.387304	-0.123557
C	-1.039627	-1.465701	-0.259221
C	-2.404921	-1.488237	-0.140299
C	-3.121769	-0.270975	0.068356
C	-2.409151	0.925157	0.151562
C	2.017979	-0.987460	-0.474774
O	4.417760	-0.323241	0.169499
C	5.243418	-1.383436	0.506532
C	2.532208	2.075018	-0.154049
H	-0.444855	-2.355702	-0.420519
H	-2.934820	-2.429942	-0.205935
C	-4.541844	-0.288372	0.187299
H	-2.922524	1.865776	0.311880
H	-0.253424	2.993472	0.228953
H	1.717067	-2.035743	-0.519785
H	3.189468	-0.702615	-0.348082
H	6.250136	-1.268875	0.057699
H	5.402310	-1.477807	1.599206
H	4.859566	-2.366403	0.152903
H	2.952340	2.048589	-1.167069
H	2.436857	3.117560	0.159574
H	3.264950	1.544433	0.467228
C	-5.749447	-0.314346	0.287565
H	-6.812425	-0.333227	0.376662

TS-coarctate

SCF Energy: -517.437852098

Num. Imaginary Frequencies: 1

Imaginary Frequency: -361.3695

C	1.263357	-1.007316	-0.000002
C	-0.085000	-0.618599	0.000007
N	-0.407110	0.692864	-0.000005
C	0.514555	1.653032	-0.000025
C	1.868104	1.347808	-0.000035
C	2.253109	-0.015609	-0.000023
C	-1.279954	-1.429482	0.000030
C	-2.423494	-0.684771	0.000034
C	-3.812773	-1.251789	0.000048
C	-2.255365	0.750055	0.000017
C	-2.973039	1.820300	0.000018
H	0.142312	2.675927	-0.000034
H	2.615870	2.131768	-0.000052
C	3.637550	-0.372270	-0.000033
H	1.534621	-2.057173	0.000008
H	-1.251270	-2.511707	0.000042
H	-2.628990	2.848628	0.000005
H	-4.365253	-0.899919	-0.876935
H	-3.793428	-2.345089	0.000048
H	-4.365240	-0.899918	0.877038
C	4.812154	-0.668289	-0.000041
H	5.845925	-0.930981	-0.000048

TS-isomerization

SCF Energy: -517.401548704

Num. Imaginary Frequencies: 1

Imaginary Frequency: -371.3408

C	1.238666	-0.802739	-0.062573
C	-0.040334	-0.188845	-0.150167
N	-0.183040	1.171500	-0.128134
C	0.917303	1.908125	-0.012947
C	2.215093	1.389936	0.085262
C	2.382112	-0.010366	0.057915
C	-1.212032	-0.983424	-0.270365
C	-2.581949	-0.437633	-0.338755
C	-3.167283	-0.096887	-1.686819
C	-3.301037	-0.259595	0.828570
C	-3.942912	-0.116910	1.866448
H	0.768300	2.986491	0.001654
H	3.071376	2.048257	0.177864
C	3.682502	-0.599893	0.150984
H	1.323776	-1.884166	-0.085147
H	-1.083562	-2.065454	-0.331028
H	-4.491257	0.026182	2.768998
H	-4.220012	0.183301	-1.602230
H	-2.615261	0.740423	-2.134944
H	-3.082264	-0.946193	-2.378039
C	4.785576	-1.094743	0.229268
H	5.755955	-1.531496	0.298882

Z-enynylpyridine

SCF Energy: -517.471110645

Num. Imaginary Frequencies: 0

C	2.389594	0.003995	-0.000020
C	1.238133	-0.795218	-0.000057
C	-0.033172	-0.190317	0.000122
N	-0.181208	1.150022	0.000342
C	0.919232	1.905154	0.000375
C	2.219705	1.399657	0.000201
C	-1.215930	-1.054227	0.000082
C	-2.532499	-0.722946	0.000091
C	-3.053794	0.604591	0.000014
C	-3.654344	1.659443	-0.000713
C	-3.593545	-1.807498	0.000140
H	0.756458	2.981380	0.000557
H	3.077175	2.063291	0.000241
C	3.693699	-0.584073	-0.000201
H	1.330791	-1.876241	-0.000226
H	-0.990968	-2.118410	0.000035
H	-4.112214	2.621994	-0.001061
H	-4.238763	-1.713650	0.880892
H	-4.238754	-1.713738	-0.880629
H	-3.142407	-2.803387	0.000196
C	4.798846	-1.080815	-0.000353
H	5.771583	-1.517870	-0.000488

3.2 Model B

carbene

SCF Energy: -441.278948956

Num. Imaginary Frequencies: 0

Imaginary Frequency: -55.9077

C	1.407871	0.140628	0.000000
N	0.000000	0.566481	0.000000
C	-0.818434	-0.545360	0.000000
C	0.004838	-1.705195	0.000000
C	1.324883	-1.305414	0.000000
C	-0.494794	1.826984	0.000000
C	-1.854360	2.037489	0.000000
C	-2.728636	0.923928	0.000000
C	-2.216232	-0.359045	0.000000
C	2.537337	0.909043	0.000000
H	0.241956	2.622172	0.000000
H	-2.237200	3.051186	0.000000
H	-3.802631	1.081185	0.000000
H	-2.864333	-1.228725	0.000000
H	-0.374708	-2.718348	0.000000
C	2.537597	-2.180223	0.000000
H	2.300951	1.988366	0.000000
H	3.435562	-1.559258	0.000000
H	2.549990	-2.829473	0.883046
H	2.549990	-2.829473	-0.883046

E-enynylpyridine

SCF Energy: -441.301576800

Num. Imaginary Frequencies: 0

C	-0.635449	-0.302414	0.000113
N	-1.076691	0.974851	0.000306
C	-2.393473	1.195162	0.000289
C	-3.356444	0.181930	0.000007
C	-2.910228	-1.140477	-0.000282
C	-1.540780	-1.385848	-0.000236
C	0.799557	-0.608786	0.000243
C	1.886567	0.209508	0.000073
C	3.180261	-0.404832	0.000271
C	4.300578	-0.872968	0.000011
H	-2.698464	2.240195	0.000437
H	-4.413740	0.426409	0.000025
H	-3.616170	-1.966086	-0.000552
H	-1.162159	-2.403480	-0.000482
H	1.011026	-1.675460	0.000485
C	1.897641	1.721665	-0.000530
H	5.277507	-1.299609	0.000082
H	2.439124	2.086554	0.880491
H	2.442522	2.085573	-0.879853
H	0.887803	2.124301	-0.002526

indoizine

SCF Energy: -557.142314999

Num. Imaginary Frequencies: 0

C	-0.632044	0.472810	0.219465
N	0.578061	-0.195536	0.140073
C	1.608436	0.739639	-0.104444
C	1.008356	1.997877	-0.179739
C	-0.379697	1.832781	0.017325
C	0.839559	-1.543301	0.242564
C	2.124842	-1.999019	0.143957
C	3.197241	-1.087132	-0.086990
C	2.934734	0.256508	-0.215096
C	-1.899249	-0.231854	0.534474
O	-2.284916	-1.102532	-0.537597
C	-3.497380	-1.785536	-0.271901
C	-1.400921	2.936263	0.035240
H	-0.019776	-2.187612	0.371262
H	2.310655	-3.063877	0.226909
H	4.212933	-1.459228	-0.171415
H	3.729567	0.971525	-0.401672
H	1.527237	2.929403	-0.359956
H	-1.803128	-0.831956	1.458275
H	-2.687325	0.513391	0.714409
H	-3.700596	-2.425818	-1.132969
H	-3.421884	-2.410684	0.632116
H	-4.335150	-1.082911	-0.141307
H	-2.333339	2.638616	-0.455378
H	-1.649707	3.245531	1.058392
H	-1.019851	3.818421	-0.487529

TS-cheletropic

SCF Energy: -557.061046928

Num. Imaginary Frequencies: 1

Imaginary Frequency: -189.5130

C	0.355516	-0.091492	-0.260505
N	-1.049219	-0.378855	-0.108196
C	-1.732259	0.808411	0.103345
C	-0.784562	1.871257	0.101745
C	0.470709	1.351696	-0.122658
C	-1.683031	-1.579882	-0.159982
C	-3.046488	-1.645126	0.002012
C	-3.781067	-0.454423	0.217773
C	-3.128181	0.763643	0.268099
C	1.343428	-1.001612	-0.453549
O	3.762699	-0.195941	0.055807
C	4.662370	-1.174215	0.438320
C	1.765871	2.080458	-0.201859
H	-1.059079	-2.447772	-0.331116
H	-3.539951	-2.608660	-0.039177
H	-4.858018	-0.500465	0.342121
H	-3.667455	1.689675	0.433182
H	-1.037295	2.911495	0.255568
H	1.085088	-2.061074	-0.476014
H	2.483834	-0.676093	-0.394024
H	5.641111	-1.047398	-0.068023
H	4.878855	-1.163529	1.526161
H	4.322733	-2.206528	0.193461
H	2.148218	2.067730	-1.230280
H	1.649736	3.119503	0.116551
H	2.541338	1.570344	0.386063

TS-coarctate

SCF Energy: -441.268050628

Num. Imaginary Frequencies: 1

Imaginary Frequency: -357.2258

C	0.481958	-0.808997	-0.000024
N	0.397535	0.538281	0.000016
C	1.470405	1.324912	0.000047
C	2.751443	0.781979	0.000046
C	2.878730	-0.617689	0.000012
C	1.746433	-1.425240	-0.000023
C	-0.838691	-1.394755	-0.000080
C	-1.832891	-0.460392	-0.000077
C	-1.414124	0.922403	-0.000048
C	-1.930197	2.102861	-0.000080
H	1.278662	2.396616	0.000074
H	3.622126	1.428336	0.000070
H	3.865798	-1.070627	0.000014
H	1.824991	-2.507652	-0.000051
H	-1.002316	-2.465069	-0.000114
C	-3.300524	-0.773400	0.000112
H	-1.407713	3.053158	-0.000062
H	-3.782900	-0.329959	-0.876777
H	-3.474196	-1.853067	0.000277
H	-3.782460	-0.329787	0.877153

TS-isomerization

SCF Energy: -441.231481326

Num. Imaginary Frequencies: 1

Imaginary Frequency: -367.1017

C	-0.592257	-0.400068	-0.236864
N	-0.698971	0.622483	0.666200
C	-1.907384	1.119497	0.906346
C	-3.087031	0.663201	0.295577
C	-2.989183	-0.387111	-0.625146
C	-1.740745	-0.926248	-0.895416
C	0.699576	-0.929497	-0.497492
C	1.943668	-0.427586	0.118837
C	2.662274	0.570781	-0.512464
C	3.307519	1.447210	-1.082795
H	-1.951166	1.931848	1.630356
H	-4.041875	1.117559	0.539057
H	-3.874999	-0.773704	-1.121043
H	-1.624713	-1.740117	-1.605097
H	0.769393	-1.772973	-1.186621
C	2.407115	-1.027857	1.423144
H	3.853444	2.224156	-1.566473
H	3.388281	-0.642559	1.710924
H	1.688718	-0.792918	2.220114
H	2.464399	-2.122603	1.353026

Z-enynylpyridine

SCF Energy: -441.300495532

Num. Imaginary Frequencies: 0

C	1.696416	-1.339481	-0.000115
C	0.581252	-0.475223	-0.000081
N	0.728226	0.865028	0.000015
C	1.964329	1.367246	0.000109
C	3.125434	0.587301	0.000095
C	2.979625	-0.800907	-0.000022
C	-0.761689	-1.059665	-0.000164
C	-1.975398	-0.451273	0.000107
C	-3.246622	-1.279856	0.000128
C	-2.196752	0.957739	0.000315
C	-2.555149	2.117557	-0.000320
H	2.034310	2.453797	0.000189
H	4.104328	1.056045	0.000162
H	3.849387	-1.451758	-0.000039
H	1.547334	-2.415323	-0.000208
H	-0.773963	-2.147539	-0.000407
H	-2.792986	3.156521	-0.000513
H	-3.856392	-1.048667	0.880862
H	-3.856267	-1.048988	-0.880782
H	-3.022009	-2.349917	0.000320

3.3 Model C

carbene

SCF Energy: -401.945689967

Num. Imaginary Frequencies: 0

C	-0.254343	-0.923846	0.000000
N	0.000000	0.433995	0.000000
C	1.260741	0.930238	0.000000
C	2.339777	0.077214	0.000000
C	2.121347	-1.321332	0.000000
C	0.832806	-1.820246	0.000000
C	-1.668424	-1.112682	0.000000
C	-2.253883	0.129546	0.000000
C	-1.271403	1.175895	0.000000
C	-1.488201	2.528927	0.000000
H	1.341285	2.011325	0.000000
H	3.343027	0.486878	0.000000
H	2.968449	-1.999834	0.000000
H	0.637339	-2.887083	0.000000
H	-2.153770	-2.078639	0.000000
H	-3.311354	0.355566	0.000000
H	-0.535486	3.091536	0.000000

E-enynylpyridine

SCF Energy: -401.976546761

Num. Imaginary Frequencies: 0

N	1.312427	0.156287	0.000000
C	2.203040	1.148472	0.000000
C	1.858864	2.505888	0.000000
C	0.504388	2.837950	0.000000
C	-0.438103	1.811701	0.000000
C	0.000000	0.474597	0.000000
H	3.249479	0.848940	0.000000
H	2.630959	3.268416	0.000000
H	0.186393	3.876587	0.000000
H	-1.501390	2.032472	0.000000
C	-0.980971	-0.615878	0.000000
C	-0.654301	-1.926952	0.000000
H	-2.028854	-0.325668	0.000000
H	0.399147	-2.199970	0.000000
C	-1.605122	-2.979590	0.000000
C	-2.393563	-3.903328	0.000000
H	-3.088122	-4.711960	0.000000

indoizine

SCF Energy: -517.812763269

Num. Imaginary Frequencies: 0

C	2.843822	0.074815	-0.210018
C	1.616000	0.773028	-0.097590
N	0.441841	0.019047	0.137803
C	0.475470	-1.355471	0.234296
C	1.666787	-2.016264	0.133551
C	2.877582	-1.293531	-0.091191
C	1.238698	2.116360	-0.159666
C	-0.155578	2.168212	0.035893
C	-0.639670	0.877162	0.222221
C	-2.013628	0.406706	0.531101
H	-0.770355	3.058745	0.050010
H	-0.479941	-1.847184	0.359274
H	1.674013	-3.097667	0.210169
H	3.816765	-1.829800	-0.177622
H	3.747265	0.648396	-0.390522
H	1.908258	2.947992	-0.325950
H	-2.038209	-0.168878	1.474949
H	-2.660026	1.286258	0.667898
O	-2.520369	-0.420011	-0.522310
C	-3.837273	-0.877136	-0.267836
H	-4.129032	-1.502076	-1.114486
H	-3.887984	-1.474891	0.656104
H	-4.543949	-0.037423	-0.180536

TS-cheletropic

SCF Energy: -517.724248147

Num. Imaginary Frequencies: 1

Imaginary Frequency: -812.1034

C	-2.974474	0.687124	0.301769
C	-1.603676	0.890319	0.062516
N	-0.793642	-0.214341	-0.167269
C	-1.285532	-1.483649	-0.155148
C	-2.620675	-1.700327	0.083506
C	-3.481166	-0.598788	0.312588
C	-0.786546	2.057010	-0.005992
C	0.494944	1.655915	-0.293333
C	0.550559	0.227676	-0.410750
C	1.641958	-0.551195	-0.680604
H	1.374756	2.274653	-0.405038
H	-0.572521	-2.277552	-0.337418
H	-2.997846	-2.715998	0.094167
H	-4.536884	-0.767958	0.496808
H	-3.609461	1.548283	0.478145
H	-1.147218	3.064275	0.147233
H	1.517084	-1.635364	-0.685606
H	2.736087	-0.088431	-0.458886
O	3.688722	0.226682	0.448316
C	4.743893	-0.670277	0.343487
H	5.697752	-0.141221	0.154540
H	4.887781	-1.277452	1.257009
H	4.620476	-1.379163	-0.504834

TS-coarctate

SCF Energy: -401.934808759

Num. Imaginary Frequencies: 1

Imaginary Frequency: -391.4520

N	-0.114091	-0.423156	-0.000113
C	0.763313	-1.424363	-0.000085
C	2.130674	-1.171038	-0.000013
C	2.559710	0.167534	0.000070
C	1.630031	1.201616	0.000075
C	0.262439	0.874706	-0.000018
H	0.343460	-2.428670	-0.000134
H	2.840465	-1.990809	-0.000015
H	3.621595	0.394745	0.000134
H	1.941482	2.241169	0.000165
C	-0.904092	1.730870	-0.000039
C	-2.057510	1.008949	-0.000016
H	-0.841309	2.811003	0.000047
H	-3.048047	1.447936	-0.000035
C	-1.953145	-0.421420	-0.000094
C	-2.711422	-1.468693	0.000184
H	-2.378996	-2.502247	0.000254

TS-isomerization

SCF Energy: -401.899191982

Num. Imaginary Frequencies: 1

Imaginary Frequency: -637.4406

N	0.451991	-0.845380	0.434368
C	1.634200	-1.428437	0.270324
C	2.789553	-0.765008	-0.174990
C	2.695137	0.601357	-0.464791
C	1.473407	1.236898	-0.302744
C	0.349072	0.488685	0.150318
H	1.676213	-2.490640	0.506798
H	3.723791	-1.305616	-0.286369
H	3.562568	1.155951	-0.811153
H	1.360601	2.295186	-0.519066
C	-0.913404	1.115766	0.325043
C	-2.129420	0.419473	0.773307
H	-0.976104	2.186922	0.127918
H	-2.351031	0.379688	1.841353
C	-3.019302	-0.171957	-0.097364
C	-3.821745	-0.688385	-0.871749
H	-4.504971	-1.154174	-1.544189

Z-enynylpyridine

SCF Energy: -401.970460178

Num. Imaginary Frequencies: 0

N	0.524427	-0.571142	0.000000
C	1.852471	-0.695911	0.000000
C	2.738959	0.386803	0.000000
C	2.200704	1.674226	0.000000
C	0.816206	1.820322	0.000000
C	0.000000	0.671205	0.000000
H	2.232837	-1.715895	0.000000
H	3.811417	0.219949	0.000000
H	2.846596	2.547550	0.000000
H	0.362971	2.807289	0.000000
C	-1.455913	0.833369	0.000000
C	-2.423357	-0.114842	0.000000
H	-1.797963	1.865705	0.000000
H	-3.453227	0.240151	0.000000
C	-2.294754	-1.527478	0.000000
C	-2.330521	-2.741097	0.000000
H	-2.296383	-3.806331	0.000000

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