Vinylnitrene Formation from 3,5-Diphenyl-isoxazole and 3-Benzoyl-2-phenylazirine

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1 Transient Spectra

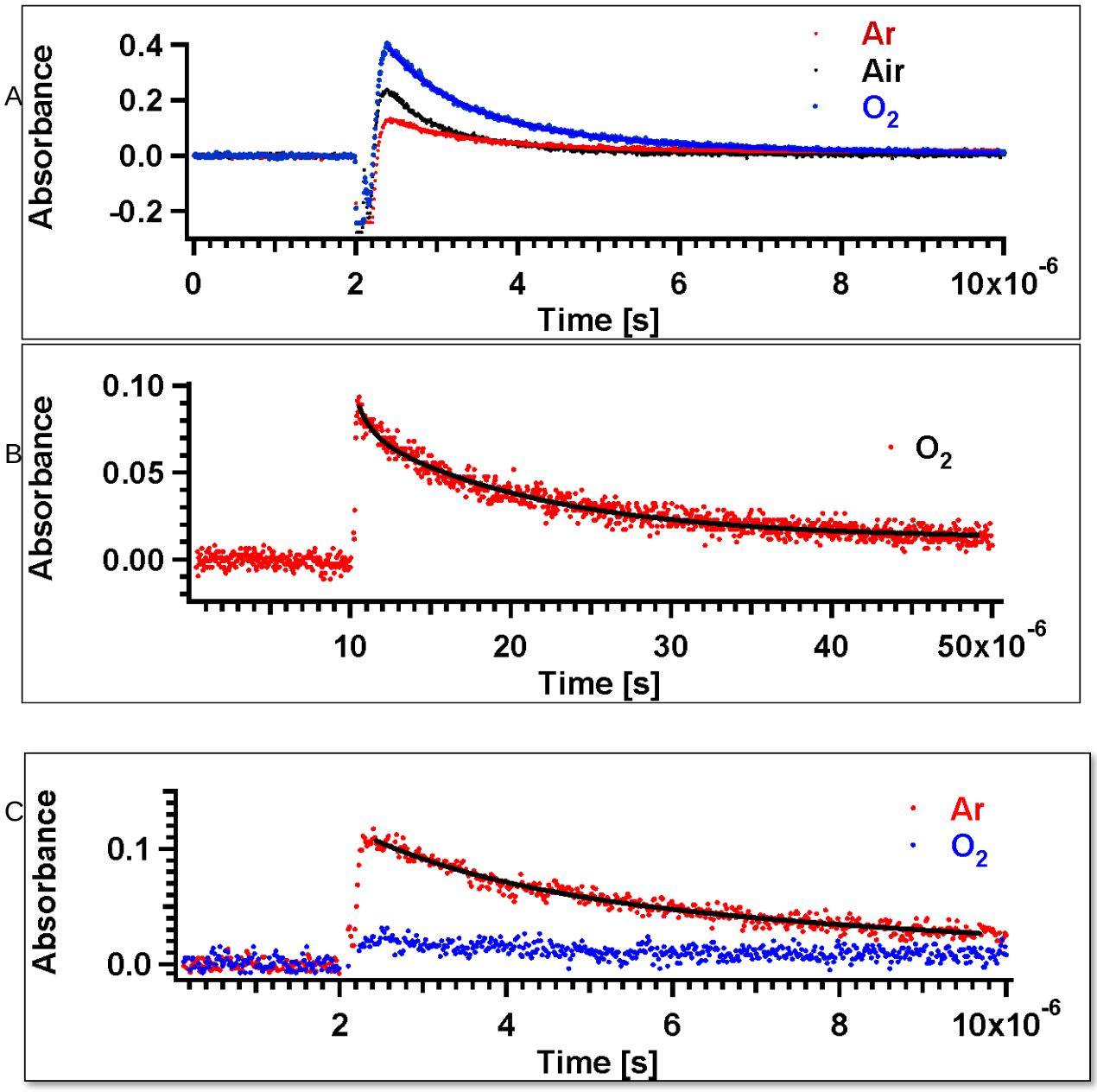
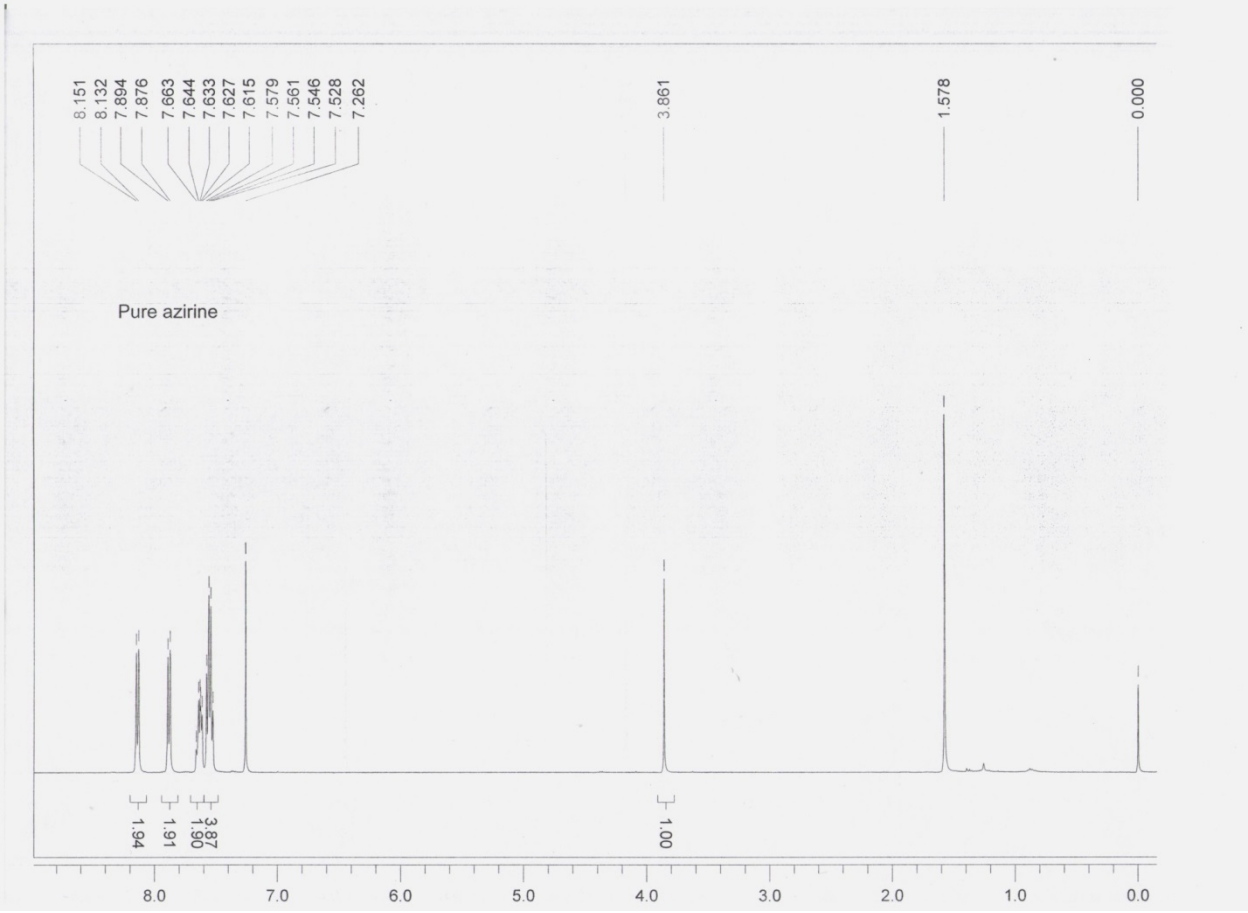


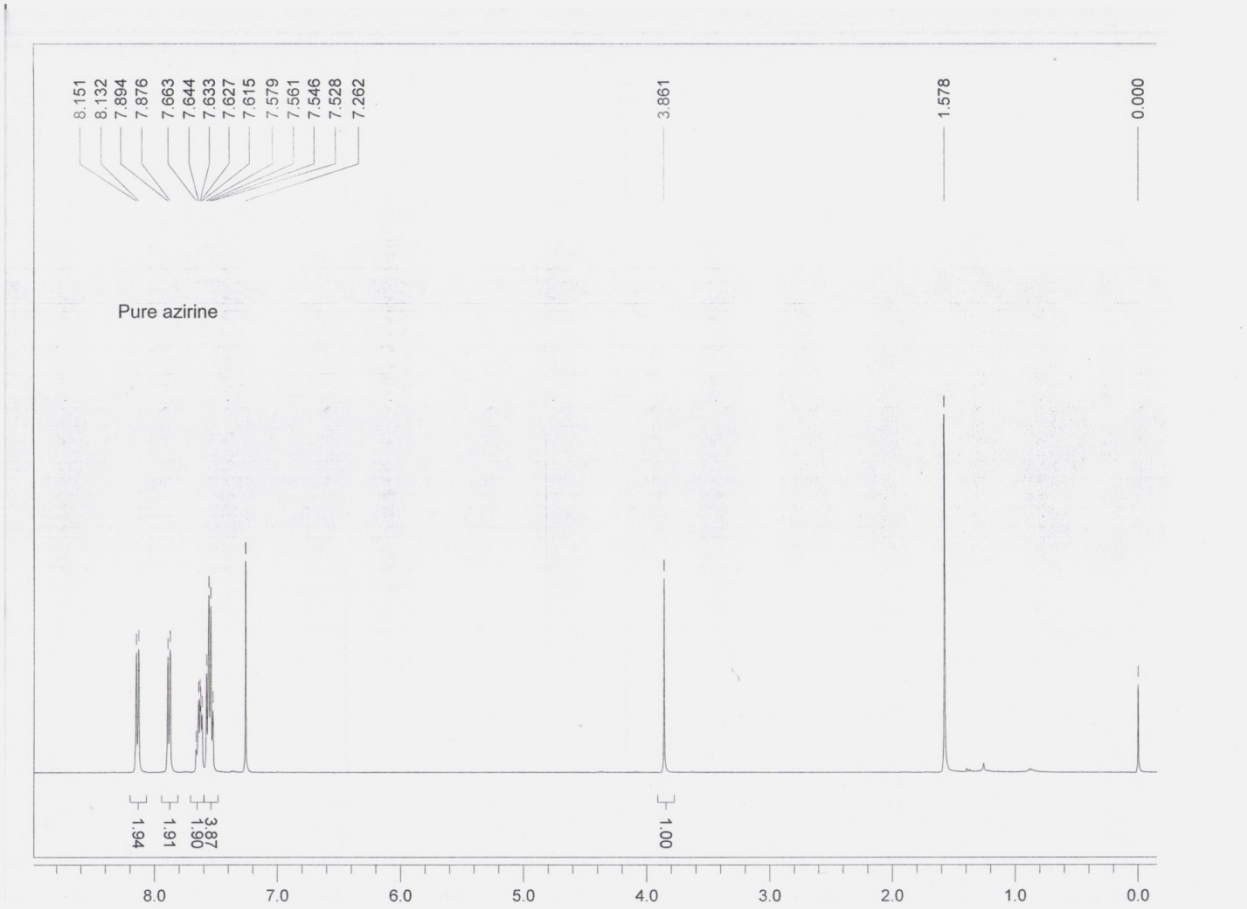
Figure S1. Kinetic traces from laser flash photolysis of 2 at A) 360 nm, B) 460 nm and C) 500 nm in argon-, air- and oxygen-saturated acetonitrile

2 Spectra

2.1 H-NMR spectrum of 1



2.2 H-NMR spectrum of 2



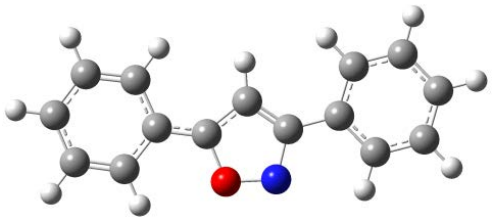
3 Calculations

3.1 Optimized 1

B3LYP/6-31+G(d) E : - 708.18451928 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.098070	-0.254776	-0.000112
2	6	0	0.008105	0.550911	0.000020
3	6	0	1.114489	-0.352295	-0.000133
4	1	0	0.032348	1.629644	0.000260
5	7	0	0.698224	-1.607334	-0.000313
6	6	0	2.557002	-0.039718	-0.000023
7	6	0	3.000214	1.292179	-0.000020
8	6	0	3.512214	-1.071778	0.000051
9	6	0	4.364747	1.588640	0.000082
10	1	0	2.280960	2.106244	-0.000117
11	6	0	4.873748	-0.773343	0.000160
12	1	0	3.176540	-2.103872	-0.000001
13	6	0	5.306658	0.557305	0.000183
14	1	0	4.689596	2.625951	0.000082
15	1	0	5.600124	-1.582034	0.000218
16	1	0	6.369029	0.787144	0.000267
17	6	0	-2.537984	0.004331	-0.000023
18	6	0	-3.019689	1.325650	-0.000210
19	6	0	-3.460120	-1.057311	0.000239
20	6	0	-4.390088	1.578852	-0.000108
21	1	0	-2.320910	2.157533	-0.000453
22	6	0	-4.830850	-0.798165	0.000333
23	1	0	-3.098513	-2.080434	0.000372
24	6	0	-5.301757	0.517899	0.000162
25	1	0	-4.746910	2.605445	-0.000254
26	1	0	-5.532678	-1.628008	0.000539
27	1	0	-6.370257	0.716407	0.000233
28	8	0	-0.694827	-1.549121	-0.000319

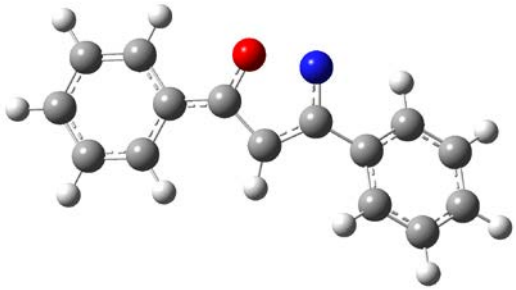
3.2 Optimized T_1 of 1



UB3LYP/6-31+G(d) E : - 708.08481538 a.u.

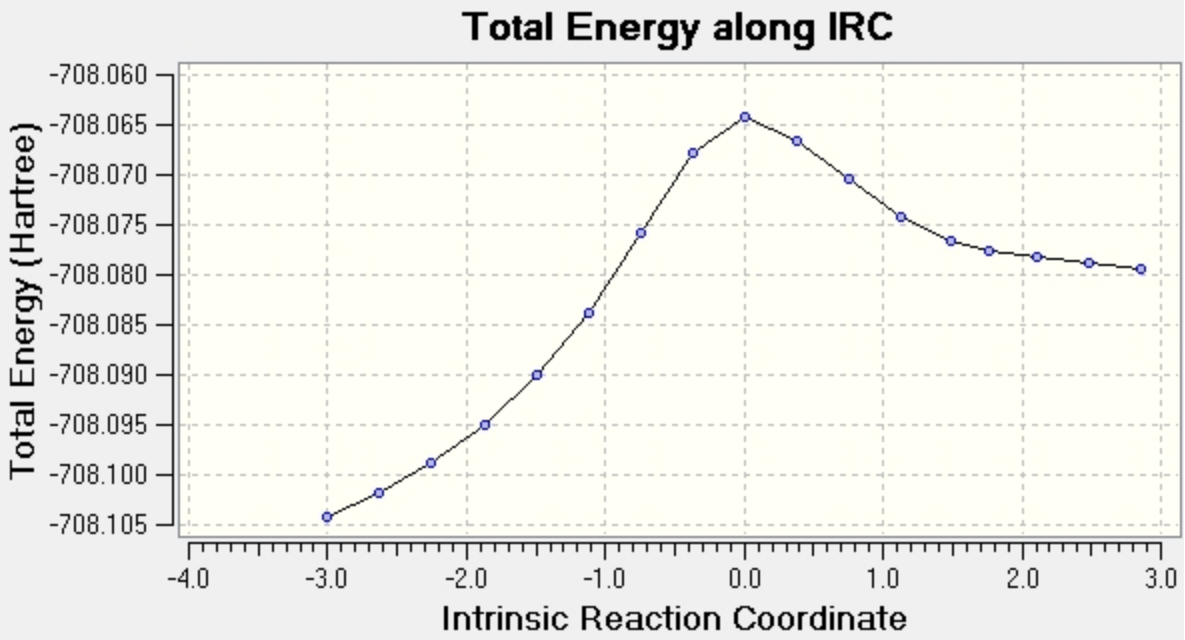
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.142654	-0.261044	-0.000001
2	6	0	0.029584	0.560785	0.000004
3	6	0	1.108375	-0.276146	-0.000009
4	8	0	-0.702028	-1.606084	-0.000016
5	1	0	0.033673	1.640875	0.000027
6	7	0	0.688325	-1.631233	-0.000022
7	6	0	2.538856	-0.000052	-0.000002
8	6	0	3.467730	-1.062464	0.000011
9	6	0	3.028114	1.323511	-0.000013
10	6	0	4.838539	-0.802859	0.000016
11	1	0	3.104412	-2.084487	0.000019
12	6	0	4.395645	1.575216	-0.000004
13	1	0	2.332082	2.157959	-0.000033
14	6	0	5.310209	0.512166	0.000011
15	1	0	5.540366	-1.632888	0.000024
16	1	0	4.753788	2.601492	-0.000011
17	1	0	6.378521	0.711606	0.000018
18	6	0	-2.505131	-0.001267	0.000000
19	6	0	-3.469590	-1.075285	0.000005
20	6	0	-3.006983	1.352134	-0.000002
21	6	0	-4.822599	-0.798463	0.000010
22	1	0	-3.113160	-2.099426	0.000005
23	6	0	-4.363536	1.597298	0.000001
24	1	0	-2.305652	2.181327	-0.000009
25	6	0	-5.291547	0.531533	0.000008
26	1	0	-5.535469	-1.619253	0.000014
27	1	0	-4.722645	2.623388	-0.000002
28	1	0	-6.358041	0.736346	0.000012

3.3 Optimized TS for T of 1 forming 4

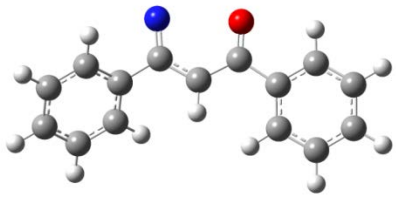


UB3LYP/6-31+G(d) E: -708.06428770 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.186949	-0.463572	-0.589743
2	6	0	0.033747	0.348799	-0.636226
3	6	0	1.113406	-0.508611	-0.412756
4	1	0	0.078328	1.429615	-0.615583
5	7	0	0.800927	-1.815174	-0.414563
6	6	0	2.500503	-0.093891	-0.093548
7	6	0	3.019886	1.108862	-0.601565
8	6	0	3.320671	-0.904755	0.710137
9	6	0	4.323470	1.501783	-0.295866
10	1	0	2.410789	1.731188	-1.252329
11	6	0	4.621659	-0.505769	1.016185
12	1	0	2.928922	-1.841448	1.094739
13	6	0	5.128868	0.698021	0.516471
14	1	0	4.711938	2.433653	-0.698797
15	1	0	5.241864	-1.138654	1.645737
16	1	0	6.144675	1.003962	0.752468
17	6	0	-2.475696	-0.041564	-0.154113
18	6	0	-2.819058	1.341462	-0.083732
19	6	0	-3.481069	-1.002007	0.166924
20	6	0	-4.096122	1.734098	0.293068
21	1	0	-2.080788	2.096772	-0.335954
22	6	0	-4.746545	-0.591900	0.551319
23	1	0	-3.231250	-2.056400	0.109079
24	6	0	-5.069396	0.776516	0.616056
25	1	0	-4.340022	2.792397	0.339525
26	1	0	-5.498206	-1.335945	0.802571
27	1	0	-6.067502	1.089260	0.909706
28	8	0	-0.878686	-1.735378	-0.733110



3.4 Optimized 4A

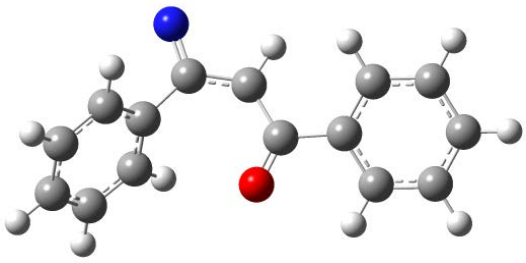


UB3LYP/6-31+G(d) E : - 708.12172110 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.274598	0.953534	-0.164318
2	6	0	-0.028560	0.295881	-0.021373
3	6	0	-1.273004	0.982606	-0.158024
4	1	0	-0.074506	-0.754057	0.244559
5	7	0	-1.361357	2.263502	-0.369394
6	6	0	-2.558869	0.207622	-0.044531
7	6	0	-2.698242	-1.051886	-0.647260
8	6	0	-3.645486	0.759929	0.651240
9	6	0	-3.901709	-1.753009	-0.544932
10	1	0	-1.875190	-1.476173	-1.216831
11	6	0	-4.845773	0.055212	0.754401
12	1	0	-3.540460	1.736313	1.114813

13	6	0	-4.976949	-1.202689	0.158451
14	1	0	-4.000678	-2.724994	-1.021281
15	1	0	-5.678485	0.488683	1.302074
16	1	0	-5.912733	-1.749664	0.238506
17	6	0	2.528548	0.138933	-0.011032
18	6	0	2.547800	-1.266211	0.022065
19	6	0	3.746109	0.835648	0.085072
20	6	0	3.755256	-1.956273	0.149384
21	1	0	1.630374	-1.839195	-0.067154
22	6	0	4.949146	0.147062	0.220252
23	1	0	3.723963	1.920189	0.051335
24	6	0	4.957416	-1.252334	0.252695
25	1	0	3.755182	-3.042935	0.166565
26	1	0	5.881966	0.699182	0.299521
27	1	0	5.896209	-1.790394	0.356272
28	8	0	1.342769	2.165547	-0.386895

3.5 Optimized 4B

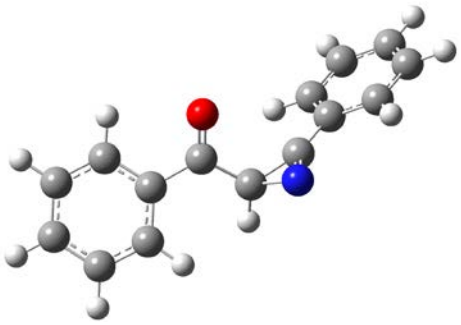


UB3LYP/6-31+G(d) E : - 708.12060076 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.827029	-0.159352	-0.212203
2	6	0	0.153271	1.106616	-0.524715
3	6	0	-1.247898	1.387294	-0.482222
4	1	0	0.768053	1.954764	-0.809995
5	7	0	-1.594725	2.616092	-0.741116
6	6	0	-2.366188	0.443585	-0.137650
7	6	0	-2.624892	-0.703442	-0.900679
8	6	0	-3.226450	0.784137	0.916539
9	6	0	-3.725310	-1.505572	-0.600031
10	1	0	-1.962267	-0.972699	-1.715838
11	6	0	-4.319084	-0.030425	1.223321

12	1	0	-3.033444	1.681035	1.498298
13	6	0	-4.571583	-1.174890	0.463955
14	1	0	-3.917931	-2.395501	-1.193416
15	1	0	-4.973195	0.234064	2.050003
16	1	0	-5.423775	-1.807773	0.698151
17	6	0	2.317765	-0.140367	-0.025375
18	6	0	3.050220	1.032029	0.228512
19	6	0	2.998093	-1.369461	-0.077927
20	6	0	4.432194	0.975445	0.421138
21	1	0	2.550701	1.993123	0.303265
22	6	0	4.378311	-1.423283	0.102307
23	1	0	2.423814	-2.272061	-0.261266
24	6	0	5.099636	-0.250054	0.352541
25	1	0	4.985159	1.888100	0.626808
26	1	0	4.893813	-2.378700	0.050004
27	1	0	6.176269	-0.292110	0.496317
28	8	0	0.203149	-1.222304	-0.129948

3.6 Optimized 2

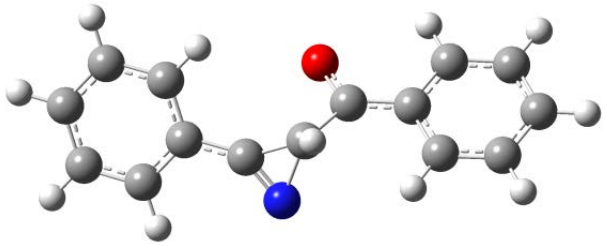


UB3LYP/6-31+G(d) E : --708.16333785

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.128687	0.987167	-0.310329
2	1	0	0.480299	1.258963	-1.302422
3	7	0	-0.776716	2.050575	0.375364
4	6	0	-1.308432	0.984413	-0.029851
5	6	0	-2.575916	0.289574	-0.122863
6	6	0	-3.741977	0.887747	0.387781
7	6	0	-2.641551	-0.975257	-0.726987
8	6	0	-4.960536	0.220534	0.290115

9	1	0	-3.678347	1.865428	0.857209
10	6	0	-3.865472	-1.637835	-0.822578
11	1	0	-1.733005	-1.431518	-1.110146
12	6	0	-5.023662	-1.041167	-0.315072
13	1	0	-5.862291	0.680151	0.685577
14	1	0	-3.915838	-2.618293	-1.288071
15	1	0	-5.976515	-1.558992	-0.388313
16	6	0	1.041946	0.207795	0.587987
17	6	0	2.467227	-0.003959	0.176754
18	6	0	3.105998	0.779231	-0.799688
19	6	0	3.197099	-1.017083	0.823100
20	6	0	4.446132	0.552462	-1.121870
21	1	0	2.574375	1.585945	-1.294218
22	6	0	4.529778	-1.250643	0.492117
23	1	0	2.698140	-1.608326	1.584723
24	6	0	5.157898	-0.465512	-0.482053
25	1	0	4.933488	1.172373	-1.869852
26	1	0	5.082184	-2.041242	0.993438
27	1	0	6.199135	-0.644808	-0.738082
28	8	0	0.611508	-0.264812	1.635404

3.7 Optimized T_{1K} of 2

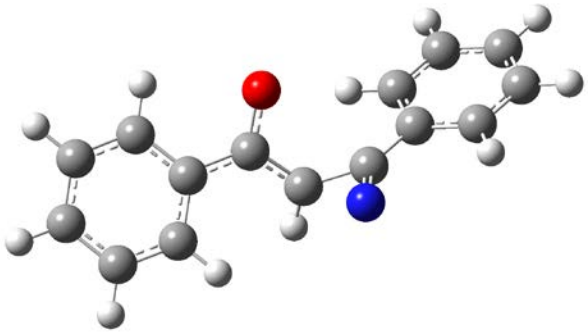


UB3LYP/6-31+G(d) E: -708.05767249 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.118779	-0.638325	0.597338
2	1	0	0.355976	-0.933091	1.622333
3	7	0	-0.492875	-1.744184	-0.310229
4	6	0	-1.244300	-0.817292	0.111445
5	6	0	-2.605952	-0.334836	0.066366
6	6	0	-3.596892	-1.087724	-0.592233
7	6	0	-2.938052	0.884557	0.680129
8	6	0	-4.906071	-0.617447	-0.634328

9	1	0	-3.326634	-2.028409	-1.063918
10	6	0	-4.252104	1.349535	0.632136
11	1	0	-2.162907	1.459680	1.178491
12	6	0	-5.234502	0.599994	-0.022348
13	1	0	-5.672997	-1.194631	-1.143540
14	1	0	-4.509669	2.294528	1.102133
15	1	0	-6.258321	0.963198	-0.057445
16	6	0	1.080371	0.334289	-0.003946
17	6	0	2.498179	0.198583	-0.012393
18	6	0	3.117992	-1.019627	0.382580
19	6	0	3.332131	1.274795	-0.430660
20	6	0	4.502278	-1.136709	0.381163
21	1	0	2.503542	-1.868489	0.668223
22	6	0	4.714056	1.134680	-0.431735
23	1	0	2.876272	2.212338	-0.736951
24	6	0	5.314355	-0.066014	-0.024112
25	1	0	4.956826	-2.075551	0.688532
26	1	0	5.334157	1.969797	-0.749290
27	1	0	6.395989	-0.168075	-0.026904
28	8	0	0.444536	1.403404	-0.438311

3.8 TS for forming 4 from T_{1K} of 2



UB3LYP/6-31+G(d) E: -708.05470934 a.u.

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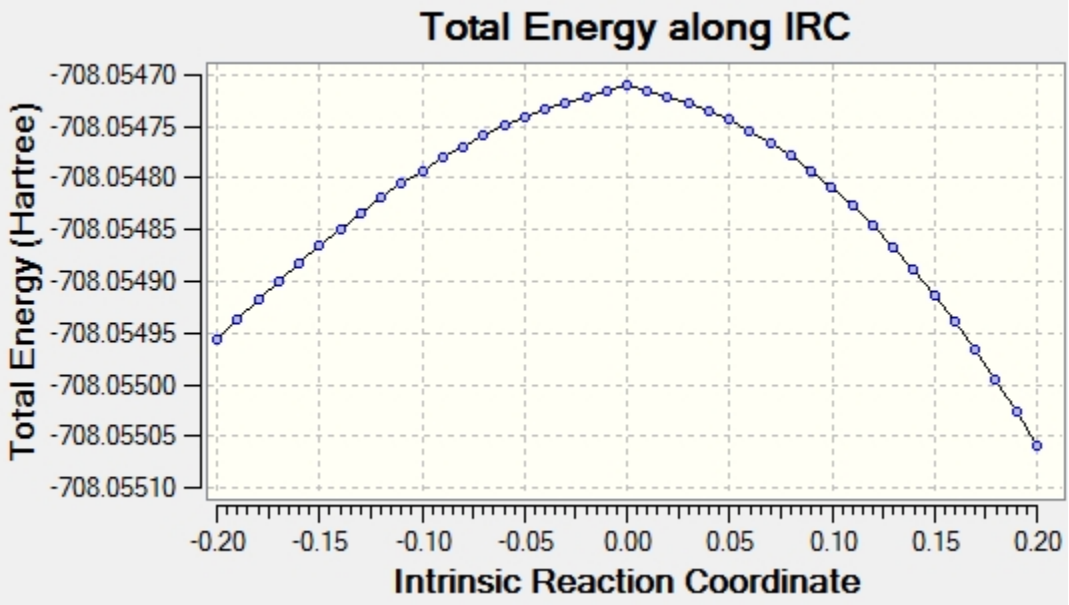
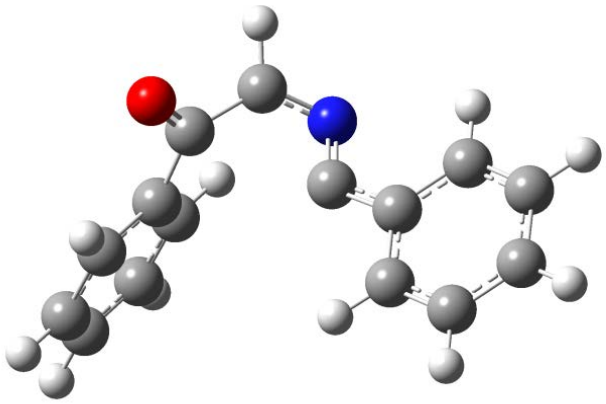
1	6	0	-0.111192	0.710675	0.430057
2	1	0	-0.389943	1.088557	1.410165
3	7	0	0.707946	1.961184	-0.520309
4	6	0	1.263449	0.946843	-0.027156
5	6	0	2.589235	0.346572	0.058349
6	6	0	3.698287	1.011875	-0.493446
7	6	0	2.757989	-0.893379	0.692616

8	6	0	4.962424	0.434317	-0.411097
9	1	0	3.554560	1.971481	-0.982668
10	6	0	4.027793	-1.467047	0.772733
11	1	0	1.893982	-1.402214	1.111388
12	6	0	5.128771	-0.804659	0.222232
13	1	0	5.820314	0.945534	-0.839626
14	1	0	4.157521	-2.429075	1.260858
15	1	0	6.117375	-1.252116	0.284570
16	6	0	-1.044684	-0.158587	-0.225996
17	6	0	-2.480635	-0.136827	-0.072861
18	6	0	-3.137156	1.005482	0.447030
19	6	0	-3.264284	-1.252279	-0.463382
20	6	0	-4.518436	1.008355	0.608678
21	1	0	-2.559630	1.890051	0.699522
22	6	0	-4.647031	-1.228458	-0.310040
23	1	0	-2.772096	-2.134126	-0.862785
24	6	0	-5.284180	-0.104791	0.231518
25	1	0	-5.006712	1.890278	1.015845
26	1	0	-5.233334	-2.094203	-0.608077
27	1	0	-6.364076	-0.091389	0.351030
28	8	0	-0.476961	-1.077453	-0.994184



3.9 TS for forming ylide 5 from 2

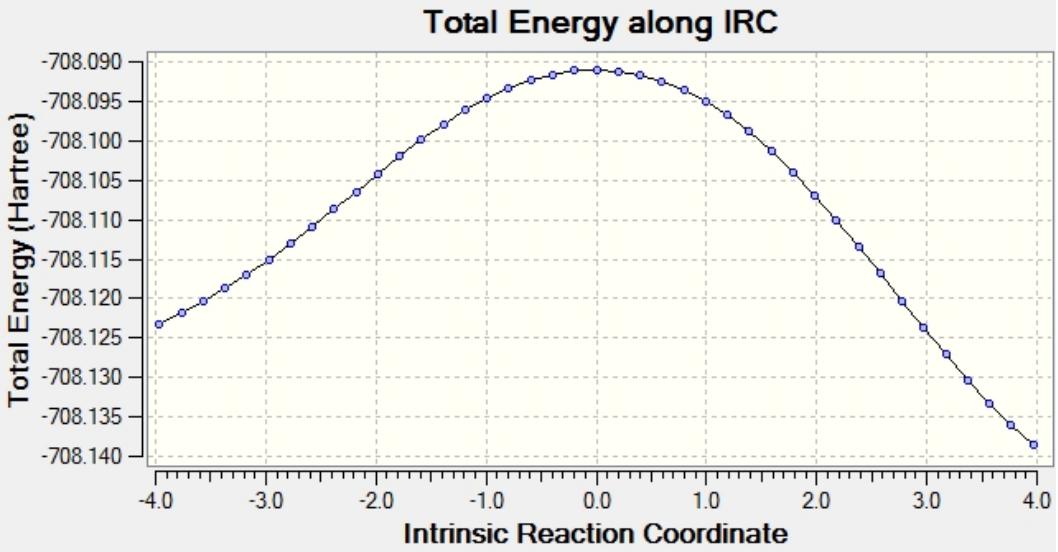


B3LYP/6-31+G(d) E: -708.09100017 a.u.

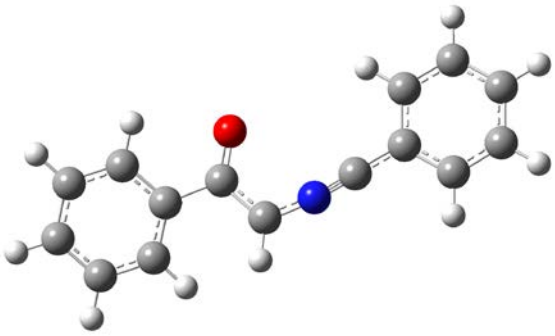
Imaginary frequency: -452 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.315619	2.143132	-0.136865
2	1	0	-0.247056	3.220148	0.024394
3	7	0	0.515517	1.622187	-1.079483
4	6	0	0.760392	0.496503	-0.492629
5	6	0	2.082375	-0.033272	-0.247786
6	6	0	2.192676	-1.316074	0.328376
7	6	0	3.256572	0.689784	-0.566533
8	6	0	3.446686	-1.871805	0.571989
9	1	0	1.282277	-1.854739	0.574217
10	6	0	4.505704	0.131499	-0.318782
11	1	0	3.163929	1.677279	-1.008317
12	6	0	4.599507	-1.147155	0.249798
13	1	0	3.529947	-2.861084	1.012986
14	1	0	5.408795	0.684003	-0.564188
15	1	0	5.578598	-1.578402	0.443369
16	6	0	-1.243318	1.413616	0.765395
17	6	0	-2.143473	0.330044	0.226194
18	6	0	-2.469279	0.213758	-1.133307
19	6	0	-2.747039	-0.533561	1.150726
20	6	0	-3.373241	-0.759387	-1.560571

21	1	0	-2.020784	0.885313	-1.859884
22	6	0	-3.641923	-1.515182	0.721321
23	1	0	-2.510091	-0.418007	2.204012
24	6	0	-3.957347	-1.631690	-0.635762
25	1	0	-3.624886	-0.835027	-2.615532
26	1	0	-4.097931	-2.184730	1.446536
27	1	0	-4.659030	-2.391601	-0.970752
28	8	0	-1.391053	1.830038	1.917519



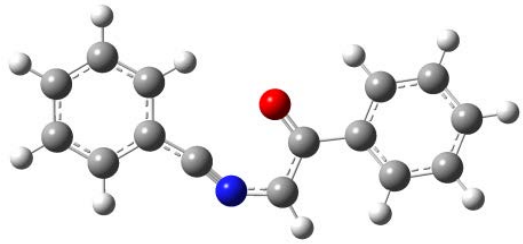
3.10 Optimized Ylide 5



B3LYP/6-31+G(d) E: -708.16038933 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.026734	-1.186487	0.213602
2	6	0	3.630958	-1.139321	0.222659
3	6	0	2.955175	0.074209	0.015541
4	6	0	3.709034	1.240530	-0.191897
5	6	0	5.102696	1.193162	-0.208245
6	6	0	5.766954	-0.021355	-0.006461
7	1	0	5.535388	-2.132222	0.383672
8	1	0	3.076838	-2.052990	0.416124
9	1	0	3.177291	2.175656	-0.336652
10	1	0	5.672364	2.103908	-0.376203
11	1	0	6.853505	-0.058999	-0.015551
12	6	0	1.455048	0.204233	0.020591
13	8	0	0.923819	1.324204	0.118037
14	6	0	0.672322	-1.000681	-0.109138
15	1	0	1.059827	-1.996241	-0.269397
16	7	0	-0.648714	-0.866141	-0.094556
17	6	0	-1.785000	-0.584243	-0.061300
18	6	0	-3.155546	-0.249895	-0.024307
19	6	0	-4.147765	-1.249957	-0.135244
20	6	0	-3.532344	1.105228	0.123714
21	6	0	-5.492122	-0.889832	-0.099300
22	1	0	-3.858216	-2.290295	-0.248305
23	6	0	-4.882797	1.439322	0.158410
24	1	0	-2.764866	1.868268	0.207737
25	6	0	-5.867234	0.450255	0.047192
26	1	0	-6.251580	-1.662156	-0.185838
27	1	0	-5.168155	2.481518	0.272508
28	1	0	-6.918621	0.721902	0.074597

3.11 TS for 5 forming 3



B3LYP/6-31+G(d) E: -708.15704847 a.u.

Imaginary frequency: - 108 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.980138	-0.740194	0.243413
2	6	0	3.615214	-1.031821	0.233494
3	6	0	2.670142	-0.018173	0.004098
4	6	0	3.122275	1.294750	-0.205245
5	6	0	4.486627	1.584811	-0.200574
6	6	0	5.420866	0.568337	0.022807
7	1	0	5.699224	-1.534140	0.429042
8	1	0	3.292398	-2.050483	0.426183
9	1	0	2.385282	2.074071	-0.370162
10	1	0	4.822005	2.605160	-0.369380
11	1	0	6.484295	0.794209	0.029727
12	6	0	1.194343	-0.271966	-0.016338
13	8	0	0.385912	0.686650	0.040357
14	6	0	0.706276	-1.616294	-0.119668
15	1	0	1.270269	-2.527646	-0.228122
16	7	0	-0.635965	-1.654350	-0.134255
17	6	0	-1.575328	-0.926789	-0.086198
18	6	0	-2.843459	-0.308819	-0.026032
19	6	0	-4.018509	-1.092250	-0.093051
20	6	0	-2.933650	1.095352	0.099568
21	6	0	-5.261607	-0.467739	-0.033561
22	1	0	-3.946131	-2.171279	-0.189680
23	6	0	-4.188242	1.694438	0.157592
24	1	0	-2.019343	1.676487	0.148753
25	6	0	-5.354499	0.922646	0.091854
26	1	0	-6.162874	-1.072699	-0.085108

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    27          1           0       -4.255466     2.774659     0.254711
    28          1           0       -6.328731     1.401174     0.138012
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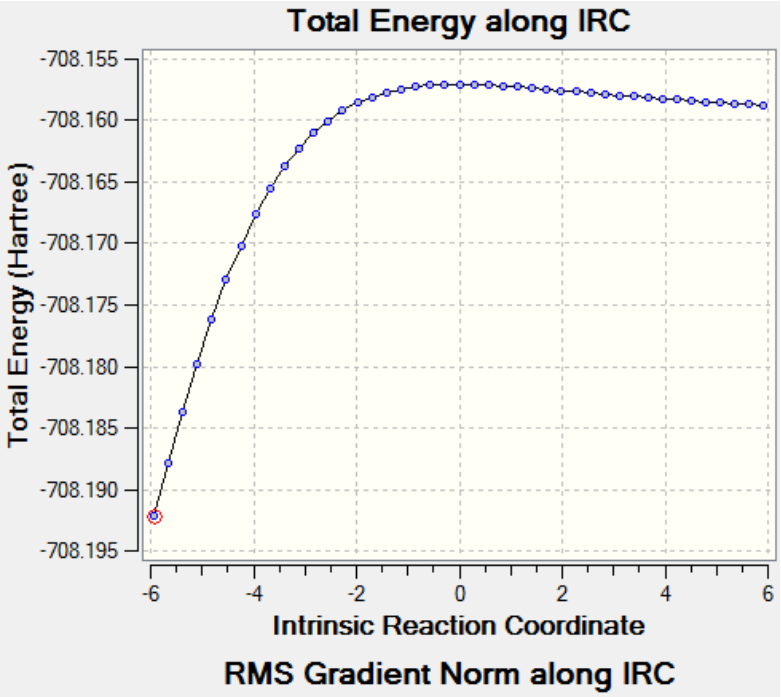
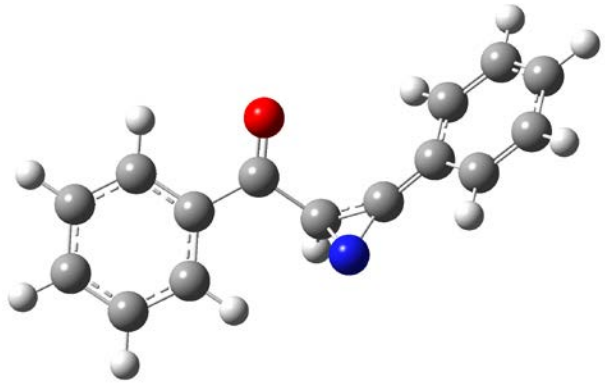


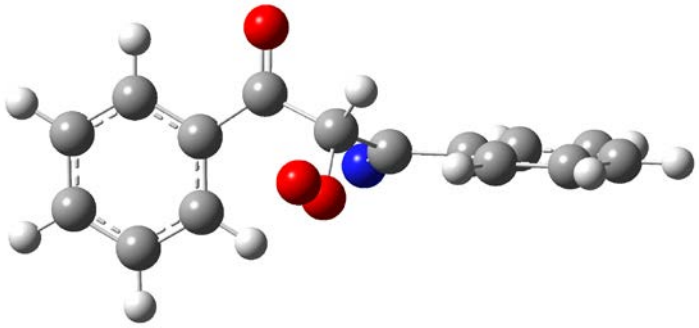
3.12 Optimized T_A of 2



UB3LYP/6-31+G(d) E: -708.06188864 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.122146	-0.541228	0.782347
2	1	0	0.508234	-0.808369	1.773658
3	7	0	-0.314400	-1.696580	-0.049601
4	6	0	-1.247527	-0.731103	0.430387
5	6	0	-2.529941	-0.318273	0.182918
6	6	0	-3.412576	-1.126797	-0.632590
7	6	0	-3.061285	0.905024	0.744187
8	6	0	-4.717053	-0.734024	-0.849635
9	1	0	-3.021825	-2.043028	-1.064759
10	6	0	-4.368060	1.268977	0.508411
11	1	0	-2.404619	1.530195	1.341524
12	6	0	-5.215983	0.459835	-0.285504
13	1	0	-5.368519	-1.350070	-1.464700
14	1	0	-4.753259	2.193093	0.932310
15	1	0	-6.244917	0.759109	-0.462428
16	6	0	1.001681	0.524639	0.089036
17	6	0	2.463818	0.252220	0.005650
18	6	0	2.999047	-1.015464	0.288782
19	6	0	3.321054	1.298353	-0.379443
20	6	0	4.374939	-1.229824	0.193552
21	1	0	2.342825	-1.838405	0.553327
22	6	0	4.693925	1.081542	-0.466212
23	1	0	2.892790	2.270644	-0.602682
24	6	0	5.222914	-0.182672	-0.178652
25	1	0	4.783456	-2.214436	0.404215
26	1	0	5.353436	1.894520	-0.758100
27	1	0	6.294543	-0.351201	-0.248660
28	8	0	0.492006	1.545847	-0.331988

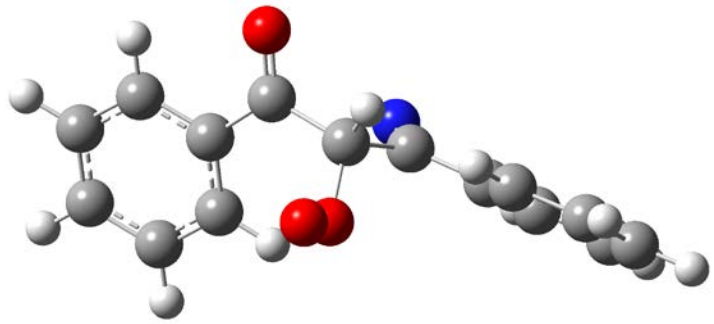
3.13 Optimized 6A



UB3LYP/6-31+G(d) E : -858.46742551 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.212926	0.265349	1.120036
2	6	0	-0.125351	0.648351	0.432294
3	6	0	-0.997993	-0.559245	0.044276
4	1	0	-0.655912	1.281905	1.145223
5	7	0	-0.424732	-1.655978	-0.203740
6	6	0	-2.482830	-0.397438	-0.023324
7	6	0	-3.077829	0.862549	-0.193604
8	6	0	-3.299721	-1.538132	0.073202
9	6	0	-4.467832	0.977122	-0.268415
10	1	0	-2.468350	1.755360	-0.287783
11	6	0	-4.685617	-1.417126	0.000649
12	1	0	-2.840249	-2.511224	0.218034
13	6	0	-5.273950	-0.159161	-0.170883
14	1	0	-4.917563	1.956879	-0.404435
15	1	0	-5.307996	-2.303978	0.084463
16	1	0	-6.355401	-0.065899	-0.224226
17	6	0	2.446714	-0.047939	0.351664
18	6	0	2.460093	-0.289715	-1.032665
19	6	0	3.650770	-0.127934	1.077008
20	6	0	3.656184	-0.611427	-1.675357
21	1	0	1.545670	-0.243643	-1.611563
22	6	0	4.843057	-0.437596	0.430008
23	1	0	3.627713	0.055848	2.146413
24	6	0	4.847464	-0.681459	-0.948931
25	1	0	3.655846	-0.806306	-2.744183
26	1	0	5.768706	-0.491400	0.996719
27	1	0	5.778246	-0.925941	-1.454528
28	8	0	1.180047	0.251661	2.340266
29	8	0	0.047107	1.434630	-0.793059
30	8	0	0.386084	2.685340	-0.513920

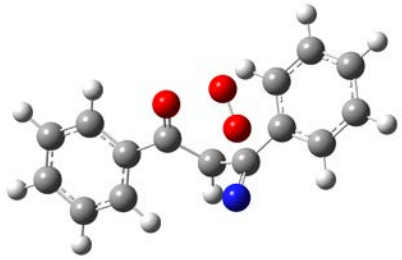
3.14 Optimized 6B



UB3LYP/6-31+G(d) E: -858.46729344 a.u.

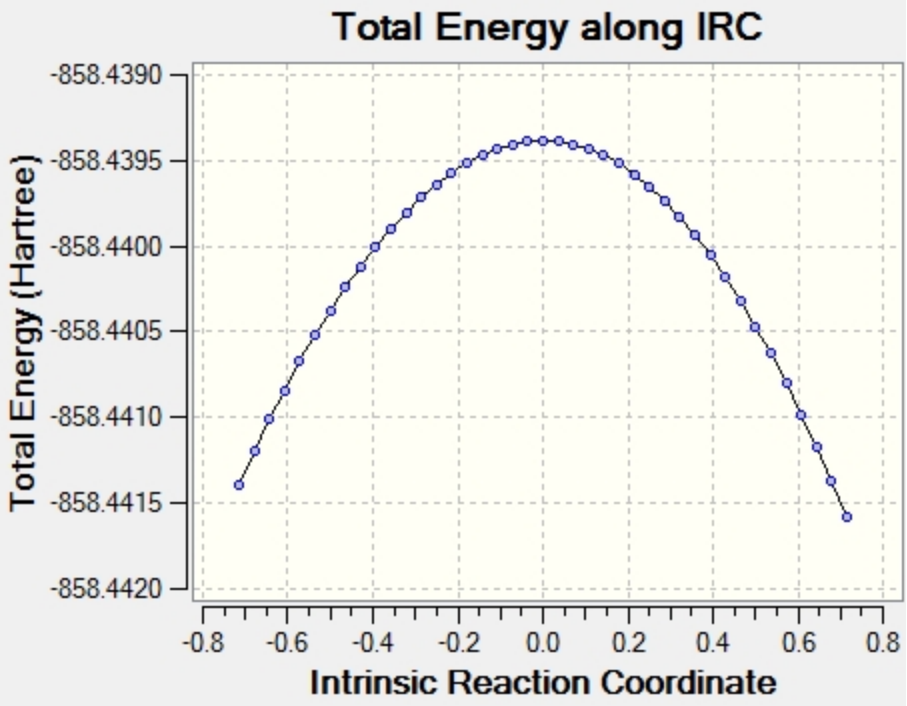
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.348587	1.006810	-0.773813
2	6	0	0.093557	0.956572	-0.201221
3	6	0	0.946987	-0.209243	-0.723180
4	1	0	0.551800	1.909572	-0.473665
5	7	0	0.402053	-1.055488	-1.485213
6	6	0	2.390983	-0.288830	-0.340587
7	6	0	3.099129	0.834575	0.113268
8	6	0	3.060710	-1.519452	-0.464155
9	6	0	4.455570	0.730035	0.428738
10	1	0	2.607180	1.795378	0.224388
11	6	0	4.413366	-1.618755	-0.146779
12	1	0	2.511188	-2.392423	-0.803399
13	6	0	5.115649	-0.493715	0.299507
14	1	0	4.992836	1.607301	0.778467
15	1	0	4.919696	-2.575428	-0.243275
16	1	0	6.170246	-0.573011	0.549670
17	6	0	-2.441299	0.157034	-0.229691
18	6	0	-2.228173	-0.888382	0.685040
19	6	0	-3.747550	0.418921	-0.683765
20	6	0	-3.302778	-1.657588	1.132700
21	1	0	-1.232164	-1.113564	1.047522
22	6	0	-4.817740	-0.345546	-0.229189
23	1	0	-3.899589	1.226102	-1.393153
24	6	0	-4.596690	-1.387199	0.680033
25	1	0	-3.128244	-2.467722	1.835319
26	1	0	-5.823407	-0.133293	-0.581913
27	1	0	-5.431935	-1.986104	1.034155
28	8	0	-1.525824	1.799851	-1.684166
29	8	0	0.118917	0.873912	1.261501
30	8	0	-0.044440	2.066260	1.815284

3.15 TS for forming 6 from 4 and O_2

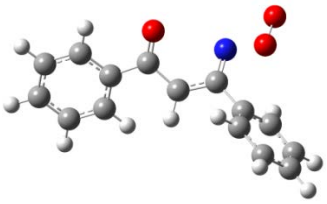


UB3LYP/6-31+G(d) E: -858.43938394 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.006832	-0.009822	-0.506997
2	6	0	-0.105024	0.768215	0.390571
3	6	0	1.236495	1.207992	-0.119937
4	1	0	-0.542196	1.450847	1.107532
5	7	0	0.997907	2.357527	-0.579518
6	6	0	2.535404	0.495537	-0.124361
7	6	0	2.614668	-0.899704	-0.248818
8	6	0	3.713869	1.257194	-0.038444
9	6	0	3.863564	-1.522202	-0.283018
10	1	0	1.708622	-1.485329	-0.349971
11	6	0	4.957158	0.627538	-0.067243
12	1	0	3.645817	2.336830	0.061512
13	6	0	5.034091	-0.763990	-0.189142
14	1	0	3.920390	-2.602550	-0.385827
15	1	0	5.864568	1.220875	0.007986
16	1	0	6.003598	-1.255099	-0.210460
17	6	0	-2.482667	0.038462	-0.293007
18	6	0	-3.121534	1.059031	0.432519
19	6	0	-3.261555	-0.978148	-0.875395
20	6	0	-4.510095	1.059322	0.575194
21	1	0	-2.550647	1.872906	0.868093
22	6	0	-4.645318	-0.981043	-0.723498
23	1	0	-2.759524	-1.757382	-1.439840
24	6	0	-5.272987	0.038326	0.002806
25	1	0	-4.994618	1.858186	1.129900
26	1	0	-5.237215	-1.775457	-1.170170
27	1	0	-6.353739	0.037584	0.118988
28	8	0	-0.501248	-0.749006	-1.349351
29	8	0	0.145842	-0.573759	1.860389
30	8	0	-0.017823	-1.775277	1.580402



3.16 Optimized 7

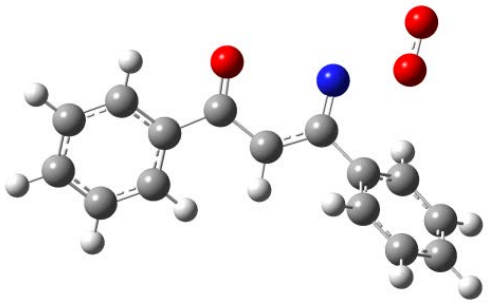


UB3LYP/6-31+G(d) E: -858.44109846 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.499804	0.643283	0.501034
2	6	0	-0.258491	-0.068003	0.142673
3	6	0	1.046442	0.519870	0.012493
4	1	0	-0.306868	-1.145885	0.020151
5	6	0	2.226778	-0.398381	0.067064
6	6	0	2.367072	-1.270413	1.157793
7	6	0	3.167710	-0.443361	-0.974188
8	6	0	3.439453	-2.162974	1.214734

9	1	0	1.646406	-1.235885	1.971137
10	6	0	4.229469	-1.346903	-0.921105
11	1	0	3.064312	0.222017	-1.825724
12	6	0	4.370754	-2.204870	0.173900
13	1	0	3.545628	-2.823749	2.070910
14	1	0	4.949231	-1.377517	-1.734641
15	1	0	5.202841	-2.902768	0.215152
16	6	0	-2.806489	0.015036	0.117893
17	6	0	-2.908273	-0.984927	-0.863544
18	6	0	-3.974366	0.474883	0.749692
19	6	0	-4.153286	-1.518702	-1.202524
20	1	0	-2.022826	-1.335431	-1.386652
21	6	0	-5.214926	-0.064952	0.417651
22	1	0	-3.886428	1.257402	1.496916
23	6	0	-5.307247	-1.063861	-0.558964
24	1	0	-4.221803	-2.284807	-1.970286
25	1	0	-6.111683	0.292440	0.916967
26	1	0	-6.275901	-1.482577	-0.819726
27	8	0	-1.464924	1.688944	1.151346
28	7	0	1.086233	1.815867	-0.194372
29	8	0	2.480550	2.254496	-0.204786
30	8	0	2.542457	3.475479	-0.671710

3.17 TS for 4 and O_2 forming 7



UB3LYP/6-31+G(d) E : - 858.42313129 a.u.

Imaginary frequency: - 346 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.545186	0.805479	0.084607
2	6	0	-0.332757	-0.016078	-0.019382

3	6	0	1.002241	0.500254	-0.113329
4	1	0	-0.424060	-1.097064	-0.004246
5	6	0	2.128353	-0.490893	-0.008393
6	6	0	2.189743	-1.374681	1.078890
7	6	0	3.108701	-0.558264	-1.008999
8	6	0	3.221959	-2.311429	1.166362
9	1	0	1.441423	-1.317447	1.865586
10	6	0	4.133457	-1.502266	-0.923368
11	1	0	3.061240	0.123518	-1.852972
12	6	0	4.193724	-2.378794	0.164053
13	1	0	3.267398	-2.985140	2.017969
14	1	0	4.886179	-1.550641	-1.705760
15	1	0	4.995080	-3.109954	0.230613
16	6	0	-2.881806	0.126031	-0.009690
17	6	0	-3.057952	-1.167973	-0.529440
18	6	0	-4.009439	0.843346	0.426439
19	6	0	-4.332929	-1.732483	-0.606133
20	1	0	-2.211313	-1.737266	-0.901060
21	6	0	-5.279473	0.275367	0.359164
22	1	0	-3.866010	1.846628	0.814995
23	6	0	-5.444704	-1.015239	-0.157163
24	1	0	-4.456731	-2.730072	-1.019160
25	1	0	-6.142296	0.837256	0.707070
26	1	0	-6.436044	-1.457739	-0.212131
27	8	0	-1.473540	2.022398	0.272685
28	7	0	1.193364	1.771217	-0.334403
29	8	0	3.075392	2.180990	0.107154
30	8	0	3.269149	3.392255	-0.007562

IRC Calculation