Supporting Information for

Early events in the photochemistry of 5-diazo Meldrum's acid: formation of a product manifold at C-N bound and pre-dissociated intersection seam regions

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Table SI1. Absolute energies of the critical points

Structure	State	CASSCF (Hartree)	CASPT2 (Hartree)	MS-CASPT2 (Hartree)	Active space CASSCF/CASPT2
DMA-S_0	S_0	-639.31861	-640.98832	-640.99173	(10,9)/(12,11)
	S_1	-639.17615	-640.85526	-640.85526	
	S_2	-639.08796	-640.80558	-640.80217	
	T_1	-639.18025	-640.85952	-640.85952	
	T_2	-639.16370	-640.84606	-640.84614	
	T_3	-639.07734	-640.76139	-640.76131	
DMA-S_1	S_0	-639.29092	-640.95521	-640.95619	(10,9)/(12,11)
	S_1	-639.24071	-640.91337	-640.91337	
	S_2	-639.10044	-640.80576	-640.80478	
	T_1	-639.24255	-640.92680	-640.92732	
	T_2	-639.15775	-640.84588	-640.84588	
	T_3	-639.06064	-640.76732	-640.76680	
DMA-T_1	T_1	-639.25365	-640.92394	-640.92401	(10,9)/(12,11)
	T_2	-639.16471	-640.84483	-640.84483	
	T_3	-639.08837	-640.76843	-640.76836	
$(S_2/S_1)_X$	S_0	-639.27058	-640.94870	-640.95652	(10,9)/(12,11)
	S_1	-639.18191	-640.87853	-640.87071	
	S_2	-639.17126	-640.84814	-640.84814	
	T_1	-639.24001	-640.91480	-640.91492	
	T_2	-639.16915	-640.85073	-640.85073	
	T_3	-639.08000	-640.76652	-640.76639	
$(S_1/S_0)_X$	S_0	-639.23434	-640.91669	-640.92271	(10,9)/(12,11)
	S_1	-639.22909	-640.90102	-640.90097	
	S_2	-639.09976	-640.80455	-640.79858	
	T_1	-639.23749	-640.91251	-640.91252	
	T_2	-639.14096	-640.82318	-640.82327	
	T_3	-639.11740	-640.82067	-640.82057	
$(S_1/S_0)_X$-D90	S_0	-639.22214	-640.89673	-640.90716	(10,9)/(12,11)
	S_1	-639.20775	-640.90215	-640.89284	
	S_2	-639.12844	-640.81264	-640.81152	
$(S_1/T_2)_X$	S_0	-639.30726	-640.97799	-640.98230	(10,9)/(12,11)
	S_1	-639.20102	-640.87542	-640.87577	
	S_2	-639.12540	-640.83840	-640.83374	
	T_1	-639.22414	-640.89136	-640.89146	
	T_2	-639.20603	-640.87388	-640.87381	
	T_3	-639.07245	-640.76196	-640.76193	
$(T_2/T_1)_X$	S_0	-639.30875	-640.97884	-640.98264	(10,9)/(12,11)
	S_1	-639.19799	-640.87253	-640.87253	
	S_2	-639.12039	-640.83751	-640.83371	
	T_1	-639.21479	-640.88474	-640.88477	

	T_2	-639.21279	-640.87882	-640.87882	
	T_3	-639.07449	-640.76275	-640.76273	
TS-T_1	T_1	-639.24801	-640.91111	-640.91119	(10,9)/(12,11)
	T_2	-639.09521	-640.76931	-640.76933	
	T_3	-639.04712	-640.72457	-640.72447	
Diazirine-S_0	S_0	-639.28426	-640.96464	-640.96402	(12,11)/(12,11)
	S_1	-639.10181	-640.79699	-640.79867	
	S_2	-638.96452	-640.68126	-640.68536	
TS-iso-S_0	S_0	-639.23813	-640.91054	-640.91057	(12,11)/(12,11)
	S_1	-639.18350	-640.88067	-640.88092	
	S_2	-639.15589	-640.83649	-640.83622	
Carbene-boatlike	S_0	-530.21607	-531.65087	-531.65155	(10,8)/(10,8)
	S_1	-530.14665	-531.59895	-531.59886	
	S_2	-530.11332	-531.57681	-531.57623	
	T_1	-530.21825	-531.65586	-531.65608	
	T_2	-530.13171	-531.58577	-531.58598	
	T_3	-530.06001	-531.51323	-531.51280	
Carbene-chairlike	S_0	-530.21388	-531.64764	-531.64878	(10,8)/(10,8)
	S_1	-530.14109	-531.58959	-531.58891	
	S_2	-530.09990	-531.55935	-531.55890	
	T_1	-530.21259	-531.64426	-531.64444	
	T_2	-530.11791	-531.56841	-531.56897	
	T_3	-530.04256	-531.48446	-531.48373	
Carbene-planar	S_0	-530.18959	-531.63285	-531.63286	(10,8)/(10,8)
	S_1	-530.18265	-531.61311	-531.61334	
	S_2	-530.14138	-531.58349	-531.58326	
	T_1	-530.23995	-531.67244	-531.67297	
	T_2	-530.15227	-531.58527	-531.58527	
	T_3	-530.08179	-531.52051	-531.51997	
Carbene-$(S_0/T_1)_X$	S_0	-530.21554	-531.65185	-531.65235	(10,8)/(10,8)
	S_1	-530.13548	-531.59024	-531.59065	
	S_2	-530.10648	-531.57922	-531.57831	
	T_1	-530.20871	-531.64800	-531.64814	
	T_2	-530.12576	-531.58690	-531.58753	
	T_3	-530.05273	-531.51256	-531.51179	
Carbene-triplet	T_1	-530.23463	-531.67284	-531.67284	(10,8)/(10,8)
	T_2	-530.14725	-531.58296	-531.58297	
	T_3	-530.09308	-531.54469	-531.54467	
Ketene-S_0	S_0	-530.31145	-531.74106	-531.74130	(10,8)/(10,8)
	S_1	-530.20793	-531.64811	-531.64798	
	S_2	-530.09463	-531.54644	-531.54634	
TS-CK-S_0	S_0	-530.20614	-531.67322	-531.67341	(10,8)/(10,8)
	S_1	-530.01577	-531.52154	-531.52154	
	S_2	-529.95553	-531.45657	-531.45638	

Table SI2. Relative energies of the critical points

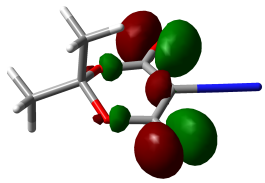
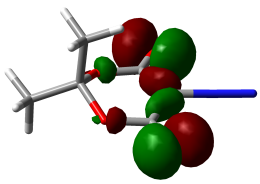
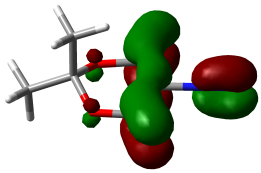
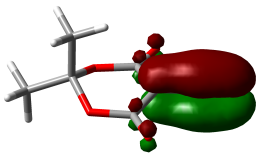
Structure	State	CASSAF (eV)	CASPT2 (eV)	MS-CASPT2 (eV)	Active space CASSCF/CASPT2
DMA-S_0	S_0	0.00	0.00	0.00	(10,9)/(12,11)
	S_1	3.88	3.62	3.71	
	S_2	6.28	4.97	5.16	
	T_1	3.76	3.50	3.60	
	T_2	4.22	3.87	3.96	
	T_3	6.56	6.17	6.27	
DMA-S_1	S_0	0.75	0.90	0.97	(10,9)/(12,11)
	S_1	2.12	2.04	2.13	
	S_2	5.94	4.97	5.09	
	T_1	2.07	1.67	1.75	
	T_2	4.38	3.88	3.97	
	T_3	7.02	6.01	6.12	
DMA-T_1	T_1	1.77	1.75	1.84	(10,9)/(12,11)
	T_2	4.19	3.90	4.00	
	T_3	6.26	5.98	6.08	
$(S_2/S_1)_X$	S_0	1.31	1.08	0.96	(10,9)/(12,11)
	S_1	3.72	2.99	3.29	
	S_2	4.01	3.81	3.91	
	T_1	2.14	2.00	2.09	
	T_2	4.07	3.74	3.84	
	T_3	6.49	6.04	6.13	
$(S_1/S_0)_X$	S_0	2.29	1.95	1.88	(10,9)/(12,11)
	S_1	2.44	2.38	2.47	
	S_2	5.95	5.00	5.26	
	T_1	2.21	2.06	2.16	
	T_2	4.83	4.49	4.58	
	T_3	5.48	4.56	4.66	
$(S_1/S_0)_X$-D90	S_0	2.62	2.49	2.30	(10,9)/(12,11)
	S_1	3.02	2.34	2.69	
	S_2	5.17	4.78	4.90	
$(S_1/T_2)_X$	S_0	0.31	0.28	0.26	(10,9)/(12,11)
	S_1	3.20	3.07	3.16	
	S_2	5.26	4.08	4.30	
	T_1	2.57	2.64	2.73	
	T_2	3.06	3.11	3.21	
	T_3	6.70	6.16	6.25	
$(T_2/T_1)_X$	S_0	0.27	0.26	0.25	(10,9)/(12,11)
	S_1	3.28	3.15	3.24	
	S_2	5.39	4.10	4.30	
	T_1	2.82	2.82	2.91	

	T_2	2.88	2.98	3.07	
	T_3	6.64	6.14	6.23	
TS-T_1	T_1	1.92	2.10	2.19	(10,9)/(12,11)
	T_2	6.08	5.96	6.05	
	T_3	7.39	7.18	7.27	
Diazirine-S_0	S_0	0.93	0.64	0.75	(12,11)/(12,11)
	S_1	5.90	5.21	5.25	
	S_2	9.63	8.36	8.34	
TS-iso-S_0	S_0	2.19	2.12	2.21	(12,11)/(12,11)
	S_1	3.68	2.93	3.02	
	S_2	4.43	4.13	4.23	
Carbene-boatlike	S_0	0.00	0.00	0.00	(10,8)/(10,8)
	S_1	1.89	1.41	1.43	
	S_2	2.80	2.02	2.05	
	T_1	-0.06	-0.14	-0.12	
	T_2	2.30	1.77	1.78	
	T_3	4.25	3.75	3.78	
Carbene-chairlike	S_0	0.06	0.09	0.08	(10,8)/(10,8)
	S_1	2.04	1.67	1.70	
	S_2	3.16	2.49	2.52	
	T_1	0.09	0.18	0.19	
	T_2	2.67	2.24	2.25	
	T_3	4.72	4.53	4.57	
Carbene-planar	S_0	0.72	0.49	0.51	(10,8)/(10,8)
	S_1	0.91	1.03	1.04	
	S_2	2.03	1.83	1.86	
	T_1	-0.65	-0.59	-0.58	
	T_2	1.74	1.79	1.80	
	T_3	3.65	3.55	3.58	
Carbene-$(S_0/T_1)_X$	S_0	0.01	-0.03	-0.02	(10,8)/(10,8)
	S_1	2.19	1.65	1.66	
	S_2	2.98	1.95	1.99	
	T_1	0.20	0.08	0.09	
	T_2	2.46	1.74	1.74	
	T_3	4.44	3.76	3.80	
Carbene-triplet	T_1	-0.51	-0.60	-0.58	(10,8)/(10,8)
	T_2	1.87	1.85	1.87	
	T_3	3.35	2.89	2.91	
Ketene-S_0	S_0	-2.38	-2.43	-2.43	(10,8)/(10,8)
	S_1	0.44	0.10	0.11	
	S_2	3.52	2.86	2.87	
TS-CK-S_0	S_0	0.48	-0.59	-0.59	(10,8)/(10,8)
	S_1	5.66	3.54	3.55	
	S_2	7.30	5.31	5.32	

Table SI3. The singlet-triplet energy gaps at MS-CASPT2 level and the corresponding SOC values at carbene geometries.

Structure	Energy gap(eV)[a]	SOC(cm^{-1})
Carbene-boatlike	0.12	6.3
Carbene-chairlike	-0.11	6.6
Carbene-planar	1.09	0.0

[a] $E(S_0)$- $E(T_1)$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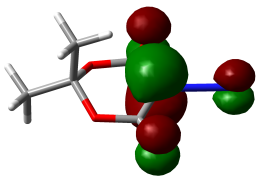	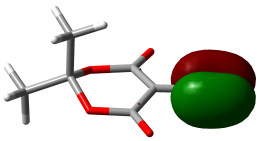	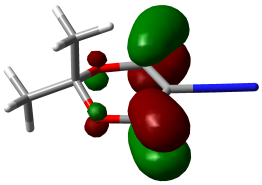	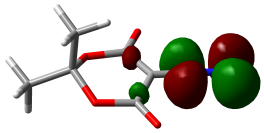
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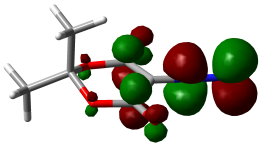	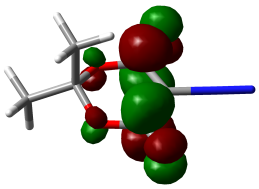	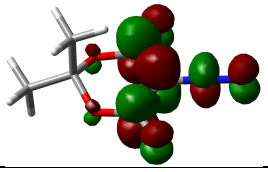	
9	**10**	**11**	

Figure SI1. Active space of the MS-CASPT2/CASSCF(14,11) calculation at the FC geometry of DMA for calculation of the $\mathbf{n_O\pi^*_{NN}}$ state.

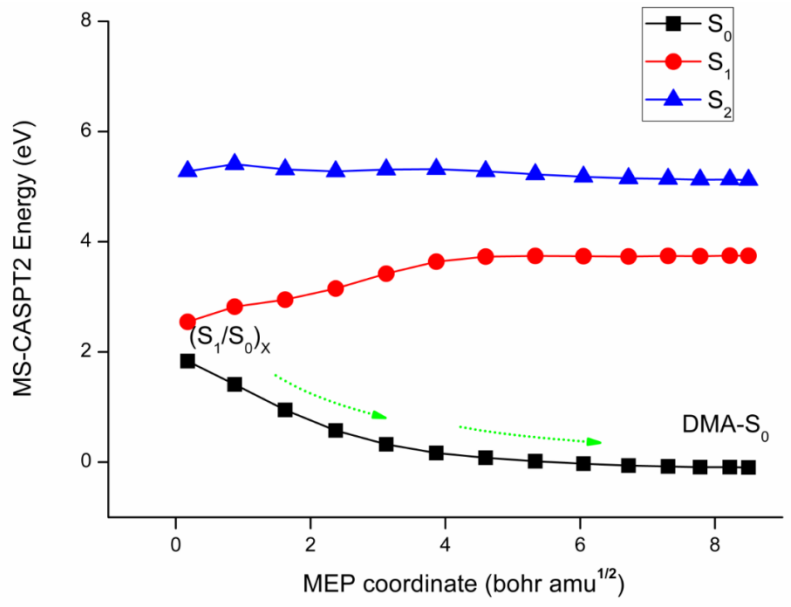

Figure SI2. MS-CASPT2 energy profile for the MEP from $(S_1/S_0)_X$ to DMA-S_0

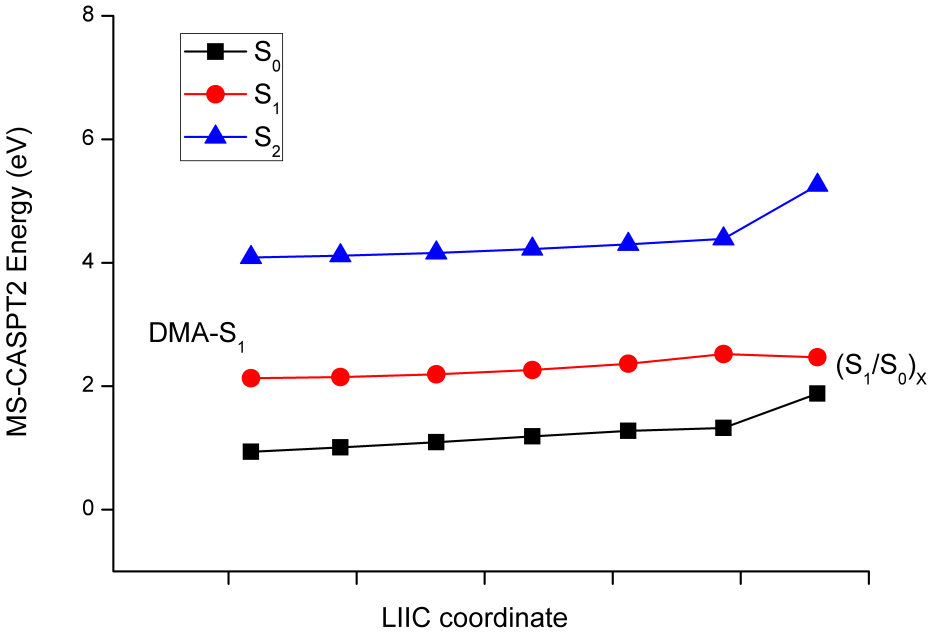

Figure SI3. MS-CASPT2 energy profile for LIIC between DMA-S_1 and $(S_1/S_0)_X$.

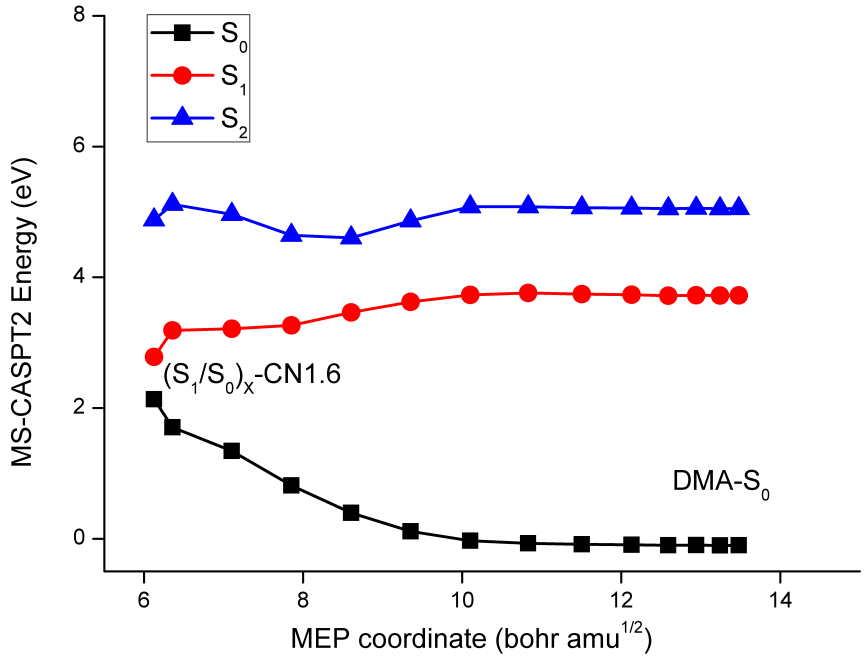

Figure SI4. MS-CASPT2 energy profile for the MEP from $(S_1/S_0)_X$ to DMA-S_0.

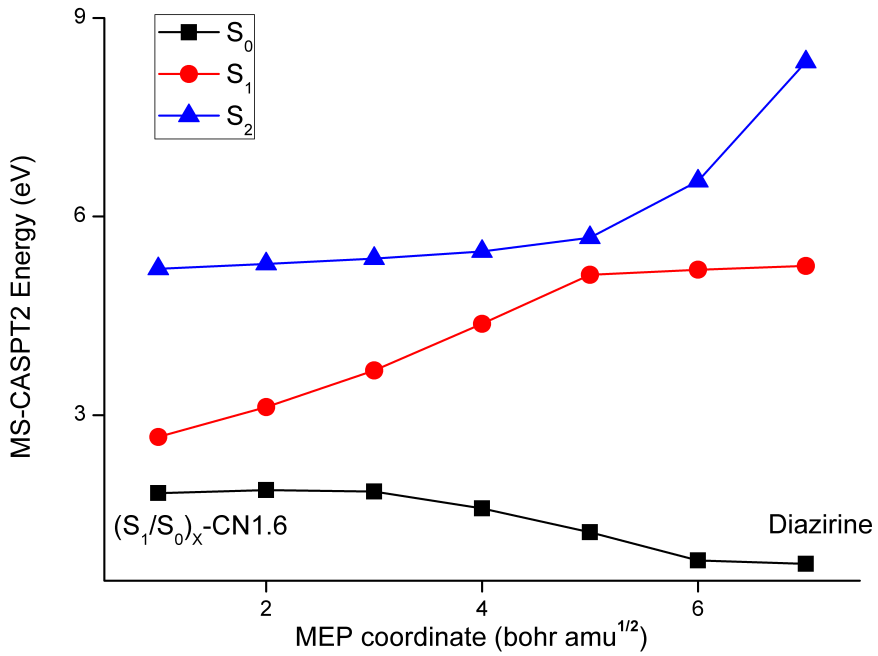

Figure SI5. MS-CASPT2 energy profile for the MEP from $(S_1/S_0)_X$ to diazirine.

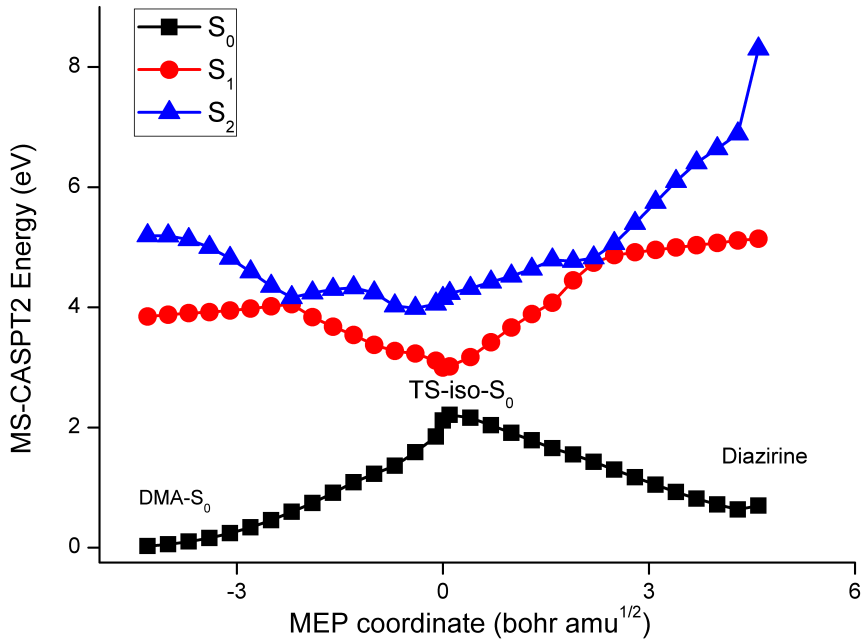

Figure SI6. MS-CASPT2 energy profiles along the MEPs for DMA-S_0 to diazirine transformation through TS-iso-S_0.

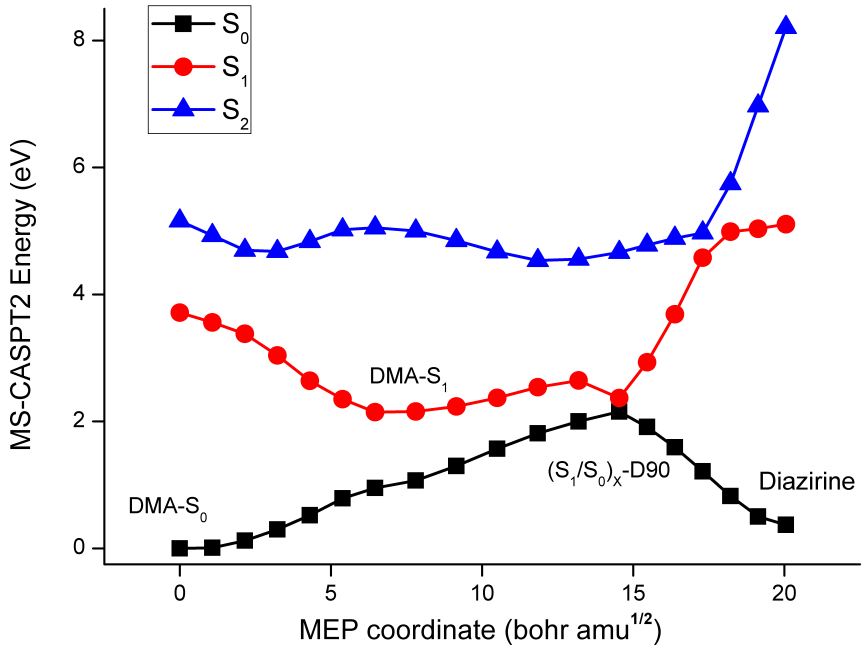

Figure SI7. MS-CASPT2 energy profile along MEP from FC to DMA-S_1, LIIC from DMA-S_1 to $(S_1/S_0)_X$-D90 and MEP from $(S_1/S_0)_X$-D90 to diazirine.

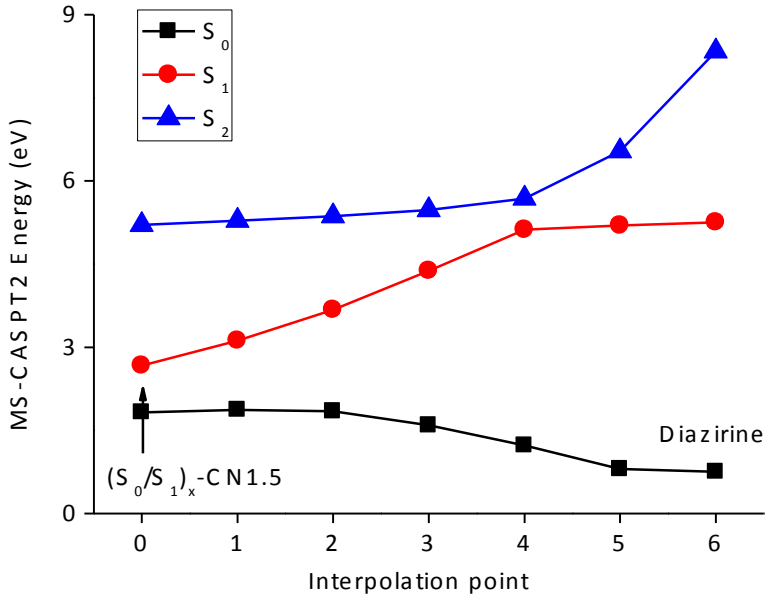

Figure SI8. MS-CASPT2 energy profile along LIIC from $(S_1/S_0)_X$-CN1.5 to diazirine.

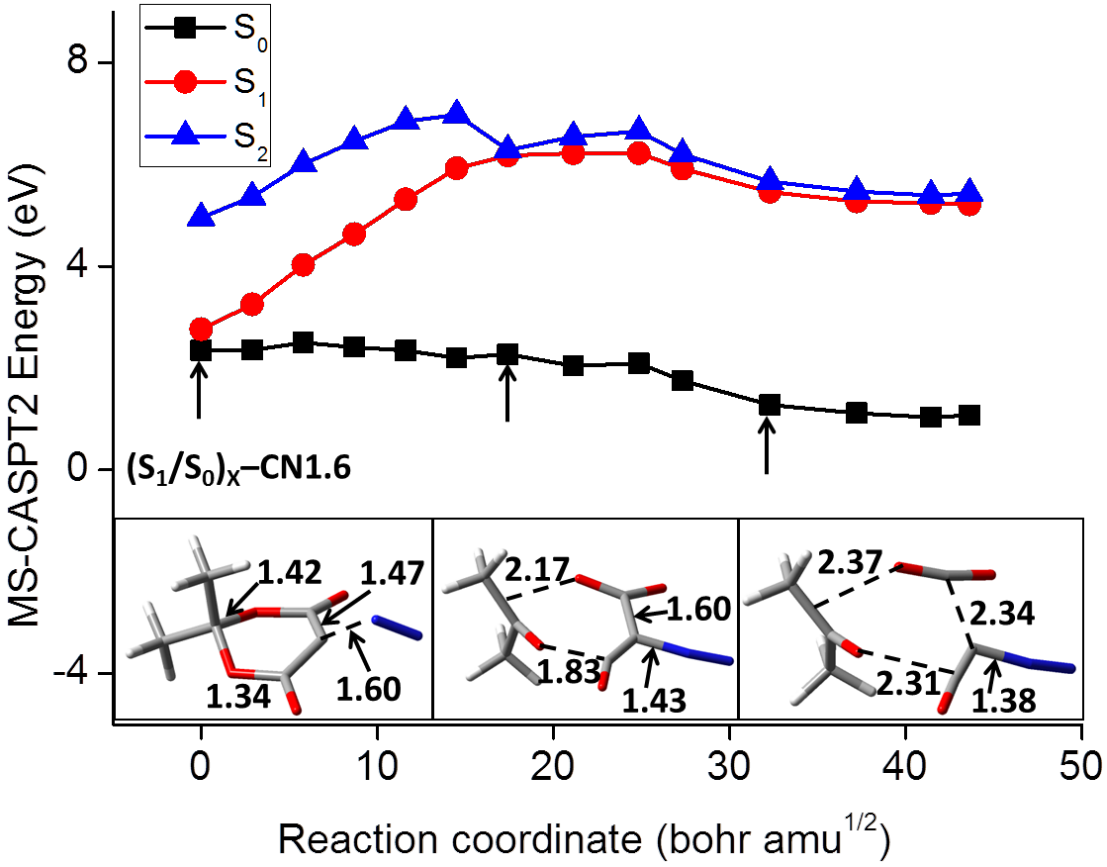

Figure SI9. MS-CASPT2 energy profile along decay path from $(S_1/S_0)_X$-CN1.6 leading to acetone formation.

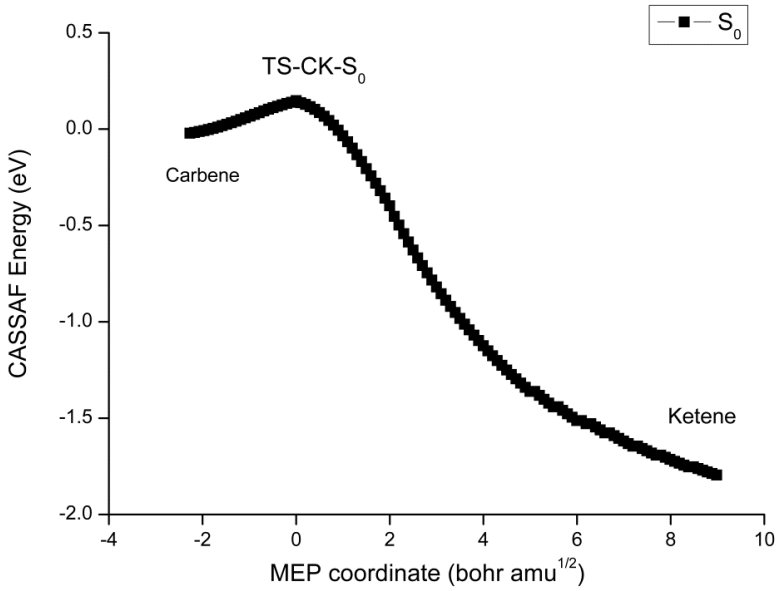

Figure SI10. CASSCF energy profile of the ground state MEP from carbene to ketene through TS-CK-S_0.

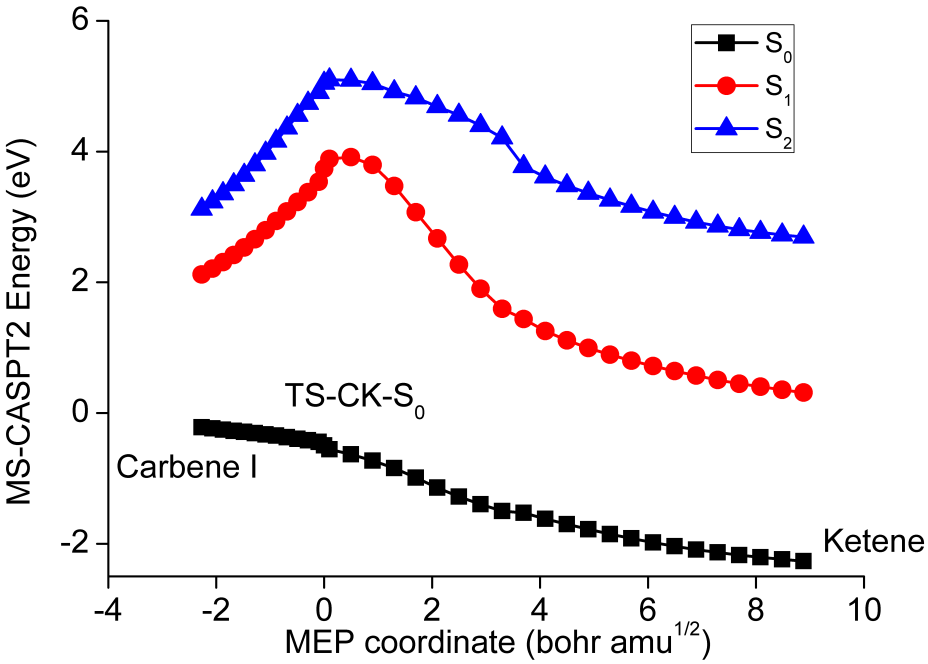

Figure SI11. MS-CASPT2 energy profile along the ground state MEP from carbene I to ketene through TS-CK-S_0.

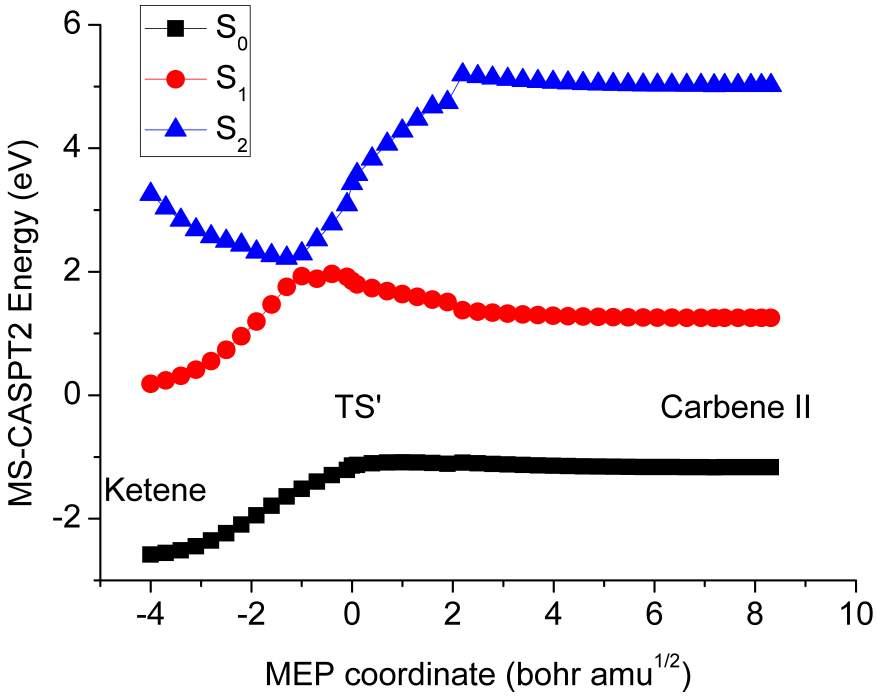

Figure SI12. MS-CASPT2 energy profile along the ground state MEP from the ketene to carbene I through TS'.

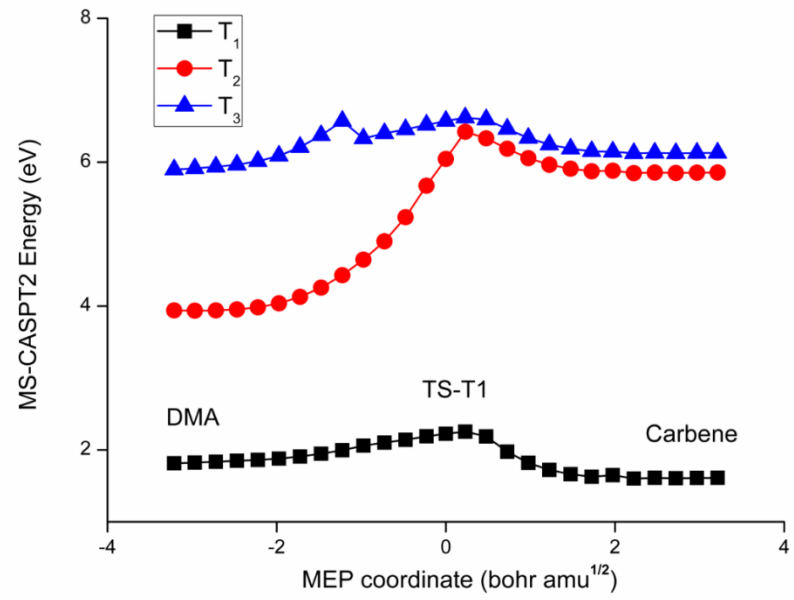

Figure SI13. MS-CASPT2 energy profile for the C-N cleavage reaction on T_1 state.

Cartesian coordinates of optimized structures

DMA-S_0

6	0.397357	-1.282465	-0.189811
6	1.059232	0.000090	-0.034318
6	0.397158	1.282571	-0.189528
6	-1.604779	-0.000113	0.073714
6	-2.934667	-0.000203	-0.645649
6	-1.749025	-0.000168	1.588713
8	0.943198	2.342531	-0.208103
8	0.943598	-2.342320	-0.208651
7	2.385987	0.000158	0.096951
7	3.492594	0.000171	0.218569
8	-0.928597	1.167226	-0.353516
8	-0.928433	-1.167351	-0.353575
1	-0.783481	-0.000068	2.080623
1	-2.292240	0.882750	1.901458
1	-2.292038	-0.883221	1.901424
1	-2.764257	-0.000067	-1.714070
1	-3.498368	-0.884109	-0.375750
1	-3.498595	0.883500	-0.375559

DMA-S_1

6	0.714045	-0.040270	-1.544381
6	1.112809	-0.126827	-0.120132
6	0.086510	0.004668	0.956124
8	-1.166524	-0.021401	0.507309
6	-1.480531	-0.564494	-0.762796
8	-0.608528	-0.035376	-1.738995
6	-1.392699	-2.083332	-0.722969
6	-2.861105	-0.062067	-1.115482
8	0.347080	0.165222	2.092802
8	1.489739	0.080177	-2.465260
7	2.449715	-0.303541	0.292726
7	3.365738	-0.391238	-0.449621
1	-0.397877	-2.429511	-0.464419
1	-2.085052	-2.465358	0.016742
1	-1.650339	-2.487218	-1.694078
1	-2.859689	1.019636	-1.128090
1	-3.141235	-0.428190	-2.095087
1	-3.578032	-0.409713	-0.383005

DMA-T_1

6	-0.23299300	1.38591900	-0.21737700
6	-1.10943900	0.20415000	-0.08785500
6	-0.55423400	-1.15734900	-0.25520800
6	1.57976000	-0.13178100	0.08328700
6	2.93203600	-0.30250000	-0.56923100
6	1.64549300	-0.15894900	1.60355000
8	-1.21070100	-2.15248900	-0.31367500
8	-0.63480100	2.50755300	-0.23436300
7	-2.46948100	0.44590100	0.18248600
7	-3.28888600	-0.39796300	0.30768400
8	0.77491300	-1.18958300	-0.40084500
8	1.06675800	1.10407800	-0.36745800
1	0.66820600	-0.03336300	2.05692500
1	2.05249800	-1.10606900	1.93470700
1	2.28391800	0.64389100	1.95077200
1	2.81843700	-0.27780300	-1.64472400
1	3.59263800	0.49810600	-0.26228900
1	3.35978700	-1.25373600	-0.27886000

$(S_1/S_2)_X$

6	0.394532	-1.274643	-0.265739
6	1.074413	-0.001346	-0.181726
6	0.394204	1.272705	-0.263283
6	-1.606222	-0.000283	0.084070
6	-2.953629	-0.000470	-0.602549
6	-1.708786	0.001481	1.601531
8	0.944711	2.336523	-0.296593
8	0.943896	-2.339028	-0.302477
7	2.512196	0.000373	-0.167612
7	3.277935	0.000237	0.710851
8	-0.940773	1.167213	-0.359979
8	-0.940954	-1.168785	-0.357996
1	-0.730660	0.001076	2.069166
1	-2.241741	0.885697	1.928077
1	-2.243773	-0.880542	1.930613
1	-2.809084	-0.002377	-1.674852
1	-3.511635	-0.883323	-0.317793
1	-3.509981	0.884405	-0.320787

$(S_1/S_0)_X$

6	0.418975	-1.398400	0.131976
6	1.123412	-0.163788	-0.234575
6	0.532585	1.171083	0.016932
6	-1.496135	0.002528	0.573063
6	-2.240731	0.115804	-0.747643
6	-2.411476	0.031429	1.779540
8	1.058438	2.220240	-0.192258
8	0.885832	-2.493925	0.009834
7	2.424428	-0.366218	-0.837250
7	2.654112	0.457068	-1.634448
8	-0.619856	1.102367	0.701852
8	-0.805995	-1.228449	0.647160
1	-1.823805	-0.080512	2.681417
1	-2.951818	0.969037	1.818440
1	-3.117368	-0.788158	1.717778
1	-1.559743	0.113033	-1.592128
1	-2.930223	-0.711511	-0.862466
1	-2.795984	1.047283	-0.764302

$(S_1/S_0)_X$-D90

6	0.540917	1.234842	0.157058
6	1.012162	-0.043076	-0.314713
6	0.423771	-1.314752	0.029427
6	-1.488992	0.02555	0.591012
6	-2.213935	0.104664	-0.744305
6	-2.429289	0.018718	1.775742
8	-0.750214	-1.180723	0.671381
8	-0.656523	1.159157	0.762842
7	2.466907	-0.079215	-0.721052
7	2.549842	-0.232495	-1.855701
8	0.909323	-2.387274	-0.175101
8	1.131256	2.269727	0.057453
1	-1.519105	0.106473	-1.575808
1	-2.871495	-0.749241	-0.84987
1	-2.800058	1.014087	-0.786269
1	-1.853156	-0.036295	2.689999
1	-3.018431	0.926989	1.782076
1	-3.088329	-0.838222	1.71875

$(S_1/T_2)x$

6	0.381735	-1.291129	0.010984
6	1.021710	-0.020743	-0.369219
6	0.478076	1.260883	0.109124
6	-1.498541	0.024842	0.632204
6	-2.210122	0.060057	-0.712849
6	-2.450742	0.028675	1.805470
8	1.024863	2.308761	-0.055647
8	0.835220	-2.361355	-0.257973
7	2.117038	-0.037533	-1.177647
7	3.253234	-0.276380	-1.444960
8	-0.673303	1.163692	0.786442
8	-0.726611	-1.153352	0.750664
1	-1.885158	0.007486	2.727354
1	-3.058764	0.923833	1.781353
1	-3.090879	-0.842998	1.760113
1	-1.511355	0.062054	-1.542653
1	-2.844856	-0.811732	-0.808977
1	-2.816896	0.953846	-0.780864

$(T_2/T_1)x$

6	0.368716	-1.273246	-0.268398
6	1.085988	0.003429	-0.077291
6	0.369090	1.285322	-0.231017
6	-1.615256	0.002083	0.040713
6	-2.981842	0.011657	-0.604359
6	-1.679310	-0.020154	1.561933
8	0.915866	2.345061	-0.239042
8	0.915260	-2.332420	-0.307373
7	2.355124	-0.003123	0.363106
7	3.550468	-0.002248	0.294769
8	-0.952015	1.166078	-0.411072
8	-0.952361	-1.148509	-0.444733
1	-0.693241	-0.027310	2.013658
1	-2.204718	0.857983	1.915575
1	-2.205700	-0.907656	1.889814
1	-2.873068	0.027931	-1.680444
1	-3.529078	-0.876326	-0.314802
1	-3.529281	0.890363	-0.288113

TS-T_1

6	0.395855	-1.215365	-0.238539
6	1.062884	0.082848	-0.098782
6	0.327736	1.339174	-0.252922
6	-1.634064	0.011916	0.051323
6	-2.987392	-0.031185	-0.620128
6	-1.721833	0.025031	1.570688
8	0.835841	2.418036	-0.284744
8	0.963847	-2.264005	-0.270961
7	2.805221	0.261565	0.193401
7	3.412032	-0.637341	0.479541
8	-0.999076	1.186866	-0.413538
8	-0.937888	-1.138844	-0.388838
1	-0.739688	0.055257	2.030671
1	-2.274163	0.897527	1.895838
1	-2.228290	-0.868073	1.914009
1	-2.854526	-0.039437	-1.693760
1	-3.517765	-0.925966	-0.320508
1	-3.564088	0.840908	-0.339827

TS-iso-S_0

6	0.40968800	-1.27171100	-0.30631200
6	1.11882900	0.00335500	-0.22177000
6	0.40747300	1.27677000	-0.31115800
6	-1.57358300	0.00065800	0.05387100
6	-2.94991600	-0.00023300	-0.56954400
6	-1.60516500	-0.00103000	1.57516700
8	0.95552300	2.33784800	-0.33425700
8	0.95857600	-2.33242800	-0.32066400
8	-0.92286100	1.16324000	-0.42381400
8	-0.92026900	-1.15949700	-0.42563200
7	2.90068700	-0.01803200	1.03485900
7	2.55229100	0.00638000	-0.13076600
1	-0.60738300	-0.00020100	2.00068600
1	-2.12420700	0.88089400	1.92827500
1	-2.12175900	-0.88519600	1.92635200
1	-2.85571400	0.00141100	-1.64724200
1	-3.49156400	-0.88504800	-0.26086300
1	-3.49389200	0.88231800	-0.25843600

Diazirine-S_0

6	0.464080	-1.288315	-0.193939
6	1.178583	0.000161	-0.024078
6	0.463876	1.288387	-0.194948
6	-1.530872	-0.000056	0.046380
6	-2.866850	-0.000378	-0.659887
6	-1.654035	0.000379	1.562923
8	1.007154	2.344993	-0.202292
8	1.007491	-2.344860	-0.200040
8	-0.853283	1.162696	-0.390321
8	-0.853087	-1.163008	-0.389485
1	-0.682000	0.000499	2.044899
1	-2.191470	0.883528	1.884157
1	-2.191454	-0.882618	1.884610
1	-2.706887	-0.000545	-1.729848
1	-3.427390	-0.884163	-0.383675
1	-3.427621	0.883359	-0.383992
7	2.385295	0.000557	0.818790
7	2.640363	0.000159	-0.352674

Ketene-S_0

6	0.882669	-0.248084	-0.137501
6	0.468754	1.150775	-0.044153
6	-1.347175	-0.222932	0.001515
6	-2.404748	-0.431711	-1.056857
6	-1.818077	-0.509395	1.414427
8	1.116598	2.142251	0.039855
8	-0.874032	1.113486	-0.072220
8	-0.226134	-1.035358	-0.310965
1	-1.004987	-0.363117	2.116277
1	-2.628588	0.158590	1.679908
1	-2.161658	-1.534198	1.488938
1	-1.996545	-0.191315	-2.029968
1	-2.728427	-1.465600	-1.054048
1	-3.257691	0.206894	-0.861703
6	2.113022	-0.716835	-0.013217
8	3.198845	-1.097765	0.061474

Carbene-boatlike

6	-0.977435	1.189952	-0.078406
6	-1.495053	0.000114	0.654990
6	-0.977897	-1.189349	-0.079103
6	1.079561	-0.000314	0.048022
6	2.324651	-0.000468	-0.807572
6	1.376004	-0.000476	1.540492
8	-1.669294	-2.082275	-0.454508
8	-1.667943	2.084134	-0.452382
8	0.344754	-1.159776	-0.309296
8	0.345209	1.159518	-0.308985
1	0.466516	-0.000171	2.133515
1	1.946009	-0.883807	1.798575
1	1.946556	0.882512	1.798545
1	2.042457	-0.000481	-1.851740
1	2.913598	0.883082	-0.597263
1	2.913257	-0.884234	-0.597194

Carbene-chairlike

6	-0.975045	1.194636	-0.101610
6	-1.619620	0.000528	-0.702902
6	-0.975508	-1.193486	-0.101114
6	1.079638	-0.000218	-0.004057
6	2.343055	-0.000323	-0.829937
6	1.320611	-0.000747	1.495957
8	-1.522099	-2.086773	0.457385
8	-1.521122	2.087830	0.457531
8	0.349588	-1.165077	-0.369532
8	0.350291	1.165285	-0.368925
1	0.383732	-0.000686	2.043186
1	1.877915	-0.885196	1.776555
1	1.878423	0.883188	1.777164
1	2.087307	0.000192	-1.881258
1	2.927195	0.882804	-0.605022
1	2.926608	-0.884017	-0.605731

Carbene-planar

6	-0.965151	1.273282	-0.072732
6	-1.599171	0.000537	0.074250
6	-0.965875	-1.272509	-0.073273
6	1.058269	-0.000202	-0.000324
6	2.331292	-0.000399	-0.815147
6	1.311574	-0.000583	1.500512
8	-1.503057	-2.345923	0.004392
8	-1.501716	2.346971	0.005390
8	0.348440	-1.167121	-0.378662
8	0.349102	1.167270	-0.378183
1	0.386866	-0.000434	2.066791
1	1.875104	-0.883899	1.773126
1	1.875610	0.882299	1.773488
1	2.082987	-0.000117	-1.868093
1	2.913585	0.883055	-0.586745
1	2.913082	-0.884277	-0.587100

Carbene-$(S_0/T_1)_X$

6	-0.974638	1.155215	-0.063480
6	-1.455685	0.000223	0.751665
6	-0.975074	-1.154867	-0.063612
6	1.087843	-0.000197	0.043002
6	2.327475	-0.000404	-0.818684
6	1.384617	-0.000286	1.535140
8	-1.713446	-1.989534	-0.482363
8	-1.712729	1.990206	-0.482085
8	0.343857	-1.156868	-0.308683
8	0.344273	1.156750	-0.308637
1	0.474011	-0.000146	2.128733
1	1.953012	-0.883992	1.794948
1	1.953319	0.883210	1.794996
1	2.039676	-0.000324	-1.861254
1	2.917378	0.883128	-0.610969
1	2.917049	-0.884167	-0.611014

Carbene-triplet

6	-0.957041	1.284071	-0.070095
6	-1.624031	0.000423	0.133973
6	-0.957403	-1.283528	-0.068921
6	1.058551	-0.000146	-0.000280
6	2.329656	-0.000165	-0.817902
6	1.313306	-0.000766	1.500169
8	-1.496065	-2.346115	-0.023910
8	-1.495977	2.346617	-0.026316
8	0.348224	-1.166325	-0.375398
8	0.348983	1.167022	-0.374338
1	0.387159	-0.000350	2.065287
1	1.875853	-0.884351	1.773799
1	1.876826	0.882063	1.774215
1	2.078823	-0.000186	-1.870288
1	2.912027	0.883640	-0.591155
1	2.912047	-0.883958	-0.591138

TS-CK-S_0

6	1.066018	-1.148613	-0.556212
6	1.444008	-0.211970	0.386250
6	0.973257	1.160476	0.062192
6	-1.055784	0.032689	0.305257
6	-1.905186	-0.306830	-0.902306
6	-1.829111	0.127431	1.601561
8	1.676274	2.104695	-0.186025
8	1.082759	-1.923715	-1.414448
8	-0.371707	1.239444	0.077198
8	-0.039251	-0.965984	0.513013
1	-1.149993	0.340178	2.417181
1	-2.557016	0.926378	1.530317
1	-2.340728	-0.806032	1.799784
1	-1.303135	-0.336915	-1.801824
1	-2.379601	-1.270201	-0.763065
1	-2.668633	0.450683	-1.027945

DMA-S_0

DMA-S_1

DMA-T_1

$(S_1/S_2)_X$

$(S_1/S_0)_X$

$(S_1/S_0)_X$-D90

(S_1/T_2)x

(T_2/T_1)x

TS-T_1

TS-iso-S_0

Diazirine-S_0

Ketene-S_0

Carbene-boatlike

Carbene-chairlike

Carbene-planar

Carbene-$(S_0/T_1)_X$

Carbene-triplet

TS-CK-S_0