Supplementary Information

for

Theoretical Study on the Photochemical Generation of Phenylborylene from Phenyldiazidoborane

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Table SI1. Absolute and relative CASPT2 energies of the critical points optimized by CASSCF.

Structure	State	CASPT2 (Hartree)	CASPT2 (eV)	Active space
1-S_0	S_0	-583.3284927	0.00	(12,12)
	S_1	-583.1609861	4.56	
	S_2	-583.1515229	4.82	
	S_3	-583.1216329	5.63	
	S_4	-583.1171281	5.75	
1-S_1	S_0	-583.3244261	0.11	(12,12)
	S_1	-583.1702636	4.31	
	S_2	-583.1547236	4.73	
	S_3	-583.1172515	5.75	
	S_4	-583.1167437	5.76	
TS1-S_0	S_0	-583.2490184	2.16	(12,12)
	S_1	-583.0683265	7.08	
	S_2	-583.0494569	7.59	
	S_3	-583.0136398	8.57	
	S_4	-582.9978595	9.00	
TS1-S_1	S_0	-583.2367581	2.50	(12,12)
	S_1	-583.1657039	4.43	
	S_2	-583.1331886	5.31	
	S_3	-583.1017790	6.17	
	S_4	-583.0267012	8.21	
TS1′-S_1	S_0	-583.2523689	2.07	(12,12)
	S_1	-583.1577166	4.65	
	S_2	-583.1113973	5.91	
	S_3	-583.0908347	6.47	
	S_4	-583.0674628	7.10	
P′-S_1	S_0	-583.2522938	2.07	(12,12)
	S_1	-583.2011313	3.47	

	S_2	-583.1585310	4.62	
	S_3	-583.1337414	5.30	
	S_4	-583.0995175	6.23	
***anti-anti*-S_1**	S_0	-583.3210576	0.20	(12,12)
	S_1	-583.1725472	4.24	
	S_2	-583.1611905	4.55	
	S_3	-583.1370227	5.21	
	S_4	-583.1260224	5.51	
TSa-S_1	S_0	-583.2415470	2.37	(12,12)
	S_1	-583.1633819	4.49	
	S_2	-583.1360680	5.24	
	S_3	-583.0986061	6.26	
	S_4	-583.0132436	8.58	
P_a-S_1	S_0	-583.24059462	2.39	(12,12)
	S_1	-583.21423918	3.11	
	S_2	-583.18603848	3.88	
	S_3	-583.14484862	5.00	
	S_4	-583.12806857	5.45	
***syn-syn*-S_1**	S_0	-583.3090656	0.53	(12,12)
	S_1	-583.1723769	4.25	
	S_2	-583.1327159	5.33	
	S_3	-583.1172182	5.75	
	S_4	-583.1073554	6.02	
TSb-S_1	S_0	-583.2355991	2.07	(12,12)
	S_1	-583.1516591	4.65	
	S_2	-583.0931768	5.91	
	S_3	-582.9975586	6.47	
	S_4	-583.0345305	7.10	
P_b-S_1	S_0	-583.2240756	2.84	(12,12)
	S_1	-583.2049349	3.36	

	S_2	-583.1548454	4.72	
	S_3	-583.1282237	5.45	
	S_4	-583.0909008	6.46	
(S_1/S_0)x-a	S_0	-473.9751628	2.39	(12,12)
	S_1	-473.9758073	2.41	
	S_2	-473.9258152	3.75	
	S_3	-473.9249885	3.77	
	S_4	-473.9126182	4.12	
2-S_0	S_0	-474.0072930	1.58	(12,12)
	S_1	-473.8826885	4.97	
	S_2	-473.8329160	6.32	
	S_3	-473.8304170	6.39	
	S_4	-473.8285090	6.44	
3-S_0	S_0	-474.0994295	-0.97	(12,12)
	S_1	-473.9309309	3.61	
	S_2	-473.9019674	4.40	
	S_3	-473.8914893	4.68	
	S_4	-473.8800855	4.99	
3-S_1	S_0	-474.0871618	-0.64	(12,12)
	S_1	-473.9415529	3.32	
	S_2	-473.8954531	4.57	
	S_3	-473.8664305	5.36	
	S_4	-473.8412979	6.05	
TS2-S_0	S_0	-474.0049351	1.60	(12,12)
	S_1	-473.8852777	4.85	
	S_2	-473.8485671	5.85	
	S_3	-473.8332528	6.27	
	S_4	-473.8262951	6.46	
4-S_0	S_0	-474.0288135	0.95	(12,12)
	S_1	-473.9041035	4.34	

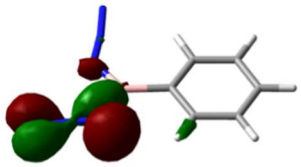
	S_2	-473.8510057	5.78	
	S_3	-473.8507464	5.79	
	S_4	-473.7929165	7.37	
TS3-S_0	S_0	-474.0030297	1.65	(12,12)
	S_1	-473.8669756	5.35	
	S_2	-473.8406450	6.07	
	S_3	-473.8246147	6.50	
	S_4	-473.8196416	6.64	
5-S_0	S_0	-364.8600421	-1.67	(10,10)
	S_1	-364.7694048	0.80	
	S_2	-364.7112030	2.38	
	S_3	-364.6789045	3.26	
	S_4	-364.6641059	3.66	
TS4-S_1	S_0	-474.0322422	0.85	(12,12)
	S_1	-473.9281722	3.68	
	S_2	-473.9206221	3.89	
	S_3	-473.8742450	5.15	
	S_4	-473.8618770	5.49	
6-S_0	S_0	-364.8083057	-0.26	(10,10)
	S_1	-364.8020791	-0.09	
	S_2	-364.7486153	1.36	
	S_3	-364.7430845	1.51	
	S_4	-364.7156549	2.26	
6-S_1	S_0	-364.8013875	-0.07	(10,10)
	S_1	-364.7967545	0.05	
	S_2	-364.7727105	0.71	
	S_3	-364.7596398	1.06	
	S_4	-364.7160772	2.25	
6-T_1	T_1	-364.8342246	-0.97	(10,10)
	T_2	-364.7590826	1.08	

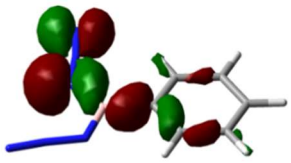
	T_3	-364.7638096	0.95	
	T_4	-364.7206300	2.12	
	T_5	-364.7183913	2.19	
$(S_1/S_0)_X$-b	S_0	-364.7984577	0.01	(10,10)
	S_1	-364.7949398	0.10	
	S_2	-364.7716450	0.74	
	S_3	-364.7570698	1.13	
	S_4	-364.7142966	2.30	
$(S_2/S_1)_X$	S_0	-474.0136942	1.36	(12,12)
	S_1	-473.8840214	4.89	
	S_2	-473.8683071	5.31	
	S_3	-473.8473518	5.88	
	S_4	-473.8450439	5.95	
TS5-S_1	S_0	-473.9891231	2.03	(12,12)
	S_1	-473.9000195	4.45	
	S_2	-473.8461131	5.92	
	S_3	-473.8431284	6.00	
	S_4	-473.8343970	6.24	
7-S_0	S_0	-364.8229587	-0.66	(10,10)
	S_1	-364.8110705	-0.34	
	S_2	-364.7447977	1.46	
	S_3	-364.7408371	1.58	
	S_4	-364.7081893	2.46	
7-S_1	S_0	-364.8146969	-0.43	(10,10)
	S_1	-364.8128576	-0.38	
	S_2	-364.7927786	0.16	
	S_3	-364.7397265	1.61	
	S_4	-364.6925512	2.89	
$(S_1/S_0)_X$-c	S_0	-364.8146969	-0.43	(10,10)
	S_1	-364.8128576	-0.38	

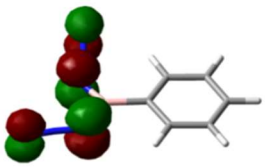
	S_2	-364.7927786	0.16	
	S_3	-364.7397265	1.60	
	S_4	-364.6925512	2.89	
TS6-S_0	S_0	-364.8177113	-0.52	(10,10)
	S_1	-364.7813099	0.47	
	S_2	-364.7222390	2.08	
	S_3	-364.7000874	2.68	
	S_4	-364.6858324	3.07	
TS7-S_0	S_0	-364.7978103	0.02	(10,10)
	S_1	-364.7317690	1.82	
	S_2	-364.7083788	2.46	
	S_3	-364.6505945	4.03	
	S_4	-364.6480420	4.10	
8-S_0	S_0	-255.5677145	-0.92	(8,8)
	S_1	-255.4749030	1.60	
	S_2	-255.4492681	2.30	
	S_3	-255.4038559	3.54	
	S_4	-255.3777881	4.25	
8-S_1	S_0	-255.5520819	-0.50	(8,8)
	S_1	-255.4795905	1.48	
	S_2	-255.4346554	2.70	
	S_3	-255.3928474	3.84	
	S_4	-255.3818350	4.14	
8-T_1	T_1	-255.5153701	0.50	(8,8)
	T_2	-255.5142155	0.54	
	T_3	-255.4381678	2.60	
	T_4	-255.4052995	3.50	
	T_5	-255.3823535	4.12	

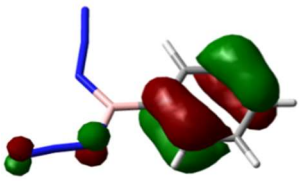
Table SI2. Relative TD-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at **1**-S_0 together with the electronic configuration (weight in the parenthesis, orbital below the Table) and oscillation strength (f).

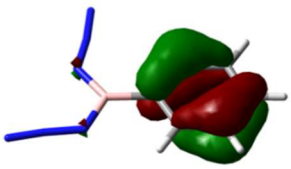
State	Electronic configuration (weight)	ΔE/eV	λ/nm	f
S_0	-	0.00	-	-
S_1	HOMO→LUMO(0.51) HOMO-1→LUMO(0.46)	4.41	281	0.0170
S_2	HOMO-1→LUMO(0.51)	4.61	269	0.3299
S_3	HOMO-2→LUMO(0.66)	4.98	249	0.1418
S_4	HOMO-3→LUMO(0.67)	4.99	249	0.0003
S_5	HOMO-2→LUMO+1(0.49)	5.14	241	0.0000
S_6	HOMO-4→LUMO(0.36)	5.21	238	0.0006
S_7	HOMO-4→LUMO(0.51)	5.26	236	0.0000
S_8	HOMO-1→LUMO+1(0.49)	5.49	226	0.0001
S_9	HOMO-2→LUMO+2(0.36)	5.59	222	0.0004
S_{10}	HOMO→LUMO+3(0.36)	5.67	219	0.0058

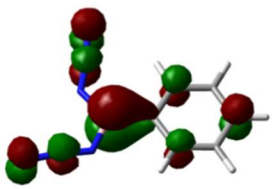

HOMO-4

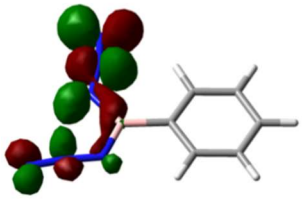

HOMO-3

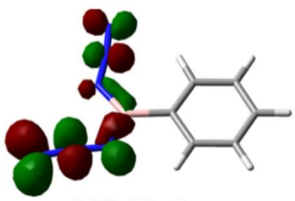

HOMO-2


HOMO-1


HOMO


LUMO


LUMO+1


LUMO+2

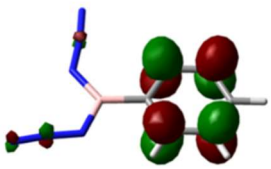

LUMO+3

Table SI3. Relative TD-CAM-B3LYP vertical excitation energy (ΔE) and wavelength (λ) at **1**-S_0 together with the electronic configuration (weight in the parenthesis, orbital below the Table) and oscillation strength (f).

State	Electronic configuration (weight)	ΔE/eV	λ/nm	f
S_0	-	0.00	-	-
S_1	HOMO-1→LUMO(0.44) HOMO→LUMO(0.49)	4.95	251	0.0355
S_2	HOMO-1→LUMO(0.45)	5.12	242	0.3576
S_3	HOMO-2→LUMO+1(0.48)	5.23	237	0.0000
S_4	HOMO-2→LUMO(0.60)	5.31	234	0.1265
S_5	HOMO-3→LUMO (0.43)	5.36	231	0.0000
S_6	HOMO-3→LUMO(0.33)	5.46	227	0.0013
S_7	HOMO-4→LUMO(0.57)	5.66	219	0.0001
S_8	HOMO-3→LUMO+1(0.29)	6.07	204	0.0059
S_9	HOMO→LUMO+3(0.48)	6.32	196	0.0706
S_{10}	HOMO-1→LUMO+3(0.50)	6.56	189	0.3312

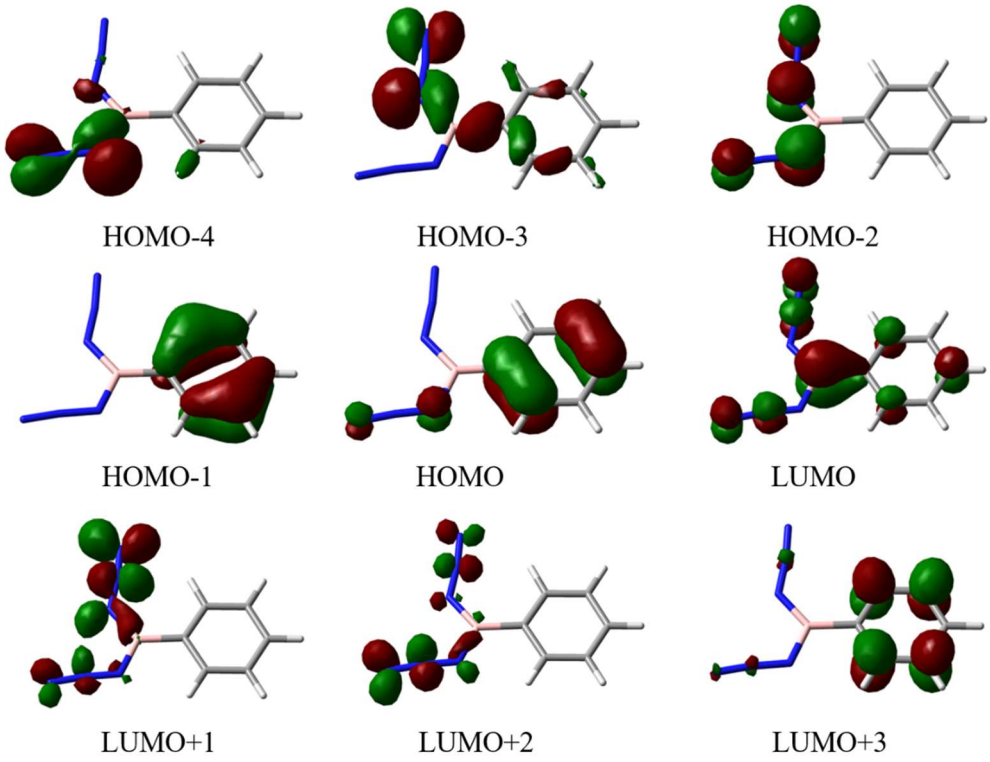
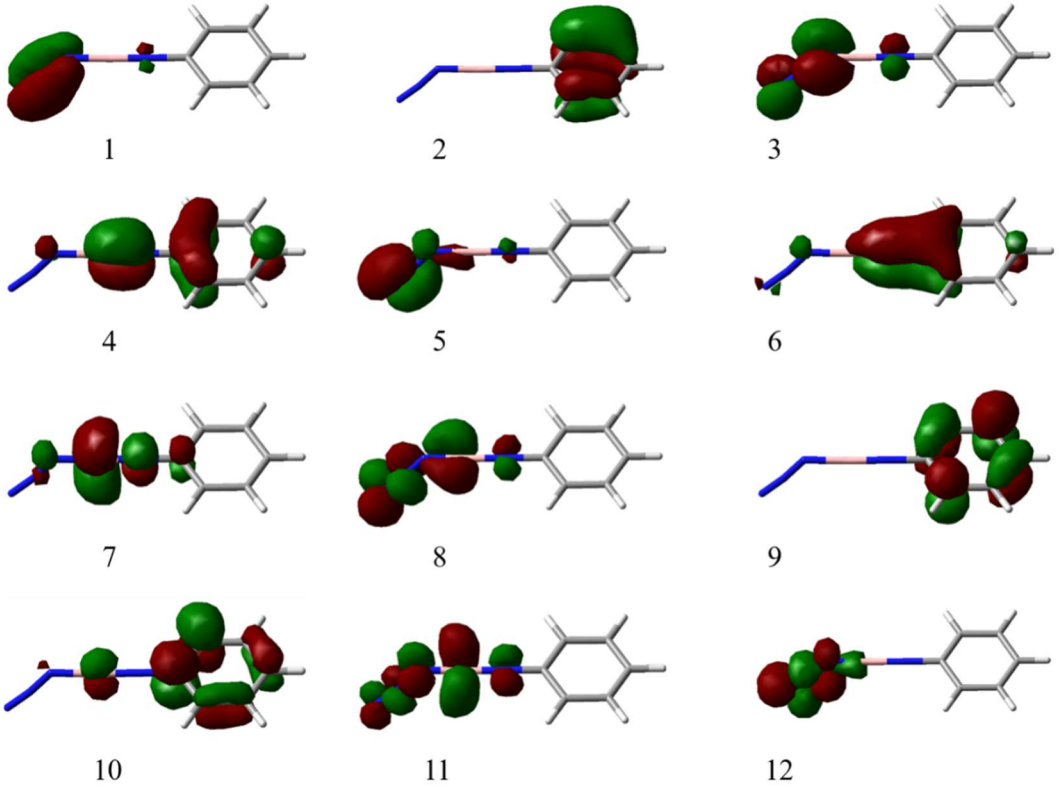


Table SI4. Relative CASPT2 vertical excitation energy (ΔE), wavelengths (λ), oscillation strength (f), and the main configuration with weight in parenthesis at **3**-S_0, where the related orbitals are shown.

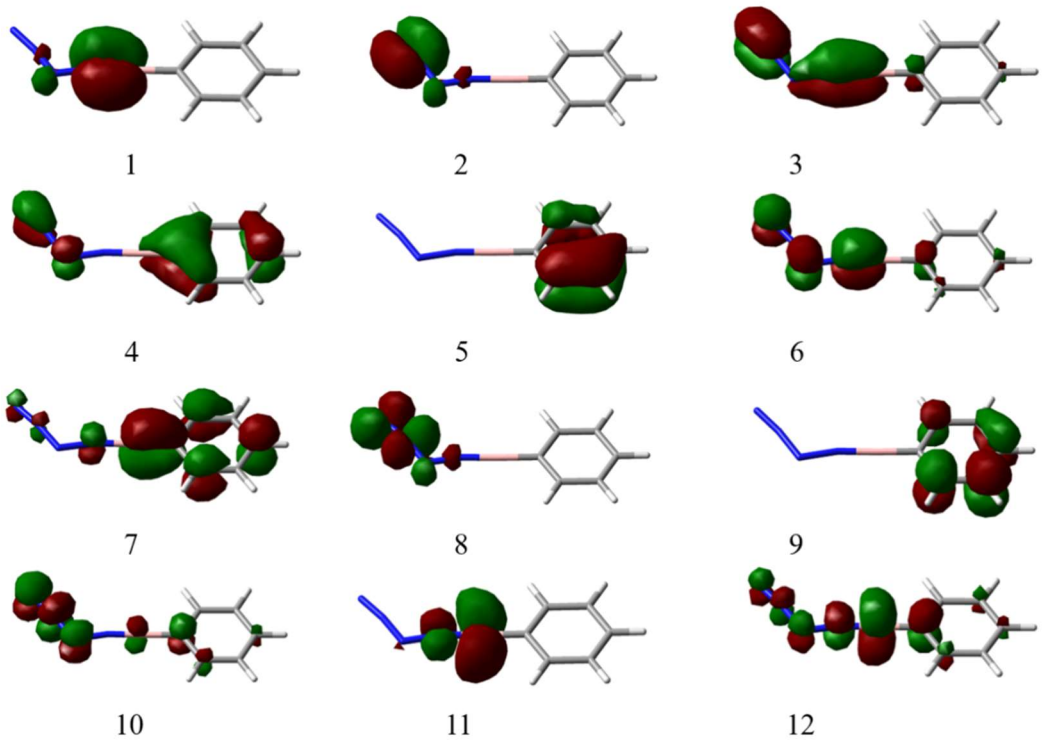
State	Configuration (weight)	ΔE/eV	λ/nm	f
S_0	222222000000(0.82)	0.00	-	-
S_1	222u2200d000(0.31) 2u2222000d00(0.24)	4.58	270	0.0104
S_2	22u22200000d(0.73)	5.37	231	0.0005
S_3	222u220d0000(0.78)	5.66	219	0.0050
S_4	222u2200000d(0.71)	5.97	208	0.0011



"u" and "d" stand for singly occupied orbitals with electrons of spin up (u) or spin down (d)

Table SI5. Relative CASPT2 vertical excitation energy (ΔE), wavelengths (λ), oscillation strength (f), and the main configuration with weight in parenthesis at **4**-S_0, where the related orbitals are shown.

State	Configuration (weight)	ΔE/eV	λ/nm	f
S_0	222222000000(0.81)	0.00	-	-
S_1	22222u0d0000(0.74)	3.39	365	0.0005
S_2	22222ud00000(0.72)	4.84	256	0.7884
S_3	2222u2d00000(0.38)	4.85	256	0.0096
S_4	u22222d00000(0.78)	6.42	193	0.0003



"u" and "d" stand for singly occupied orbitals with electrons of spin up (u) or spin down (d)

Table SI6. Key bond length (in angstrom (Å)), angle and dihedral angle (in degree (°)) of **1**-S_0 and **1**-S_1 optimized by TD-B3LYP, TD-CAM-B3LYP and CASSCF methods.

1	B3LYP			CAM-B3LYP			CASSCF		
	S_0	S_1	$\Delta(S_1-S_0)$	S_0	S_1	$\Delta(S_1-S_0)$	S_0	S_1	$\Delta(S_1-S_0)$
C1-C2	1.39	1.45	0.06	1.39	1.42	0.03	1.39	1.44	0.05
C2-C3	1.41	1.40	-0.01	1.40	1.42	0.02	1.39	1.44	0.05
C3-C4	1.41	1.41	0.00	1.40	1.43	0.03	1.41	1.48	0.07
C4-C5	1.39	1.44	0.05	1.39	1.42	0.03	1.39	1.47	0.08
C5-C6	1.40	1.39	-0.01	1.39	1.40	0.01	1.39	1.47	0.08
C1-C6	1.40	1.39	-0.01	1.39	1.40	0.01	1.39	1.41	0.02
C3-B12	1.55	1.59	0.04	1.55	1.52	-0.03	1.58	1.55	-0.03
B12-N13	1.45	1.45	0.00	1.44	1.46	0.02	1.44	1.44	0.00
B12-N14	1.45	1.43	-0.02	1.44	1.45	0.01	1.45	1.45	0.00
N13-N15	1.24	1.23	-0.01	1.23	1.22	-0.01	1.25	1.25	0.00
N15-N17	1.14	1.14	0.00	1.12	1.13	0.01	1.11	1.11	0.00
N14-N16	1.23	1.22	-0.01	1.22	1.22	0.00	1.24	1.24	0.00
N16-N18	1.14	1.15	0.01	1.12	1.13	0.01	1.12	1.12	0.00
C1-C2-C3	121	123	2	121	123	2	122	124	2
C2-C3-C4	117	114	-3	118	112	-6	117	116	-1
C3-C4-C5	121	123	2	121	123	2	121	120	-1
C4-C5-C6	120	121	1	120	122	2	120	119	-1
C5-C6-C1	120	117	-3	120	116	-4	119	118	-1
C6-C1-C2	120	122	2	120	122	2	120	123	3
C2-C3-B12	124	125	1	124	126	2	124	125	1
C4-C3-B12	119	121	2	119	121	2	118	119	1
N13-B12-N14	115	120	5	115	117	2	115	116	1
N13-B12-C3	117	114	-3	117	117	0	116	117	1
N14-B12-C3	128	126	-2	128	126	-2	129	128	-1
B12-N13-N15	122	125	3	121	122	1	117	117	0
N13-N15-N17	173	175	2	174	175	1	174	174	0
B12-N14-N16	128	131	3	128	127	-1	125	123	-2
N14-N16-N18	172	174	2	173	174	1	172	173	1
C2-C3-B12-N14	3	0	-3	0	10	10	1	21	20

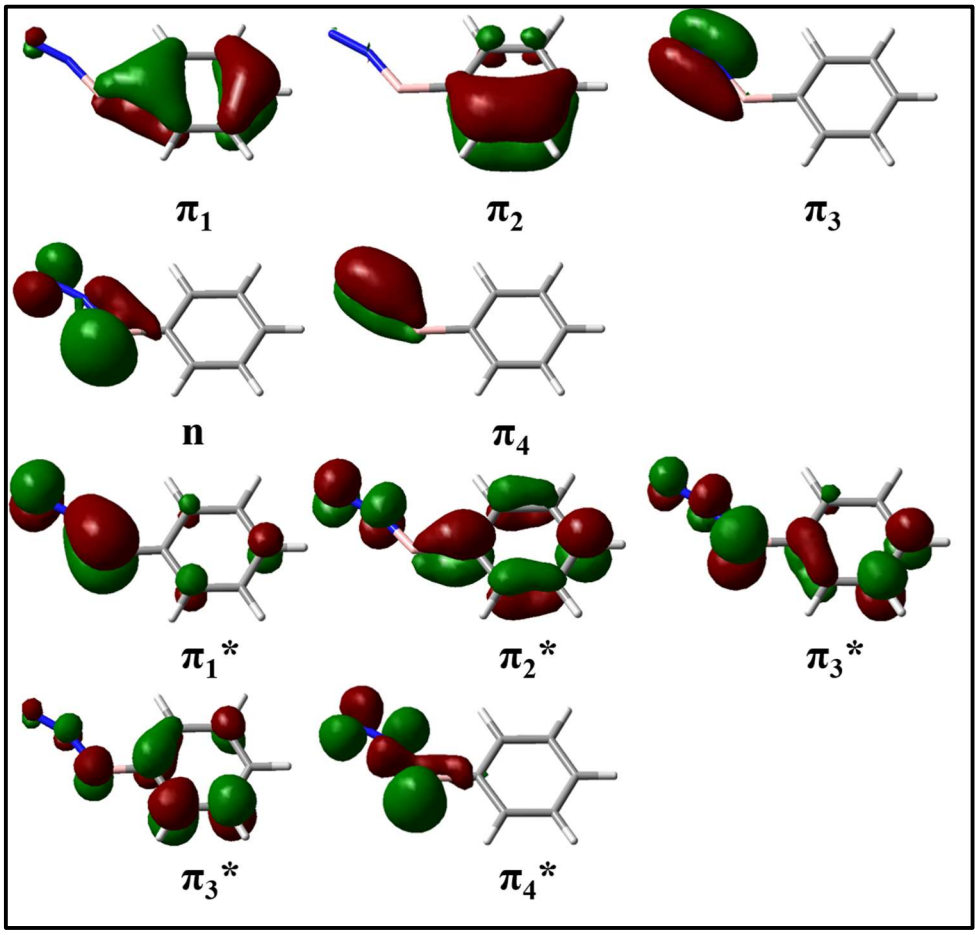


Figure SI1. The (10,10) active orbitals of **7** in the CASPT2 calculations.

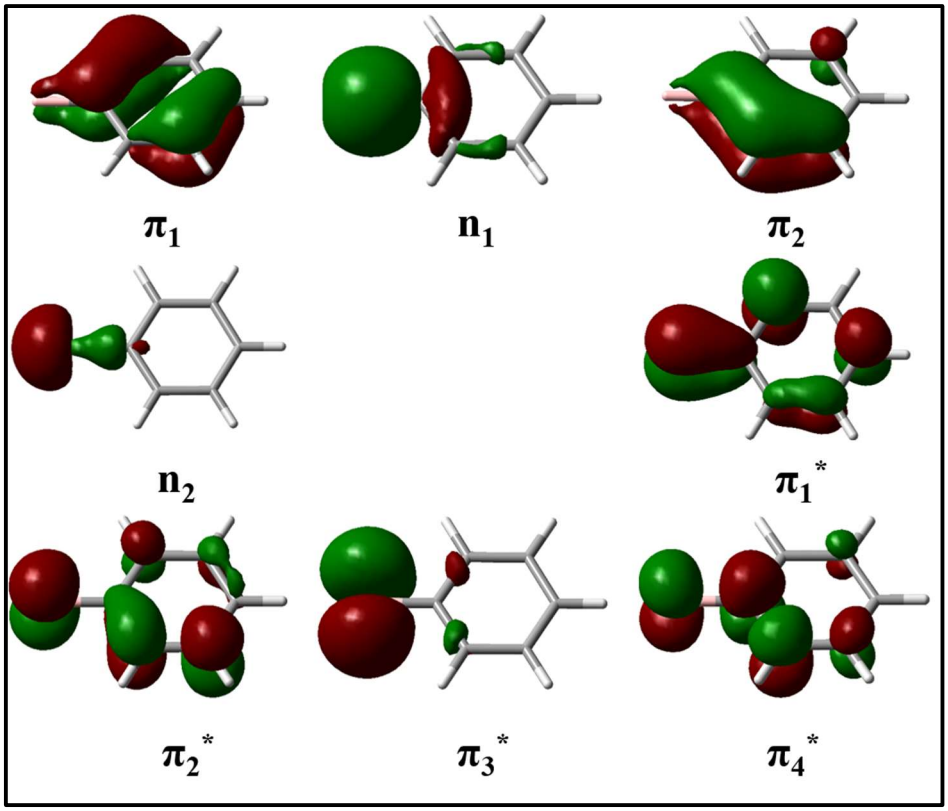
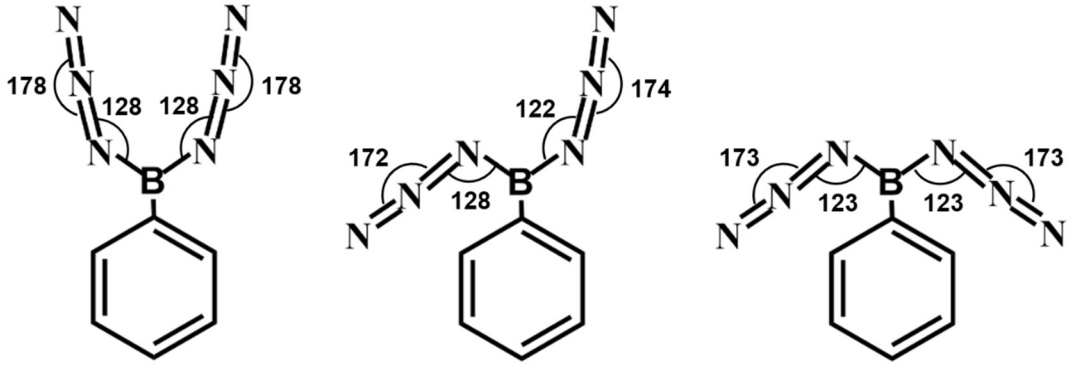


Figure SI2. The (8,8) active orbitals of **8** in the CASPT2 calculations.



anti-anti *syn-anti* *syn-syn*

Figure SI3. DFT-optimized ground-state structure of **1**. Angles are given in °.

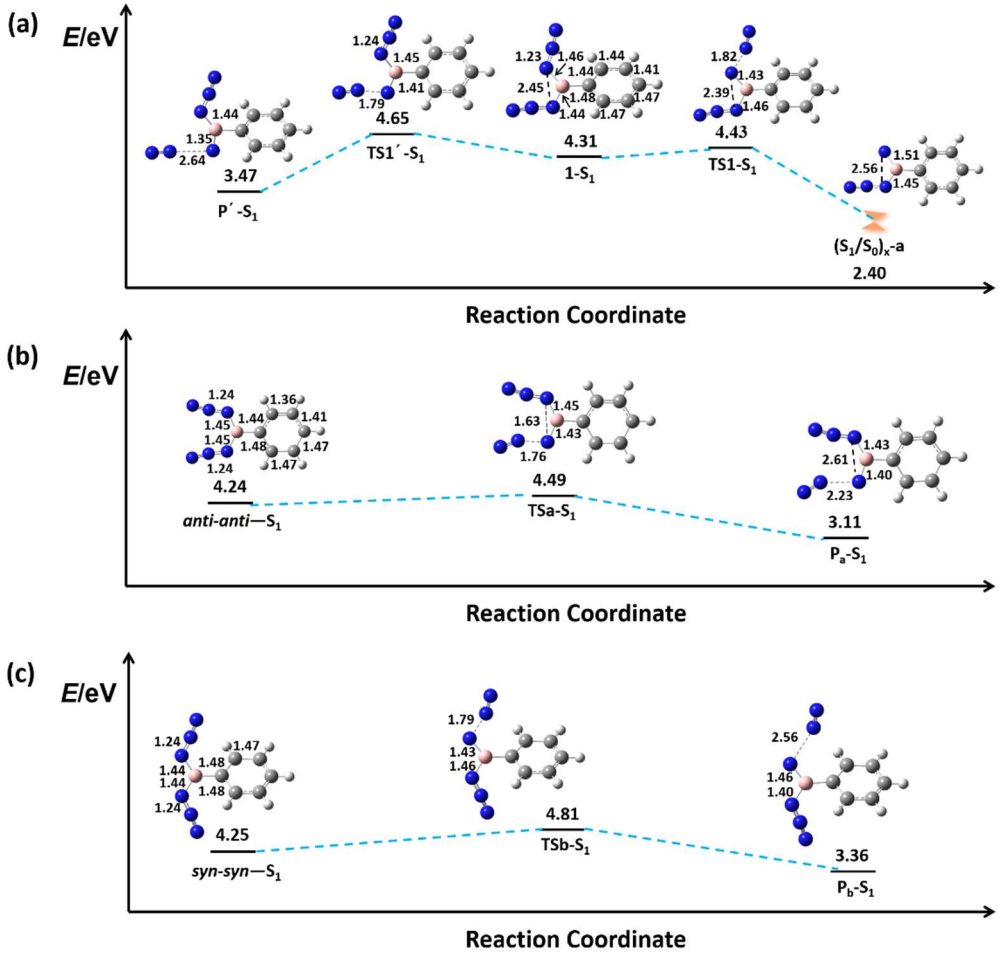


Figure SI4. CASPT2//CASSCF energy profiles with key structures (distance in Å) for the first dinitrogen extrusion from (a) *syn-anti* conformer, (b) *anti-anti* conformer, and (c) *syn-syn* conformer of $PhBN_6$ in S_1 state.

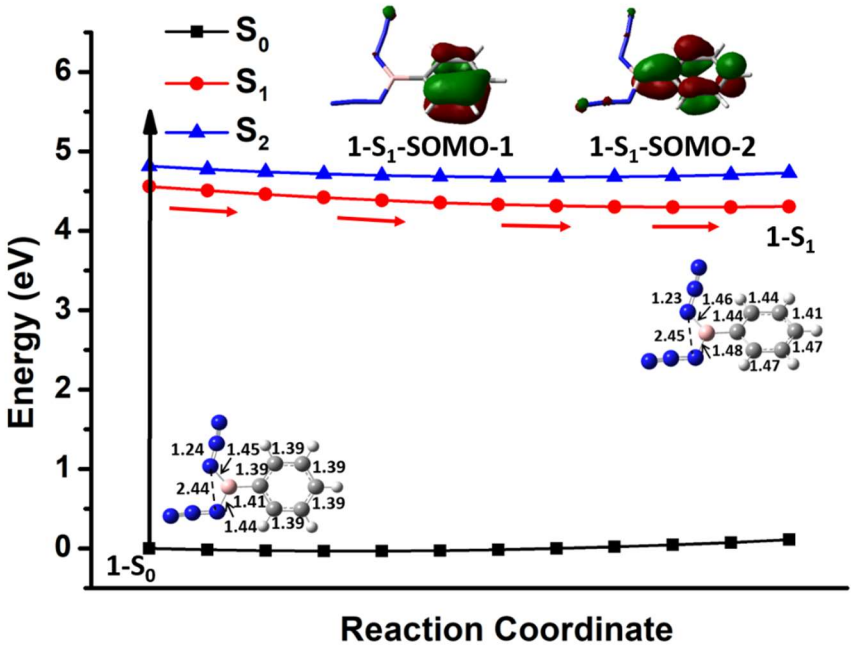


Figure SI5. Energy plot from **1**-S_0 to **1**-S_1. Bond lengths are given in Å.

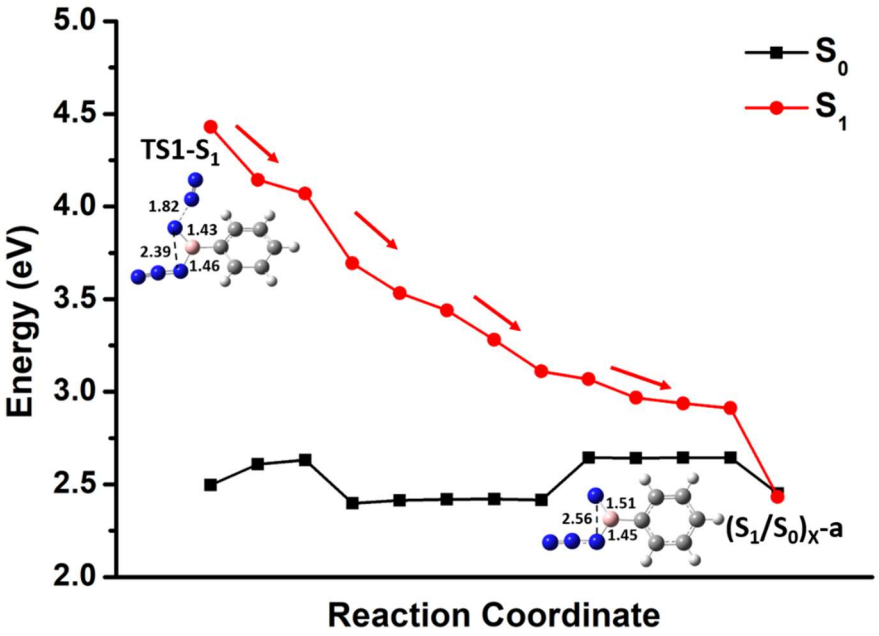


Figure SI6. Energy plot from **TS1**-S_1 to $(S_1/S_0)_x$-a. Bond lengths are given in Å.

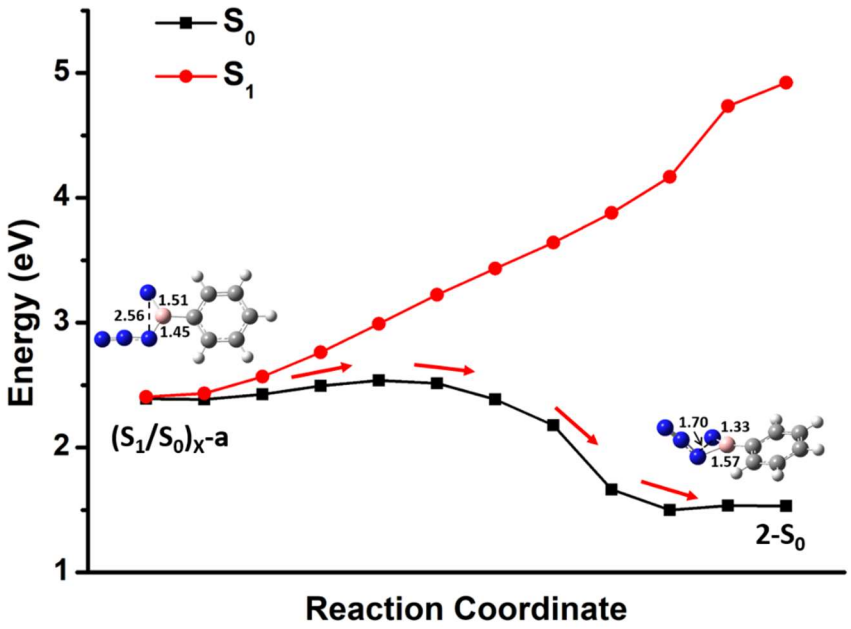


Figure SI7. Energy plot from $(S_1/S_0)_x$-a to **2**-S_0. Bond lengths are given in Å.

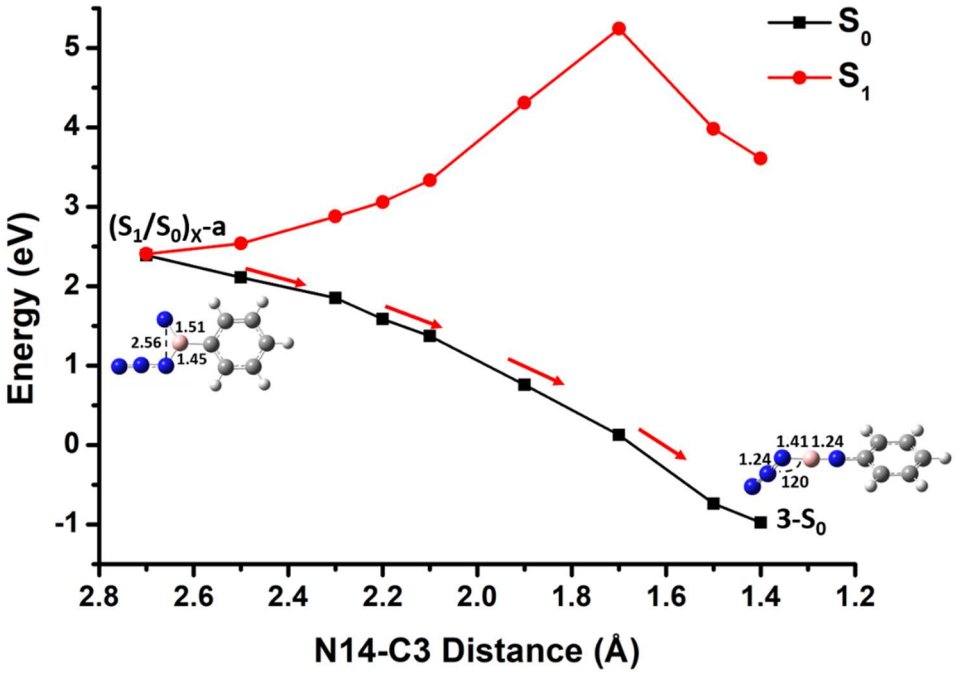


Figure SI8. Energy plot along the shorten C-N distance from $(S_1/S_0)_x$-a. Bond lengths are given in Å and angles are in °.

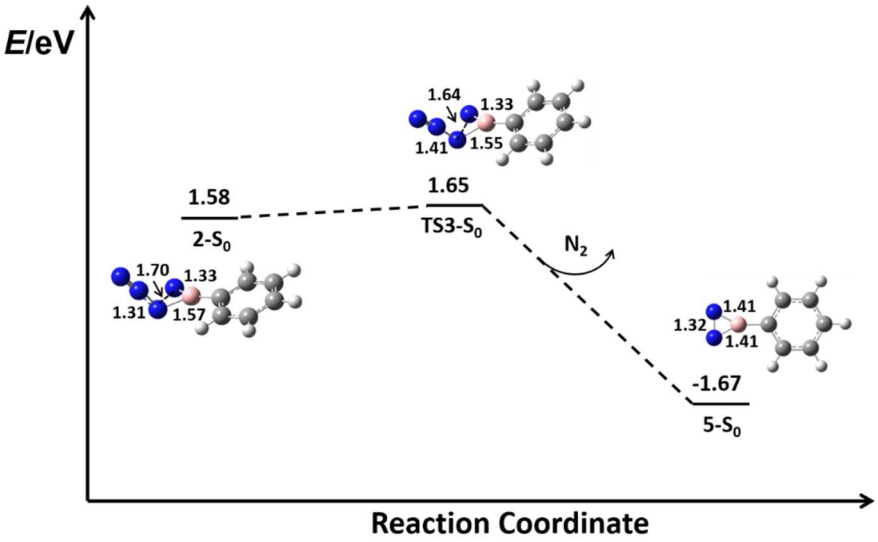


Figure SI9. CASPT2//CASSCF energy profiles for the dinitrogen extrusion reaction of **2**-S_0 to the diazirine derivative **5**-S_0. Distances are given in Å.

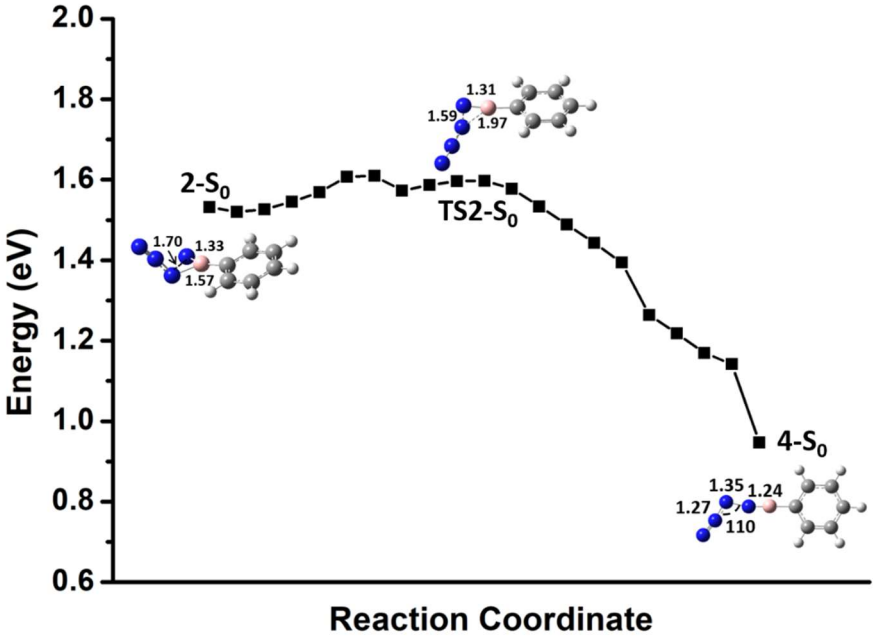


Figure SI10. Energy plot from **2**-S_0 to **4**-S_0 via **TS2**-S_0. Bond lengths are given in Å and angles are in °.

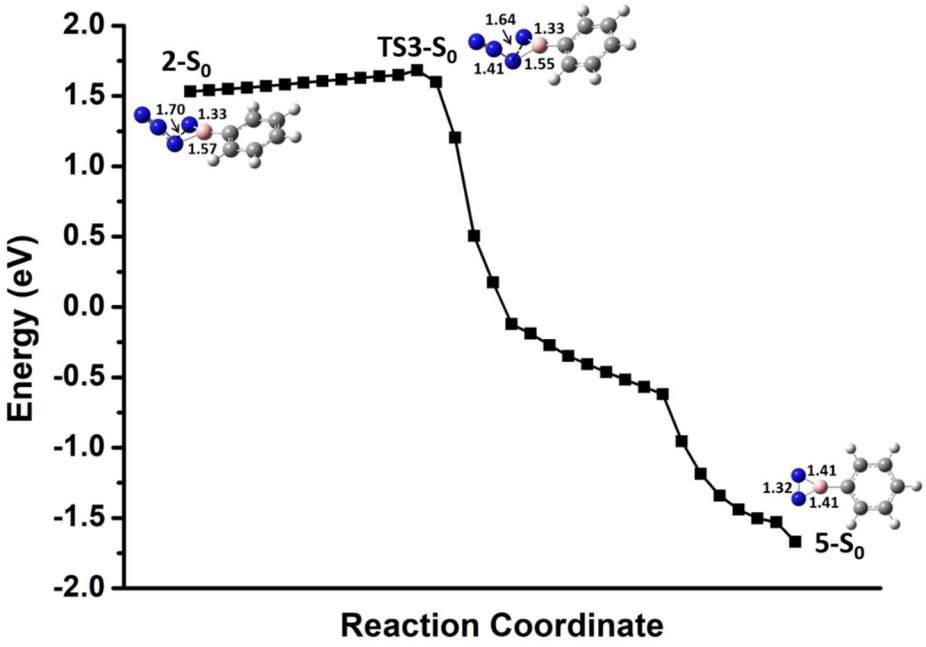


Figure SI11. Energy plot from **2**-S_0 to **5**-S_0 via **TS3**-S_0. Bond lengths are given in Å.

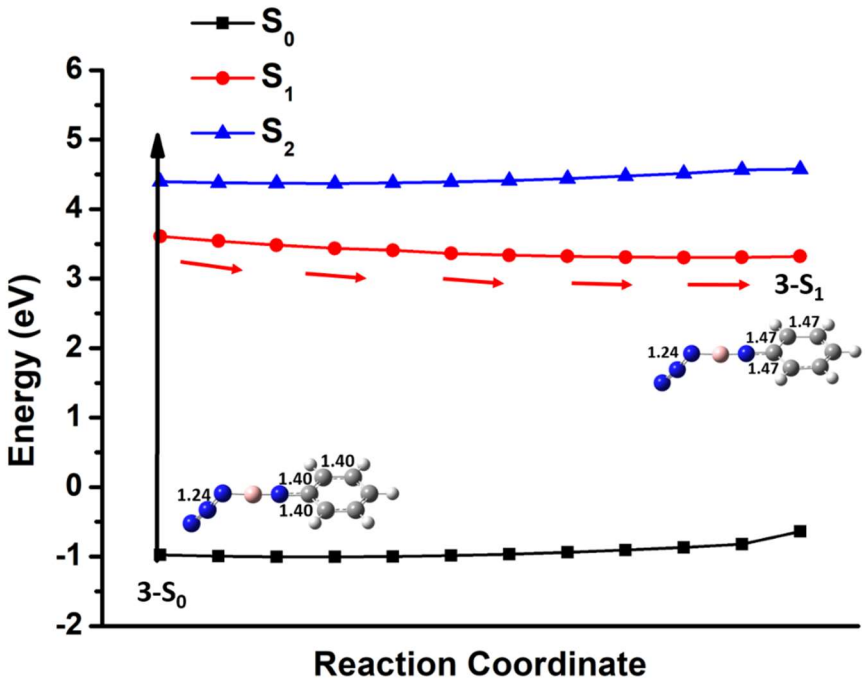


Figure SI12. Energy plot from **3**-S_0 to **3**-S_1. Bond lengths are given in Å.

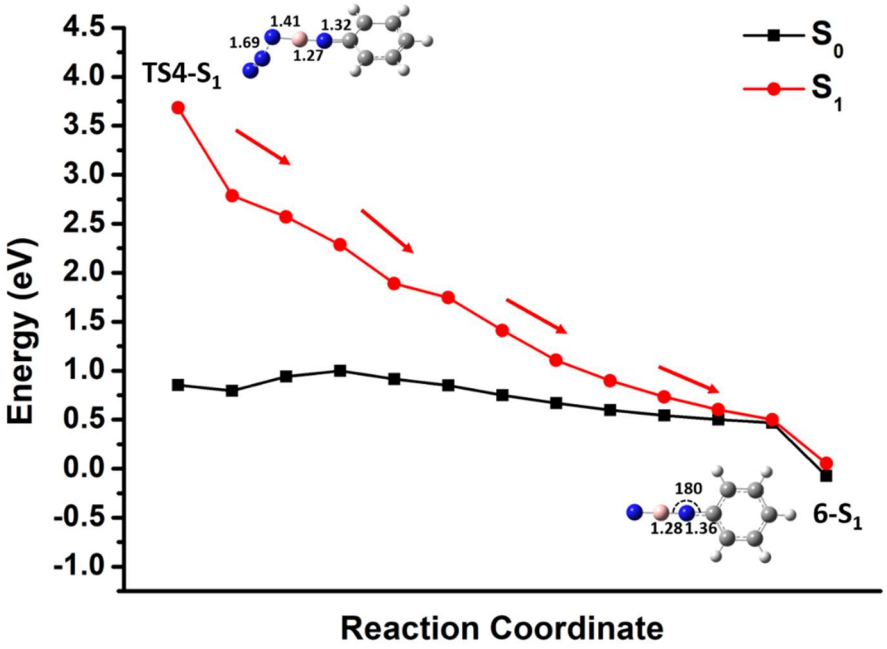


Figure SI13. Energy plot from **TS4**-S_1 to **6**-S_1. Bond lengths are given in Å and angles are in °.

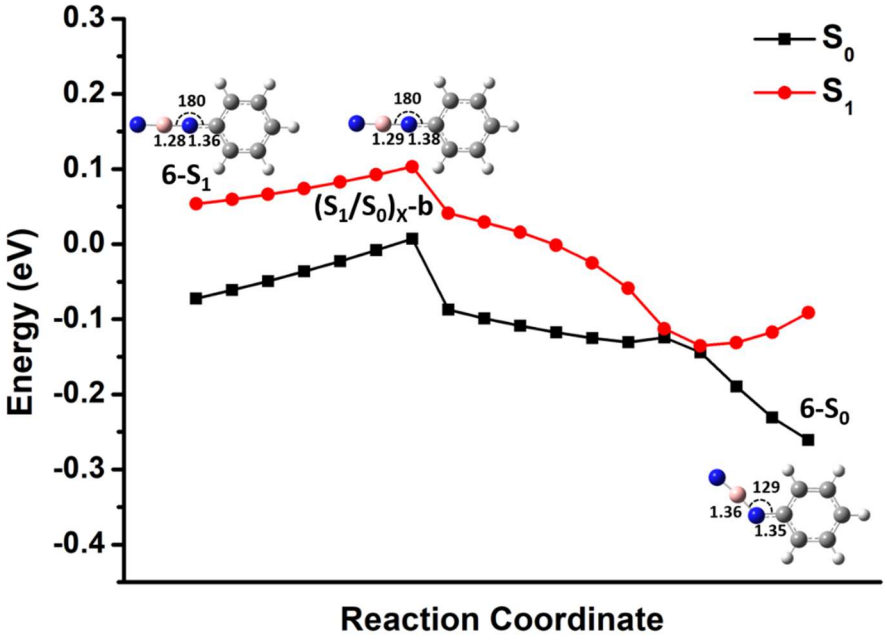


Figure SI14. Energy plot from to **6**-S_1 and **6**-S_0 *via* $(S_1/S_0)_X$-b. Bond lengths are given in Å and angles are in °.

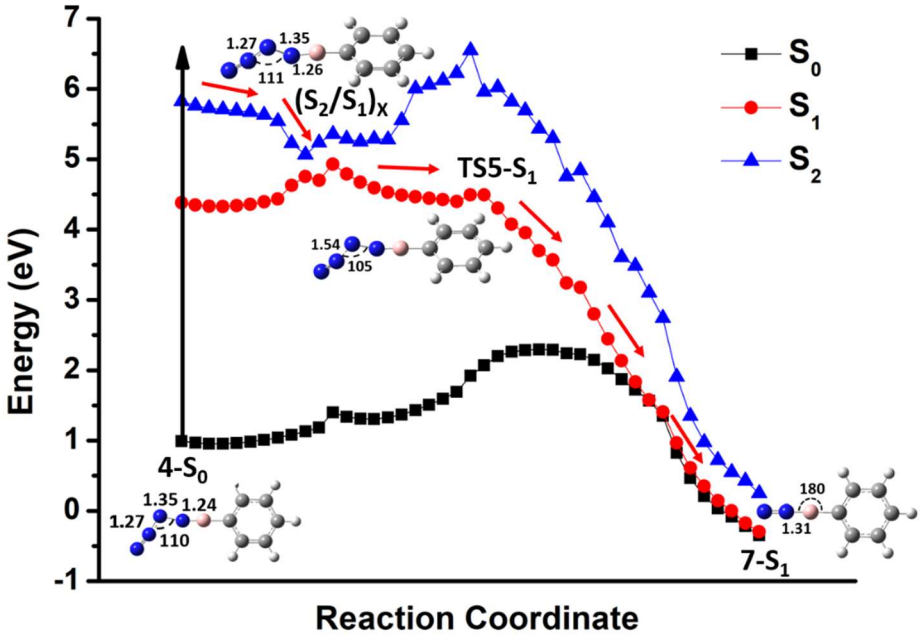


Figure SI15. Energy plot from **4**-S_0 to **7**-S_1 via $(S_2/S_1)_X$ and **TS5**-S_1. Bond lengths are given in Å.

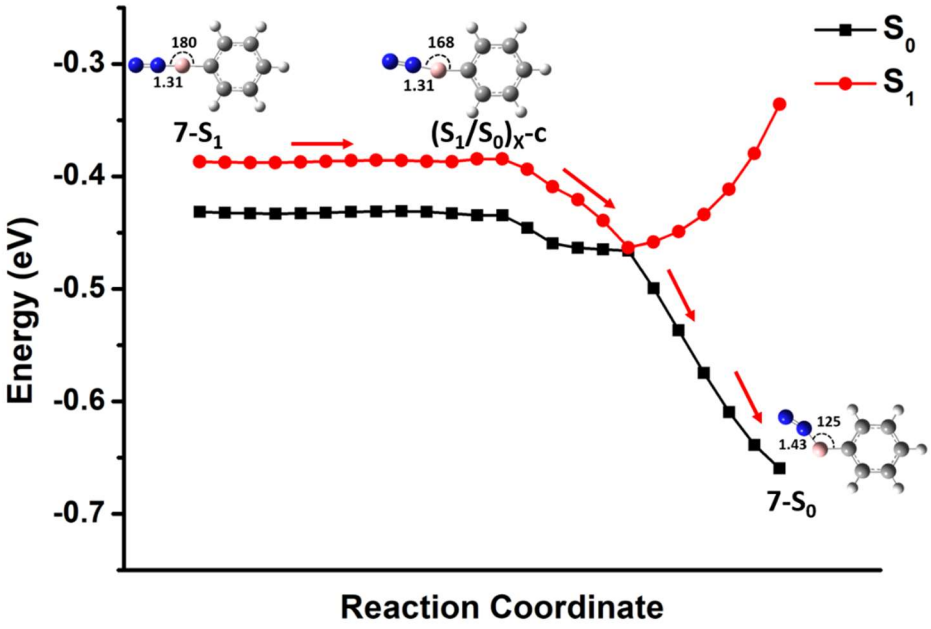


Figure SI16. Energy plot from **7**-S_1 to **7**-S_0. Bond lengths are given in Å and angles are in °.

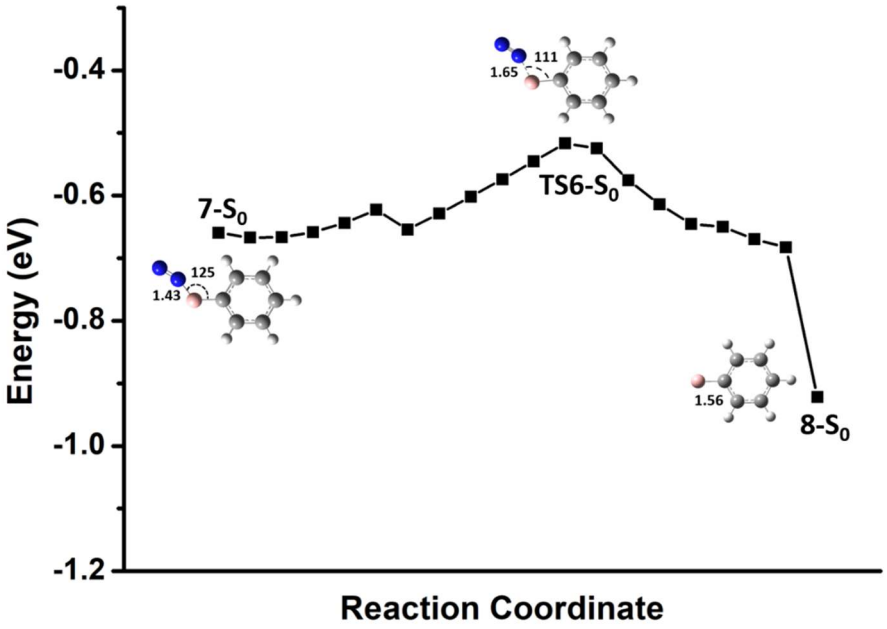


Figure SI17. Energy plot from **7**-S_0 to **8**-S_0 via **TS6**-S_0. Bond lengths are given in Å and angles are in °.

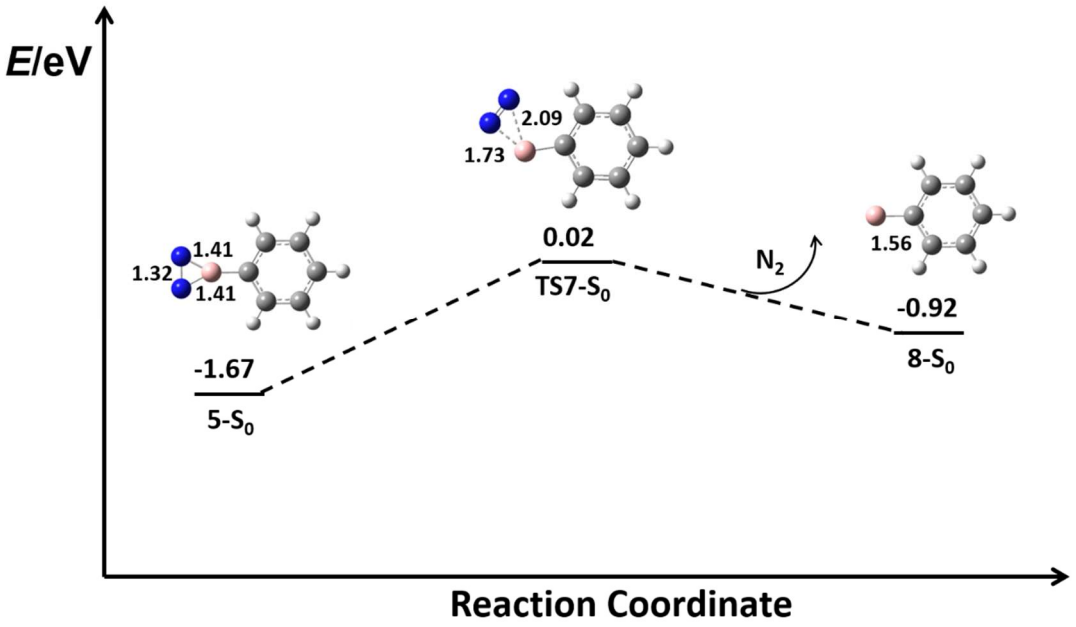


Figure SI18. CASPT2//CASSCF energy profiles for the dinitrogen extrusion reaction of **5**-S_0 to **8**-S_0. Distances are given in Å.

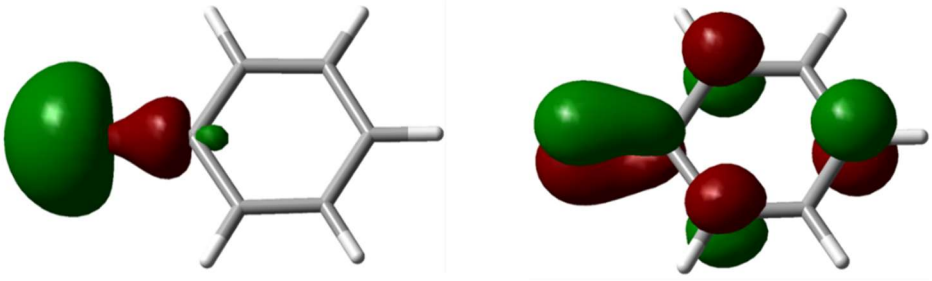


Figure SI19. The key molecular orbitals of **8**. For S_0 state, the left orbital is the HOMO orbital and the right is the LUMO orbital. For T_1 and S_1 states, these two orbitals are singly occupied.

Cartesian coordinates of optimized structure by CASSCF and DFT

	1-S_0(CASSCF)				**1**-S_1(CASSCF)		
C	2.934360	0.821643	0.007995	C	2.953876	0.843230	-0.265151
C	1.550094	0.918741	0.007757	C	1.522043	0.940273	-0.302249
C	0.734144	-0.210466	0.000423	C	0.672606	-0.210983	-0.061489
C	1.369154	-1.466512	-0.006697	C	1.353105	-1.468244	0.185875
C	2.754676	-1.576414	-0.006649	C	2.784494	-1.559079	0.232400
C	3.544693	-0.427898	0.000737	C	3.592929	-0.402690	0.012618
H	3.532681	1.715275	0.013981	H	3.543335	1.720430	-0.453238
H	1.126095	1.904806	0.014119	H	1.092639	1.889859	-0.554968
H	0.768666	-2.355940	-0.011983	H	0.767713	-2.352318	0.340189
H	3.215826	-2.548081	-0.012058	H	3.245080	-2.508136	0.429994
H	4.617326	-0.506238	0.001001	H	4.662015	-0.469425	0.045497
B	-0.841985	-0.167645	0.000891	B	-0.882709	-0.172465	-0.088595
N	-1.513966	-1.441553	0.006254	N	-1.565730	-1.422375	-0.288986
N	-1.715554	0.986976	-0.004227	N	-1.732514	0.999764	0.069219
N	-2.765276	-1.423569	0.008141	N	-2.818223	-1.394279	-0.273731
N	-1.329695	2.163172	-0.011430	N	-1.283834	2.082737	0.451999
N	-3.874551	-1.525606	0.010288	N	-3.928087	-1.488004	-0.279106
N	-1.135080	3.263550	-0.017931	N	-1.007130	3.095947	0.800337
	TS1-S_0(CASSCF)				**TS1**-S_1(CASSCF)		
C	2.837780	0.775949	-0.544686	C	2.855995	0.814590	-0.418873
C	1.460146	0.836876	-0.579222	C	1.495603	0.877387	-0.465747
C	0.669911	-0.215741	-0.101069	C	0.634939	-0.213077	-0.091941
C	1.323884	-1.346051	0.407006	C	1.309781	-1.470104	0.308690
C	2.715202	-1.406473	0.462154	C	2.776367	-1.527093	0.383635
C	3.475777	-0.343400	-0.014986	C	3.551266	-0.337040	0.011222
H	3.420781	1.593883	-0.929732	H	3.426389	1.674130	-0.726134
H	0.990899	1.707182	-1.004792	H	1.047874	1.782937	-0.833141
H	0.744060	-2.181074	0.756627	H	0.728647	-2.340075	0.530589
H	3.199419	-2.277939	0.865652	H	3.267068	-2.428364	0.690717
H	4.549751	-0.387494	0.017797	H	4.621276	-0.354251	0.050369
B	-0.901408	-0.189032	-0.156966	B	-0.914722	-0.169338	-0.158779
N	-1.569297	-1.396573	-0.617573	N	-1.593520	-1.418882	-0.489667
N	-1.816026	0.849758	0.168431	N	-1.842728	0.898704	0.026370
N	-2.814322	-1.481129	-0.580792	N	-2.835296	-1.499328	-0.422223
N	-0.836426	2.183339	0.949976	N	-0.919527	2.295569	0.748906
N	-3.910168	-1.693105	-0.601458	N	-3.932083	-1.709272	-0.400746
N	-0.568353	3.095263	1.504246	N	-0.705719	3.247750	1.257363

TS1′-S_1(CASSCF)				**P′**-S_1(CASSCF)			
C	0.000037	-0.562649	-0.030152	C	0.023422	-0.607265	-0.083733
C	0.039895	-0.605029	1.404615	C	0.080320	-0.670870	1.352157
C	1.170924	-0.082843	2.143566	C	1.177138	-0.077994	2.087594
C	2.267485	0.465988	1.372666	C	2.237013	0.531679	1.310864
C	2.222822	0.513679	-0.060155	C	2.194332	0.551416	-0.119545
C	1.088719	0.001549	-0.767204	C	1.084002	-0.006141	-0.824227
H	-0.852062	-0.959909	-0.547381	H	-0.821846	-1.030486	-0.595460
H	-0.780428	-1.057710	1.929486	H	-0.723108	-1.165174	1.886505
H	3.128616	0.849771	1.883557	H	3.080039	0.959383	1.823074
H	3.048177	0.934731	-0.601090	H	3.003484	0.999665	-0.660389
H	1.056431	0.035882	-1.838085	H	1.048902	0.023573	-1.893881
B	1.213012	-0.144482	3.714562	B	1.147471	-0.119591	3.677698
N	2.443789	-0.662436	4.165599	N	2.291048	-0.827636	3.787631
N	0.135655	0.241972	4.610894	N	0.156512	0.339470	4.615901
N	2.336629	-0.551389	5.948344	N	2.451677	-0.672549	6.418787
N	-0.846659	0.821393	4.129189	N	-0.827203	0.933699	4.153104
N	2.501728	-0.596149	7.034762	N	2.551024	-0.642416	7.515104
N	-1.768663	1.343973	3.813341	N	-1.748121	1.467578	3.855331
anti-anti-S_1(CASSCF)				**TSa**-S_1(CASSCF)			
C	3.115967	1.213121	-0.000841	C	-0.008161	0.026675	0.045899
C	1.751538	1.193654	0.001979	C	0.021656	0.007474	1.407526
C	0.971180	-0.017115	0.003186	C	1.238172	-0.021613	2.175080
C	1.733352	-1.280806	0.002709	C	2.502507	-0.039499	1.405537
C	3.202940	-1.254334	-0.000443	C	2.465953	-0.015038	-0.064670
C	3.893404	0.038875	-0.002472	C	1.164934	0.020387	-0.742715
H	3.620607	2.164124	-0.002042	H	-0.961934	0.048109	-0.452480
H	1.222550	2.128515	0.002884	H	-0.908085	0.013463	1.944937
H	1.217837	-2.218046	0.004263	H	3.446607	-0.082412	1.907675
H	3.757389	-2.171926	-0.001446	H	3.378274	-0.028146	-0.626526
H	4.963393	0.080389	-0.005174	H	1.114067	0.040353	-1.812219
B	-0.566213	0.002538	0.002922	B	1.197951	-0.013528	3.731258
N	-1.229012	-1.289627	0.002301	N	2.509892	0.153240	4.268344
N	-1.204520	1.306569	0.003005	N	-0.102954	-0.154799	4.357082
N	-2.458826	-1.428896	-0.001859	N	2.463441	0.032578	6.027330
N	-2.430727	1.470115	-0.000338	N	-0.295670	-0.033076	5.569023
N	-3.544521	-1.701153	-0.005621	N	2.854519	-0.006028	7.055591
N	-3.510917	1.763912	-0.003331	N	-0.608552	0.057828	6.640327

	P$_a$-S$_1$(CASSCF)				***syn-syn***-S$_1$(CASSCF)		
C	-0.010090	0.027117	0.040466	C	-2.468210	-0.842459	-0.849781
C	0.018959	0.007903	1.401677	C	-1.048825	-0.861462	-0.880241
C	1.235733	-0.023014	2.166606	C	-0.235335	0.011468	0.002869
C	2.501512	-0.040855	1.399901	C	-1.021991	0.889956	0.897705
C	2.465291	-0.015198	-0.069799	C	-2.494116	0.854608	0.871691
C	1.164006	0.020558	-0.747074	C	-3.165994	-0.026348	-0.015891
H	-0.963319	0.048804	-0.458843	H	-2.997782	-1.498022	-1.517752
H	-0.910147	0.014149	1.940121	H	-0.555382	-1.494871	-1.591389
H	3.445579	-0.085524	1.901892	H	-0.529463	1.502705	1.626123
H	3.377407	-0.028223	-0.631863	H	-3.045754	1.497033	1.529506
H	1.113318	0.040660	-1.816570	H	-4.240089	-0.040133	-0.023702
B	1.192543	-0.013622	3.721798	B	1.325093	0.002096	-0.004798
N	2.509975	0.158813	4.228116	N	2.138844	1.187498	0.120566
N	-0.102189	-0.155319	4.355638	N	2.125966	-1.190847	-0.136204
N	2.462663	0.030786	6.074566	N	1.609933	2.307957	0.012718
N	-0.292587	-0.032934	5.568265	N	1.587483	-2.306867	-0.027316
N	2.863796	-0.008004	7.097886	N	1.265744	3.367494	-0.069295
N	-0.606525	0.057769	6.639047	N	1.235232	-3.363662	0.055100
	TSb-S$_1$(CASSCF)				**P$_b$**-S$_1$(CASSCF)		
C	2.473342	-0.895270	0.792078	C	2.462870	-0.886955	0.806025
C	1.054276	-0.940662	0.813348	C	1.045677	-0.964955	0.820866
C	0.234954	-0.000994	0.006003	C	0.208305	-0.072457	-0.018760
C	1.006004	0.951030	-0.823330	C	0.956905	0.905850	-0.833462
C	2.479025	0.933922	-0.792703	C	2.429718	0.926406	-0.793620
C	3.159180	-0.002245	0.029288	C	3.131925	0.011373	0.035149
H	3.012922	-1.594556	1.405477	H	3.014284	-1.565963	1.431730
H	0.561483	-1.647670	1.451936	H	0.565947	-1.673426	1.467751
H	0.500676	1.610317	-1.500069	H	0.435213	1.568098	-1.494309
H	3.025441	1.629700	-1.398456	H	2.960249	1.635623	-1.398902
H	4.233509	0.000423	0.041713	H	4.205766	0.038981	0.049899
B	-1.321894	-0.063975	0.022444	B	-1.334645	-0.234900	-0.037555
N	-2.270735	1.000804	0.065474	N	-2.279370	0.798945	-0.138828
N	-2.081040	-1.307958	-0.017235	N	-2.062641	-1.498297	0.037451
N	-1.321864	2.465621	0.462677	N	-1.085321	2.962813	0.540746
N	-1.535979	-2.324139	-0.473520	N	-1.529673	-2.486852	-0.496630
N	-1.058465	3.487564	0.774350	N	-0.978749	3.970599	0.971968
N	-1.152201	-3.300601	-0.859499	N	-1.147825	-3.433571	-0.949543

$(S_1/S_0)_X$-a(CASSCF)				**2**-S_0(CASSCF)			
C	3.386586	-0.359922	-0.008939	C	3.331999	-0.306131	-0.261787
C	2.503712	-1.438184	-0.023514	C	2.697552	-1.374390	0.371776
C	1.124583	-1.222623	-0.015046	C	1.355646	-1.302679	0.674407
C	0.619753	0.074718	0.020794	C	0.602097	-0.164185	0.355396
C	1.543628	1.141986	0.034294	C	1.247788	0.903423	-0.280162
C	2.892570	0.947506	0.015246	C	2.605930	0.835143	-0.587136
B	-0.917855	0.423774	0.006803	B	-0.905105	-0.095516	0.697813
N	-1.841346	-0.675890	0.204804	N	-2.026524	0.966061	0.411028
N	-3.058833	-0.365642	0.036808	N	-2.684223	0.740636	-0.702870
N	-4.156393	-0.208936	-0.077416	N	-3.322803	0.654558	-1.602826
N	-1.445246	1.822128	-0.172055	N	-2.041891	-0.527794	1.230464
H	2.888336	-2.442097	-0.044833	H	3.258559	-2.256298	0.625163
H	0.452857	-2.061246	-0.029974	H	0.878673	-2.133336	1.164314
H	1.156609	2.147245	0.047885	H	0.694032	1.792455	-0.526470
H	3.565432	1.785917	0.024058	H	3.090426	1.663423	-1.072629
H	4.447501	-0.538123	-0.018919	H	4.379740	-0.364760	-0.496480
3-S_0(CASSCF)				**3**-S_1(CASSCF)			
C	3.620123	-0.330869	0.161280	C	3.640506	-0.318675	0.151042
C	2.788031	-1.234820	0.817419	C	2.835273	-1.262517	0.840303
C	1.408689	-1.151664	0.669117	C	1.369918	-1.201542	0.705294
C	0.850834	-0.156731	-0.141294	C	0.795774	-0.156134	-0.147662
C	1.691624	0.744857	-0.794785	C	1.701865	0.781878	-0.827786
C	3.070778	0.649790	-0.638045	C	3.104961	0.651389	-0.640985
B	-1.748566	0.016891	-0.422927	B	-1.776553	0.037445	-0.421841
N	-3.143602	0.065380	-0.641589	N	-3.171255	0.069657	-0.636772
N	-3.864125	0.684063	0.159463	N	-3.899290	0.686501	0.160878
N	-4.619881	1.201087	0.797738	N	-4.662237	1.197958	0.794542
N	-0.517780	-0.068553	-0.291127	N	-0.535922	-0.053106	-0.301311
H	3.210529	-2.001833	1.441368	H	3.281332	-2.017176	1.455464
H	0.758562	-1.845289	1.169806	H	0.727112	-1.896954	1.203182
H	1.260820	1.507179	-1.417273	H	1.285990	1.545122	-1.453630
H	3.708935	1.349966	-1.147256	H	3.755528	1.344455	-1.143187
H	4.686922	-0.398840	0.278107	H	4.708892	-0.377688	0.262471

TS2-S_0(CASSCF)				**4**-S_0(CASSCF)			
C	3.404417	-0.419582	-0.235307	C	3.531441	-0.401406	-0.027349
C	2.532530	-1.453128	0.104753	C	2.719706	-1.503021	0.225387
C	1.214193	-1.176389	0.395982	C	1.335026	-1.384193	0.124201
C	0.730629	0.138066	0.357526	C	0.746632	-0.163062	-0.230588
C	1.614377	1.173221	0.016667	C	1.584696	0.932614	-0.480150
C	2.945711	0.894516	-0.279799	C	2.954160	0.816338	-0.380537
B	-0.732427	0.446735	0.683671	B	-0.784024	-0.031825	-0.342648
N	-2.285244	0.805082	-0.469340	N	-3.358779	-0.014124	-0.472453
N	-3.144206	-0.107500	-0.615089	N	-3.882538	1.089051	-0.808721
N	-3.937217	-0.868148	-0.815587	N	-4.484612	1.986591	-1.091136
N	-1.929584	0.803459	1.081305	N	-2.010610	0.107805	-0.442601
H	2.889228	-2.466711	0.139296	H	3.158290	-2.446013	0.498552
H	0.549926	-1.980296	0.658606	H	0.714570	-2.240203	0.320942
H	1.260615	2.187501	-0.017869	H	1.154626	1.879847	-0.753914
H	3.616820	1.692206	-0.541913	H	3.579368	1.669256	-0.576305
H	4.432129	-0.638422	-0.462901	H	4.600358	-0.488774	0.049526
TS3-S_0(CASSCF)				**TS4**-S_0(CASSCF)			
C	3.326289	-0.312869	-0.276940	C	3.622732	-0.282846	0.202347
C	2.687424	-1.380096	0.354053	C	2.801642	-1.234809	0.858480
C	1.349516	-1.295617	0.673927	C	1.343572	-1.202110	0.667749
C	0.605481	-0.146495	0.375960	C	0.765992	-0.174445	-0.204138
C	1.255912	0.919984	-0.257355	C	1.696369	0.774763	-0.845807
C	2.608990	0.839708	-0.582298	C	3.095588	0.673982	-0.609595
B	-0.897834	-0.063023	0.736322	B	-1.786831	-0.118239	-0.617086
N	-2.042601	0.943265	0.465354	N	-3.175153	-0.175176	-0.843460
N	-2.673962	0.692819	-0.767143	N	-3.825294	0.813205	0.370771
N	-3.305018	0.611163	-1.668076	N	-4.503614	1.374956	1.031128
N	-2.038366	-0.485833	1.272141	N	-0.534256	-0.104295	-0.416425
H	3.241185	-2.270980	0.591578	H	3.233497	-1.983446	1.493045
H	0.868451	-2.125579	1.160975	H	0.701170	-1.914474	1.143415
H	0.709130	1.817725	-0.487880	H	1.293082	1.529582	-1.491414
H	3.096926	1.667387	-1.065477	H	3.747105	1.379545	-1.093242
H	4.370372	-0.380949	-0.525139	H	4.686291	-0.32558	0.354233

	5-S_0(CASSCF)				**6**-S_0(CASSCF)		
C	-1.882643	-1.211933	-0.000018	C	-2.183965	-0.901305	0.000303
C	-0.488641	-1.210599	0.000006	C	-0.856721	-1.306837	0.000036
C	0.228866	-0.000850	0.000027	C	0.189746	-0.348435	-0.000279
C	-0.488536	1.208713	0.000036	C	-0.149248	1.034105	-0.000378
C	-1.882122	1.207702	0.000026	C	-1.477453	1.425880	-0.000044
C	-2.579460	-0.001703	-0.000007	C	-2.499875	0.463056	0.000493
H	-2.419662	-2.143162	-0.000051	H	-2.969361	-1.634524	0.000499
H	0.044447	-2.144527	-0.000007	H	-0.588116	-2.346177	-0.000187
H	0.043899	2.142982	0.000043	H	0.638248	1.765388	-0.000798
H	-2.430849	2.158035	0.000032	H	-1.726563	2.471107	-0.000167
H	-3.654646	-0.001594	-0.000028	H	-3.527903	0.775718	0.000758
B	1.764982	-0.000975	0.000009	N	1.455755	-0.804351	-0.000216
N	3.007098	0.658258	-0.000115	B	2.625179	-0.101400	0.000329
N	3.007036	-0.660321	0.000048	N	3.832140	0.406404	0.000570
	6-S_1(CASSCF)				**6**-T_1(CASSCF)		
C	-2.084332	-0.911878	0.000916	C	-2.081211	-0.910268	0.000273
C	-0.712119	-1.138521	0.001830	C	-0.713748	-1.139248	0.000254
C	0.177547	-0.047712	-0.000343	C	0.185795	-0.048481	0.000093
C	-0.325944	1.266787	0.001471	C	-0.327460	1.268812	-0.000100
C	-1.700131	1.481098	0.000429	C	-1.697953	1.478935	-0.000081
C	-2.581811	0.395322	-0.000519	C	-2.580835	0.395214	0.000115
H	-2.761828	-1.745831	-0.000039	H	-2.764340	-1.751797	0.000407
H	-0.313101	-2.135596	0.000912	H	-0.312304	-2.145104	0.000371
H	0.365146	2.088839	0.001048	H	0.368325	2.098749	-0.000260
H	-2.082519	2.485220	-0.000220	H	-2.083733	2.491858	-0.000219
H	-3.642872	0.565677	-0.001965	H	-3.650717	0.566942	0.000122
N	1.515544	-0.262574	-0.000708	N	1.516001	-0.261971	0.000034
B	2.793621	-0.466005	-0.000865	B	2.779310	-0.464716	-0.000023
N	4.114663	-0.676196	-0.001028	N	4.124734	-0.680297	-0.000071

$(S_2/S_1)_X$(CASSCF)				**TS5**-S_1(CASSCF)			
C	3.593956	-0.556038	0.009235	C	3.598888	-0.490857	-0.144090
C	2.599067	-1.558143	0.168689	C	2.690775	-1.624055	0.068218
C	1.277287	-1.295395	0.021803	C	1.241339	-1.379399	0.084822
C	0.749527	0.013345	-0.314748	C	0.727338	-0.005131	-0.111751
C	1.743924	1.093989	-0.493170	C	1.708346	1.031429	-0.309907
C	3.169735	0.808941	-0.328757	C	3.050232	0.796369	-0.323780
B	-0.738440	0.251169	-0.438841	B	-0.759954	0.292152	-0.105642
N	-3.115835	0.785428	0.049897	N	-3.236969	0.826245	0.211571
N	-4.096374	0.766879	-0.764505	N	-4.036106	0.792762	-1.102990
N	-5.067292	0.808540	-1.305305	N	-4.812785	0.834981	-1.884951
N	-1.971615	0.442706	-0.575322	N	-1.984075	0.526354	-0.134576
H	2.908194	-2.562224	0.423134	H	3.072262	-2.614746	0.211346
H	0.565315	-2.098931	0.164898	H	0.562891	-2.192006	0.243139
H	1.411116	2.096579	-0.713880	H	1.357312	2.037439	-0.452095
7-S_0(CASSCF)				**7**-S_1(CASSCF)			
C	-2.271253	-0.907784	0.000124	C	-2.030716	-1.210198	0.000010
C	-0.937825	-1.312521	0.000005	C	-0.637100	-1.208239	-0.000496
C	0.109411	-0.369099	0.000064	C	0.084107	0.002178	-0.000706
C	-0.231338	1.000501	-0.000014	C	-0.641252	1.210081	-0.000488
C	-1.563486	1.407526	0.000043	C	-2.034869	1.207248	0.000013
C	-2.583867	0.453086	0.000150	C	-2.731913	-0.002674	0.000310
H	-3.057216	-1.641233	0.000180	H	-2.564126	-2.143654	0.000327
H	-0.698781	-2.360425	-0.000002	H	-0.105763	-2.142893	-0.000479
H	0.548408	1.740183	-0.000150	H	-0.113116	2.146546	-0.000476
H	-1.806072	2.454905	-0.000013	H	-2.571491	2.138862	0.000340
H	-3.612138	0.767639	0.000190	H	-3.807232	-0.004521	0.000858
B	1.565114	-0.867287	-0.000040	B	1.610866	0.004676	-0.000240
N	2.720894	-0.031654	-0.000106	N	2.919526	0.000564	0.000260
N	3.840434	0.267399	-0.000145	N	4.100572	-0.001596	0.000879

$(S_1/S_0)_X$-b(CASSCF)				$(S_1/S_0)_X$-c(CASSCF)			
C	-2.086306	-0.909302	0.000646	C	-2.206623	-0.920332	-0.004200
C	-0.711817	-1.133903	0.000117	C	-0.840859	-1.192887	-0.004344
C	0.166034	-0.045685	-0.001115	C	0.106821	-0.147646	-0.000620
C	-0.327555	1.262463	-0.000490	C	-0.369333	1.181633	0.003752
C	-1.703356	1.478878	0.000012	C	-1.735393	1.451603	0.005255
C	-2.583774	0.395258	-0.000037	C	-2.657536	0.401803	0.000955
H	-2.763863	-1.742910	0.001058	H	-2.913195	-1.730612	-0.007597
H	-0.307576	-2.128892	0.000536	H	-0.504535	-2.213645	-0.005835
H	0.367507	2.081182	-0.000439	H	0.331134	1.996897	0.004722
H	-2.086303	2.482541	0.000078	H	-2.078754	2.470393	0.009001
H	-3.644856	0.565404	0.000175	H	-3.711909	0.611300	0.001393
N	1.525732	-0.263812	-0.000696	B	1.599166	-0.442230	-0.001735
B	2.792186	-0.464911	-0.000075	N	2.912856	-0.411687	-0.000705
N	4.125811	-0.677682	0.001149	N	4.090445	-0.453355	0.000244
TS6-S_0(CASSCF)				**TS7**-S_0(CASSCF)			
C	-2.285255	-0.900715	0.000340	C	-1.911987	-1.197721	-0.024079
C	-0.959914	-1.334258	0.000894	C	-0.541723	-1.350361	-0.047492
C	0.112729	-0.419207	0.001248	C	0.329255	-0.244991	-0.019657
C	-0.200998	0.957290	0.001127	C	-0.250466	1.037780	0.033108
C	-1.523154	1.395070	-0.000060	C	-1.631922	1.194975	0.056404
C	-2.567093	0.465772	-0.000424	C	-2.465359	0.077856	0.028086
H	-3.087215	-1.616894	0.000277	H	-2.550774	-2.062327	-0.046050
H	-0.745791	-2.388052	0.000837	H	-0.126032	-2.341618	-0.087875
H	0.589165	1.685961	0.001777	H	0.374633	1.907611	0.055733
H	-1.740826	2.448162	-0.000660	H	-2.056856	2.181864	0.096657
H	-3.587584	0.805048	-0.001292	H	-3.533346	0.201805	0.046631
B	1.537099	-1.052756	-0.003364	B	1.823593	-0.686111	-0.052909
N	2.701127	0.122495	0.000832	N	2.709884	1.202940	0.000323
N	3.779994	0.433321	-0.001245	N	3.307009	0.210284	-0.038867
C	-2.285255	-0.900715	0.000340	C	-1.911987	-1.197721	-0.024079
C	-0.959914	-1.334258	0.000894	C	-0.541723	-1.350361	-0.047492

	8-S_0(CASSCF)				**8**-S_1(CASSCF)		
C	-0.966522	-1.211577	-0.000010	C	0.952143	-1.231804	-0.000009
C	0.424185	-1.215905	-0.000035	C	-0.413593	-1.256369	-0.000191
C	1.152455	-0.008380	0.000055	C	-1.190174	-0.003395	-0.000010
C	0.424024	1.217717	-0.000017	C	-0.417552	1.259438	-0.000188
C	-0.972616	1.212832	-0.000008	C	0.949742	1.229646	0.000023
C	-1.663427	0.002557	0.000027	C	1.669213	-0.000371	0.000194
H	-1.508806	-2.140132	-0.000016	H	1.497056	-2.158223	-0.000037
H	0.950736	-2.154960	-0.000049	H	-0.934632	-2.193148	-0.000412
H	0.955581	2.153890	-0.000039	H	-0.935718	2.197723	-0.000474
H	-1.514600	2.141526	-0.000020	H	1.496342	2.155225	-0.000004
H	-2.738839	0.000324	0.000024	H	2.740349	0.000292	0.000330
B	2.711577	0.002202	0.000080	B	-2.639510	0.001035	0.000772

	8-T_1(CASSCF)		
C	0.964488	-1.207284	0.000015
C	-0.424307	-1.217878	0.000053
C	-1.162975	-0.007015	0.000094
C	-0.421047	1.223965	0.000049
C	0.971621	1.209950	0.000005
C	1.671626	0.002099	0.000005
H	1.499841	-2.140147	-0.000029
H	-0.941020	-2.161983	0.000013
H	-0.943032	2.164833	0.000015
H	1.509057	2.141674	-0.000037
H	2.746737	-0.000672	-0.000027
B	-2.697323	-0.007494	-0.000162

	1-S_0(B3LYP)				**1**-S_0(CAM-B3LYP)		
C	2.936384	0.823247	0.001480	C	2.925686	0.830236	0.002460
C	1.548094	0.927225	0.001559	C	1.542394	0.931070	0.002650
C	0.728805	-0.217570	0.000199	C	0.730244	-0.210133	0.000379
C	1.366339	-1.474754	-0.001220	C	1.365648	-1.459852	-0.002036
C	2.752715	-1.582887	-0.001357	C	2.746923	-1.565920	-0.002340
C	3.541846	-0.432463	-0.000003	C	3.530315	-0.419051	-0.000085
H	3.544999	1.720407	0.002576	H	3.532219	1.727862	0.004306
H	1.114978	1.918865	0.002782	H	1.107691	1.921954	0.004767
H	0.759825	-2.372868	-0.002246	H	0.757872	-2.356337	-0.003709
H	3.219513	-2.561502	-0.002499	H	3.214869	-2.543117	-0.004291
H	4.623190	-0.514151	-0.000085	H	4.611094	-0.498729	-0.000277
B	-0.823978	-0.158810	0.000232	B	-0.822166	-0.164339	0.000510
N	-1.544432	-1.417412	0.000326	N	-1.525085	-1.425212	0.000855
N	-1.662737	1.024389	0.000214	N	-1.671516	1.004005	0.000145
N	-2.775210	-1.458536	0.000419	N	-2.754654	-1.456817	0.000748
N	-1.319233	2.199464	-0.000762	N	-1.332349	2.178225	-0.001285
N	-3.892075	-1.615395	0.000574	N	-3.864592	-1.596212	0.000759
N	-1.147415	3.316991	-0.001576	N	-1.160400	3.286291	-0.002581