

Supporting Information

Triplet States of Tetrazoles. Nitrenes and Carbenes from Matrix Photolysis of Tetrazoles. and Phenylcyanamide as a Source of Phenylnitrene

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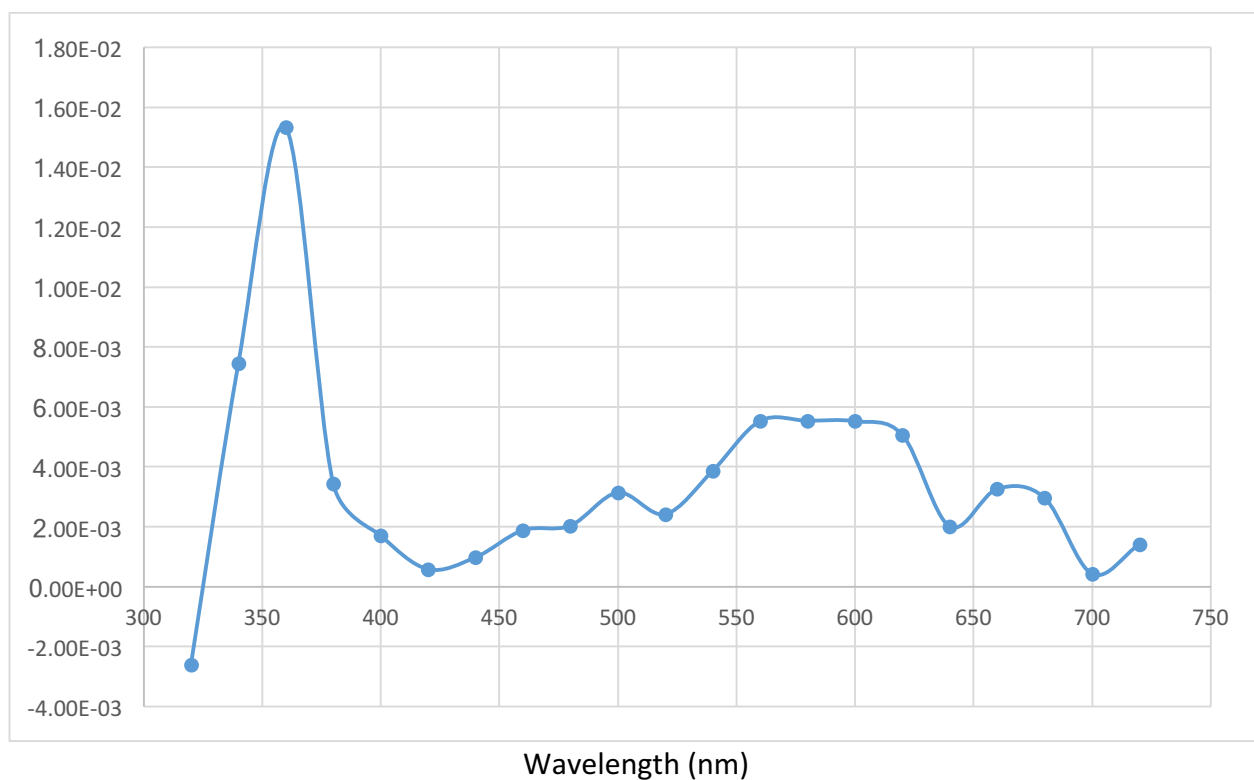


Figure S1. UV/Vis absorption spectrum during LFP of 5-(*p*-tolyl)tetrazole **1b/2b**. 1.9 mm in CH₃CN at 298 K. using laser photolysis at 266 nm (8.2 mJ. 14 ns pulse width). Lifetimes under N₂: 360 nm. ~10 us and 45.5 us (two components); 540 nm. 9.7 us; 560 nm. 11.4 us. All signals were quenched in aerated solution. being replaced by (product) species with longer-lifetimes.

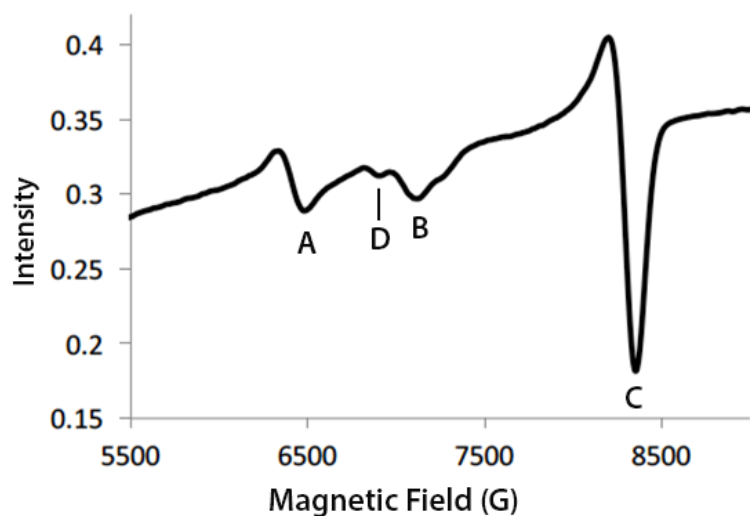


Figure S2. ESR spectrum resulting from photolysis of 1-methyl-5-phenyltetrazole **19**. 10 mM in MTHF. at 266 nm (15 mJ per pulse. 6 K) for 10 min. Labeling of peaks as in the reference.¹ where a 5 mJ laser pulse was used: A (6404 G) and B (7109 G). X_2 and Y_2 transitions of *N*-methylbenzimidoylnitrene $\text{PhC(=NCH}_3\text{)-N}$ **20** ($|D/hc| = 0.9602$. $|E/hc| = 0.0144 \text{ cm}^{-1}$); C. methylnitrene $\text{CH}_3\text{-N}$ **23** (8265 and 8352 G. $|D/hc| = 1.611$. $|E/hc| = 0.0018 \text{ cm}^{-1}$). D. new signal ascribed to XY_2 transition of phenylnitrene **14a** (6859 G. $|D/hc| = 0.998$. $|E/hc| = 0.0012 \text{ cm}^{-1}$. Microwave frequency = 9.404459 GHz.

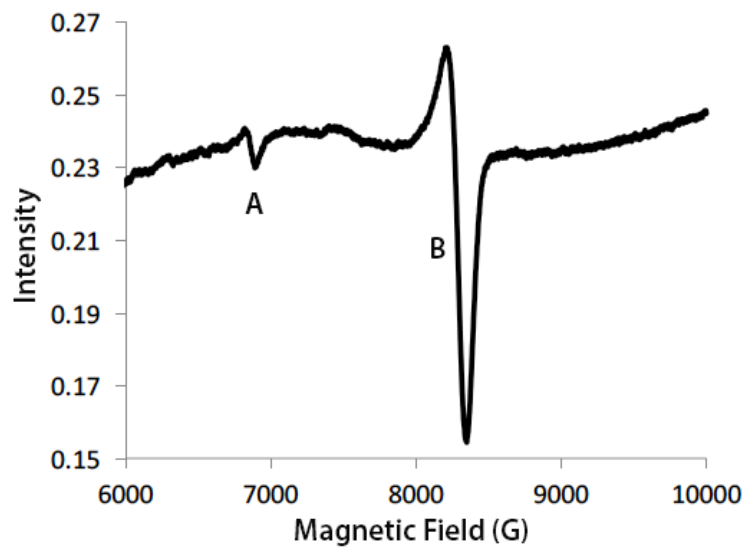


Figure S3. ESR spectrum resulting from photolysis of 2-methyl-5-phenyltetrazole **24**. 10 mM in MTHF. at 266 nm (15 mJ per pulse. 6 K) for 11 h (the spectrum was clearly observable after 1 h). A. phenylnirene **14a** ; B. methylnitrene **23**.

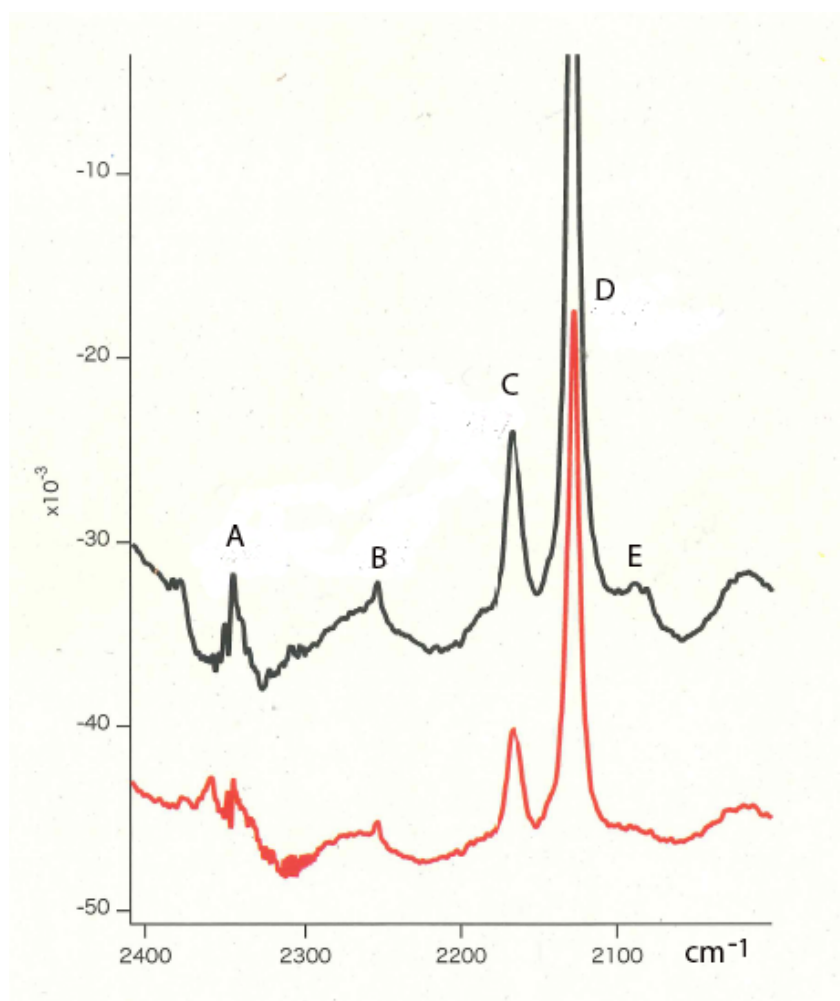


Figure S4. Ar matrix IR spectrum of the photolysis products from 1-phenyltetrazole **2a** in Ar at 10 K. Red (lower) trace: photolysis at 172 nm for 40 s. Black (upper trace): subsequent photolysis at 266 nm for 40 min. A: 2347 cm^{-1} (CO_2); B: 2256 cm^{-1} (PhNHCN ; NH stretch at 3404 cm^{-1} also present (not shown)); C: 2167 cm^{-1} ($\text{PhN}=\text{C}=\text{NH}$); D: 2129 cm^{-1} ($\text{PhN}=\text{C}=\text{NH}$); E: 2087 cm^{-1} (tentatively assigned to a trace of PhN_3 ; band at 1601 cm^{-1} also present (not shown)). Interpretations in agreement with the literature.²

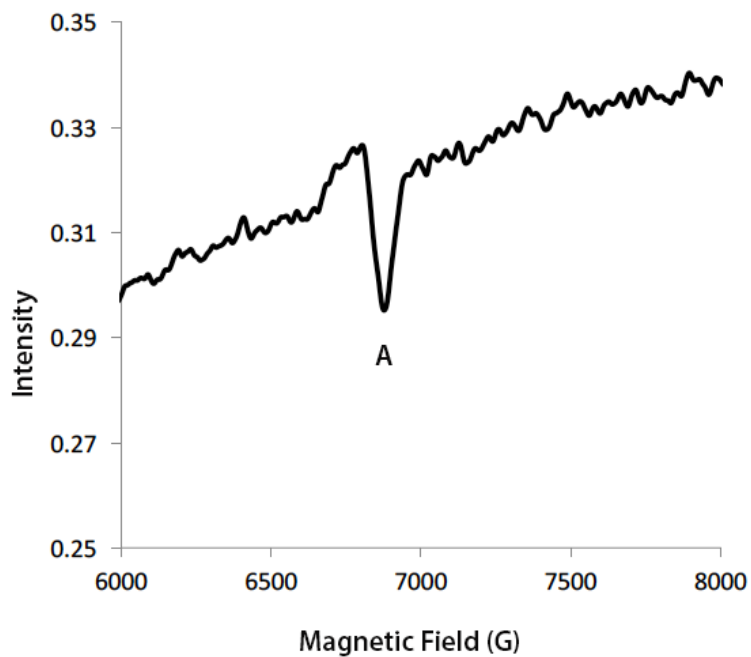


Figure S5. ESR spectrum resulting from photolysis of 5-amino-1-phenyltetrazole (10 mM in MTHF) for 2 h at 266 nm (5 mJ/pulse). A. XY_2 transition of phenylnitrene ($|D/hc| = 0.998$; $|E/hc| = 0.001 \text{ cm}^{-1}$).

Computational Methods. Ground-state geometries, energies and spin densities were determined at the DFT level using the (U)B3LYP exchange-correlation functional with the 6-311G(d,p) basis set. Calculations were performed using Gaussian 09 and Molpro program packages.^{3,4} Excited-states calculations were performed within the TDDFT U-B3LYP/6-311G(d,p) level of theory by using the Orca 3.0.3 software.⁵

5-phenyl-2H-tetrazole **1a**

Table S1. Spin densities in 5-phenyl-2H-tetrazole **1aT**

		alpha	beta	NPA
	n°	Nat. Charge	Nat. Charge	Spin Density
N	1	-0.17328	-0.05830	0.11498
C	2	0.08417	0.10914	0.02497
N	3	-0.32473	0.06158	0.38631
N	4	-0.15743	-0.04490	0.11253
N	5	0.00646	-0.03500	-0.04146
C	6	-0.22929	0.21363	0.44292
C	7	-0.19381	0.00185	0.19566
C	8	-0.11097	-0.12771	-0.01674
C	9	-0.39038	0.22385	0.61423
C	10	-0.08051	-0.16039	-0.07988
C	11	-0.23873	0.04365	0.28238
H	12	0.21398	0.20996	-0.00402
H	13	0.12399	0.11526	-0.00873
H	14	0.11383	0.11541	0.00158
H	15	0.11716	0.09917	-0.01799
H	16	0.11462	0.11438	-0.00024
H	17	0.12492	0.11842	-0.00650

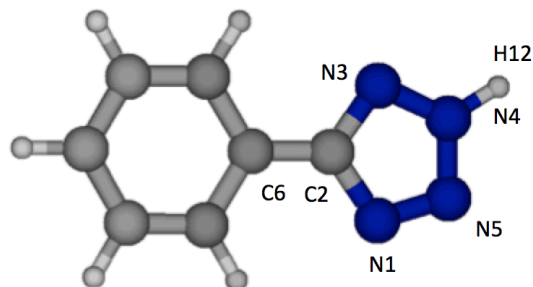


Figure S6. Structure of 5-phenyl-2H-tetrazole **1aT**

Table S2. Calculated absorption spectrum of 5-phenyl-2H-tetrazole **1aT**

State	Energy (cm ⁻¹)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	11432.5	874.7	0.002102402	0.06054	-0.22736	-0.06682	0.06622
2	12709.2	786.8	0.009232418	0.23915	-0.45025	-0.03924	0.18679
3	17298.6	578.1	0.002307710	0.04392	-0.01330	0.17672	0.11185
4	19008.5	526.1	0.000137003	0.00237	0.01809	-0.02320	0.03883
5	22238.8	449.7	0.056500801	0.83641	0.80327	0.41905	-0.12476
6	24406.0	409.7	0.000899286	0.01213	0.04102	-0.05237	0.08778
7	28052.5	356.5	0.002225186	0.02611	0.04677	-0.12222	-0.09481
8	29013.0	344.7	0.000002652	0.00003	0.00196	-0.00265	0.00439
9	30401.1	328.9	0.000044810	0.00049	0.00825	-0.01044	0.01756
10	31865.3	313.8	0.000020393	0.00021	-0.00628	0.00649	-0.01137
11	32980.5	303.2	0.000739765	0.00738	0.05396	0.06539	0.01401
12	35325.2	283.1	0.000037828	0.00035	0.00679	-0.00896	0.01504
13	36575.3	273.4	0.790962237	7.11940	2.32392	1.26961	-0.32694
14	38584.8	259.2	0.000002915	0.00002	-0.00200	0.00210	-0.00406
15	38701.2	258.4	0.071917693	0.61177	-0.59258	-0.50980	-0.02701
16	38731.5	258.2	0.000884610	0.00752	-0.03596	0.03792	-0.06919
17	39653.7	252.2	0.000393647	0.00327	0.02162	-0.02697	0.04553
18	41307.1	242.1	0.015706446	0.12518	0.31559	-0.01893	-0.15882
19	41532.5	240.8	0.001876038	0.01487	0.07211	-0.04335	0.08827
20	41544.6	240.7	0.015271445	0.12102	-0.30776	-0.14685	0.06882
21	45178.9	221.3	0.001397899	0.01019	-0.09341	-0.01287	0.03599
22	46211.9	216.4	0.000361576	0.00258	0.01947	-0.02432	0.04007
23	46641.6	214.4	0.076081930	0.53701	-0.65101	0.04811	0.33299
24	47030.3	212.6	0.001098004	0.00769	-0.03274	0.04180	-0.06976
25	47362.8	211.1	0.001923516	0.01337	0.04301	-0.05548	0.09188
26	47737.1	209.5	0.008337107	0.05750	-0.08955	0.11376	-0.19115
27	48093.0	207.9	0.016764794	0.11476	0.08876	0.29529	0.14031
28	48108.6	207.9	0.002029422	0.01389	0.04005	-0.06710	0.08821
29	49095.7	203.7	0.000047973	0.00032	0.00635	-0.00956	0.01378
30	49125.0	203.6	0.043651369	0.29253	-0.23522	0.36178	0.32606

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

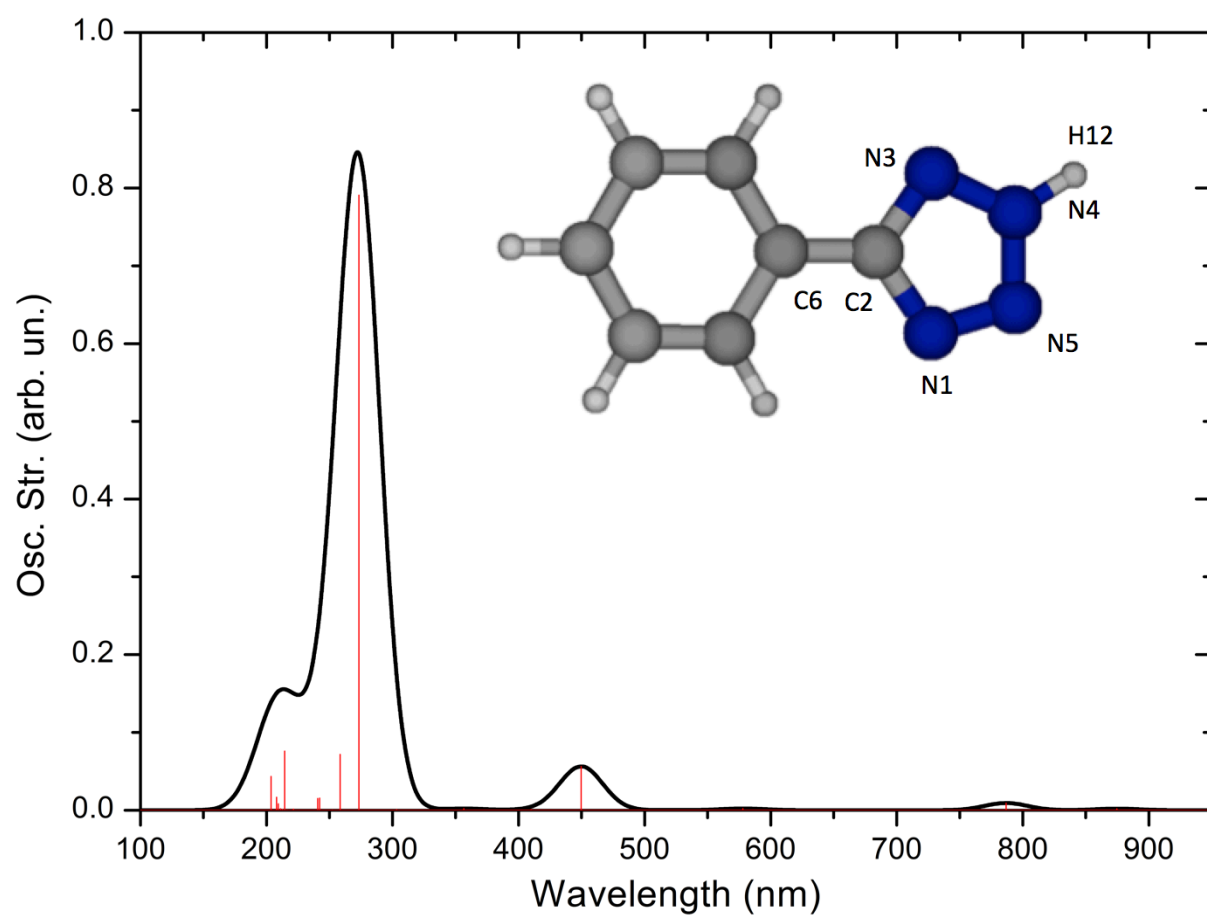


Figure S7. Calculated absorption spectrum of 5-phenyl-2H-tetrazole **1aT**

Table S3. Calculated absorption spectrum of 5-phenyl-2H-tetrazole **1aS**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	29350.7	340.7	0.000000000	0.00000	-0.00000	0.00000	0.00000
2	34624.4	288.8	0.000000000	0.00000	-0.00000	0.00000	0.00000
3	35333.7	283.0	0.000000000	0.00000	-0.00000	0.00000	-0.00000
4	37253.0	268.4	0.000000000	0.00000	0.00000	0.00000	0.00000
5	39191.6	255.2	0.000000000	0.00000	0.00000	-0.00000	-0.00000
6	39562.9	252.8	0.000000000	0.00000	0.00000	0.00000	-0.00000
7	40091.9	249.4	0.015137417	0.12430	0.30752	-0.04177	-0.16729
8	42396.4	235.9	0.124131014	0.96389	-0.85641	-0.46531	0.11803
9	43081.3	232.1	0.000000000	0.00000	0.00000	0.00000	-0.00000
10	44162.1	226.4	0.000000000	0.00000	-0.00000	-0.00000	0.00000
11	44751.6	223.5	0.070161658	0.51614	0.58952	0.40965	-0.02812
12	45479.4	219.9	0.000000000	0.00000	-0.00000	0.00000	-0.00000
13	45613.7	219.2	0.005429109	0.03918	-0.07393	0.09400	-0.15774
14	45617.9	219.2	0.000000000	0.00000	0.00000	0.00000	0.00000
15	45881.8	218.0	0.339372138	2.43507	-1.37436	-0.70763	0.21323
16	47787.8	209.3	0.000000000	0.00000	0.00000	0.00000	0.00000
17	49242.2	203.1	0.009493913	0.06347	0.09310	-0.12016	0.20091
18	50959.5	196.2	0.000025036	0.00016	0.00463	-0.00591	0.01027
19	51468.5	194.3	0.000000000	0.00000	0.00000	0.00000	0.00000
20	52448.9	190.7	0.000000000	0.00000	0.00000	0.00000	-0.00000
21	52580.5	190.2	0.000000000	0.00000	0.00000	0.00000	0.00000
22	53797.0	185.9	0.210391727	1.28750	0.19150	-0.91788	-0.63900
23	54646.8	183.0	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
24	55281.4	180.9	0.000245234	0.00146	0.01290	-0.01854	0.03082
25	55487.6	180.2	0.003204622	0.01901	-0.05338	0.06528	-0.10910
26	55816.1	179.2	0.000000000	0.00000	0.00000	0.00000	-0.00000
27	55878.7	179.0	0.372256295	2.19317	-1.35972	-0.47380	0.34617
28	56078.6	178.3	0.000000000	0.00000	0.00000	0.00000	-0.00000
29	56462.2	177.1	0.000000000	0.00000	0.00000	0.00000	-0.00000
30	56596.2	176.7	0.001273304	0.00741	-0.03175	0.04121	-0.06856

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

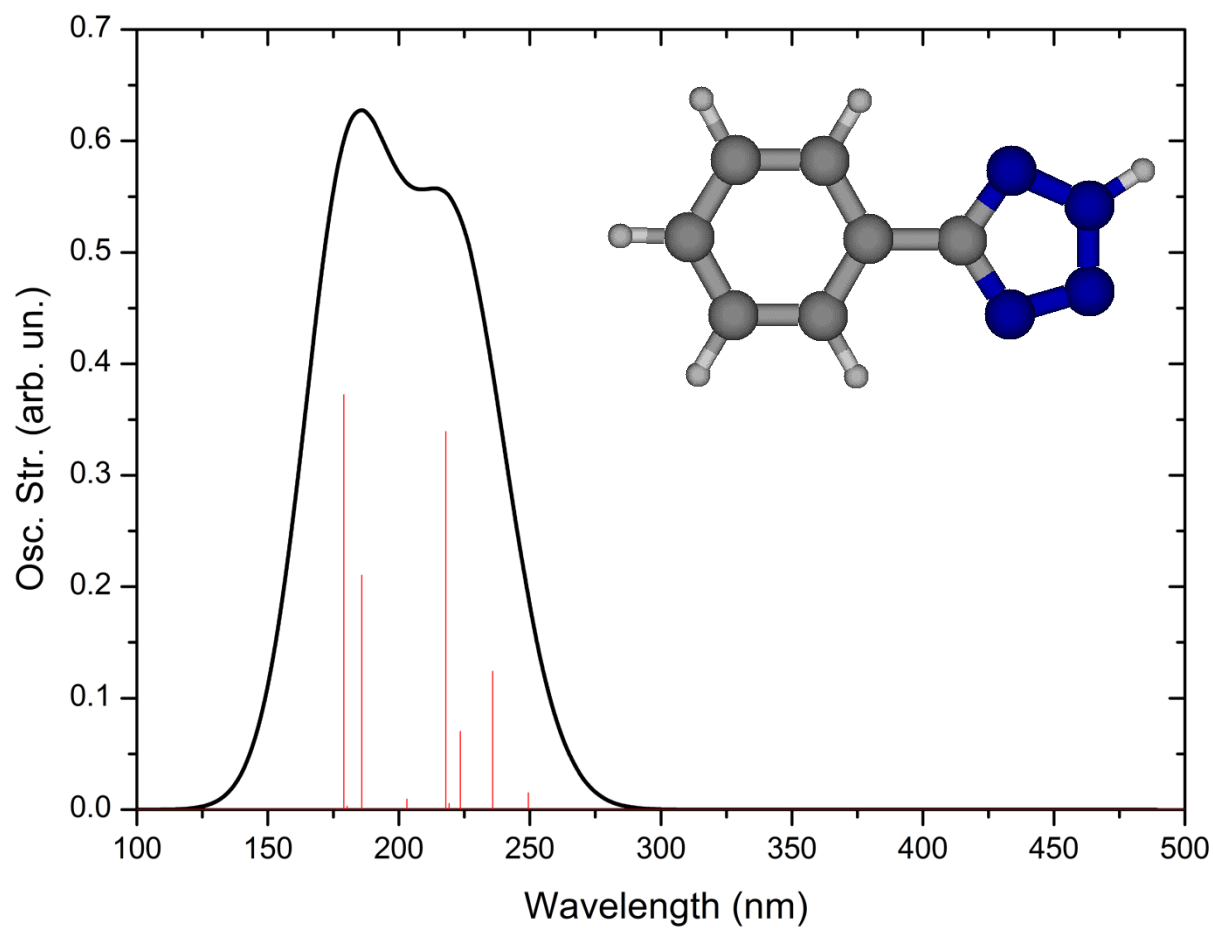


Figure S8. Calculated absorption spectrum of 5-phenyl-2H-tetrazole **1aS**

5-phenyl-1H-tetrazole **2a**

Table S4. Spin densities in 5-phenyl-1H-tetrazole **2aT**

		alpha	beta	NPA
	n°	Nat. Charge	Nat. Charge	Spin Density
N	1	-0.27362	-0.11462	0.15900
C	2	0.09503	0.15266	0.05763
N	3	-0.25284	0.00746	0.26030
N	4	0.00933	-0.06886	-0.07819
N	5	-0.16260	0.10543	0.26803
C	6	-0.22260	0.17373	0.39633
C	7	-0.22962	0.01366	0.24328
C	8	-0.08399	-0.13619	-0.05220
C	9	-0.38229	0.21192	0.59421
C	10	-0.08938	-0.15469	-0.06531
C	11	-0.21307	0.03958	0.25265
H	12	0.12824	0.12025	-0.00799
H	13	0.11579	0.11698	0.00119
H	14	0.11494	0.11586	0.00092
H	15	0.11036	0.10261	-0.00775
H	16	0.21764	0.21298	-0.00466
H	17	0.11868	0.10124	-0.01744

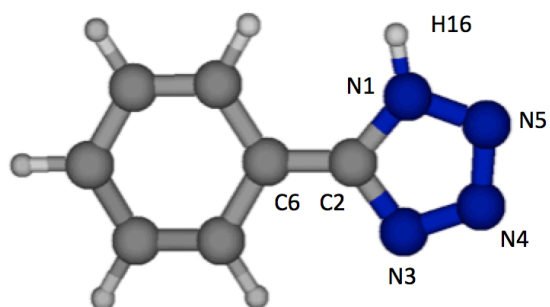


Figure S9. Structure of 5-phenyl-1H-tetrazole **2aT**

Table S5. Calculated absorption spectrum of 5-phenyl-1H-tetrazole **2aT**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	11645.7	858.7	0.000070602	0.00200	-0.04122	-0.01046	0.01368
2	12950.5	772.2	0.000385972	0.00981	0.03709	-0.03939	0.08297
3	16304.6	613.3	0.006603065	0.13333	-0.22816	0.20339	0.19976
4	18047.6	554.1	0.007334509	0.13379	-0.28639	-0.22648	0.02185
5	18912.1	528.8	0.000470540	0.00819	-0.03416	0.03579	-0.07578
6	22135.0	451.8	0.057993080	0.86253	-0.79240	-0.46413	0.13863
7	25979.1	384.9	0.024178746	0.30640	0.33189	0.43913	0.05842
8	26993.4	370.5	0.000110267	0.00134	0.01195	-0.01636	0.03057
9	28737.4	348.0	0.000016194	0.00019	0.00500	-0.00571	0.01131
10	32751.2	305.3	0.013531533	0.13602	-0.29511	-0.21922	0.02958
11	33598.4	297.6	0.000131614	0.00129	-0.01363	0.01452	-0.02989
12	34258.3	291.9	0.000006326	0.00006	-0.00307	-0.00517	0.00497
13	36358.7	275.0	0.877522838	7.94558	-2.39127	-1.43783	0.40005
14	36501.8	274.0	0.000030343	0.00027	-0.00650	-0.01055	0.01097
15	39745.9	251.6	0.000434304	0.00360	0.02293	-0.02356	0.05016
16	40060.6	249.6	0.000000857	0.00001	-0.00208	0.00016	-0.00165
17	40193.3	248.8	0.012193990	0.09988	-0.12655	0.23521	0.16894
18	40550.3	246.6	0.000683744	0.00555	0.02875	-0.02953	0.06207
19	41016.3	243.8	0.006233240	0.05003	-0.16152	-0.15473	-0.00046
20	42923.6	233.0	0.028286349	0.21695	0.40218	0.22208	-0.07669
21	43751.9	228.6	0.001553074	0.01169	0.03995	-0.04339	0.09059
22	45290.7	220.8	0.001017125	0.00739	-0.03272	0.03467	-0.07156
23	45723.0	218.7	0.005573897	0.04013	-0.04487	-0.18342	-0.06691
24	46910.7	213.2	0.072332606	0.50762	0.31419	-0.51079	-0.38471
25	47293.2	211.4	0.000339583	0.00236	-0.01856	0.01934	-0.04056
26	48250.6	207.3	0.000495970	0.00338	-0.02247	0.02301	-0.04847
27	49054.9	203.9	0.000502573	0.00337	0.02180	-0.02308	0.04863
28	49406.1	202.4	0.006018505	0.04010	-0.07579	0.07933	-0.16753
29	49854.8	200.6	0.046820770	0.30918	0.49730	0.21649	-0.12249
30	50009.3	200.0	0.000005643	0.00004	0.00195	0.00302	-0.00492

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

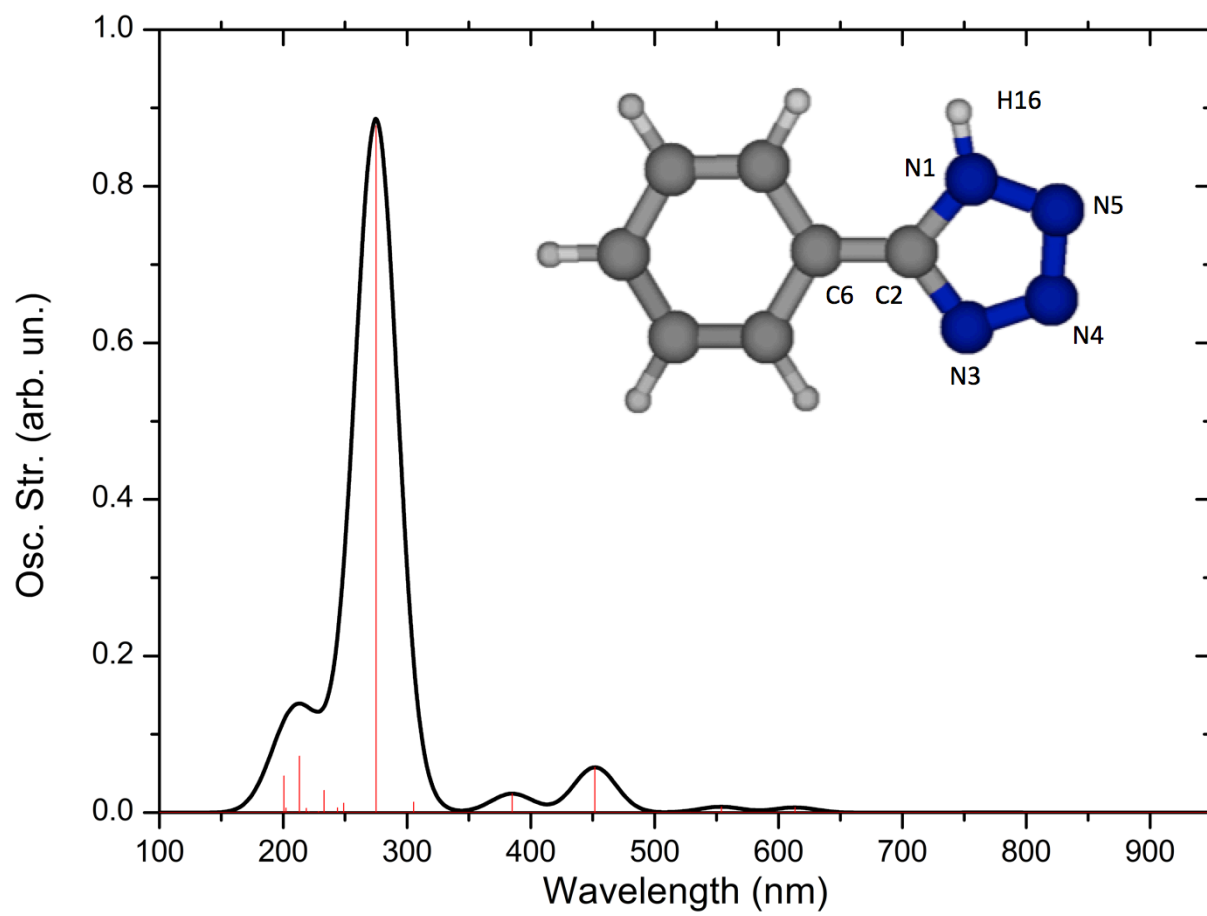


Figure S10. Calculated absorption spectrum of 5-phenyl-1H-tetrazole **2aT**

Table S6. Calculated absorption spectrum of 5-phenyl-1H-tetrazole **2aS**

State	Energy (cm ⁻¹)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	29043.0	344.3	0.000000000	0.00000	0.00000	-0.00000	0.00000
2	34962.8	286.0	0.000000000	0.00000	-0.00000	0.00000	-0.00000
3	36487.1	274.1	0.000000000	0.00000	0.00000	0.00000	-0.00000
4	38882.2	257.2	0.000000000	0.00000	0.00000	-0.00000	-0.00000
5	38933.2	256.9	0.000000000	0.00000	0.00000	0.00000	-0.00000
6	39668.8	252.1	0.000000000	0.00000	-0.00000	0.00000	0.00000
7	40214.6	248.7	0.017344606	0.14199	0.21511	0.30507	0.05148
8	40289.5	248.2	0.000000000	0.00000	0.00000	0.00000	-0.00000
9	41263.6	242.3	0.000707956	0.00565	-0.00564	-0.04353	0.06100
10	43258.8	231.2	0.000000000	0.00000	0.00000	0.00000	-0.00000
11	43288.4	231.0	0.539330138	4.10165	1.71975	1.03360	-0.27526
12	44156.8	226.5	0.000000000	0.00000	-0.00000	0.00000	-0.00000
13	44556.6	224.4	0.005037143	0.03722	0.00452	0.10555	-0.16142
14	47028.5	212.6	0.000000000	0.00000	-0.00000	-0.00000	0.00000
15	47335.5	211.3	0.000000000	0.00000	0.00000	-0.00000	0.00000
16	49969.4	200.1	0.003917518	0.02581	-0.03867	0.08206	-0.13259
17	50512.1	198.0	0.057338755	0.37370	0.17792	-0.49193	-0.31631
18	51103.2	195.7	0.000000000	0.00000	0.00000	0.00000	0.00000
19	51416.7	194.5	0.070758689	0.45306	0.01578	0.60716	0.29011
20	52087.2	192.0	0.000000000	0.00000	0.00000	0.00000	0.00000
21	52228.4	191.5	0.000000000	0.00000	0.00000	-0.00000	-0.00000
22	52294.6	191.2	0.001396929	0.00879	-0.04318	0.01216	-0.08235
23	52508.3	190.4	0.000176037	0.00110	0.00309	0.02988	-0.01418
24	53237.2	187.8	0.011973118	0.07404	-0.15890	0.06410	-0.21138
25	53441.4	187.1	0.000000000	0.00000	0.00000	0.00000	-0.00000
26	53527.3	186.8	0.167666788	1.03121	0.92071	0.32483	-0.27926
27	54548.3	183.3	0.000000000	0.00000	0.00000	0.00000	-0.00000
28	54847.9	182.3	0.120229277	0.72165	-0.74064	-0.38535	0.15688
29	54848.6	182.3	0.000000000	0.00000	0.00000	0.00000	-0.00000
30	55589.6	179.9	0.006908326	0.04091	-0.01664	0.08304	-0.18368

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

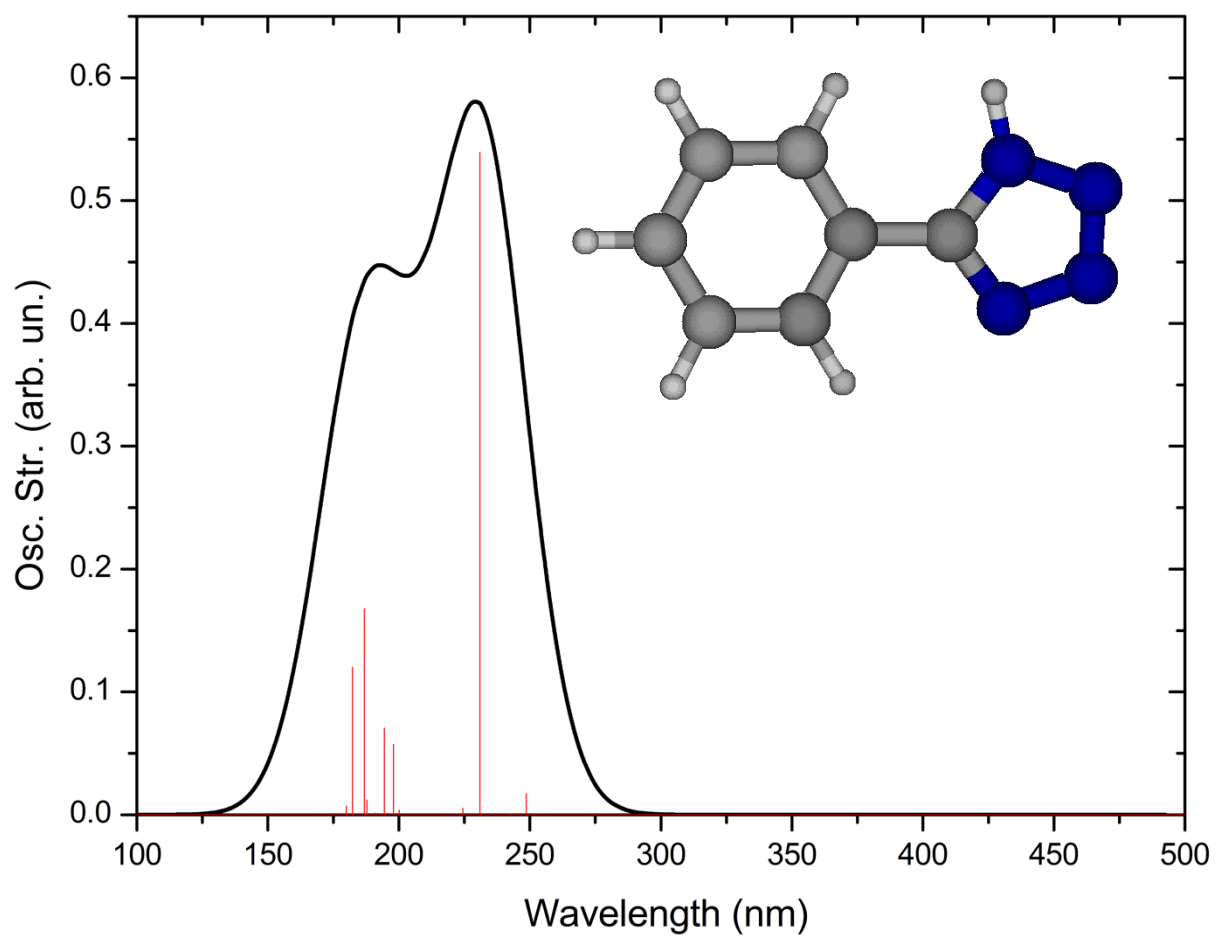


Figure S11. Calculated absorption spectrum of 5-phenyl-1H-tetrazole **2aS**

Table S7. Electronic energies (hartree) calculated at 0K for the phenyl-XH-tetrazole (X=1,2) systems

Reference energy = **1aS**

μ	State	Energy (u.a.)	
S	1aS	-489.438538	0.0
T	1aT	-489.319841	74.5
S	2aS	-489.433282	3.3
T	2aT	-489.316876	76.3
			kcal/mol

5-(*p*-tolyl)tetrazole **1b**

Table S8. Spin densities in 5-(*p*-tolyl)tetrazole **1bT**

		alpha	beta	NPA
	n°	Nat. Charge	Nat. Charge	Spin Density
C	1	-0.20624	-0.01135	0.19489
C	2	-0.10029	-0.12274	-0.02245
C	3	-0.29174	0.31207	0.60381
C	4	-0.10003	-0.12895	-0.02892
C	5	-0.21484	0.00680	0.22164
C	6	-0.21563	0.24530	0.46093
H	7	0.12335	0.11695	-0.00640
H	8	0.11277	0.11272	-0.01063
C	9	-0.31900	-0.34615	-0.45892
H	10	0.11286	0.11292	0.43192
H	11	0.12520	0.11792	0.00506
C	12	0.08871	0.09789	-0.02731
H	13	0.10132	0.13227	0.04356
H	14	0.09980	0.13434	0.03302
H	15	0.11383	0.11462	0.01482
N	16	-0.31947	0.04876	-0.06507
N	17	-0.15428	-0.05013	0.26934
N	18	0.00784	-0.04057	0.11371
N	19	-0.17750	-0.06232	-0.07016
H	20	0.21340	0.20967	0.38717

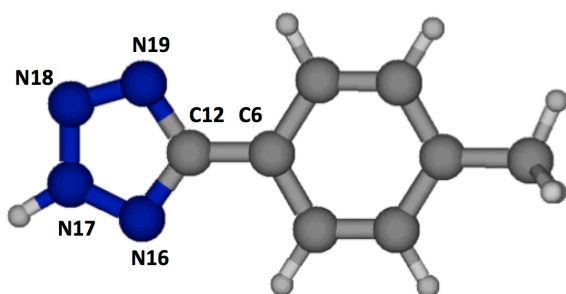


Figure S12. Structure of 5-(*p*-tolyl)tetrazole **1bT**

Table S9. Calculated Adsorption spectrum of 5-(*p*-tolyl)tetrazole **1bT**

State	Energy (cm ⁻¹)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	11269.4	887.4	0.008117668	0.23714	0.20815	-0.43969	0.02213
2	13194.8	757.9	0.006721982	0.16771	0.13245	-0.38714	0.01719
3	16816.6	594.7	0.001195798	0.02341	-0.15266	-0.00769	-0.00664
4	19972.5	500.7	0.000135506	0.00223	-0.00134	-0.00106	0.04723
5	21849.7	457.7	0.047176078	0.71081	-0.04772	0.84134	-0.02596
6	25492.6	392.3	0.000860900	0.01112	-0.00460	0.00295	0.10530
7	28847.8	346.6	0.002330076	0.02659	0.16187	0.01883	0.00590
8	29283.8	341.5	0.000051394	0.00058	0.00208	0.00056	0.02394
9	29648.2	337.3	0.000096136	0.00107	-0.00184	0.00533	0.03218
10	30868.6	324.0	0.001859966	0.01984	-0.00590	0.01503	0.13991
11	32908.8	303.9	0.000375178	0.00375	-0.02348	-0.05658	0.00105
12	35098.7	284.9	0.974786000	9.14311	-0.01910	-3.02226	0.09303
13	36020.0	277.6	0.001371126	0.01253	0.00059	-0.11003	-0.02062
14	36032.9	277.5	0.000900630	0.00823	-0.00105	-0.08764	0.02336
15	36318.7	275.3	0.000321346	0.00291	0.00567	0.02741	0.04614
16	37787.7	264.6	0.020188633	0.17589	-0.14858	-0.39215	0.00554
17	38836.9	257.5	0.000617659	0.00524	-0.00290	0.00150	0.07228
18	40069.2	249.6	0.000901302	0.00741	-0.00195	-0.00484	0.08589
19	41248.6	242.4	0.004893666	0.03906	-0.03582	0.19424	-0.00674
20	41475.5	241.1	0.000324920	0.00258	0.03867	0.03289	0.00122
21	43153.4	231.7	0.000093447	0.00071	0.00405	0.00236	0.02628
22	44285.4	225.8	0.015727624	0.11692	-0.05100	0.33810	0.00240
23	45292.9	220.8	0.001479533	0.01075	-0.01157	-0.03454	-0.09709
24	45828.2	218.2	0.018761897	0.13478	0.21412	0.29821	-0.00021
25	46217.9	216.4	0.069482825	0.49493	0.58915	-0.38297	0.03413
26	46266.2	216.1	0.000673578	0.00479	-0.03581	0.04336	-0.04038
27	47059.2	212.5	0.001696686	0.01187	-0.01365	-0.04586	0.09787
28	47230.5	211.7	0.005576579	0.03887	-0.00545	0.02408	0.19560
29	47697.1	209.7	0.003441992	0.02376	-0.00845	0.00039	0.15390
30	48298.9	207.0	0.003488695	0.02378	-0.15272	-0.02126	-0.00180

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

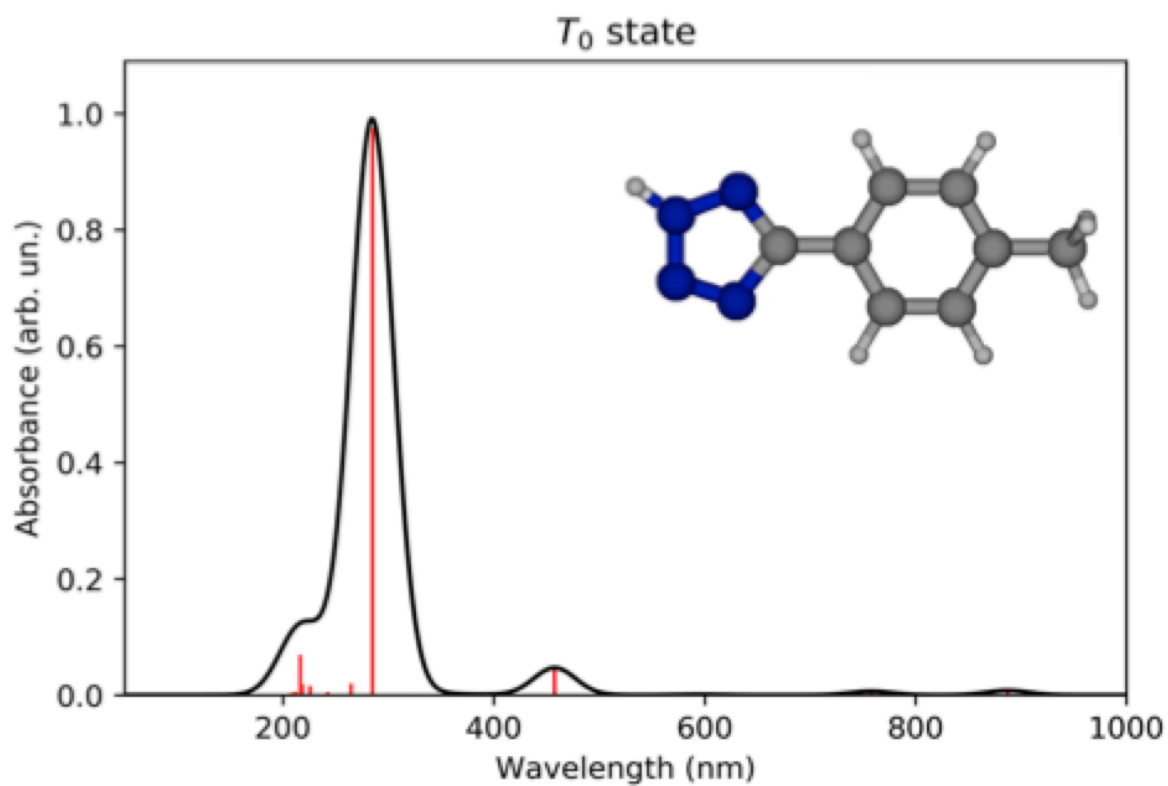


Figure S13. Calculated absorption spectrum of 5-(*p*-tolyl)tetrazole **1bT**

Table S10. Calculated adsorption spectrum of 5-(*p*-tolyl)tetrazole **1bS**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	27764.5	360.2	0.000000000	0.00000	-0.00000	0.00000	-0.00000
2	33995.4	294.2	0.000000000	0.00000	0.00000	-0.00000	0.00000
3	35528.9	281.5	0.000000000	0.00000	0.00000	-0.00000	0.00000
4	36975.8	270.4	0.000000000	0.00000	0.00000	-0.00000	0.00000
5	37490.9	266.7	0.000000000	0.00000	-0.00000	0.00000	0.00000
6	37993.0	263.2	0.000000000	0.00000	0.00000	0.00000	-0.00000
7	39334.5	254.2	0.010688786	0.08946	-0.14347	0.26193	-0.01646
8	40253.8	248.4	0.000000000	0.00000	0.00000	-0.00000	-0.00000
9	41453.9	241.2	0.394999741	3.13695	0.06760	-1.76886	0.05922
10	42472.0	235.4	0.000000000	0.00000	0.00000	-0.00000	-0.00000
11	42637.1	234.5	0.003851382	0.02974	-0.00686	-0.06268	0.16050
12	42736.8	234.0	0.000000000	0.00000	-0.00000	-0.00000	0.00000
13	43990.7	227.3	0.230575470	1.72555	0.05038	1.31227	-0.03098
14	45965.3	217.6	0.000000000	0.00000	-0.00000	0.00000	-0.00000
15	46531.0	214.9	0.098530486	0.69711	-0.30452	0.77648	-0.03829
16	46824.6	213.6	0.010735886	0.07548	-0.02446	0.01512	0.27323
17	47302.9	211.4	0.000000000	0.00000	0.00000	-0.00000	0.00000
18	47597.9	210.1	0.000331470	0.00229	-0.00878	0.01896	0.04308
19	49753.2	201.0	0.000000000	0.00000	0.00000	0.00000	0.00000
20	50376.5	198.5	0.000000000	0.00000	0.00000	0.00000	-0.00000
21	51280.7	195.0	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
22	52299.6	191.2	0.202459009	1.27442	1.00517	0.51382	0.00709
23	52518.2	190.4	0.005287207	0.03314	-0.09334	-0.06173	-0.14360
24	52881.5	189.1	0.000000000	0.00000	0.00000	-0.00000	0.00000
25	53332.0	187.5	0.002041752	0.01260	0.01948	-0.02288	-0.10817
26	53868.9	185.6	0.000000000	0.00000	-0.00000	0.00000	-0.00000
27	53952.8	185.3	0.000000000	0.00000	-0.00000	0.00000	0.00000
28	54062.6	185.0	0.126105072	0.76791	-0.44146	0.75568	-0.04440
29	54606.9	183.1	0.000417098	0.00251	-0.00275	0.01619	-0.04738
30	55371.9	180.6	0.000000000	0.00000	0.00000	-0.00000	-0.00000

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

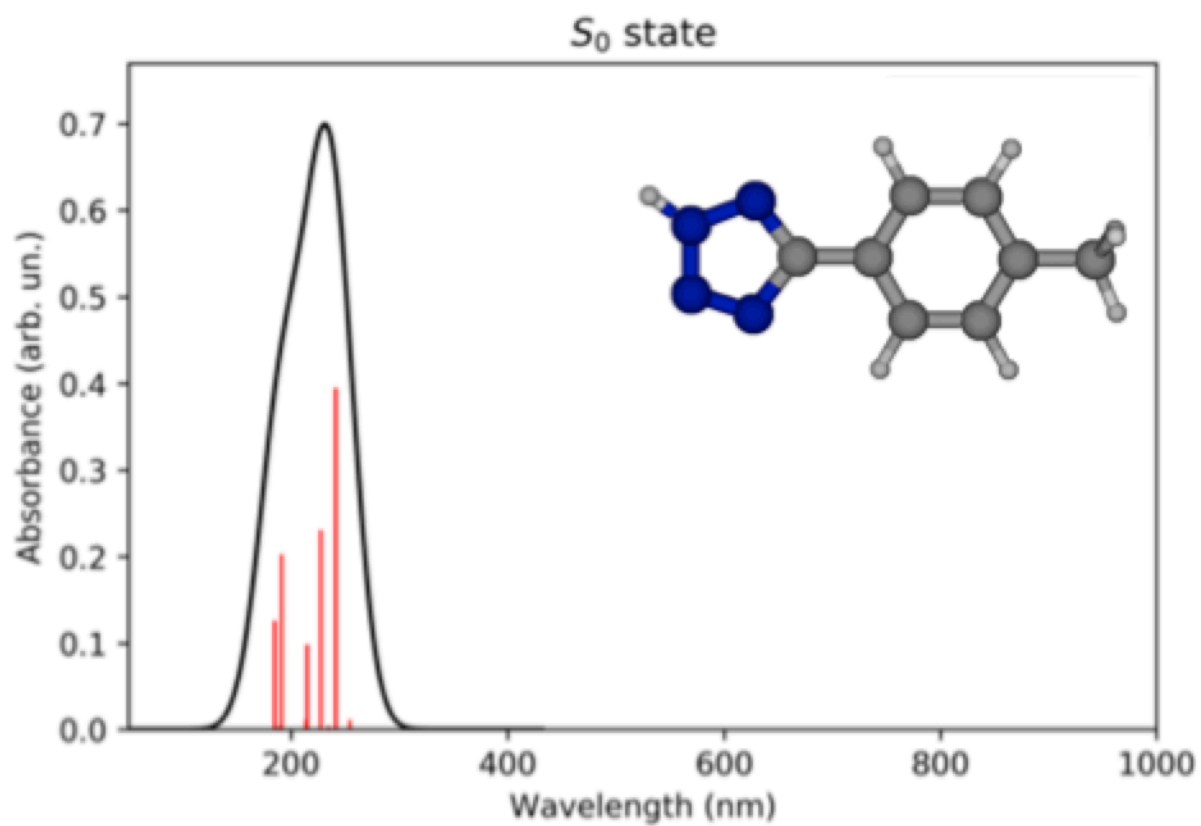


Figure S14. Calculated absorption spectrum of 5-(*p*-tolyl)tetrazole **1bS**

5-(*p*-tolyl)tetrazole **2b**

Table S11. Spin densities in 5-(*p*-tolyl)tetrazole **2bT**

		alpha	beta	NPA
	n°	Nat. Charge	Nat. Charge	Spin Density
C	1	-0.23536	-0.03201	0.20335
C	2	-0.20335	-0.10079	0.10256
C	3	0.01682	0.30210	0.28528
C	4	-0.23313	-0.14972	0.08341
C	5	-0.19453	0.03478	0.22931
C	6	0.00688	0.21627	0.20939
H	7	0.21406	0.10411	-0.10995
H	8	0.22707	0.11322	-0.10084
C	9	-0.66418	-0.34497	-0.57204
H	10	0.22915	0.11515	0.77933
H	11	0.24864	0.12013	-0.10902
C	12	0.23683	0.13521	-0.11343
H	13	0.23474	0.13293	-0.10390
H	14	0.23495	0.13358	-0.10116
H	15	0.23082	0.11574	-0.11921
N	16	-0.39232	-0.12075	-0.35157
N	17	-0.06297	0.08746	0.47978
N	18	-0.06396	-0.07144	-0.00847
N	19	-0.25973	-0.00356	0.06040
H	20	0.42960	0.21258	0.47231

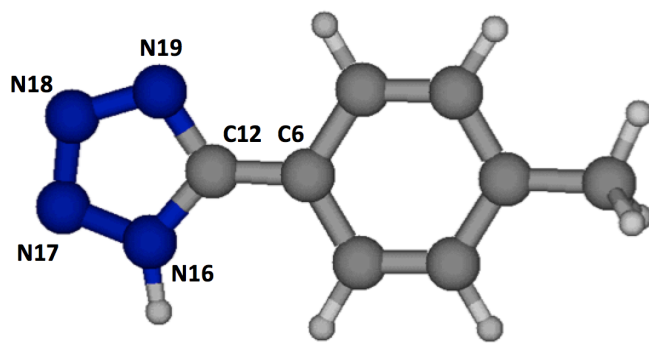


Figure S15. Structure of 5-(*p*-tolyl)tetrazole **2bT**

Table S12. Calculated adsorption spectrum of 5-(*p*-tolyl)tetrazole **2bT**

State	Energy (cm ⁻¹)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	12124.1	824.8	0.001063632	0.02888	-0.10830	0.12492	-0.03931
2	14029.2	712.8	0.000396996	0.00932	0.02650	-0.00619	-0.09260
3	15866.5	630.3	0.004137590	0.08585	0.27928	-0.03311	0.08220
4	18120.4	551.9	0.009014738	0.16378	0.04448	0.40202	-0.01356
5	19646.4	509.0	0.000467433	0.00783	-0.02424	0.00523	0.08496
6	22176.7	450.9	0.067342040	0.99969	-0.02106	-0.99786	0.05929
7	26294.9	380.3	0.016011661	0.20047	-0.21835	0.38072	-0.08858
8	26346.6	379.6	0.000257317	0.00322	0.01896	-0.01324	-0.05177
9	28894.2	346.1	0.000000727	0.00001	-0.00010	0.00028	0.00286
10	32541.1	307.3	0.030675517	0.31034	-0.02559	0.55503	-0.04032
11	32613.9	306.6	0.001564125	0.01579	0.03337	0.00362	-0.12109
12	34416.0	290.6	0.000225130	0.00215	-0.01248	0.00647	0.04423
13	34832.8	287.1	0.965143643	9.12176	0.16833	3.01176	-0.15074
14	36813.1	271.6	0.000030703	0.00027	0.00473	0.00312	-0.01557
15	37859.1	264.1	0.000163092	0.00142	0.00791	-0.00909	-0.03568
16	38723.0	258.2	0.000015054	0.00013	-0.00309	0.00646	0.00876
17	39947.5	250.3	0.000487370	0.00402	0.01733	-0.00372	-0.06085
18	40168.2	249.0	0.002317702	0.01900	-0.11318	0.06937	-0.03706
19	40981.7	244.0	0.001464028	0.01176	-0.08060	0.06724	-0.02727
20	41022.5	243.8	0.000464064	0.00372	-0.01683	0.00440	0.05849
21	42526.2	235.1	0.029241242	0.22637	0.10448	0.46417	-0.00069
22	42651.3	234.5	0.000151191	0.00117	0.00709	-0.00434	-0.03313
23	44902.0	222.7	0.019428615	0.14245	-0.02308	0.37562	-0.02865
24	45381.6	220.4	0.001025945	0.00744	0.02370	-0.00646	-0.08270
25	45799.0	218.3	0.090180972	0.64824	-0.71786	-0.31377	-0.18565
26	46913.7	213.2	0.001618908	0.01136	0.04632	-0.03415	-0.08971
27	47121.7	212.2	0.022056215	0.15409	0.21313	-0.31709	0.09012
28	47364.1	211.1	0.000103514	0.00072	0.01254	-0.00822	-0.02224
29	48316.4	207.0	0.000536142	0.00365	0.01651	-0.00445	-0.05797
30	49078.6	203.8	0.004788034	0.03212	-0.04943	0.01240	0.17181

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

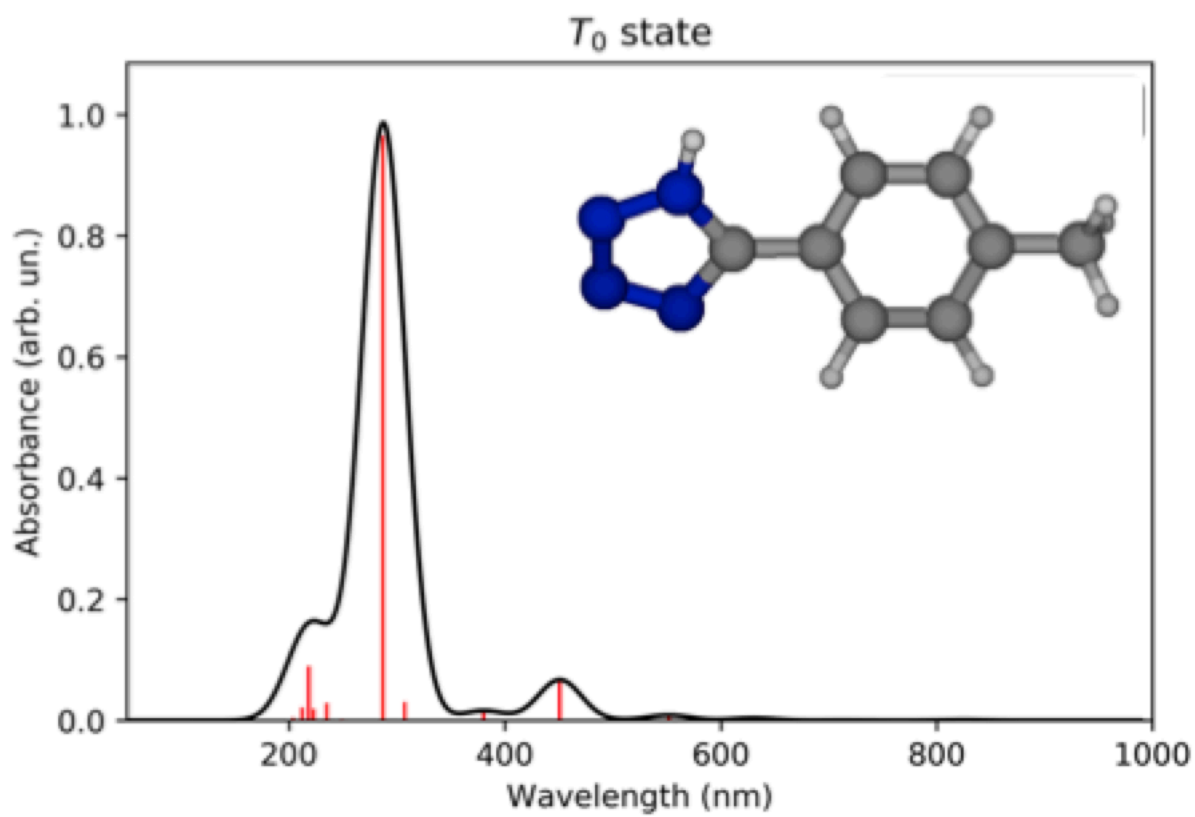


Figure S16. Calculated absorption spectrum of 5-(*p*-tolyl)tetrazole **2bT**

Table S13. Calculated adsorption spectrum of 5-(*p*-tolyl)tetrazole **2bS**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	28436.5	351.7	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
2	35121.3	284.7	0.000000000	0.00000	0.00000	0.00000	-0.00000
3	36204.1	276.2	0.000000000	0.00000	-0.00000	0.00000	-0.00000
4	38021.8	263.0	0.000000000	0.00000	-0.00000	0.00000	-0.00000
5	39192.2	255.2	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
6	39592.1	252.6	0.000000000	0.00000	-0.00000	0.00000	-0.00000
7	39750.7	251.6	0.029225897	0.24205	0.06691	-0.48360	0.06081
8	39836.2	251.0	0.000000000	0.00000	0.00000	-0.00000	0.00000
9	41613.8	240.3	0.003033292	0.02400	0.01031	-0.14542	-0.05239
10	42204.9	236.9	0.630470457	4.91787	-0.10997	-2.21118	0.12822
11	43456.1	230.1	0.000000000	0.00000	0.00000	0.00000	0.00000
12	43943.1	227.6	0.000000000	0.00000	-0.00000	0.00000	0.00000
13	44907.6	222.7	0.004812253	0.03528	0.05009	-0.06955	-0.16713
14	47216.7	211.8	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
15	47300.2	211.4	0.000000000	0.00000	0.00000	0.00000	0.00000
16	49701.1	201.2	0.040270930	0.26675	0.43347	-0.21452	0.18120
17	50053.6	199.8	0.003776878	0.02484	-0.04880	0.04431	0.14317
18	50723.2	197.1	0.104556633	0.67861	-0.70984	0.29918	-0.29193
19	50890.1	196.5	0.000000000	0.00000	-0.00000	0.00000	-0.00000
20	50988.9	196.1	0.000000000	0.00000	0.00000	-0.00000	0.00000
21	51291.0	195.0	0.002073753	0.01331	-0.09174	0.05459	-0.04376
22	52177.8	191.7	0.002332383	0.01472	0.02046	0.01993	-0.11790
23	52258.5	191.4	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
24	52484.6	190.5	0.000000000	0.00000	0.00000	-0.00000	0.00000
25	52922.5	189.0	0.148126706	0.92144	0.17993	0.94287	-0.00805
26	53290.6	187.7	0.011448724	0.07073	0.04911	-0.10257	-0.24040
27	53643.4	186.4	0.000000000	0.00000	0.00000	0.00000	0.00000
28	54417.1	183.8	0.000000000	0.00000	0.00000	0.00000	-0.00000
29	54900.5	182.1	0.138919257	0.83303	-0.12854	-0.90361	0.00068
30	54959.2	182.0	0.000000000	0.00000	0.00000	0.00000	-0.00000

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

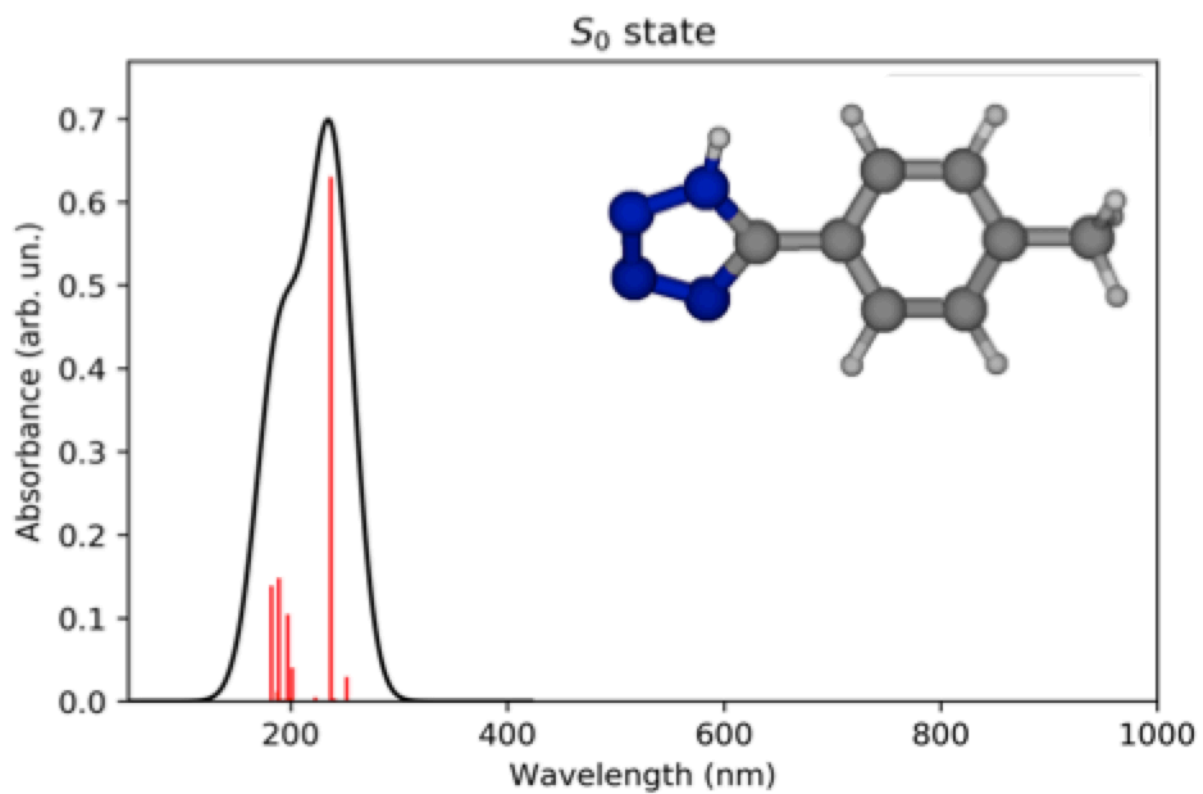


Figure S17. Calculated absorption spectrum of 5-(*p*-tolyl)tetrazole **2bS**

1-Phenyltetrazole **2d**

Table S14. Spin densities in 1-phenyltetrazole **2dT**

		Alpha	beta	NPA
	n°	Nat. Charge	Nat. Charge	Spin Density
C	1	-0.21927	-0.00729	0.21198
C	2	-0.16599	0.35917	0.52516
C	3	-0.21383	0.00772	0.22155
C	4	-0.10293	-0.13291	-0.02998
C	5	-0.40309	0.25138	0.65447
C	6	-0.10168	-0.12193	-0.02025
N	7	-0.11533	-0.08395	0.03138
N	8	-0.12239	-0.00295	0.11944
N	9	-0.09136	0.03045	0.12181
N	10	-0.15216	-0.13327	0.01889
C	11	-0.03532	0.14965	0.18497
H	12	0.11820	0.11141	-0.00679
H	13	0.11766	0.11733	-0.00033
H	14	0.11964	0.10056	-0.01908
H	15	0.11819	0.11804	-0.00015
H	16	0.13362	0.12660	-0.00702
H	17	0.11605	0.10999	-0.00606

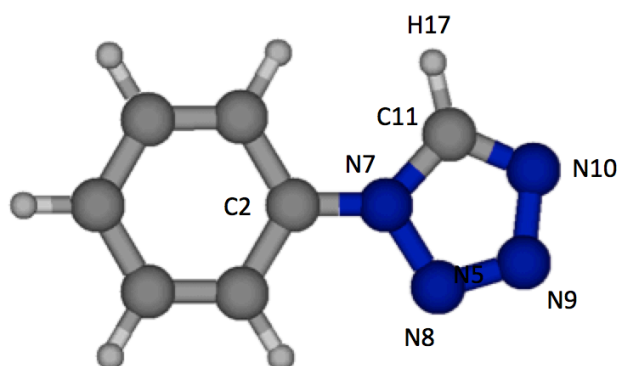


Figure S18. Structure of 1-phenyltetrazole **2dT**

Table S15. Calculated adsorption spectrum of 1-phenyltetrazole **2dT**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	8641.3	1157.2	0.001296261	0.04938	0.18219	0.11727	-0.04938
2	10262.9	974.4	0.000305592	0.00980	0.02890	0.09455	0.00531
3	13261.2	754.1	0.002062389	0.05120	-0.08908	-0.20653	-0.02463
4	15083.3	663.0	0.002925419	0.06385	-0.15815	0.19503	-0.02837
5	17192.4	581.7	0.046216432	0.88499	0.82023	0.45557	-0.06831
6	17566.1	569.3	0.009939277	0.18627	-0.41265	-0.12087	-0.03723
7	23716.8	421.6	0.012048193	0.16724	-0.13152	0.37751	0.08617
8	28327.3	353.0	0.107709185	1.25177	-1.02138	-0.44107	0.11834
9	29588.2	338.0	0.103555129	1.15220	-0.97799	-0.44226	-0.01178
10	30345.6	329.5	0.117059256	1.26995	-1.00163	-0.51614	0.01677
11	33376.9	299.6	0.008537147	0.08421	0.26211	0.11156	0.05530
12	33799.2	295.9	0.108406469	1.05590	-0.91500	-0.46738	0.01520
13	34250.7	292.0	0.003522875	0.03386	0.16809	0.04776	-0.05767
14	34810.3	287.3	0.232794353	2.20161	1.33562	0.64624	0.01082
15	37062.5	269.8	0.000826327	0.00734	0.07184	0.01589	-0.04389
16	37262.0	268.4	0.000706841	0.00624	0.07795	0.01018	0.00809
17	39276.3	254.6	0.017125854	0.14355	-0.34689	0.07697	0.13148
18	39584.6	252.6	0.000355322	0.00296	0.05197	-0.01336	0.00872
19	40121.1	249.2	0.006508087	0.05340	-0.19812	-0.08474	0.08347
20	40710.2	245.6	0.022157651	0.17918	0.25278	0.33615	-0.04780
21	41043.8	243.6	0.003038880	0.02437	-0.14303	0.05566	0.02863
22	41338.9	241.9	0.004932758	0.03928	-0.18052	-0.07004	-0.04231
23	42083.2	237.6	0.003141173	0.02457	0.09925	0.07387	0.09626
24	42336.6	236.2	0.003865139	0.03006	-0.04994	-0.13639	0.09465
25	43777.0	228.4	0.004258732	0.03203	-0.17650	-0.02777	0.01020
26	44441.1	225.0	0.001410734	0.01045	-0.07383	-0.07070	0.00109
27	45121.9	221.6	0.016021356	0.11689	0.26556	0.21390	0.02482
28	45469.8	219.9	0.005337337	0.03864	0.13948	-0.12764	-0.05381
29	45992.8	217.4	0.039597544	0.28344	-0.26643	0.44508	-0.11979
30	46593.2	214.6	0.015478237	0.10936	-0.04388	-0.32221	0.06018

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

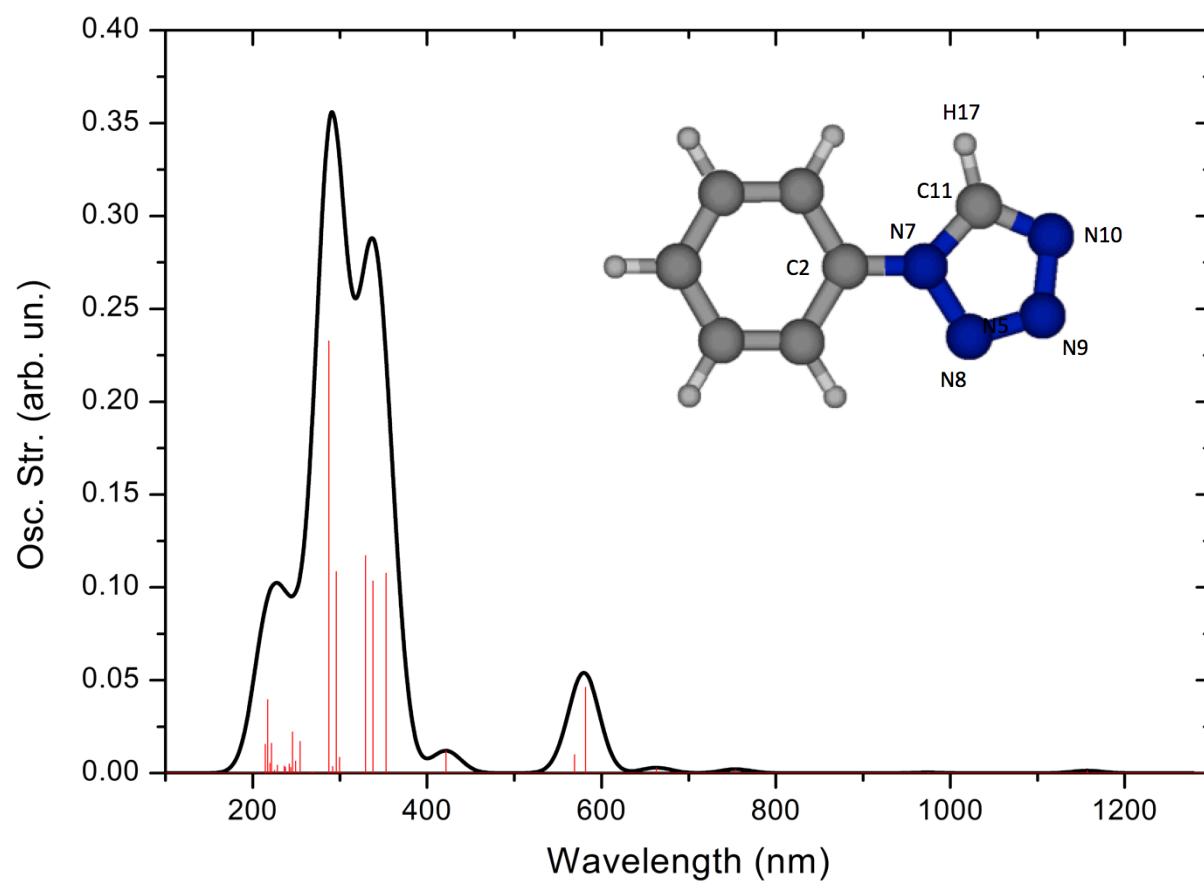


Figure S19. Calculated absorption spectrum of 1-phenyltetrazole **2dT**

Table S16. Calculated adsorption spectrum of 1-phenyltetrazole **2dS**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	31483.8	317.6	0.000000000	0.00000	0.00000	-0.00000	0.00000
2	36751.4	272.1	0.000000000	0.00000	-0.00000	0.00000	-0.00000
3	37055.6	269.9	0.000000000	0.00000	-0.00000	-0.00000	0.00000
4	38224.9	261.6	0.000000000	0.00000	0.00000	0.00000	-0.00000
5	39330.1	254.3	0.000000000	0.00000	0.00000	-0.00000	-0.00000
6	39868.4	250.8	0.000000000	0.00000	-0.00000	0.00000	-0.00000
7	41431.7	241.4	0.000000000	0.00000	0.00000	0.00000	-0.00000
8	41565.9	240.6	0.004098603	0.03246	0.14251	0.10586	-0.03078
9	42589.9	234.8	0.081956774	0.63351	0.71892	0.34129	-0.01337
10	43954.7	227.5	0.000000000	0.00000	0.00000	0.00000	-0.00000
11	44958.9	222.4	0.252890115	1.85179	1.24090	0.55817	-0.01995
12	45283.3	220.8	0.000000000	0.00000	0.00000	0.00000	-0.00000
13	45620.9	219.2	0.024749701	0.17860	0.25452	0.26326	-0.21099
14	48892.1	204.5	0.000000000	0.00000	0.00000	-0.00000	0.00000
15	50464.2	198.2	0.031107368	0.20293	-0.20731	0.39254	-0.07658
16	50469.0	198.1	0.000000000	0.00000	0.00000	-0.00000	0.00000
17	50658.3	197.4	0.000000000	0.00000	-0.00000	0.00000	-0.00000
18	51136.7	195.6	0.000000000	0.00000	0.00000	-0.00000	0.00000
19	51371.7	194.7	0.041476442	0.26580	-0.27935	0.39620	-0.17547
20	52207.8	191.5	0.014934582	0.09417	0.04618	0.27569	0.12663
21	52718.9	189.7	0.031289439	0.19539	0.43861	-0.02620	-0.04824
22	52824.9	189.3	0.000000000	0.00000	0.00000	0.00000	-0.00000
23	52890.1	189.1	0.009239912	0.05751	-0.02226	-0.22476	0.08062
24	53002.7	188.7	0.000000000	0.00000	0.00000	0.00000	-0.00000
25	53774.7	186.0	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
26	54659.6	183.0	0.027955481	0.16837	-0.19294	-0.29688	0.20739
27	54787.7	182.5	0.001736591	0.01043	0.01028	-0.06015	0.08192
28	54891.6	182.2	0.000000000	0.00000	-0.00000	-0.00000	0.00000
29	55558.4	180.0	0.158428628	0.93877	-0.83452	-0.49172	0.02341
30	55681.6	179.6	0.000000000	0.00000	-0.00000	-0.00000	-0.00000

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

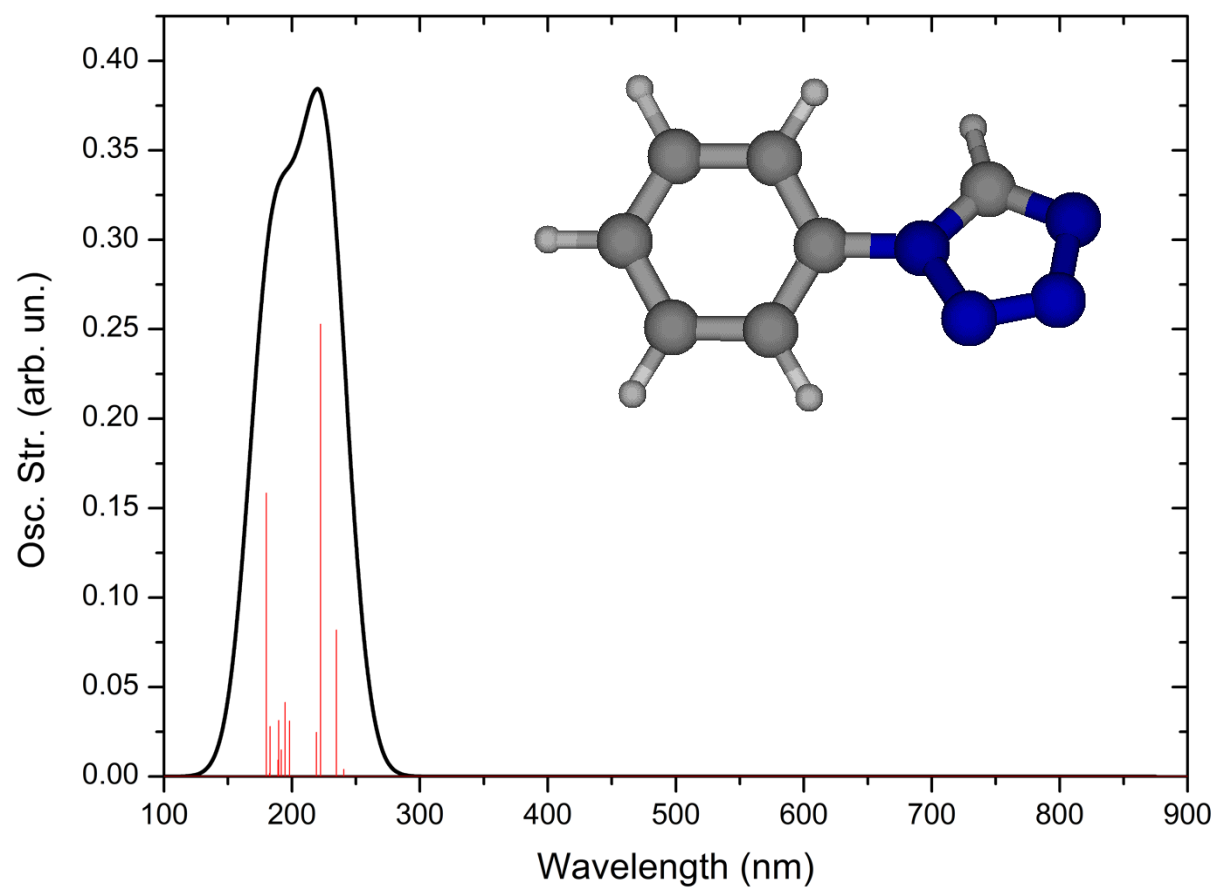


Figure S20. Calculated absorption spectrum of 1-phenyltetrazole **2dS**

Table S17. Electronic energies (hartree) calculated at 0K for both phenyl-1H-tetrazole and 1-phenyltetrazole systems.

Reference energy = **1aS**

μ	State	Energy (u.a.)	
S	1aS	-489.438538	0.0
T	1aT	-489.319841	74.5
S	2aS	-489.433282	3.3
T	2aT	-489.316876	76.3
S	2dS	-489.421959	10.4
T	2dT	-489.296985	88.8
			kcal/mol

Table S18. Cartesian coordinates for **2dT** (a) and **2dS** (b) 1-phenyltetrazole systems.

(a)

C	5.470990	0.598605	-0.670321
C	4.238676	1.405086	-0.708463
C	4.336411	2.876228	-0.797110
C	5.556491	3.454268	-0.841678
C	6.760831	2.661649	-0.804241
C	6.668263	1.221573	-0.717368
N	3.022569	0.818569	-0.663735
N	1.837785	1.555174	-0.697906
N	0.876133	0.695752	-0.638943
N	1.335932	-0.580204	-0.566788
C	2.644986	-0.508288	-0.581728
H	5.407486	-0.478950	-0.605300
H	7.581093	0.638204	-0.689921
H	7.730132	3.139898	-0.840901
H	5.639387	4.532703	-0.906778
H	3.417180	3.442189	-0.823352
H	3.327638	-1.336796	-0.538066

(b)

C	5.430971	0.664008	-0.486182
C	4.275103	1.424631	-0.659693
C	4.349349	2.795435	-0.904964
C	5.597932	3.403241	-0.979875
C	6.761471	2.651395	-0.824954
C	6.674077	1.283183	-0.579471
N	2.997253	0.799124	-0.587043
N	1.893417	1.463031	-0.153187
N	0.913754	0.633261	-0.219475
N	1.322560	-0.578431	-0.689690
C	2.608781	-0.455082	-0.910976
H	5.363230	-0.392866	-0.258921
H	7.573766	0.694374	-0.445544
H	7.731142	3.130426	-0.890038
H	5.659778	4.468691	-1.167295
H	3.436905	3.363249	-1.026240
H	3.262492	-1.212012	-1.309052

5-(3-pyridyl)tetrazole **28**

Table S19. Spin densities in 5-(3-pyridyl)tetrazole **28T**

		Alpha	beta	NPA Spin Density
n°	Nat. Charge	Nat. Charge		
C 1	-0.23102	0.01678		0.24780
C 2	-0.09778	-0.14581		-0.04803
C 3	-0.29884	0.32375		0.62259
N 4	-0.19939	-0.24949		-0.05010
C 5	-0.06259	0.17579		0.23838
C 6	-0.25645	0.19415		0.45060
H 7	0.12561	0.11762		-0.00799
H 8	0.11620	0.11683		-0.00878
H 9	0.11476	0.10586		-0.01034
C 10	0.09833	0.11372		-0.00104
N 11	-0.31465	0.05875		-0.03958
N 12	-0.15787	-0.04194		0.27271
N 13	0.01031	-0.03382		0.12405
N 14	-0.17403	-0.05596		-0.06627
H 15	0.11200	0.09245		0.26648
H 16	0.21540	0.21130		0.09930

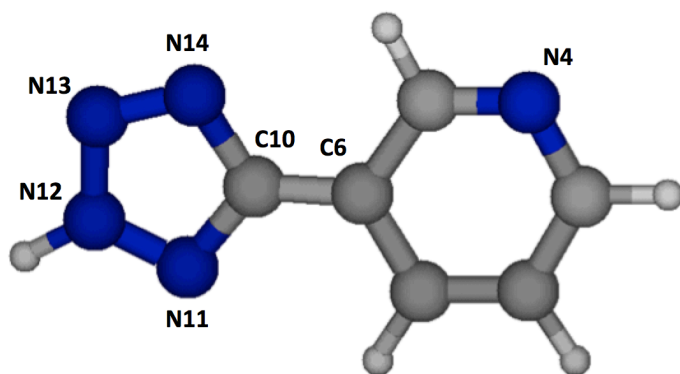


Figure S21. Structure of 5-(3-pyridyl)tetrazole **28T**

Table S20. Calculated adsorption spectrum of 5-(3-pyridyl)tetrazole **28T**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	8690.8	1150.6	0.000010112	0.00038	-0.00498	0.00028	0.01893
2	12053.6	829.6	0.002800150	0.07648	-0.22492	0.13779	-0.08308
3	14700.4	680.3	0.013618361	0.30498	-0.02268	-0.55005	0.04371
4	17454.4	572.9	0.017406788	0.32831	0.19664	-0.52680	0.11011
5	19069.0	524.4	0.000157531	0.00272	-0.01528	0.00380	0.04972
6	23867.9	419.0	0.023613227	0.32570	0.04337	0.56770	-0.03914
7	24410.3	409.7	0.000855682	0.01154	0.03156	-0.01005	-0.10219
8	27901.2	358.4	0.002612788	0.03083	0.16660	-0.01620	0.05301
9	31709.2	315.4	0.000058088	0.00060	-0.00738	0.00472	0.02294
10	34497.6	289.9	0.000141365	0.00135	0.00599	0.03189	-0.01720
11	34820.3	287.2	0.173497567	1.64035	0.06237	1.27552	-0.09748
12	35174.8	284.3	0.000227164	0.00213	0.01350	0.00444	-0.04387
13	35288.3	283.4	0.000009635	0.00009	-0.00291	0.00151	0.00889
14	37588.2	266.0	0.666117144	5.83410	0.04133	2.40609	-0.20772
15	37707.1	265.2	0.000391721	0.00342	0.00961	0.04750	-0.03273
16	38495.4	259.8	0.001752396	0.01499	0.03752	0.00999	-0.11610
17	38951.4	256.7	0.039989483	0.33799	-0.17055	-0.55578	-0.00338
18	39108.7	255.7	0.000707124	0.00595	-0.02326	-0.00464	0.07342
19	41241.6	242.5	0.000302373	0.00241	0.01376	-0.00523	-0.04687
20	41941.0	238.4	0.000097373	0.00076	-0.00770	0.00198	0.02648
21	42490.4	235.3	0.003134396	0.02429	0.14019	-0.04719	0.04904
22	42939.1	232.9	0.001404767	0.01077	0.03157	-0.00919	-0.09843
23	43570.0	229.5	0.001797621	0.01358	-0.03440	0.01094	0.11081
24	43983.7	227.4	0.005713557	0.04277	-0.19529	0.02472	-0.06338
25	45250.1	221.0	0.001169286	0.00851	-0.07626	0.04333	-0.02854
26	45988.7	217.4	0.000048354	0.00035	0.00576	-0.00165	-0.01761
27	46247.4	216.2	0.006808019	0.04846	0.06613	-0.01959	-0.20906
28	46912.4	213.2	0.000008117	0.00006	-0.00095	-0.00050	0.00747
29	47047.8	212.5	0.046378476	0.32453	-0.47762	0.25848	-0.17203
30	47786.9	209.3	0.000036473	0.00025	0.00356	-0.00155	-0.01537

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

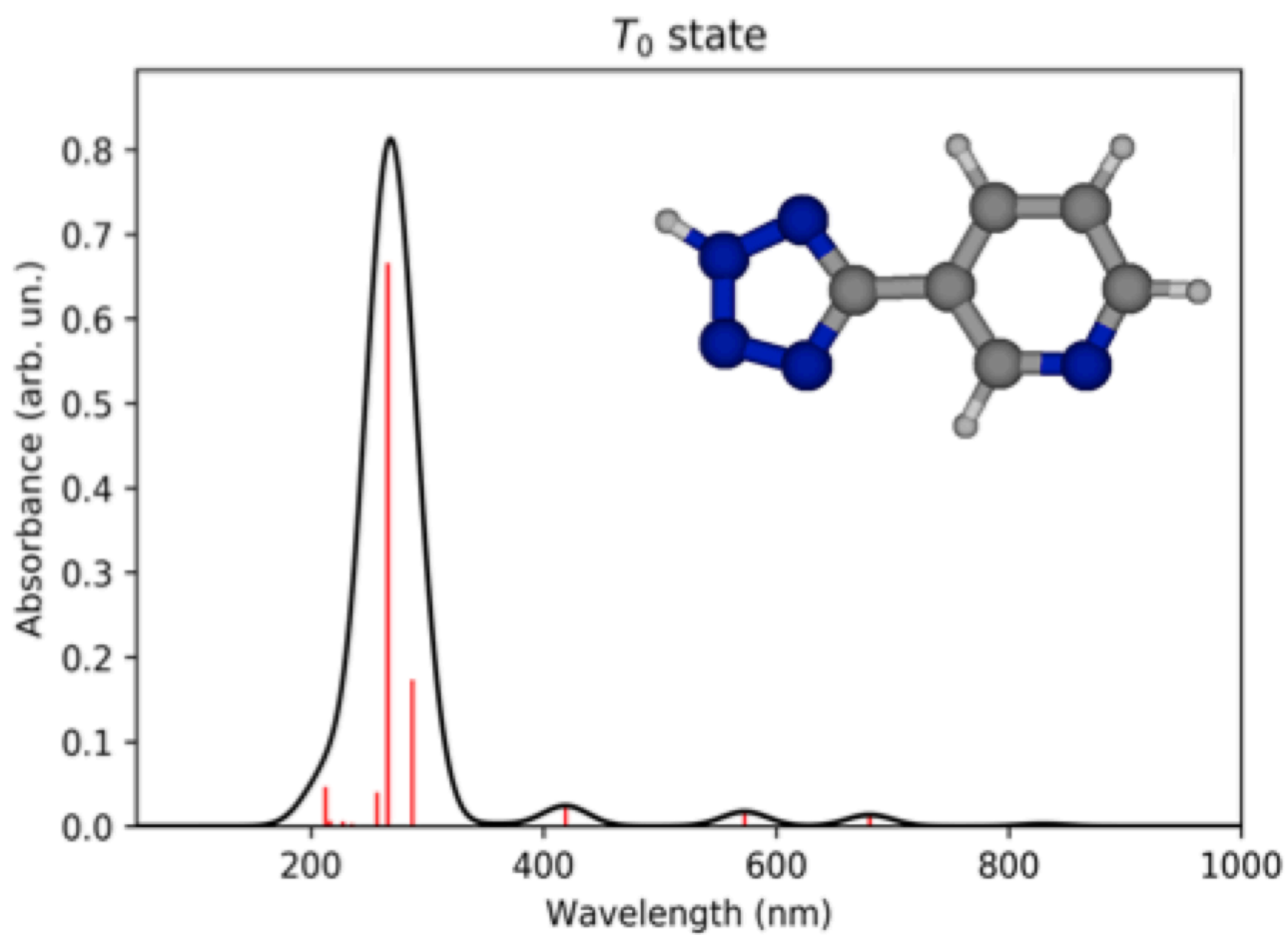


Figure S22. Calculated absorption spectrum of 5-(3-pyridyl)tetrazole **28T**

Table S21. Calculated adsorption spectrum of 5-(3-pyridyl)tetrazole **28S**

State	Energy (cm-1)	Wavelength (nm)	fosc (au**2)	T2 (au)	TX (au)	TY (au)	TZ (au)
1	29741.6	336.2	0.000000000	0.00000	0.00000	0.00000	-0.00000
2	32265.7	309.9	0.000000000	0.00000	0.00000	0.00000	-0.00000
3	34866.7	286.8	0.000000000	0.00000	-0.00000	-0.00000	0.00000
4	35803.0	279.3	0.001021592	0.00939	0.02873	-0.00870	-0.09216
5	36650.3	272.8	0.000000000	0.00000	-0.00000	-0.00000	0.00000
6	37062.1	269.8	0.000000000	0.00000	-0.00000	0.00000	-0.00000
7	37764.6	264.8	0.000000000	0.00000	0.00000	0.00000	0.00000
8	39020.5	256.3	0.000000000	0.00000	-0.00000	0.00000	0.00000
9	39479.4	253.3	0.002546661	0.02124	-0.04354	0.01331	0.13843
10	40959.8	244.1	0.102374706	0.82283	0.00177	0.90330	-0.08296
11	41732.4	239.6	0.000000000	0.00000	0.00000	-0.00000	-0.00000
12	43728.7	228.7	0.000000000	0.00000	0.00000	-0.00000	-0.00000
13	43824.9	228.2	0.000000000	0.00000	0.00000	-0.00000	0.00000
14	44256.8	226.0	0.004571912	0.03401	-0.05471	0.01567	0.17541
15	44612.6	224.2	0.000000000	0.00000	-0.00000	-0.00000	0.00000
16	45013.2	222.2	0.075952861	0.55549	-0.21360	0.70182	-0.13163
17	45240.2	221.0	0.000000000	0.00000	0.00000	0.00000	-0.00000
18	45501.1	219.8	0.342878433	2.48081	-0.05686	-1.56889	0.12710
19	45694.5	218.8	0.001411932	0.01017	0.03044	-0.00639	-0.09594
20	48814.1	204.9	0.000000000	0.00000	0.00000	-0.00000	0.00000
21	49201.4	203.2	0.010818986	0.07239	0.07988	-0.02330	-0.25586
22	49766.5	200.9	0.000000000	0.00000	0.00000	-0.00000	0.00000
23	50175.7	199.3	0.057472617	0.37709	0.25775	-0.54192	0.13032
24	50764.4	197.0	0.000018950	0.00012	0.00304	-0.00066	-0.01064
25	51517.7	194.1	0.000000000	0.00000	0.00000	0.00000	0.00000
26	52130.2	191.8	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
27	53766.7	186.0	0.000000000	0.00000	-0.00000	-0.00000	-0.00000
28	53943.5	185.4	0.119059286	0.72661	0.76444	0.31383	0.20916
29	54009.1	185.2	0.000213688	0.00130	-0.00010	0.00735	0.03533
30	54462.3	183.6	0.000000000	0.00000	-0.00000	0.00000	-0.00000

The 30 low-lying electronic excited states were calculated in a space dimension maximum set to 300. The UV-vis spectra were obtained by summing the electronic transitions so obtained, which were individually enveloped by 20 nm of FWHM real-space Gaussian functions in the 100-800 nm range.

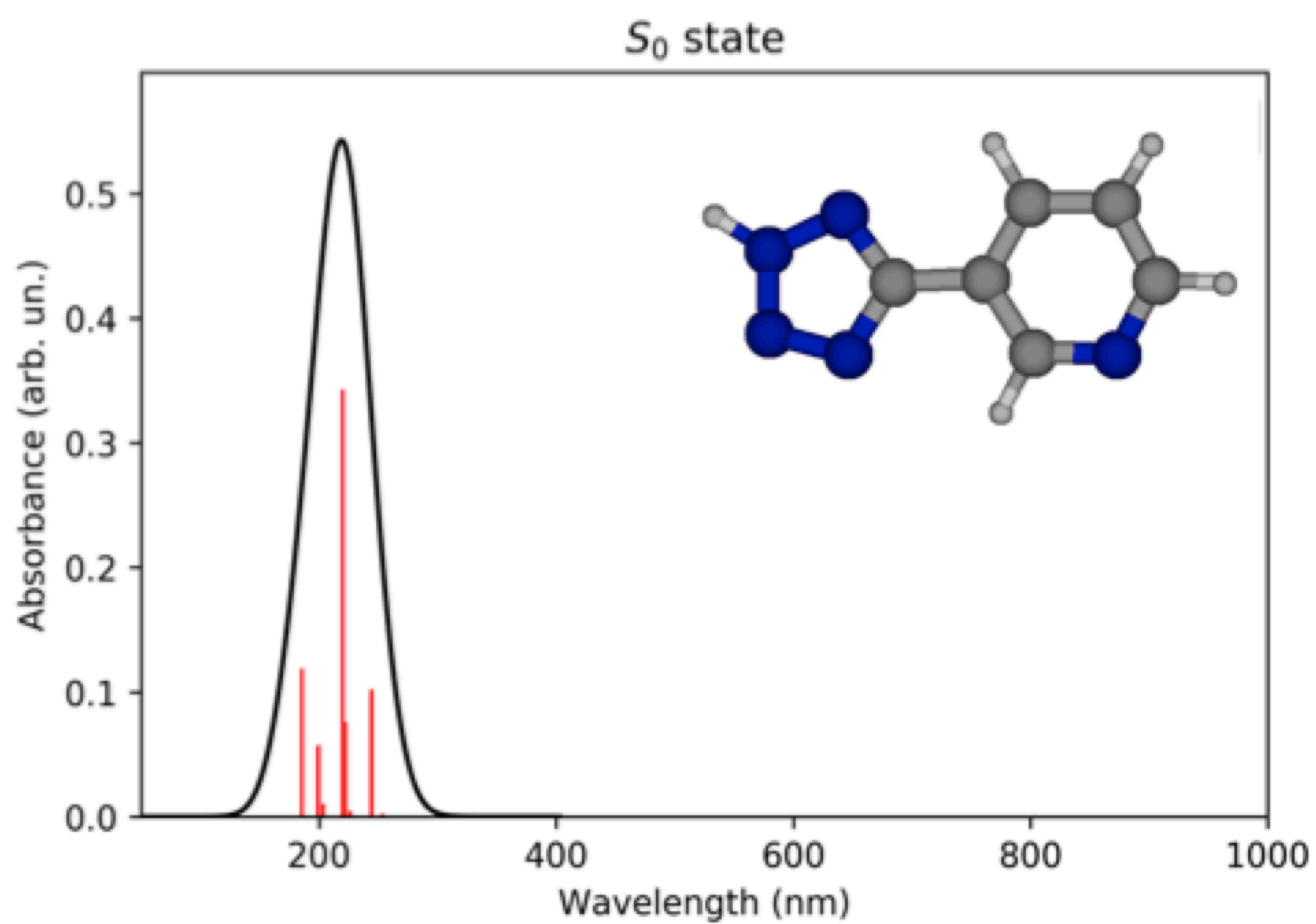
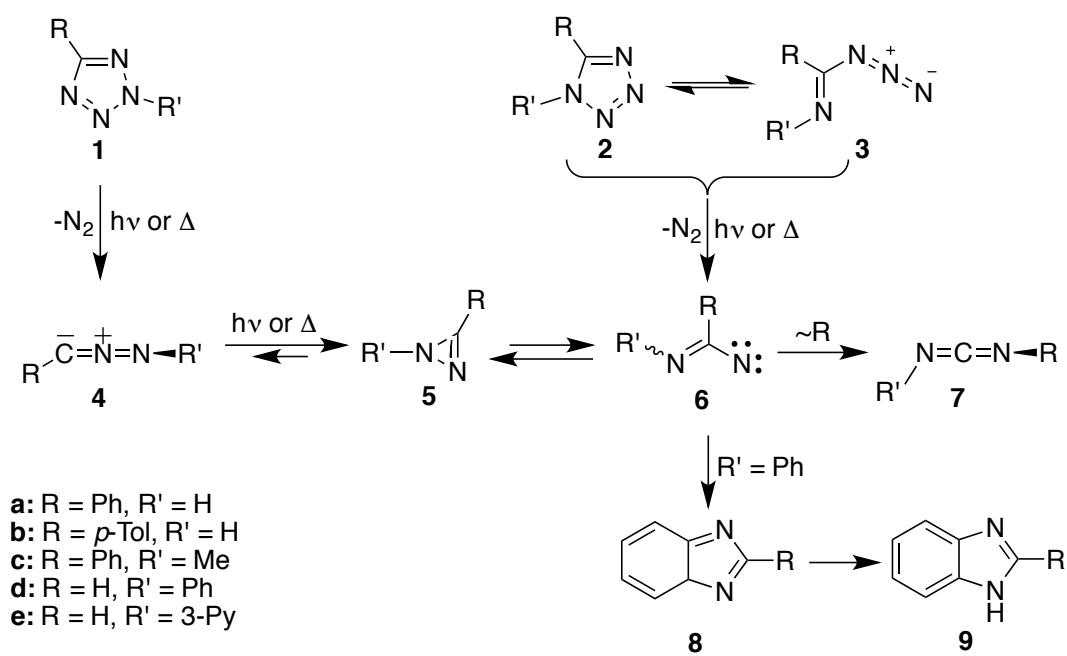


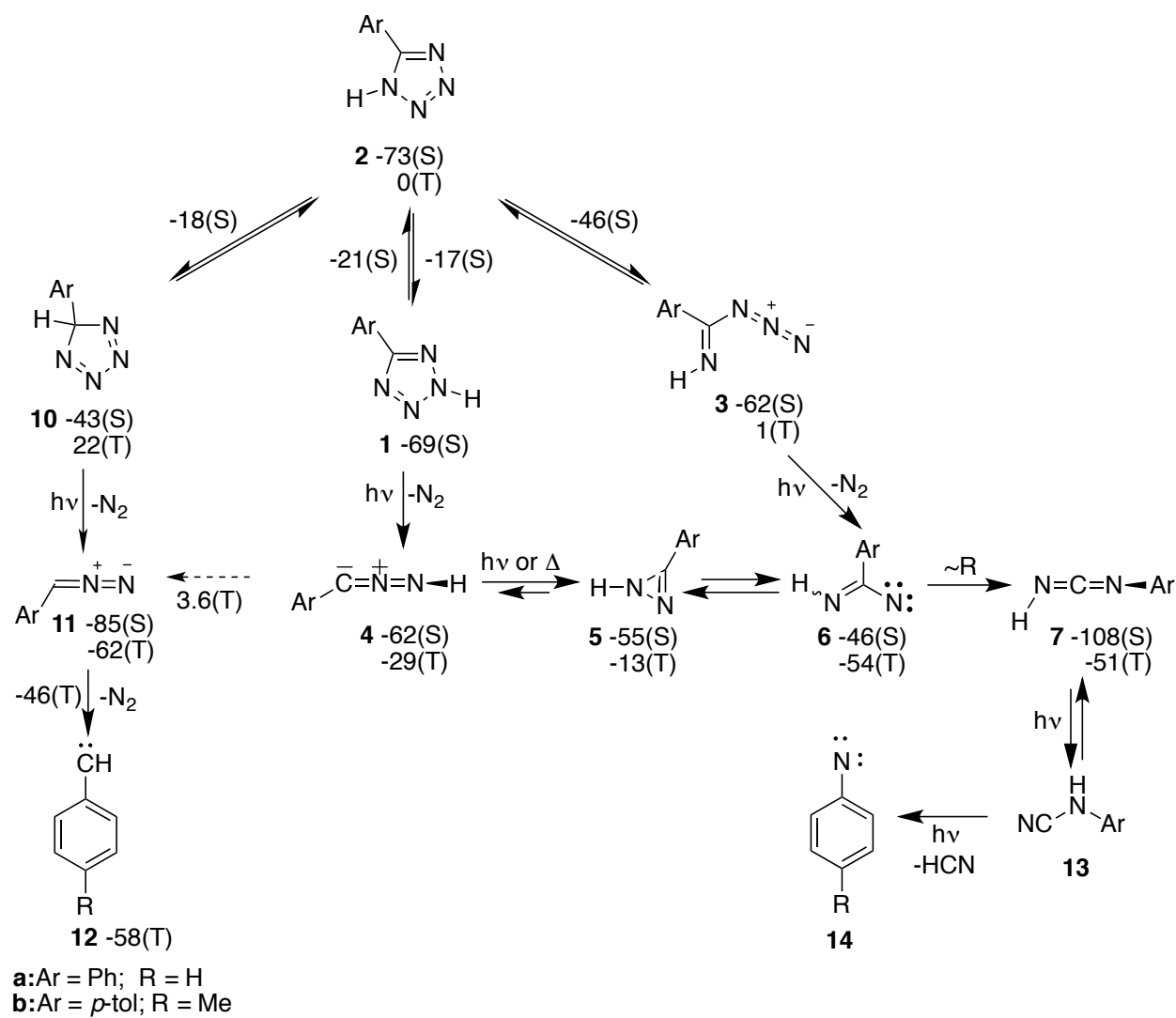
Figure S23. Calculated absorption spectrum of 5-(3-pyridyl)tetrazole **28S**

numbering summary:

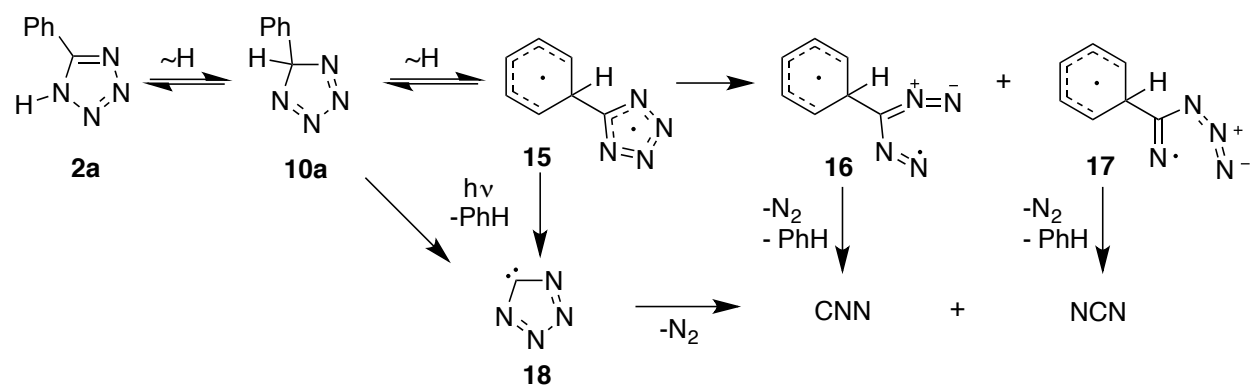
the numbering used in the paper is recalled below. This numbering is identical to the one used in the SI.



Scheme S1. Primary photochemical and thermal reactions of tetrazoles.



Scheme S2. Formation of arylcarbenes **11** and arylnitrenes **13** from 5-aryltetrazoles.



Scheme S3. Possible mechanism of formation of triplet CNN and NCN.

Table S22. Relative energies (kcal/mol) and transition states calculated at the U-B3LYP/6-311G(d,p) level of theory related to the photochemistry of 5-phenyl-1H-tetrazole **2a**.

Reference energy = **2aT**

μ	state	energy (u.a.)	kcal/mol	Slide															
				1		5	7	8	9	10	11	12	13	14	15	16	17	18	19
T	2a	-489.316876	0.0	1		5	7	8	9	10	11	12	13	14	15	16	17	18	19
T	10a	-489.279210	23.6	1		5	7	8	9	10	11	12	13	14	15	16	17	18	19
T	10a	-489.282371	21.7	1		5	7	8	9	10	11	12	13	14	15	16	17	18	19
T	TS 2a-10a	-489.212625	65.4	1															
T	TS 2a-50	-489.261600	34.7	1															
T	TS 10a-53	-489.240283	48.1	1															
T	TS 10a-53	-489.232171	53.2	1															
T	TS 2a-58	-489.234078	52.0	1															
D	H	-0.502156																	
S	N2	-109.555930																	
D	50	-488.764119	31.8	1	3														
S	benzene	-232.308539																	
D	benzene	-231.619424																	
D	53	-257.625633	45.1	1	3					10									
D	58	-257.613913	52.4	1	3														
D	TS 53-57	-257.624089	46.0	1															
D	TS 53-55	-257.595960	63.7	1															
D	57	-257.644435	33.3	1															
D	51	-488.759282	34.8	1															
D	55	-257.637879	37.4	1															
D	TS 57-54	-257.636527	38.2	1															
D	TS 51-52	-488.746442	42.8	1															
D	TS 55-56	-257.584081	71.1	1															
D	TS 53-57	-257.570371	79.7	1															
D	56	-148.170938	-18.5	1										14			17	18	
D	52	-379.240687	11.4	1															
D	54	-148.115703	16.2	1												16			
S	18	-256.929498	166.8		3														
S	TS 18-18''	-256.925353	169.4		3														
S	TS 18-18'	-256.916565	174.9		3														
S	18'	-256.917602	174.3		3														
S	TS 18'-NNC	-256.917600	174.3		3														
S	18''	-257.071263	77.8		3														
S	TS 18''-NCN	-257.024746	107.0		3														

S	10a	-489.385857	-43.3		4	7	8	9	10								
S	TS 10a-2a	-489.334972	-11.4		4					11							
S	2a	-489.433282	-73.0		4	7	8	9	10								
S	TS 10a-15	-489.305664	7.0		4	7	8	9	10								
S	15	-489.309629	4.5		4	7	8	9	10								
S	15	-489.315110	1.1		4	7	8	9	10								
T	15	-489.286427	19.1		4	7	8	9	10	11							
T	15	-489.286774	18.9		4	7	8	9	10	11							
S	TS 15-61	-489.311190	3.6		4												
S	TS 15-60	-489.314942	1.2		4												
S	60	-489.327265	-6.5		4												
S	61	-489.327553	-6.7		4												
T	61	-489.246426	44.2		4												
S	TS 15-11	-489.275075	26.2		4												
S	11	-379.896745	-85.2		4	5		9									
S	5a	-379.849101	-55.3			5	7										
S	64	-379.872297	-69.9			5											
S	65	-379.752078	5.6			5											
S	4a	-379.860106	-62.2			5	7										
S	4a	-379.859609	-61.9			5	7										
S	TS 4a-5a	-379.772293	-7.1			5	7										
S	TS 4a-64	-379.765562	-2.9			5	7										
S	TS 5a-65	-379.739895	13.2			5											
S	TS 11-65	-379.738928	13.8			5											
S	TS 4a-65	-379.670754	56.6			5											
S	TS 2a-3a	-489.389445	-45.5				7										
S	3a	-489.415033	-61.6				7										
S	TS 3a-6a	-489.361568	-28.0				7										
S	6a	-379.824641	-40.0				7										
S	6a	-379.833658	-45.6				7										
S	TS 6a-7a	-379.791194	-19.0				7										
S	TS 6a-5a	-379.830035	-43.4				7										
S	TS 6a-7a	-379.813756	-33.1				7										
S	7a	-379.932741	-107.8				7										
S	63	-324.573246						8									
S	NNNH	-164.830536	-54.5					8									
S	TS 2a-63	-489.357839	-25.7					8									
S	TS 10a-11	-489.385625	-43.1						9								
T	TS 10a-15	-489.216921	62.7							11							
T	TS 15-16	-489.278960	23.8							11							
T	TS 15-16	-489.281010	22.5							11							

T	16	-489.296207	13.0							11							
T	TS 16-66	-489.288742	17.7							11							
T	66	-379.770452	-6.0							11	12				16		
T	TS 15-17	-489.252670	40.3							11							
T	TS 15-17	-489.251320	41.1							11							
T	17	-489.292520	15.3							11							
T	17'	-489.286094	19.3							11							19
T	TS 17-67	-489.243715	45.9							11							
T	TS 17'-67	-489.240212	48.1							11							
T	67	-379.762009	-0.7							11	12						
T	TS 15-NNC	-489.243839	45.8							11							
T	TS 67-68	-379.725501	22.2								12						
T	68	-147.422662	18.7								12						
S	68	-147.466517	-8.9								12						
T	TS 68-NCN	-147.418564	21.2								12						
T	TS 68-NNC	-147.405388	29.5								12						
T	TS 66-NCN	-379.759089	1.2								12				16		
T	TS 10a -77	-489.253382	39.8									13					
T	77	-379.761882	-0.6									13					
T	TS 77-11	-379.715784	28.3									13					
T	TS 2a-69	-489.275195	26.2										14				
T	69	-489.332057	-9.5										14				
T	TS 69-6a	-489.320683	-2.4										14				
T	6a	-379.837688	-48.2										14			17	18
T	6a	-379.846431	-53.6										14			17	18
T	TS 6a-56	-379.784075	-14.5										14			17	
T	TS 69-62	-489.249398	42.3										14				
D	62	-488.752923	38.8										14				
T	TS 2a-70	-489.294767	13.9											15			
T	70	-489.296924	12.5											15			
T	TS 70-70'	-489.288085	18.1											15			
T	70'	-489.302552	9.0											15			
T	TS 70'-71	-489.287232	18.6											15			
T	71	-379.761882	-0.6											15			
T	TS 71-72	-379.727204	21.2											15			
T	72	-379.752655	5.2											15			
T	TS 71-11	-379.715783	28.3											15			
T	11	-379.859418	-61.8									13		15	16		18
T	TS 10a-11	-489.279250	23.6												16		
T	TS 11-4a	-379.755155	3.6												16		
T	TS 11-66	-379.726849	21.4												16		

T	TS 11-12a	-379.834280	-46.0													16			
T	12a	-270.296827	-57.6													16			
T	4a	-379.807604	-29.3													16	17	18	
T	4a	-379.799961	-24.5													16	17	18	
T	TS 2a-3a	-489.266649	31.5														17		
T	3a	-489.315834	0.7														17		
T	TS 3a-73	-489.244559	45.4														17		
T	73	-489.300493	10.3														17		19
T	TS 3a-6a	-489.312452	2.8														17		
T	TS 6a-5a	-379.751240	6.1														17	18	
T	5a	-379.780911	-12.5														17	18	
T	TS 4a-5a	-379.723922	23.2														17	18	
T	7a	-379.842160	-51.0														17	18	
T	7a	-379.836881	-47.7														17	18	
T	TS 6a-7a	-379.770491	-6.0															18	
T	TS 4a-72'	-379.748653	7.7															18	
T	72'	-379.768010	-4.4															18	
T	64	-379.775878	-9.4															18	19
T	64	-379.762289	-0.8															18	19
T	TS 5a-64	-379.720759	25.2															18	
T	TS 11-64	-379.774458	-8.5															18	
T	TS 7a-13	-379.775271	-9.0															18	
T	TS 13-76	-379.790041	-18.3															18	
T	TS 7a-76	-379.789992	-18.2															18	
D	76	-379.294436	-22.4															18	
T	13	-379.845664	-53.2															18	
T	13	-379.843450	-51.8															18	
S	13	-379.830655	-43.7																
T	TS 13-14	-379.812791	-32.5															18	
S	TS 13-14	-379.780020	-12.0																
T	14	-286.377175	-42.8															18	
S	14	-286.325246	-10.2																
S	HCN	-93.452018																	
T	TS 10a-73	-489.246419	44.2																19
T	TS 73-29	-489.286530	19.0																19
D	N3	-164.180985																	19
D	74	-325.124973	6.9																19
T	TS 73-17	-489.238038	49.5																19
T	TS 73-64	-489.241639	47.2																19
T	TS 64-75	-379.720320	25.5																19
D	75	-148.099792	26.2																19

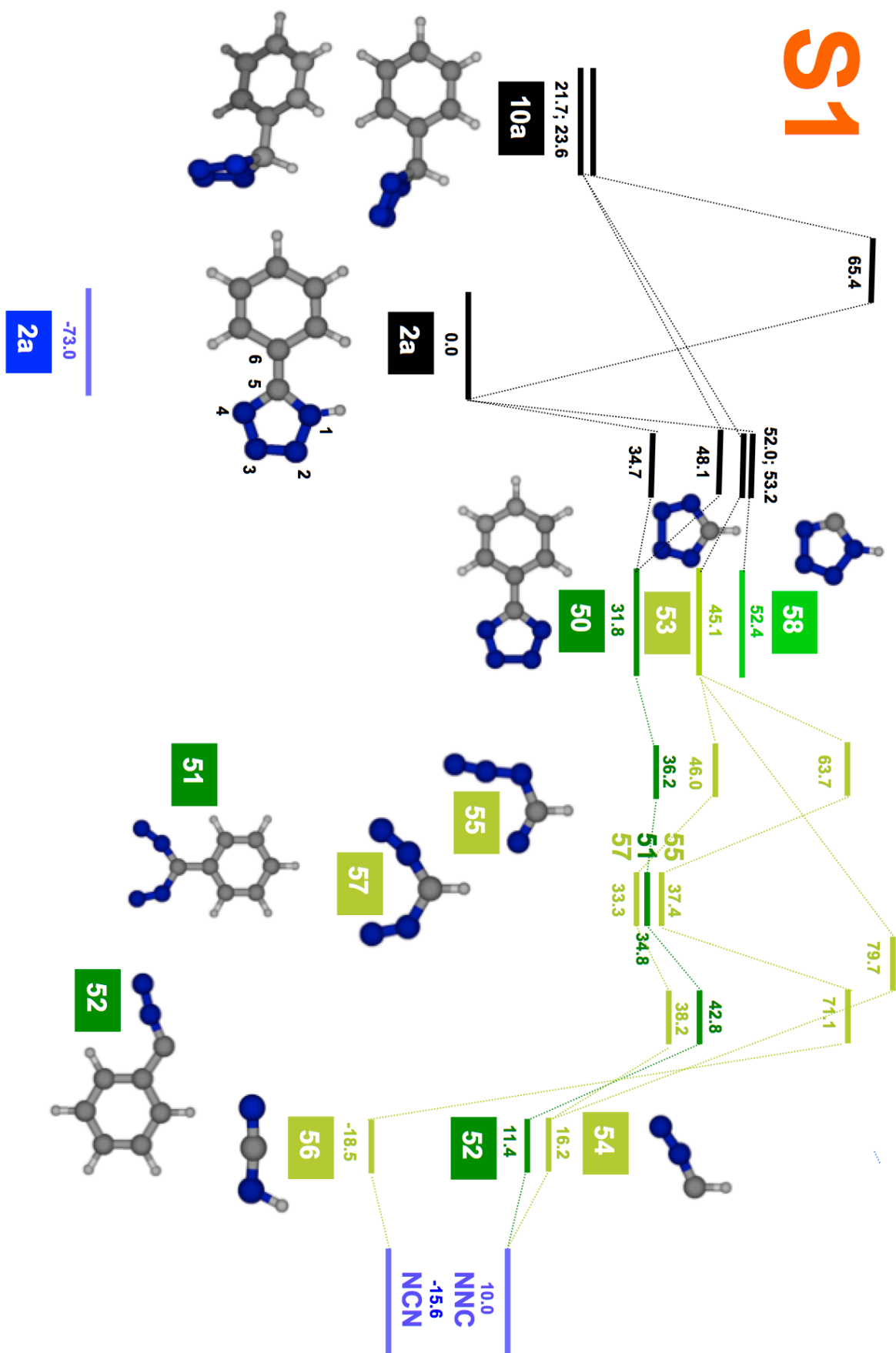


Figure S24. Reaction pathway (doublet) –slide 1 (green : doublet ; blue : singlet; black : triplet).

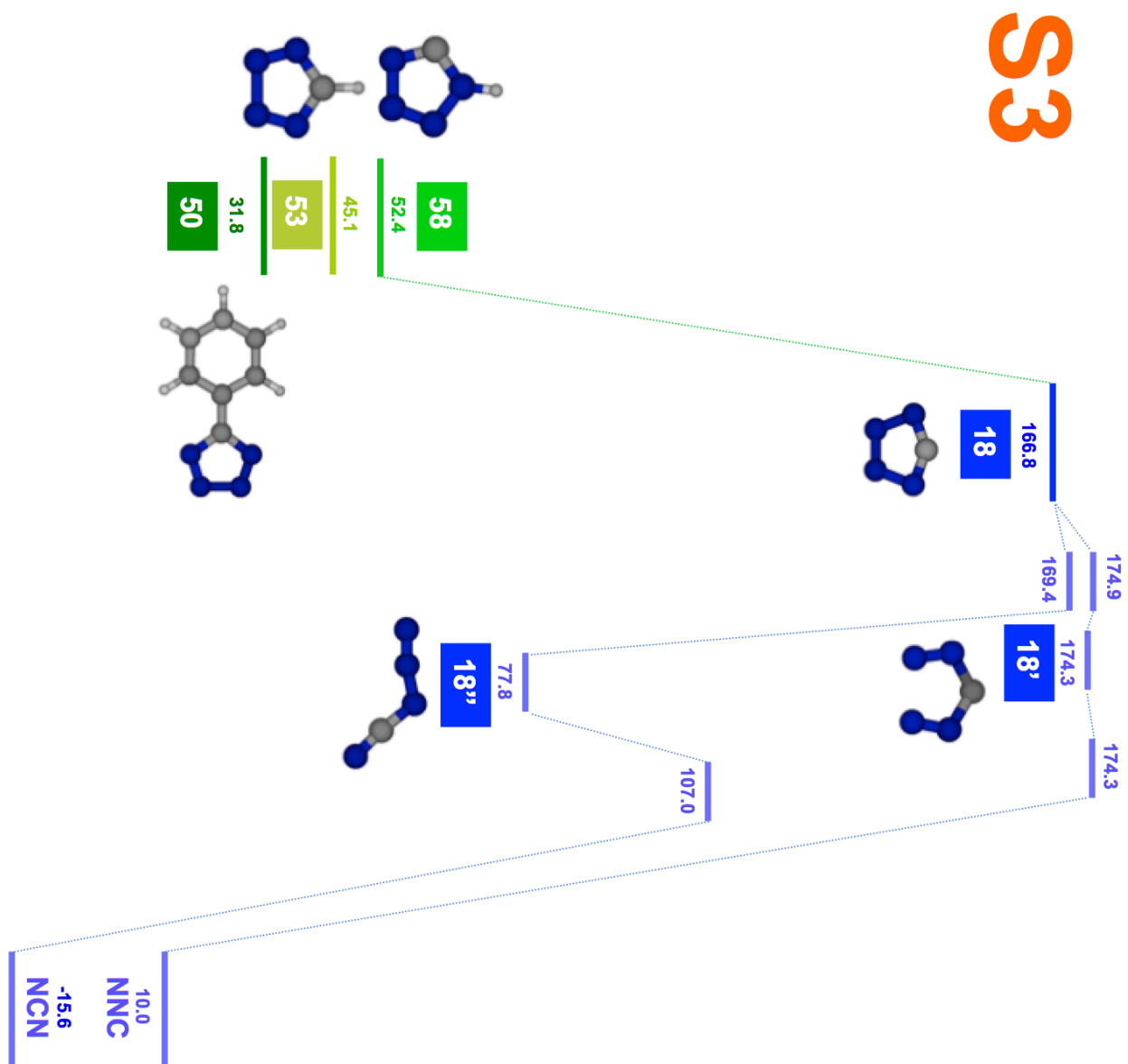


Figure S25. Reaction pathway (doublet) –slide 3 (green : doublet ; blue : singlet; black : triplet)

Singlet pathways

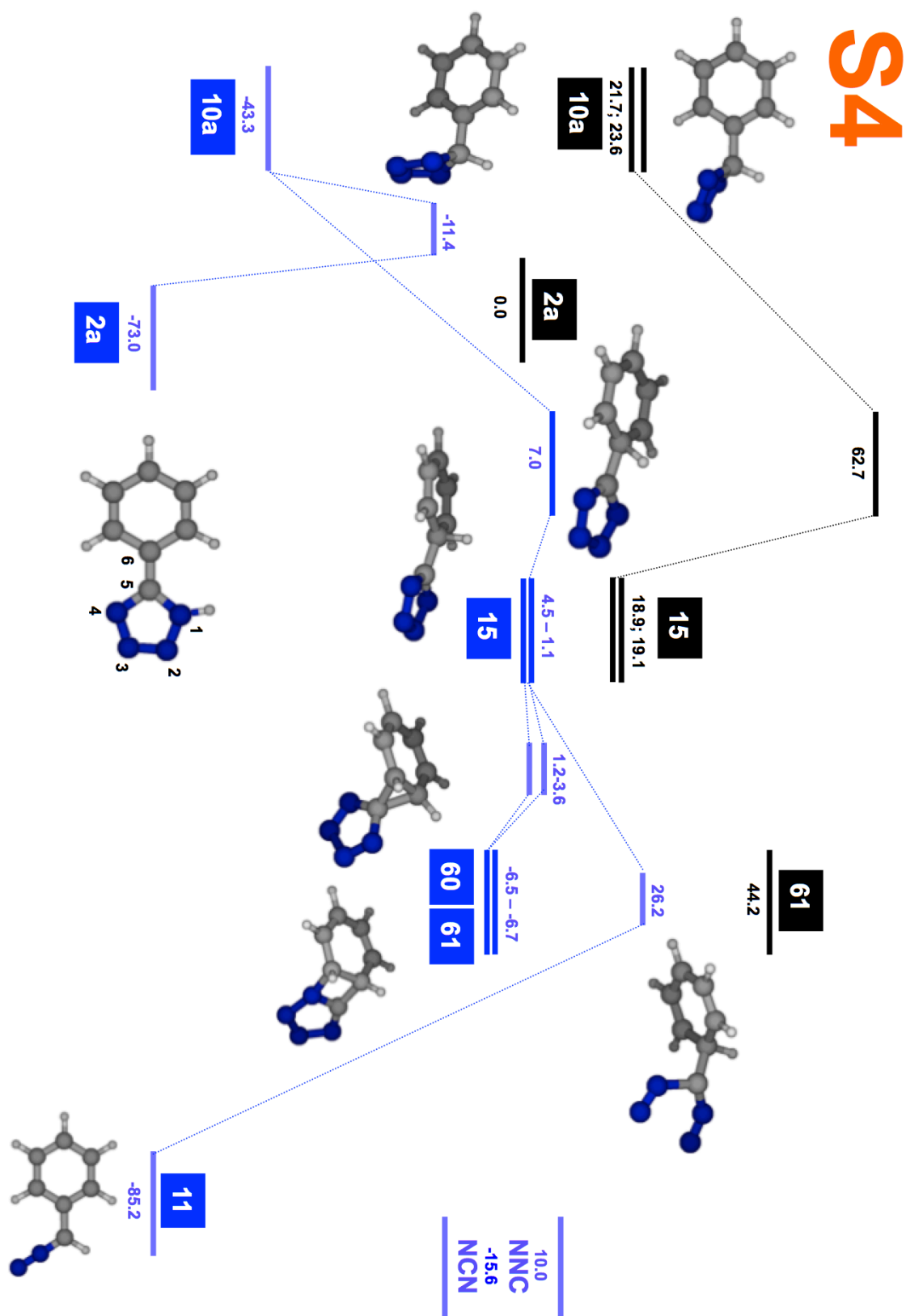


Figure S26. Reaction pathway (singlet) –slide 4 (green : doublet ; blue : singlet; black : triplet)

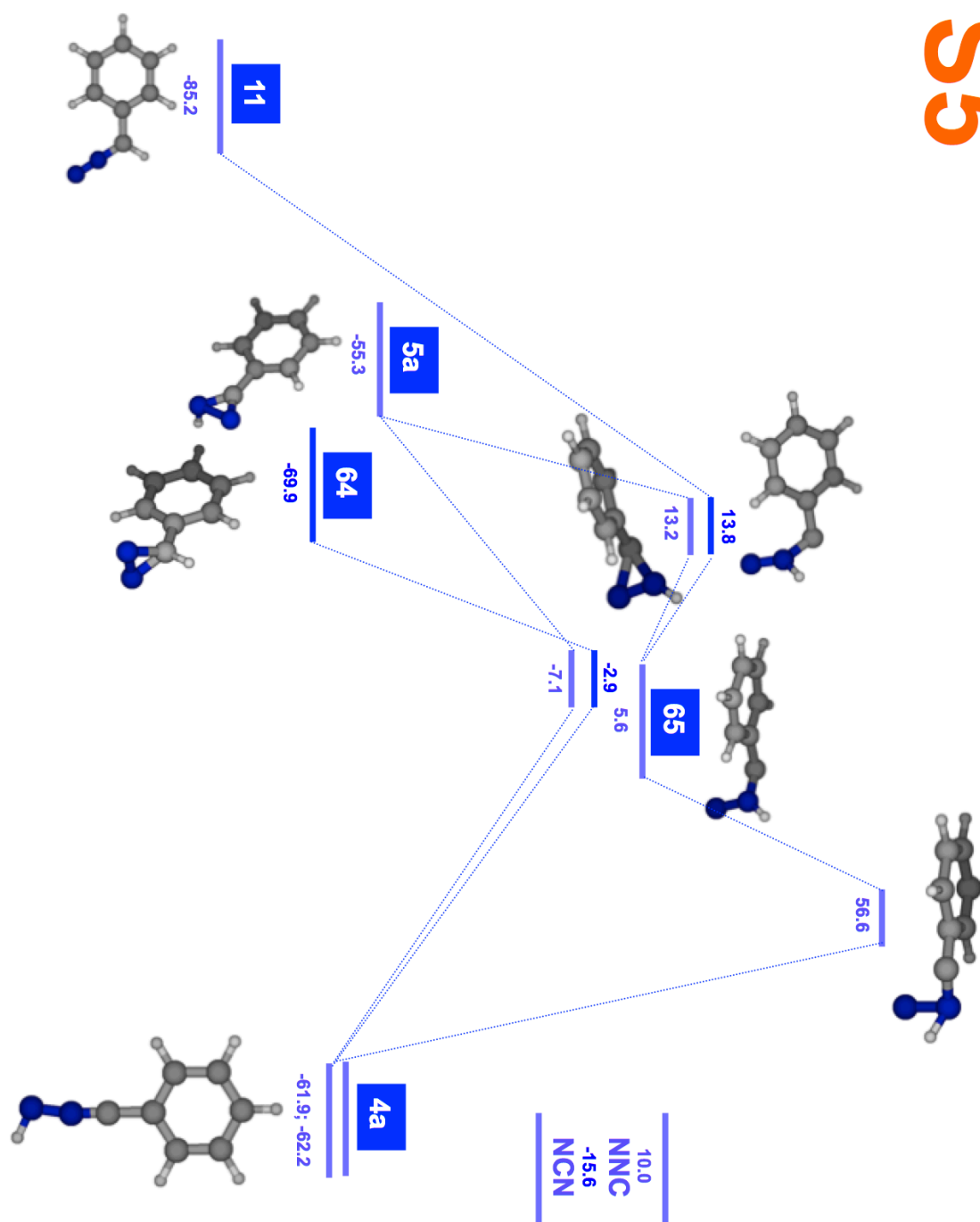


Figure S27. Reaction pathway (singlet) –slide 5 (green : doublet ; blue : singlet; black : triplet)

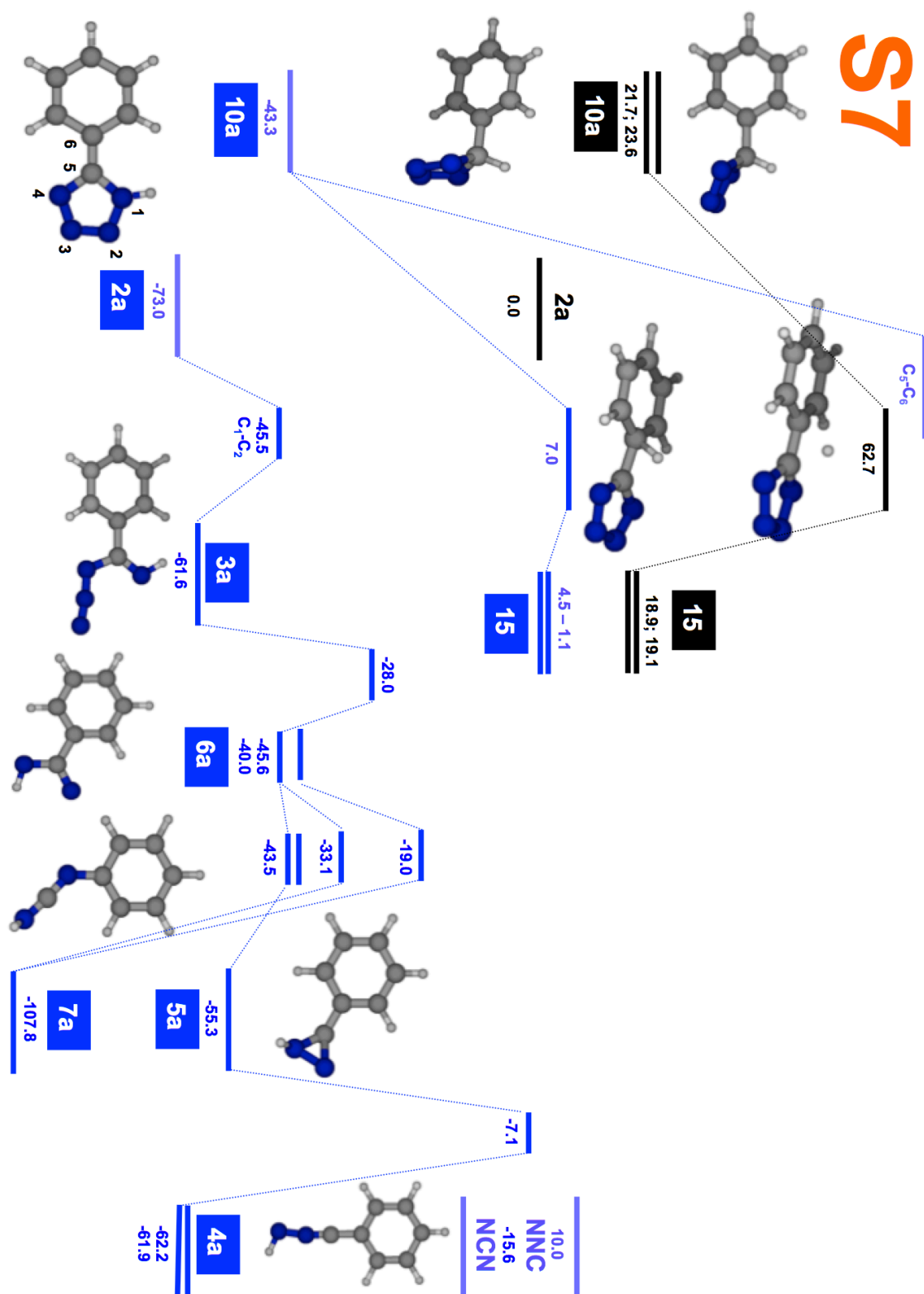


Figure S29. Reaction pathway (singlet) –slide 7 (green : doublet ; blue : singlet; black : triplet)

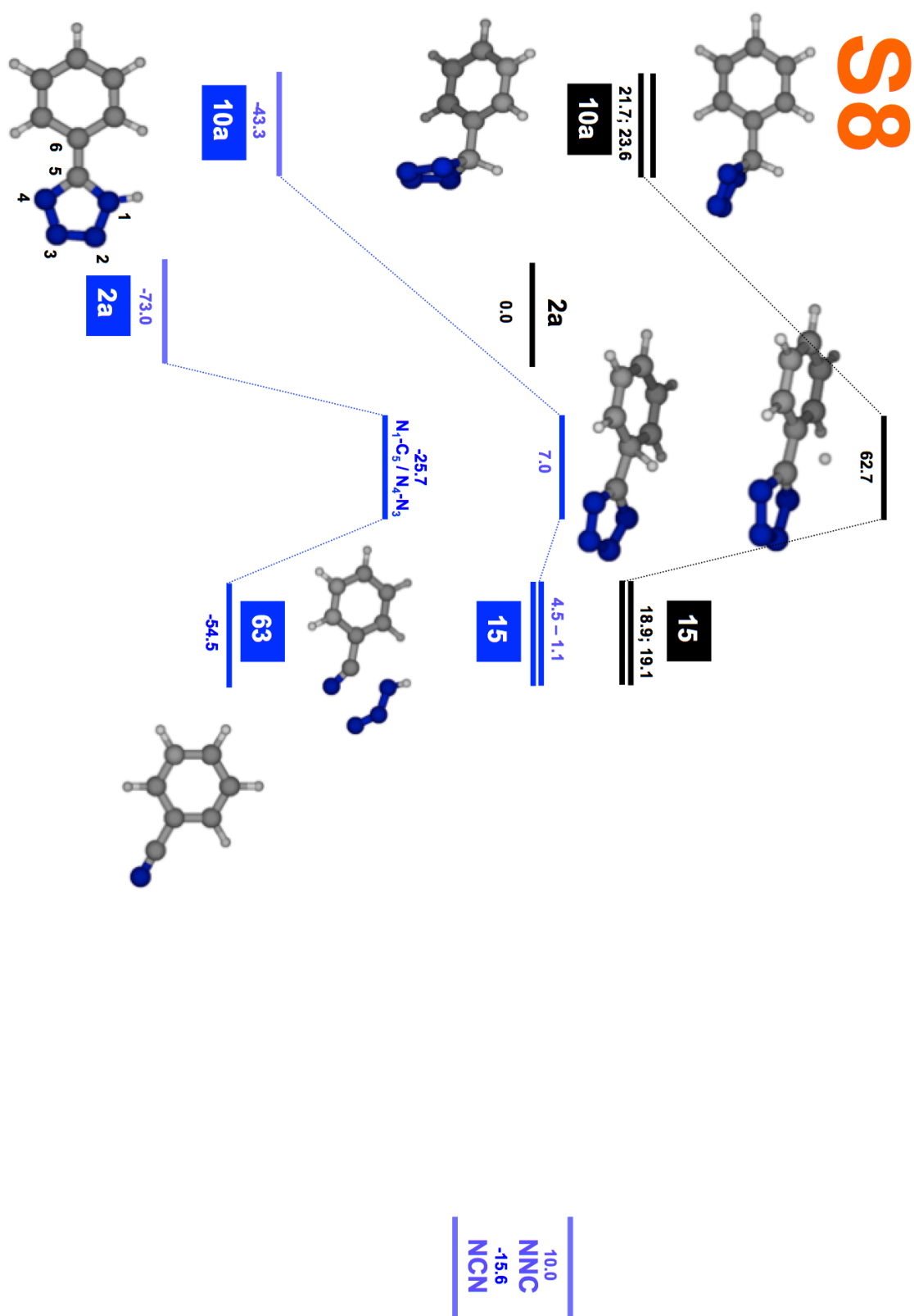


Figure S30. Reaction pathway (singlet) –slide 8 (green : doublet ; blue : singlet; black : triplet)

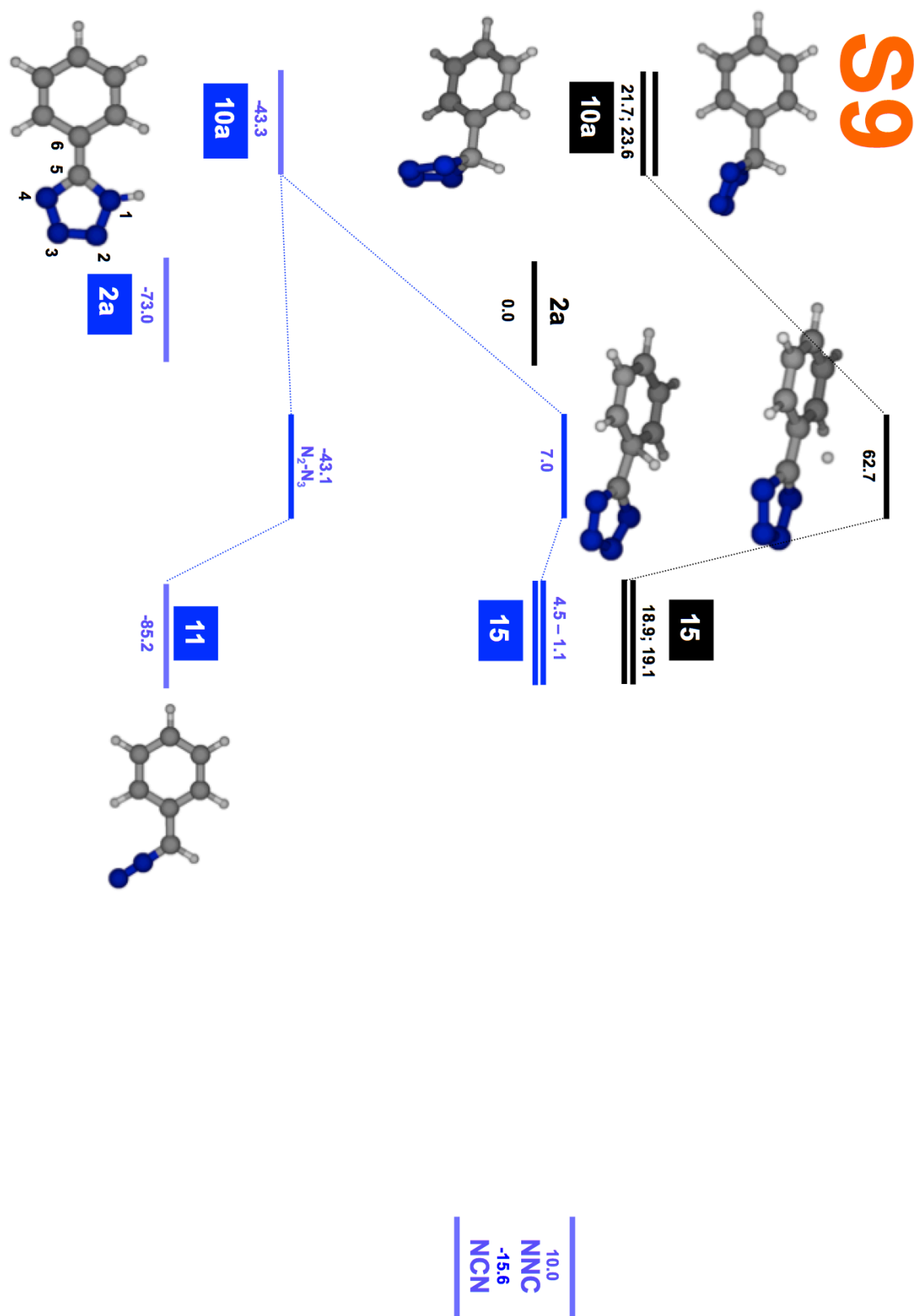


Figure S31. Reaction pathway (singlet) –slide 9 (green : doublet ; blue : singlet; black : triplet)

Triplet pathways

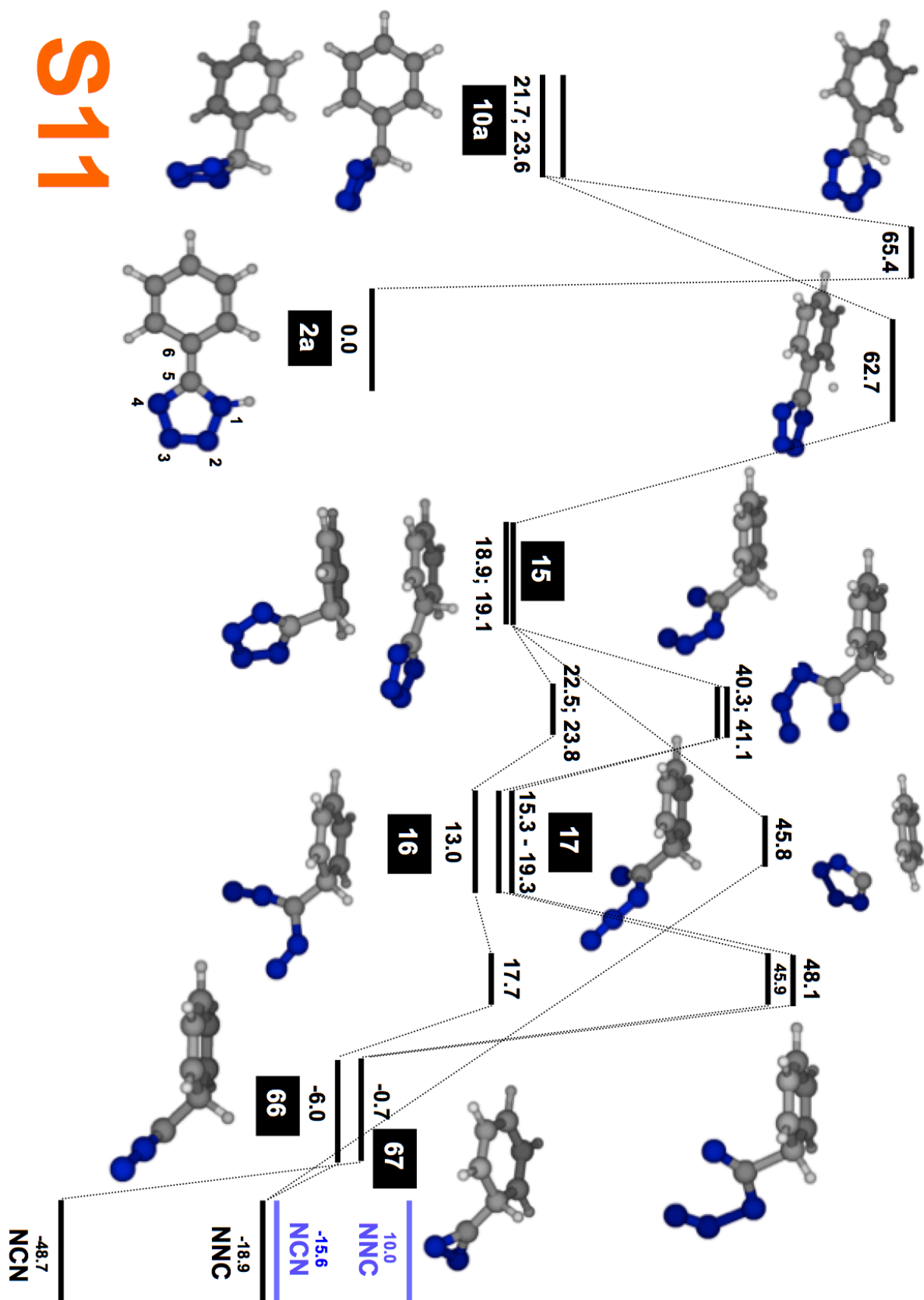


Figure S33. Reaction pathway (triplet) –slide 11 (green : doublet ; blue : singlet; black : triplet)

S12

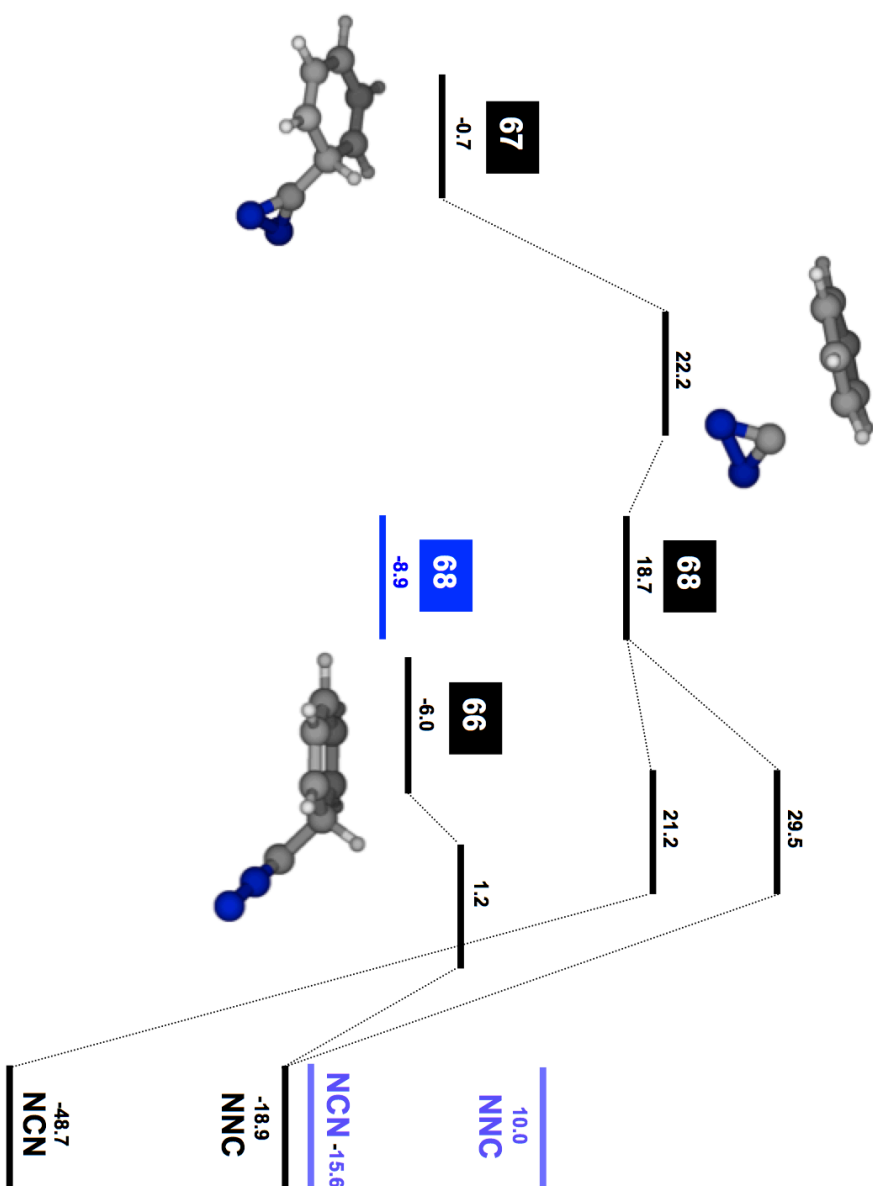


Figure S34. Reaction pathway (triplet) –slide 12 (green : doublet ; blue : singlet; black : triplet)

S13

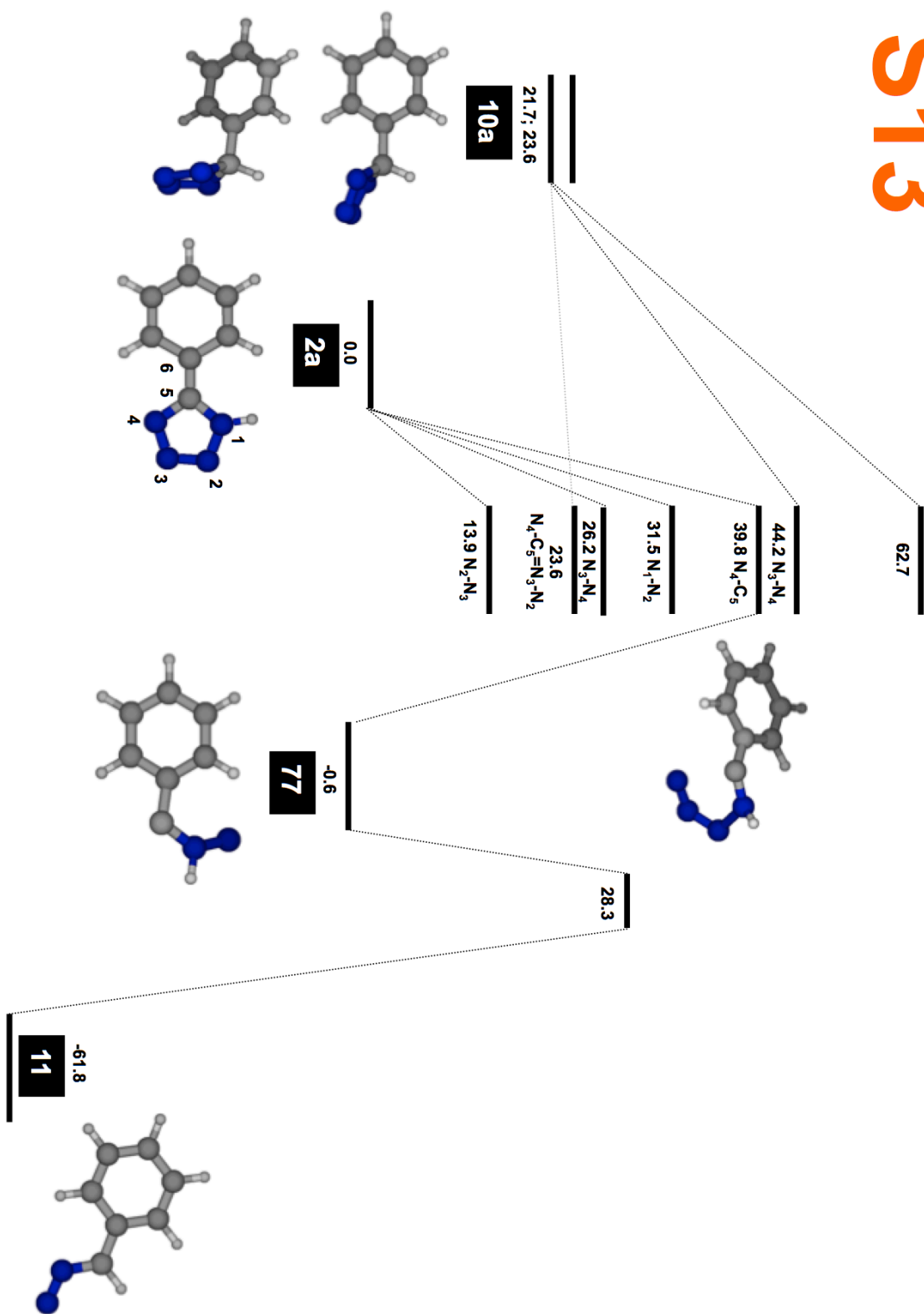


Figure S35. Reaction pathway (triplet) –slide 13 (green : doublet ; blue : singlet; black : triplet)

S14

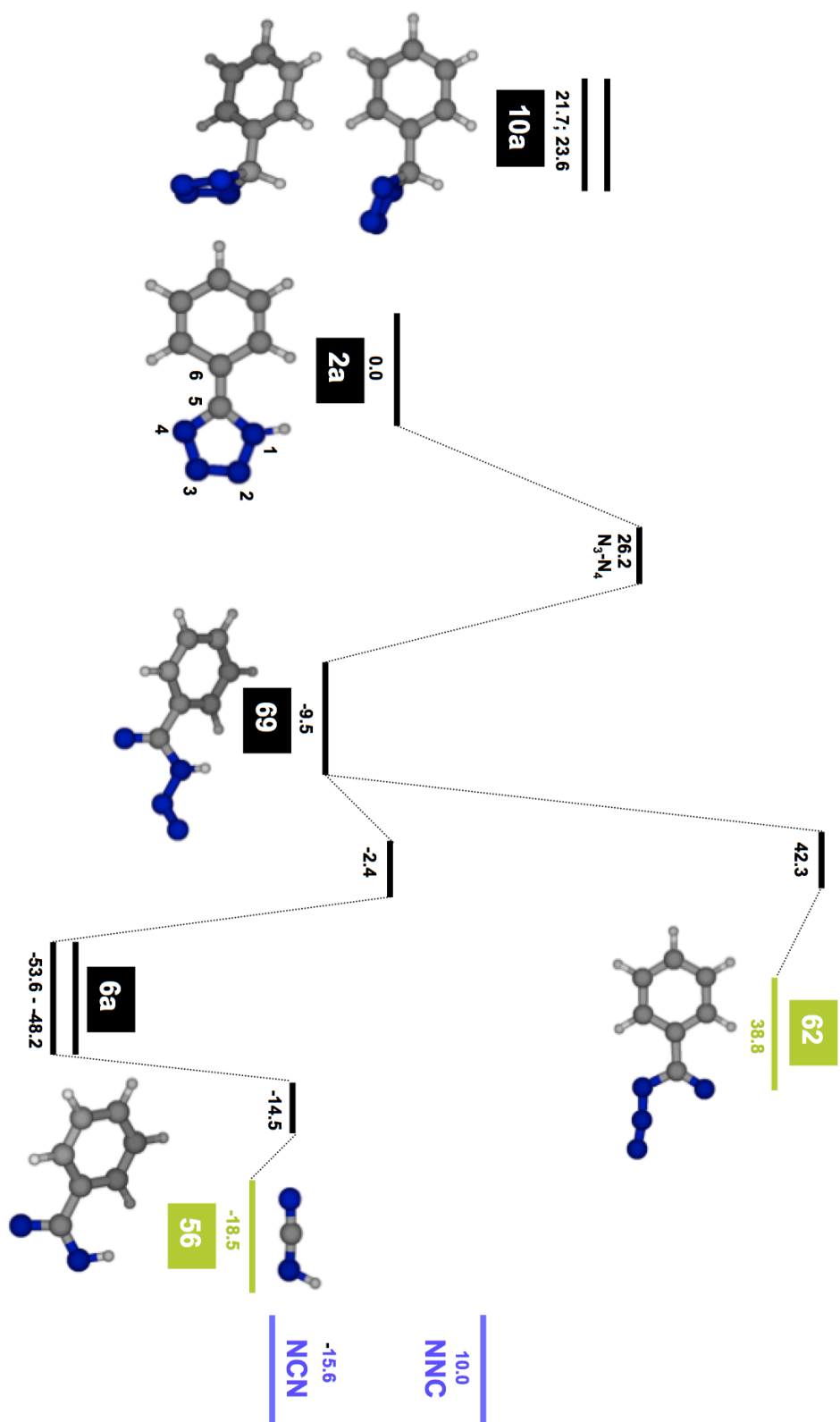


Figure S36. Reaction pathway (triplet) –slide 14 (green : doublet ; blue : singlet; black : triplet)

S15

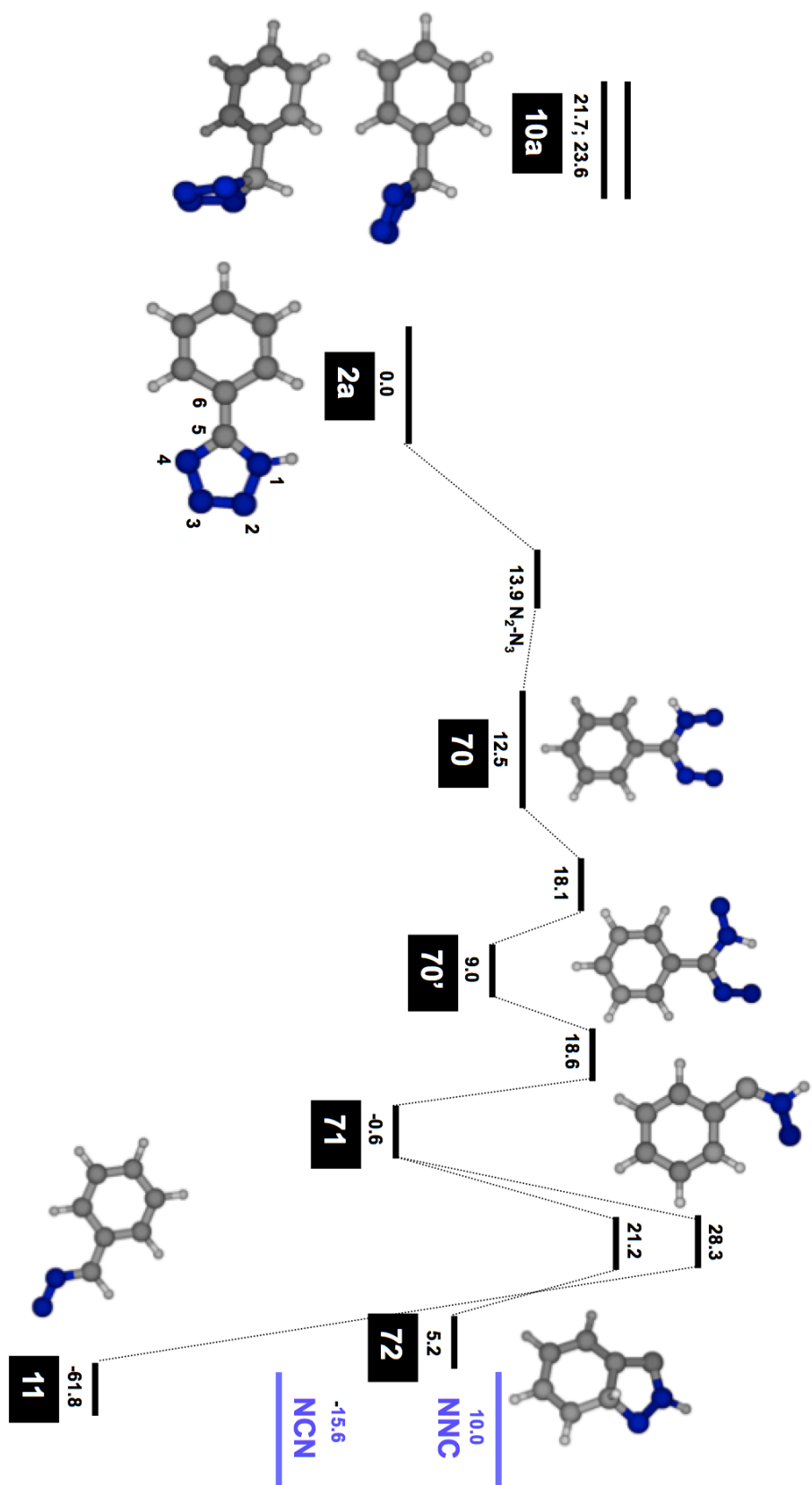


Figure S37. Reaction pathway (triplet) –slide 15 (green : doublet ; blue : singlet; black : triplet)

S16

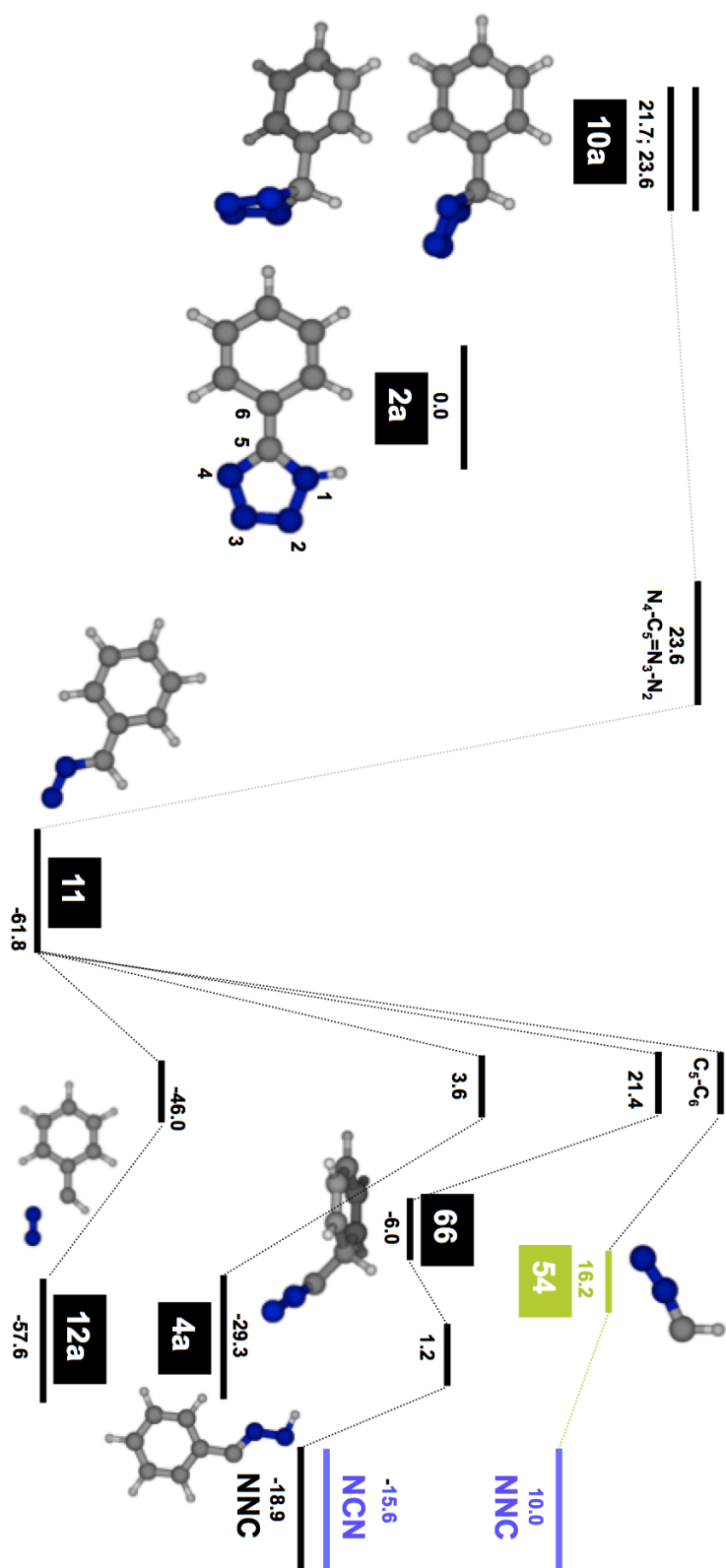


Figure S38. Reaction pathway (triplet) –slide 16 (green : doublet ; blue : singlet; black : triplet)

S17

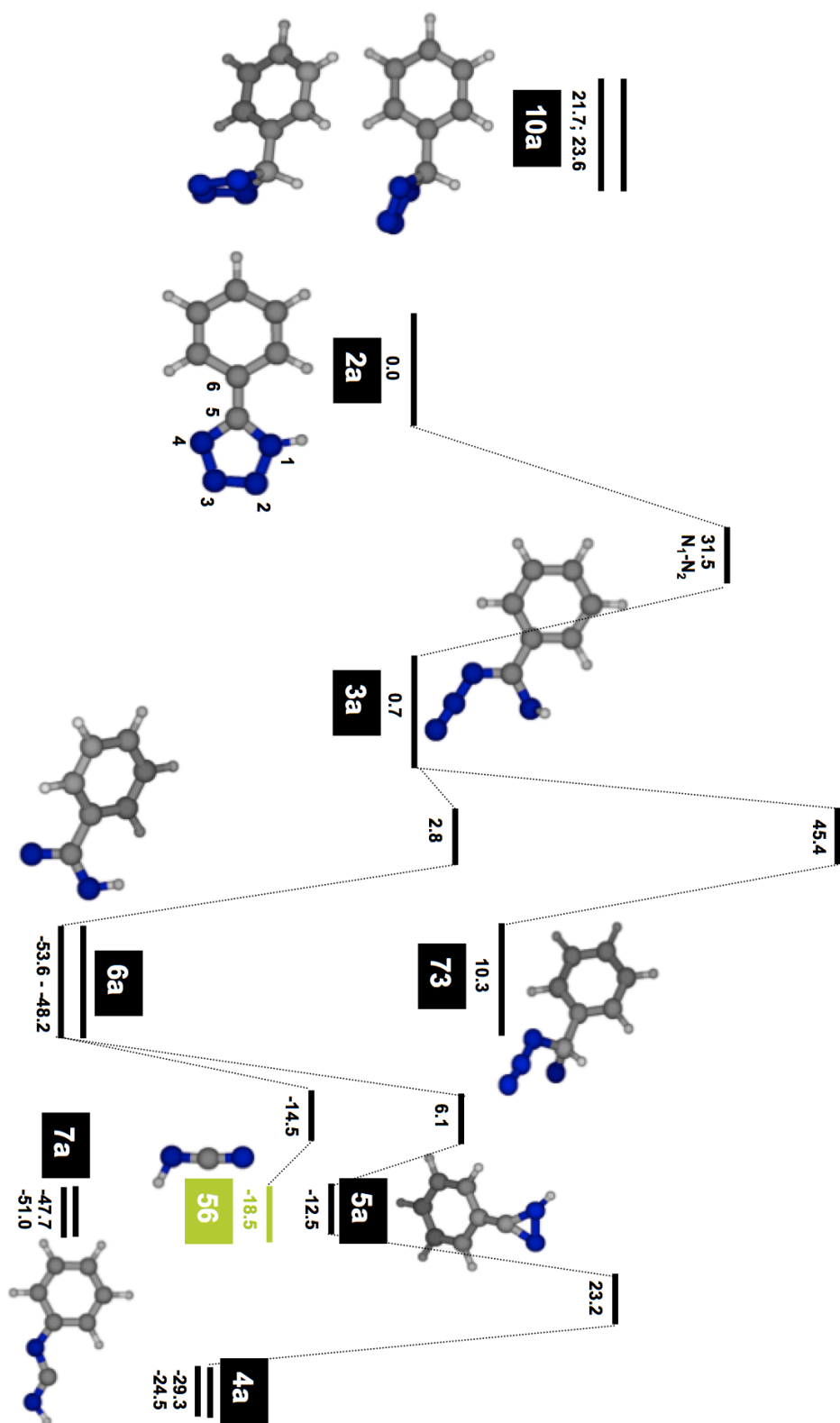


Figure S39. Reaction pathway (triplet) –slide 17 (green : doublet ; blue : singlet; black : triplet)

S18

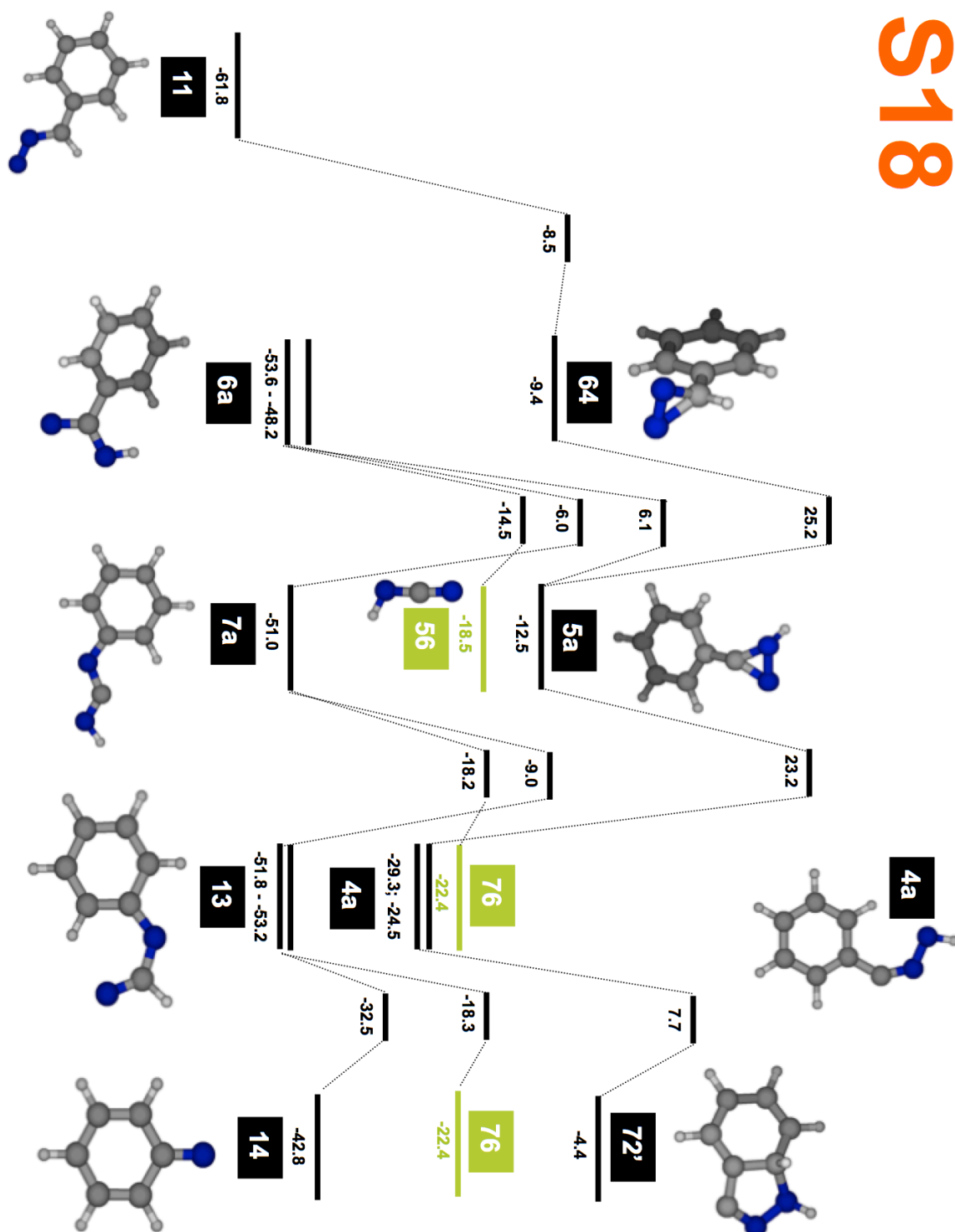


Figure S40. Reaction pathway (triplet) –slide 18 (green : doublet ; blue : singlet; black : triplet)

S19

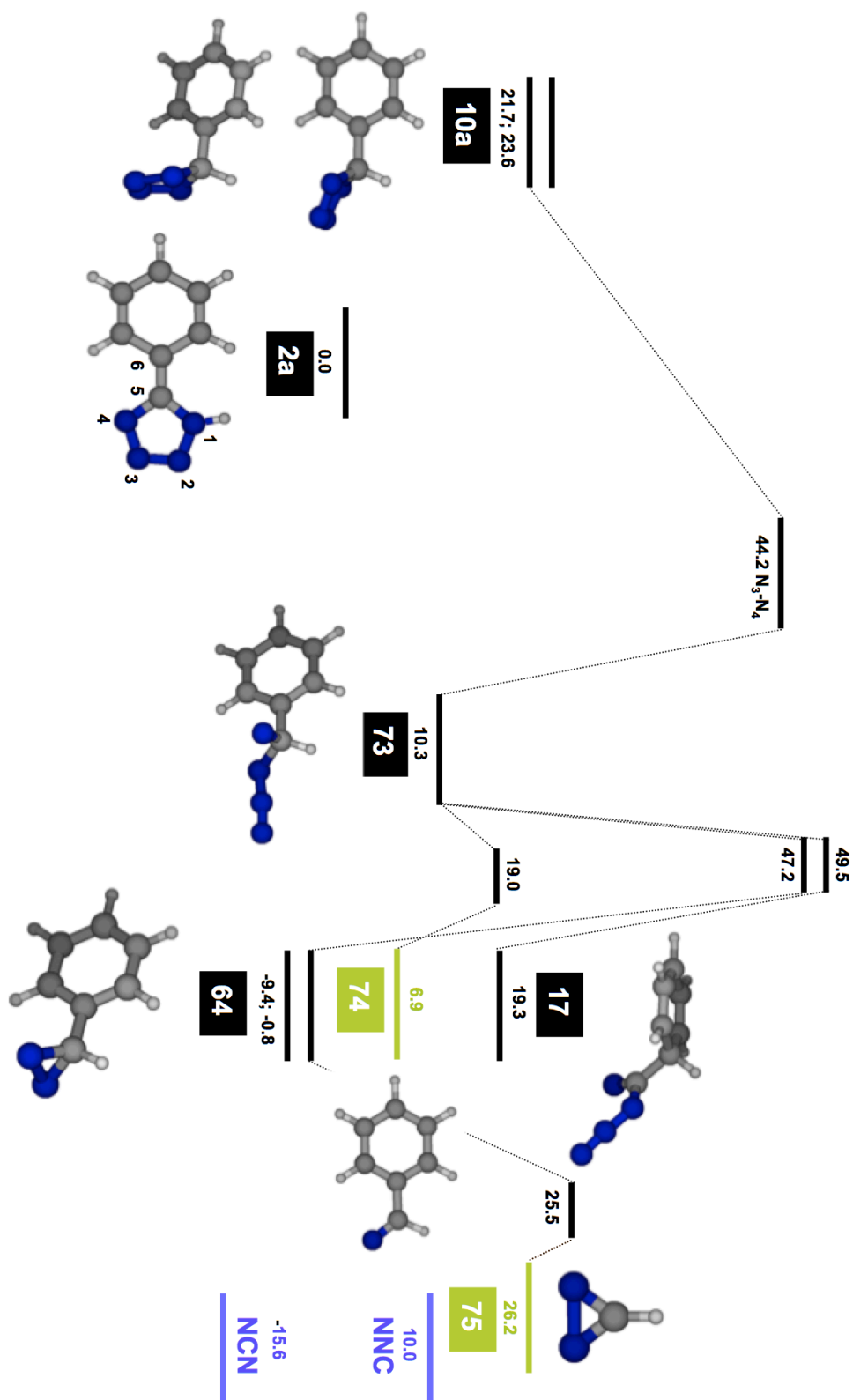
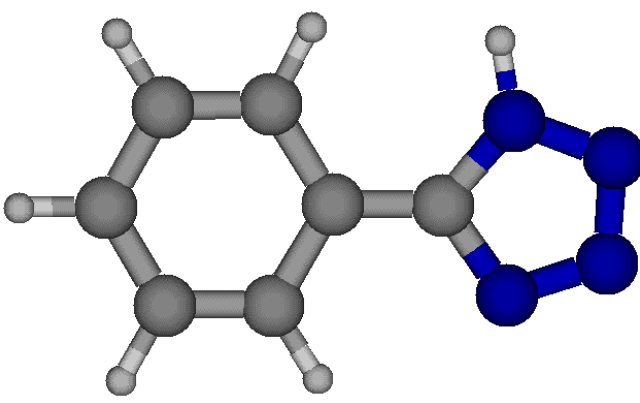


Figure S41. Reaction pathway (triplet) –slide 19 (green : doublet ; blue : singlet; black : triplet)

Table S23. Cartesian coordinates related to the photochemistry of 5-phenyl-1H-tetrazole **2a**

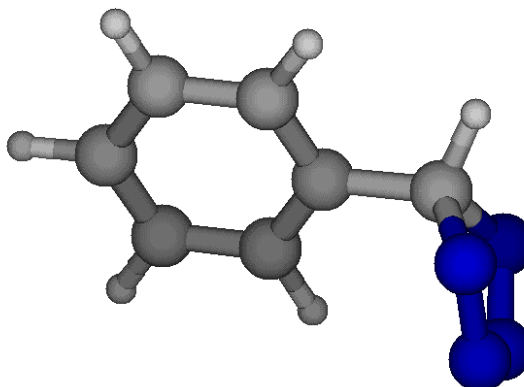
Compound **2aT** - B3LYP/6-311G(d,p) - E=-489.316876 u.a.

N	2.608280	-0.434422	-0.966005
C	2.971141	0.828830	-0.530647
N	1.876339	1.284128	0.180680
N	0.965167	0.339766	0.145218
N	1.364425	-0.718343	-0.537132
C	4.148115	1.511072	-0.739743
C	5.269931	0.948633	-1.514179
C	6.406463	1.666287	-1.688017
C	6.550008	2.980225	-1.129776
C	5.473625	3.547919	-0.373396
C	4.319536	2.866196	-0.174407
H	3.497226	3.278953	0.393612
H	5.590818	4.541239	0.044640
H	7.227064	1.245869	-2.258606
H	5.180805	-0.042187	-1.943819
H	3.112867	-1.111566	-1.512698
H	7.465820	3.536143	-1.280653



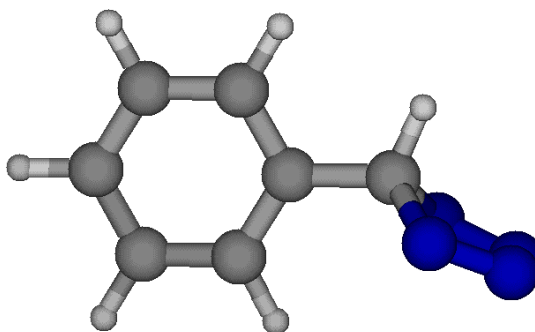
Compound **10aT** - B3LYP/6-311G(d,p) - **E=-489.279210 u.a.**

N	-1.887207	0.377970	-1.012246
C	-1.063276	-0.553044	-0.239220
N	-1.796691	-0.439323	1.041040
C	0.418765	-0.205913	-0.147447
C	0.876647	1.105551	-0.290080
C	2.236617	1.382222	-0.175488
C	3.143100	0.356265	0.081860
C	2.687764	-0.953112	0.220640
C	1.329819	-1.234211	0.101430
H	0.180305	1.909608	-0.495045
H	2.586807	2.401240	-0.292006
H	3.388592	-1.756491	0.416047
H	0.976866	-2.254374	0.207366
H	4.201037	0.575495	0.168559
H	-1.195567	-1.563479	-0.627736
N	-2.280028	0.832054	1.067415
N	-2.328968	1.309511	-0.113532



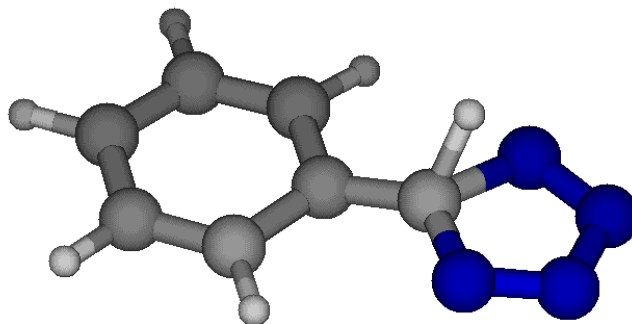
Compound **10aT** - B3LYP/6-311G(d,p) - **E=-489.282371 u.a.**

C	2.858319	-0.134107	-0.290075
C	2.731958	1.162207	-0.806904
C	1.467216	1.645681	-1.153844
C	0.340718	0.846570	-0.987462
C	0.472789	-0.442010	-0.472255
C	1.732866	-0.930562	-0.124179
C	3.942851	2.014521	-0.983045
N	4.741344	2.190320	0.263483
N	6.004669	2.343765	-0.159013
N	6.155391	1.886572	-1.339350
N	5.006475	1.385293	-1.815989
H	3.839040	-0.508151	-0.021512
H	1.834842	-1.932403	0.276207
H	-0.637206	1.226923	-1.258322
H	1.366597	2.648836	-1.554528
H	-0.404458	-1.065327	-0.342070
H	3.691852	3.004554	-1.397911



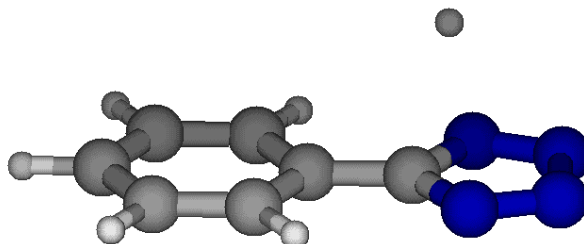
Compound TS **2aT** – **10aT** - B3LYP/6-311G(d,p) - **E=-489.212625 u.a.**

C	1.624934	1.739153	-0.630089
C	2.902269	1.008562	-0.630039
C	2.875542	-0.456405	-0.493456
C	1.689360	-1.109144	-0.513497
C	0.449698	-0.387562	-0.624927
C	0.459072	1.049791	-0.653052
C	4.109355	1.700875	-0.864957
N	5.481931	1.116928	-0.684582
N	6.246682	2.193287	-0.616121
N	5.523994	3.327501	-0.704651
N	4.259717	3.091311	-0.875609
H	3.815953	-0.979517	-0.376155
H	1.662144	-2.188858	-0.422003
H	-0.485266	1.581323	-0.675506
H	1.658615	2.820282	-0.635991
H	-0.489321	-0.924666	-0.647622
H	4.708105	1.222716	-1.816967



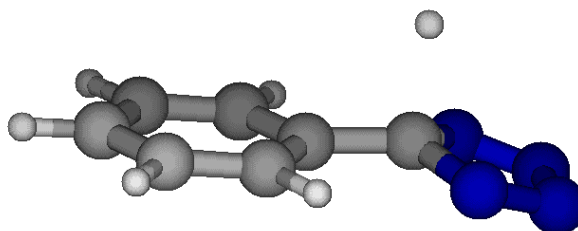
Compound TS **2aT** – **50D** - B3LYP/6-311G(d,p) - **E=-489.261600 u.a.**

N	1.844809	1.082354	-0.045230
C	1.027066	-0.037934	-0.032939
N	1.817276	-1.176006	0.004150
N	3.023877	-0.807141	-0.011778
N	3.056077	0.671841	-0.045753
C	-0.387583	-0.021916	-0.022991
C	-1.091003	1.209866	-0.063600
C	-2.473673	1.212464	-0.048482
C	-3.178832	0.004521	0.004498
C	-2.494616	-1.218068	0.044832
C	-1.113989	-1.240353	0.033432
H	-0.564444	-2.171980	0.068578
H	-3.050491	-2.146953	0.087326
H	-3.012434	2.151849	-0.078738
H	-0.530240	2.134153	-0.107412
H	1.501794	2.169530	1.217105
H	-4.262676	0.014577	0.014919



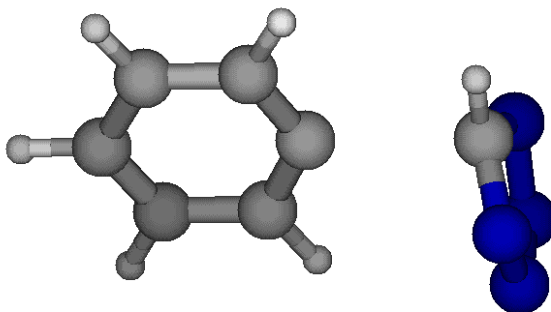
Compound TS **10aT** – **53D** - B3LYP/6-311G(d,p) - **E=-489.240283 u.a.**

C	1.013457	1.097131	-0.381311
C	0.383159	-0.101562	0.016190
C	1.165704	-1.190824	0.455798
C	2.546142	-1.093094	0.452599
C	3.165336	0.089980	0.033697
C	2.394715	1.182513	-0.379900
C	-1.057811	-0.233222	-0.081761
N	-1.766946	-1.249848	0.570813
N	-2.952676	-0.875805	0.698221
N	-3.046496	0.532734	0.183445
N	-1.908324	0.872984	-0.205096
H	0.400837	1.937969	-0.680644
H	2.879627	2.100745	-0.688925
H	3.147857	-1.930181	0.785781
H	0.668937	-2.091416	0.793491
H	4.246420	0.166812	0.047069
H	-1.059095	-0.799495	-1.630456



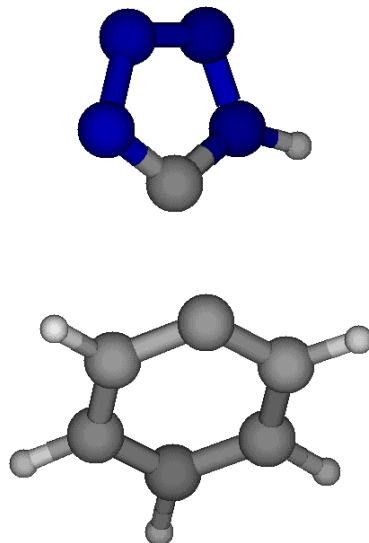
Compound TS **10aT** – **53D** - B3LYP/6-311G(d,p) - **E=-489.232171 u.a.**

C	0.804043	0.997561	0.000234
C	0.585341	-0.364346	-0.000061
C	1.567905	-1.330603	-0.000274
C	2.893190	-0.883564	-0.000181
C	3.171122	0.485541	0.000116
C	2.138325	1.422105	0.000324
C	-1.690409	-1.057540	-0.000287
N	-2.159194	-0.438431	1.091834
N	-2.628819	0.828074	0.625525
N	-2.628695	0.828117	-0.626163
N	-2.158978	-0.438359	-1.092462
H	-0.008026	1.714475	0.000391
H	2.362508	2.483141	0.000554
H	3.703770	-1.604306	-0.000341
H	1.341185	-2.391148	-0.000506
H	4.201224	0.822570	0.000185
H	-1.375672	-2.087937	-0.000289



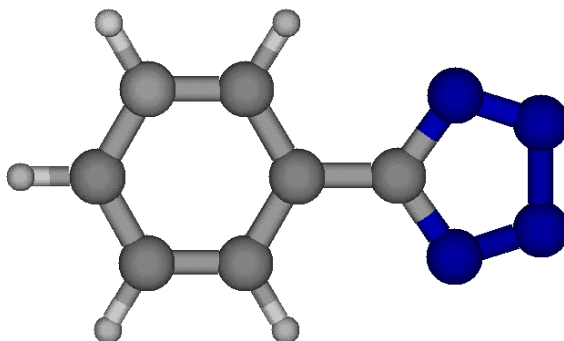
Compound TS **2aT** – **58D** - B3LYP/6-311G(d,p) - **E=-489.234078 u.a.**

N	1.787632	-0.427357	-0.926314
C	1.050240	0.289955	-0.055968
N	1.829051	1.123436	0.572043
N	3.091872	0.912544	0.055088
N	3.079431	-0.010674	-0.841388
C	-0.833417	-0.348713	1.078847
C	-1.339650	0.932792	1.298457
C	-2.398577	1.332731	0.486195
C	-2.963987	0.435544	-0.426461
C	-2.496276	-0.879456	-0.529499
C	-1.443060	-1.310903	0.275808
H	-1.099059	-2.339060	0.254613
H	-2.973856	-1.574011	-1.212377
H	-2.795391	2.337803	0.577649
H	-0.885029	1.604135	2.016463
H	1.519214	-1.143130	-1.582061
H	-3.798903	0.753659	-1.039942



Compound **50D** - B3LYP/6-311G(d,p) - E=-488.764119 u.a.

N	1.772708	1.130273	0.000000
C	0.975840	0.000000	0.000000
N	1.772708	-1.130273	0.000000
N	2.976367	-0.743982	0.000000
N	2.976367	0.743982	0.000000
C	-0.443537	0.000000	0.000000
C	-1.157298	1.224745	0.000000
C	-2.539434	1.215796	0.000000
C	-3.234253	0.000000	0.000000
C	-2.539434	-1.215796	0.000000
C	-1.157298	-1.224745	0.000000
H	-0.598909	-2.151823	0.000000
H	-3.086677	-2.150800	0.000000
H	-3.086677	2.150800	0.000000
H	-0.598909	2.151823	0.000000
H	-4.318215	0.000000	0.000000



Compound **C₆H₆ A_g(S)** - B3LYP/6-311G(d,p) - **E=-232.308539 u.a.**

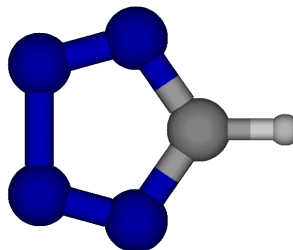
C	-0.499801	-1.301273	0.000000
C	0.877035	-1.083477	0.000000
C	1.376836	0.217796	0.000000
C	0.499801	1.301273	0.000000
C	-0.877035	1.083477	0.000000
C	-1.376836	-0.217796	0.000000
H	-0.888687	-2.313548	0.000000
H	1.559248	-1.926399	0.000000
H	2.447935	0.387149	0.000000
H	0.888687	2.313548	0.000000
H	-1.559248	1.926399	0.000000
H	-2.447935	-0.387149	0.000000

Compound **C₆H₆ A₁(D)** - B3LYP/6-311G(d,p) - **E=-231.587849 u.a.**

C	0.000000	-1.379130	0.000000
C	1.223911	-0.666924	0.000000
C	1.257536	0.694583	0.000000
C	0.000000	1.529074	0.000000
C	-1.257536	0.694583	0.000000
C	-1.223911	-0.666924	0.000000
H	2.201432	1.227933	0.000000
H	2.157378	-1.220151	0.000000
H	-2.157378	-1.220151	0.000000
H	-2.201432	1.227933	0.000000
H	0.000000	-2.461636	0.000000

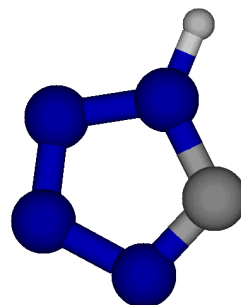
Compound **53D** - B1 - (c_2v) - B3LYP/6-311G(d,p) - **E=-257.625633 u.a.**

N	1.138399	-0.325611	0.000000
C	0.000000	-1.103937	0.000000
N	-1.138399	-0.325611	0.000000
N	-0.809650	0.877497	0.000000
N	0.809650	0.877497	0.000000
H	0.000000	-2.183570	0.000000



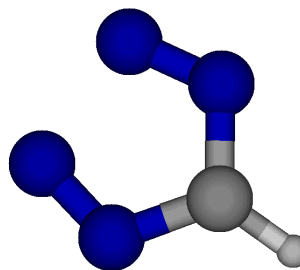
Compound **58D** – A' (Cs) - B3LYP/6-311G(d,p) - **E=-257.613913 u.a.**

N	0.976645	-0.526657	0.000000
C	-0.232962	-1.111866	0.000000
N	-1.172914	-0.248681	0.000000
N	-0.508847	0.980435	0.000000
N	0.767725	0.814299	0.000000
H	1.906102	-0.916504	0.000000



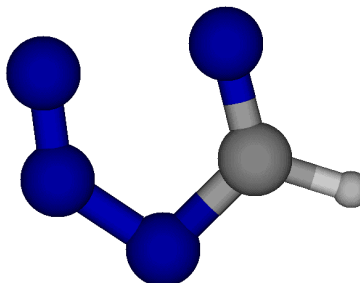
Compound TS **53D – 57D** - B3LYP/6-311G(d,p) - **E=-257.624089 u.a.**

C	1.747104	-0.829383	0.095965
N	1.285339	0.461879	0.026513
N	2.168345	1.294296	-0.059338
N	3.120275	-0.850777	0.030320
N	3.623419	0.252924	-0.055215
H	1.122508	-1.705072	0.062652



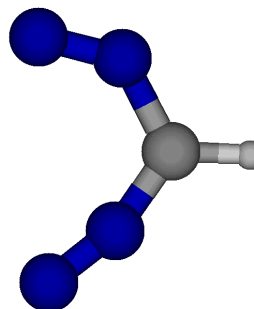
Compound TS **53D** – **55D** - B3LYP/6-311G(d,p) - E=-257.595960 u.a.

N	3.327749	0.625426	-0.042520
N	2.944853	-1.307071	0.046810
C	1.673340	-1.165335	0.066690
N	1.101426	0.090897	0.025135
N	2.196666	0.880582	-0.030659
H	1.001966	-2.016525	0.117403



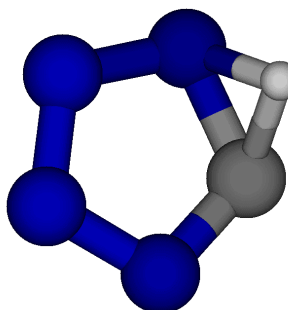
Compound **57D** - B3LYP/6-311G(d,p) - E=-257.644435 u.a.

N	1.553862	0.825476	0.053746
N	1.263440	-0.308223	0.013710
C	0.007769	-0.965016	-0.020944
N	-1.065037	-0.212654	-0.007819
N	-1.765610	0.683910	0.015436
H	-0.041470	-2.034890	-0.056702



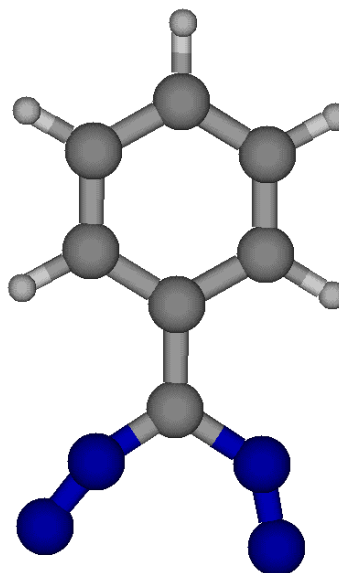
Compound TS **53D** – **58D** - B3LYP/6-311G(d,p) - E=-257.521988 u.a.

N	0.810499	0.701722	0.046531
N	1.065287	-0.532625	-0.402017
C	-0.225285	-1.123248	-0.338701
N	-1.171560	-0.268740	0.018738
N	-0.504871	0.863464	0.225857
H	0.744706	-1.456505	0.449592



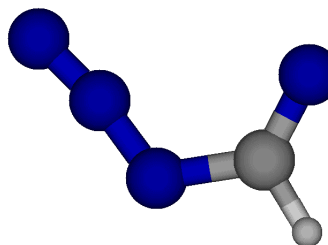
Compound **51D** - B3LYP/6-311G(d,p) - E=-488.759282 u.a.

C	-1.144513	-1.244699	-0.002956
C	-0.374090	-0.073096	-0.000116
C	-1.028197	1.168559	0.003137
C	-2.416276	1.232063	0.003519
C	-3.177943	0.064737	0.000688
C	-2.532919	-1.170236	-0.002542
C	1.081703	-0.152608	-0.000565
N	1.883470	0.890309	0.001895
N	2.823751	1.535220	0.003224
N	2.895444	-1.689390	-0.004718
N	1.761633	-1.403728	-0.003793
H	-0.651572	-2.209013	-0.005479
H	-3.113363	-2.085879	-0.004766
H	-2.904545	2.199962	0.006049
H	-0.450669	2.086754	0.005373
H	-4.260197	0.117627	0.000997



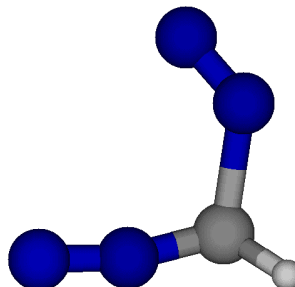
Compound **55D** - B3LYP/6-311G(d,p) - E=-257.637879 u.a.

N	0.961843	1.735118	-0.092807
N	0.497403	-1.776121	0.064627
C	-0.611249	-1.190477	0.062799
N	-0.843028	0.208329	0.008443
N	0.159750	0.945862	-0.043261
H	-1.551289	-1.744916	0.105284



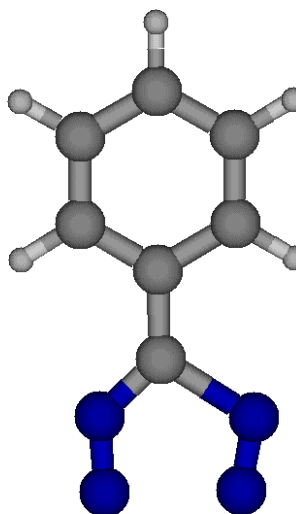
Compound TS **57D** – **54D** - B3LYP/6-311G(d,p) - E=-257.636526 u.a.

C	1.678806	-0.733927	-0.196988
N	1.367542	0.498355	0.024276
N	1.340462	1.641343	0.107482
N	3.342676	-0.987480	0.015750
N	4.187993	-0.247873	-0.118119
H	1.149508	-1.546548	0.268495



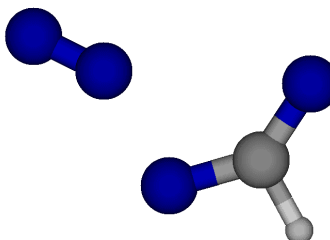
Compound TS **51D** – **52D** - B3LYP/6-311G(d,p) - E=-488.746442 u.a.

C	-1.125007	-1.209473	0.000993
C	-0.418552	0.019227	-0.000544
C	-1.149745	1.235036	-0.000495
C	-2.532520	1.211314	0.000989
C	-3.218817	-0.008139	0.002305
C	-2.509289	-1.212382	0.002337
C	0.992434	0.001943	-0.001866
N	1.880598	0.977754	-0.003107
N	3.073629	0.916398	-0.003980
N	3.069614	-1.226452	-0.002446
N	1.935445	-1.446391	-0.001632
H	-0.565320	-2.135324	0.001114
H	-3.043595	-2.155081	0.003420
H	-3.085430	2.143368	0.001155
H	-0.609231	2.173111	-0.001514
H	-4.302499	-0.018325	0.003217



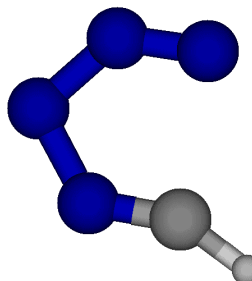
Compound TS **55D** – **56D** - B3LYP/6-311G(d,p) - E=-257.584081 u.a.

C	-0.616459	-1.168055	-0.082528
N	0.444117	-1.854360	0.028818
N	-0.976223	0.115134	-0.129853
N	0.621547	1.029939	0.008375
N	1.108365	2.012415	-0.074842
H	-1.594258	-1.700305	-0.110167



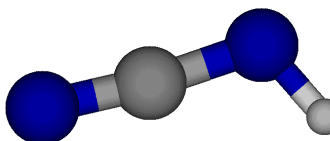
Compound TS **53D** – **57D** - B3LYP/6-311G(d,p) - E=-257.570371 u.a.

C	1.099573	-0.133516	0.032351
N	1.312927	1.048590	-0.032450
N	2.529610	1.690879	-0.083451
N	3.428204	0.672835	-0.043891
N	3.259282	-0.480954	0.018441
H	0.455726	-0.986702	0.085714



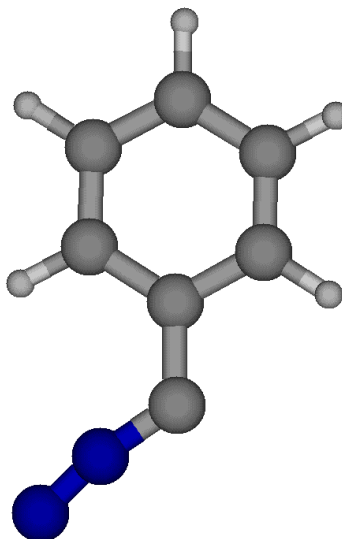
Compound **56D** - B3LYP/6-311G(d,p) - E=-148.170938 u.a.

C	-1.305457	0.164698	0.007432
N	-0.898800	-1.041903	-0.010842
N	-1.573659	1.323404	0.022564
H	-1.666957	-1.716968	-0.007465



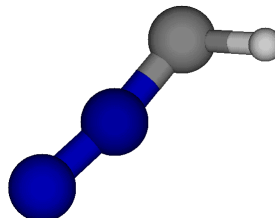
Compound **52D** - B3LYP/6-311G(d,p) - E=-379.240687 u.a.

C	-1.136270	-1.235483	-0.002924
C	-0.380209	-0.073211	-0.000126
C	-1.005646	1.193799	0.003170
C	-2.421194	1.247207	0.003544
C	-3.169221	0.081572	0.000735
C	-2.531029	-1.162849	-0.002505
C	-0.169501	2.358817	0.005960
N	-0.630531	3.548579	0.009028
N	-0.865225	4.678204	0.011885
H	0.702264	-0.110320	-0.000402
H	-0.644191	-2.201183	-0.005439
H	-4.252031	0.134199	0.001051
H	-2.916389	2.211990	0.006056
H	-3.121061	-2.072251	-0.004695



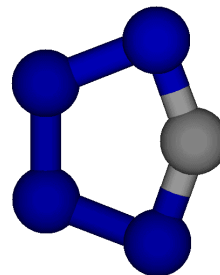
Compound **54D** - B3LYP/6-311G(d,p) - E=-148.115703 u.a.

C	-0.217762	-1.146745	-0.279575
N	-1.183203	-0.354071	-0.030780
N	-1.960848	0.494052	0.075201
H	-0.278251	-2.124298	0.198040



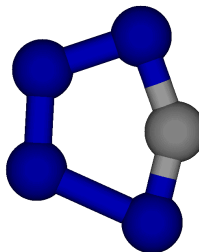
Compound **18S** – A1 - (c_{2v}) - B3LYP/6-311G(d,p) - E=-256.929498 u.a.

C	0.000000	-0.892853	0.000000
N	-1.195621	-0.456675	0.000000
N	-0.688058	0.839494	0.000000
N	0.688058	0.839494	0.000000
N	1.195621	-0.456675	0.000000



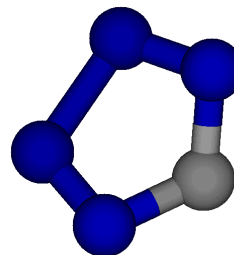
Compound TS **18S** – **18''S** - B3LYP/6-311G(d,p) - **E=-256.925353 u.a.**

N	1.193833	-0.357976	0.000000
C	-0.042847	-0.803910	0.000000
N	-1.221451	-0.502520	0.000000
N	-0.539389	1.001280	0.000000
N	0.761536	0.923264	0.000000



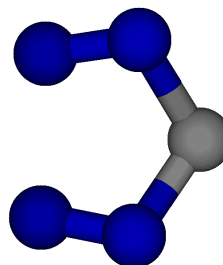
Compound TS **18S** – **18'S** - B3LYP/6-311G(d,p) - **E=-256.916565 u.a.**

C	1.727408	-0.767092	-0.107795
N	1.146658	0.477235	0.157343
N	2.067932	1.253950	-0.094073
N	3.496710	0.267459	-0.102023
N	3.098743	-0.870567	0.146481



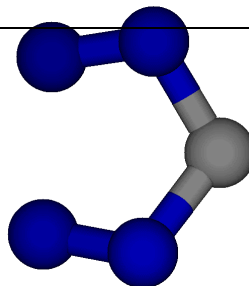
Compound **18'S** - B3LYP/6-311G(d,p) - **E=-256.917602 u.a.**

N	1.200421	-0.368081	0.129821
C	-0.028378	-1.114395	-0.181221
N	-1.217570	-0.306346	0.130054
N	-0.989919	0.841248	-0.049008
N	1.031629	0.789582	-0.049618



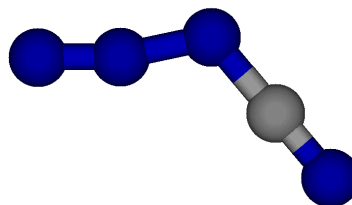
Compound TS **18'S** – **NNC** (S) - B3LYP/6-311G(d,p) - **E=-256.917600 u.a.**

C	0.018719	-1.116754	-0.293337
N	0.393025	-0.888670	-1.683134
N	-0.565679	-0.689195	-2.350901
N	-1.196448	-0.327264	0.057087
N	-1.893556	-0.222186	-0.888780



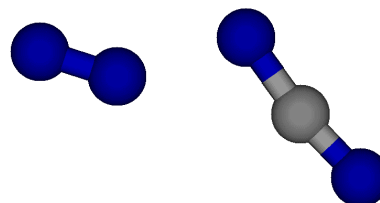
Compound **18''S** - B3LYP/6-311G(d,p) - **E=-257.071263 u.a.**

N	0.693377	-0.248026	0.000000
C	-0.338136	-1.120882	0.000000
N	-1.222225	-1.868990	0.000000
N	0.413724	2.103543	0.000000
N	0.425385	0.981078	0.000000



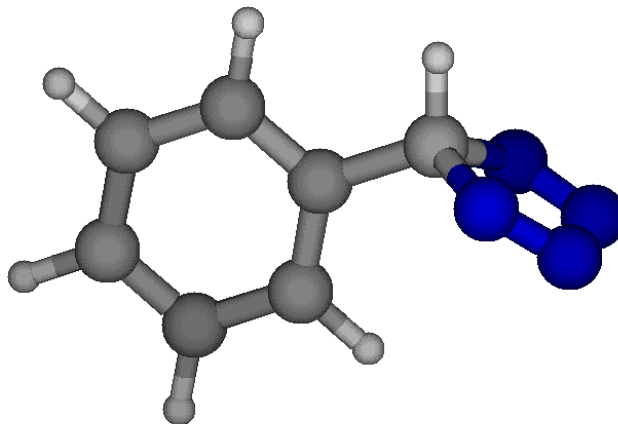
Compound TS **18''S** – **NCN** (S) - B3LYP/6-311G(d,p) - **E=-257.024746 u.a.**

C	-0.334651	-1.123391	0.000000
N	-1.195043	-1.937699	0.000000
N	0.710131	-0.382718	0.000000
N	0.181809	1.368272	0.000000
N	0.518715	2.415371	0.000000



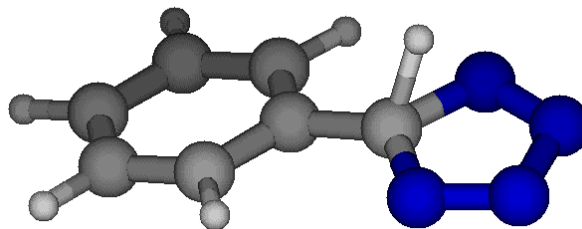
Compound **10aS** - B3LYP/6-311G(d,p) - **E=-489.385857 u.a.**

C	2.908925	-0.065236	-0.309235
C	2.738470	1.221706	-0.828618
C	1.459576	1.667264	-1.163267
C	0.356657	0.835749	-0.981615
C	0.530816	-0.444728	-0.464251
C	1.808154	-0.894185	-0.128303
C	3.932097	2.117778	-1.023693
N	4.691713	2.379586	0.255183
N	5.829234	2.085606	0.307245
N	6.064108	1.371102	-1.542236
N	4.971229	1.527596	-1.947470
H	3.900749	-0.416046	-0.047684
H	1.945028	-1.890873	0.274567
H	-0.634097	1.188160	-1.243651
H	1.324538	2.665084	-1.566334
H	-0.326013	-1.093334	-0.322123
H	3.644079	3.087452	-1.435284



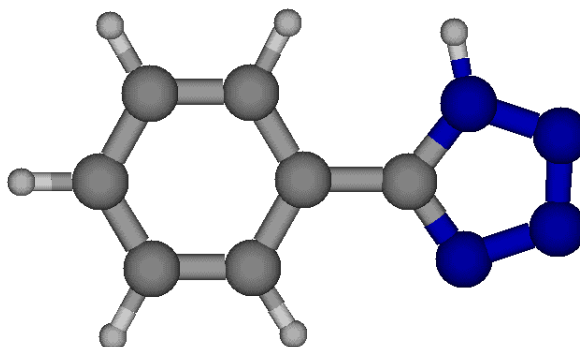
Compound TS **10aS – 2aS** - B3LYP/6-311G(d,p) - **E=-489.334972 u.a.**

C	4.393712	2.815894	-0.136641
C	4.242411	1.547952	-0.707879
C	5.248962	1.021128	-1.524468
C	6.401451	1.762247	-1.763438
C	6.554013	3.025310	-1.193994
C	5.548352	3.550351	-0.383915
C	3.009859	0.777777	-0.439910
N	2.721853	-0.524302	-0.983193
N	1.432526	-0.696095	-0.756203
N	0.920725	0.403071	-0.185953
N	1.846514	1.295824	0.040833
H	3.603558	3.216476	0.485788
H	5.662090	4.534289	0.055735
H	7.178231	1.354872	-2.399841
H	5.120461	0.044437	-1.974670
H	3.298391	-0.265442	0.202168
H	7.452635	3.600670	-1.384493



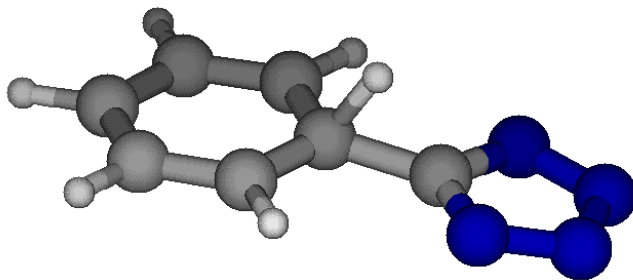
Compound **2aS** - B3LYP/6-311G(d,p) - E=-489.433282 u.a.

N	2.620259	-0.425655	-0.933394
C	2.923163	0.826697	-0.519924
N	1.866886	1.285235	0.130248
N	0.935077	0.300585	0.101712
N	1.367056	-0.734070	-0.531241
C	4.178785	1.543311	-0.744243
C	5.229037	0.986909	-1.485370
C	6.408407	1.698935	-1.676516
C	6.551512	2.972947	-1.131182
C	5.508784	3.532831	-0.393514
C	4.328821	2.826046	-0.199152
H	3.511387	3.248217	0.371148
H	5.615930	4.523799	0.032017
H	7.214422	1.259046	-2.252086
H	5.136757	-0.001840	-1.922026
H	3.160329	-1.101106	-1.450437
H	7.471020	3.526855	-1.280966



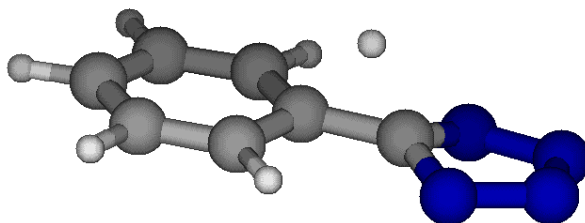
Compound TS **10aS -15S** - B3LYP/6-311G(d,p) - E=-489.305664 u.a.

C	1.117285	-1.236188	0.087231
C	0.390070	-0.000196	0.157640
C	1.116824	1.236001	0.085641
C	2.490082	1.218857	-0.034242
C	3.178061	0.000188	-0.097387
C	2.490535	-1.218659	-0.032686
C	-1.122002	-0.000457	0.017772
N	-1.866992	1.122414	-0.007733
N	-3.099280	0.679337	-0.132080
N	-3.099131	-0.679844	-0.134476
N	-1.866816	-1.123168	-0.011232
H	0.554060	-2.159908	0.134561
H	3.038413	-2.151616	-0.084247
H	3.037615	2.151958	-0.086802
H	0.553328	2.159557	0.132897
H	4.257706	0.000326	-0.192576
H	-0.137459	0.000837	1.211986



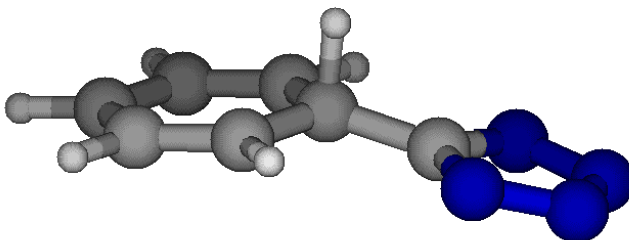
Compound TS **10aT -15T** - B3LYP/6-311G(d,p) - E=-489.216921 u.a.

C	1.130212	1.228924	-0.024319
C	0.410617	0.000002	-0.097898
C	1.130236	-1.228842	-0.023097
C	2.510471	-1.210887	0.030543
C	3.213476	0.000095	0.046003
C	2.510454	1.211041	0.029374
C	-1.065634	0.000030	-0.066284
N	-1.847331	-1.086982	0.161025
N	-3.192075	-0.623492	0.040501
N	-3.192017	0.624023	0.040208
N	-1.847358	1.087351	0.160620
H	0.580217	2.161520	-0.018750
H	3.051316	2.149315	0.074490
H	3.051354	-2.149106	0.076538
H	0.580233	-2.161422	-0.016640
H	4.295852	0.000125	0.085526
H	-0.367777	0.000069	-1.371066



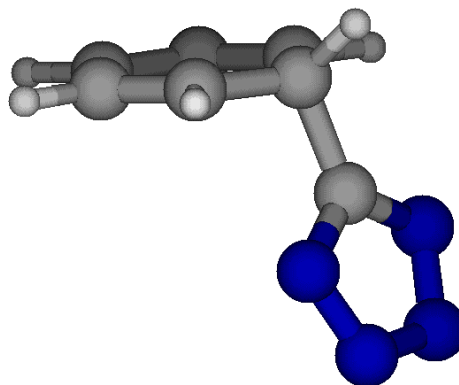
Compound **15S** - B3LYP/6-311G(d,p) - E=-489.309629 u.a.

N	-1.839993	-1.108430	-0.045254
C	-1.113392	0.010615	0.040570
N	-1.838825	1.128937	-0.062422
N	-3.077329	0.678308	-0.256406
N	-3.078007	-0.659558	-0.246145
C	0.353829	0.011821	0.300535
C	1.103080	-1.236368	0.153698
C	2.463919	-1.219456	-0.033569
C	3.139270	0.006886	-0.145131
C	2.465231	1.235544	-0.052597
C	1.104421	1.256810	0.134372
H	0.531074	-2.153568	0.234343
H	3.015662	-2.147941	-0.114439
H	3.017993	2.162057	-0.147846
H	0.533365	2.175738	0.200827
H	4.212989	0.005138	-0.298070
H	0.332830	0.020721	1.440610



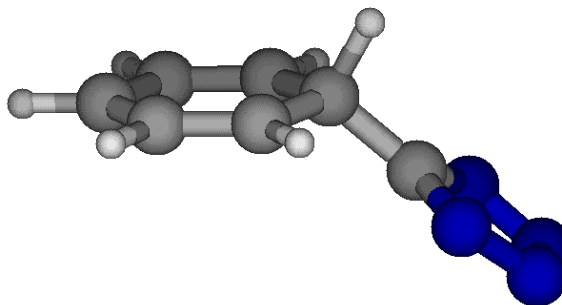
Compound **15S** - B3LYP/6-311G(d,p) - E=-489.315110 u.a.

C	-1.071621	-1.248431	0.621870
C	-0.448616	0.004421	1.103404
C	-1.033017	1.246994	0.554346
C	-2.009971	1.216765	-0.412071
C	-2.525903	-0.013786	-0.837920
C	-2.056803	-1.237917	-0.329457
C	0.917160	0.021220	0.387202
N	1.650888	1.129688	0.192464
N	2.713973	0.680952	-0.452990
N	2.605708	-0.648420	-0.653155
N	1.467959	-1.084365	-0.143253
H	-0.605063	2.181328	0.892347
H	-2.382506	2.137897	-0.842313
H	-2.473824	-2.167484	-0.695991
H	-0.686309	-2.179793	1.014605
H	-3.303031	-0.024232	-1.594919
H	-0.307543	0.028008	2.189067



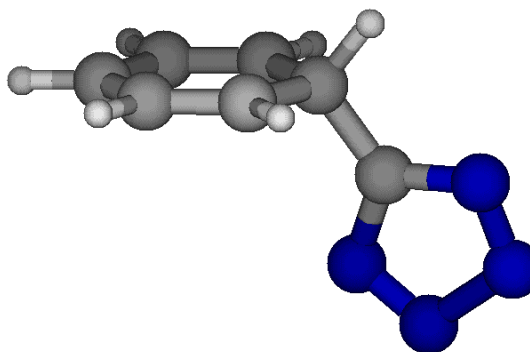
Compound **15T** - B3LYP/6-311G(d,p) - E=-489.286427 u.a.

N	1.805222	1.133119	-0.021048
C	1.042281	0.000270	0.197599
N	1.805259	-1.132660	-0.020603
N	2.960440	-0.774998	-0.357898
N	2.960449	0.775419	-0.358179
C	-0.366274	0.000370	0.691677
C	-1.105916	1.265853	0.326586
C	-2.361152	1.223515	-0.198920
C	-3.022926	-0.000467	-0.461386
C	-2.360931	-1.224057	-0.197622
C	-1.105690	-1.265614	0.327927
H	-0.599708	-2.204663	0.509547
H	-2.863491	-2.157359	-0.428696
H	-2.863874	2.156488	-0.430971
H	-0.600093	2.205176	0.507229
H	-0.237632	0.000993	1.802325
H	-4.021207	-0.000783	-0.879539



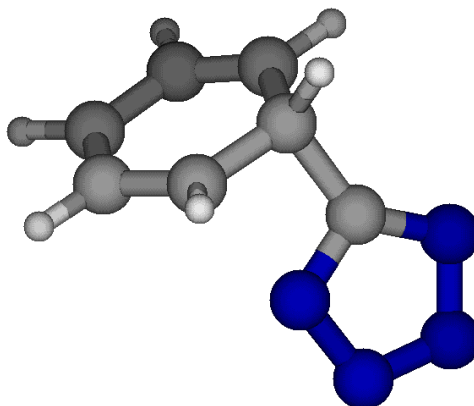
Compound **15T** - B3LYP/6-311G(d,p) - E=-489.286774 u.a.

N	-1.279093	-0.748619	-0.836012
C	-1.005462	0.044927	0.267550
N	-2.169034	0.611905	0.744251
N	-3.124220	0.224957	0.022017
N	-2.512494	-0.706616	-1.055015
C	0.358067	0.307357	0.819394
C	1.156346	-0.969038	0.930206
C	2.334933	-1.144991	0.269715
C	2.884868	-0.137318	-0.557576
C	2.218458	1.105489	-0.678004
C	1.038612	1.355740	-0.044338
H	0.541470	2.313790	-0.136295
H	2.669186	1.891245	-1.275397
H	2.870751	-2.080592	0.389172
H	0.748254	-1.753050	1.556933
H	0.178768	0.732285	1.819977
H	3.818840	-0.307005	-1.076979



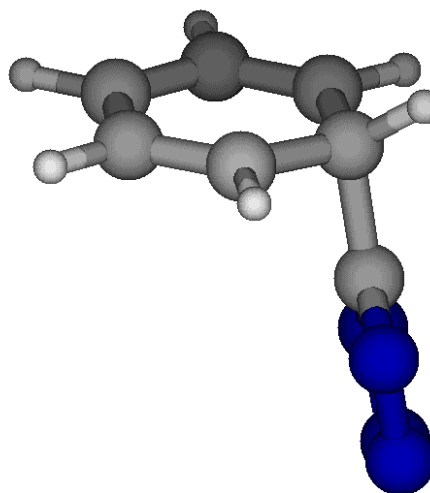
Compound TS **15S** – **61S** - B3LYP/6-311G(d,p) - E=-489.311190 u.a.

C	-0.786692	-0.887714	0.922725
C	-0.404170	0.570786	0.941671
C	-1.233436	1.452951	0.067272
C	-2.225605	0.956778	-0.700548
C	-2.542095	-0.444510	-0.660237
C	-1.855645	-1.337025	0.121400
C	0.976165	0.378105	0.339272
N	2.034544	1.097034	0.045315
N	2.853101	0.166463	-0.528724
N	2.315315	-1.024634	-0.576701
N	1.093786	-0.909570	-0.019315
H	-0.966931	2.503168	0.039774
H	-2.796814	1.604583	-1.354108
H	-2.132876	-2.383342	0.138852
H	-0.411435	-1.517093	1.716256
H	-3.369082	-0.801122	-1.265385
H	-0.340184	0.970913	1.960826



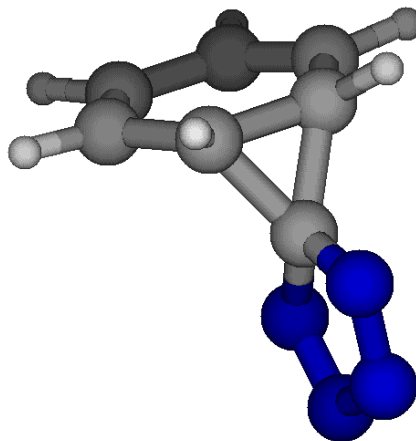
Compound TS **15S** – **60S** - B3LYP/6-311G(d,p) - E=-489.314942 u.a.

C	1.180313	-0.935185	0.582744
C	0.391572	0.265994	0.931243
C	0.757942	1.488762	0.193343
C	1.689070	1.465856	-0.835075
C	2.375888	0.291096	-1.109695
C	2.121064	-0.909360	-0.401142
C	-0.970241	0.147126	0.213929
N	-1.328977	-0.930206	-0.505799
N	-2.551671	-0.640384	-0.907933
N	-2.899851	0.592178	-0.470634
N	-1.914069	1.111470	0.232970
H	0.240933	0.400859	2.004830
H	0.959488	-1.851765	1.115338
H	3.119810	0.284228	-1.899079
H	1.887396	2.363817	-1.406327
H	2.671182	-1.806140	-0.656994
H	0.222025	2.392896	0.448703



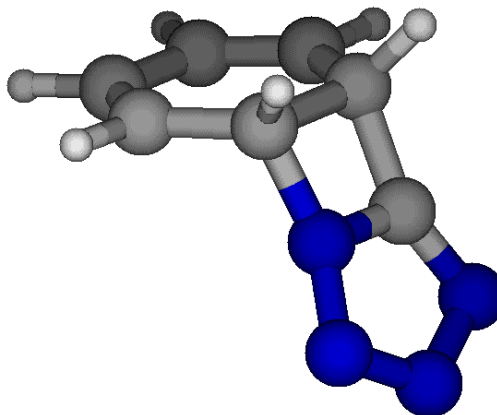
Compound **60S** - B3LYP/6-311G(d,p) - E=-489.327265 u.a.

C	-1.460482	-1.423474	0.241216
C	-0.446858	-0.703708	1.016854
C	-0.454704	0.791257	0.945817
C	-1.474908	1.424132	0.105938
C	-2.334557	0.682455	-0.622119
C	-2.327146	-0.762787	-0.553453
C	0.736704	0.015633	0.273251
N	1.985527	0.052500	0.909983
N	2.864875	0.014039	0.017096
N	2.186984	-0.052133	-1.296242
N	0.947361	-0.049345	-1.105036
H	-0.082636	1.347450	1.797267
H	-1.535816	2.505652	0.115244
H	-3.071722	-1.313562	-1.116182
H	-1.510544	-2.499854	0.352579
H	-3.084499	1.169742	-1.234115
H	-0.070297	-1.172701	1.917430



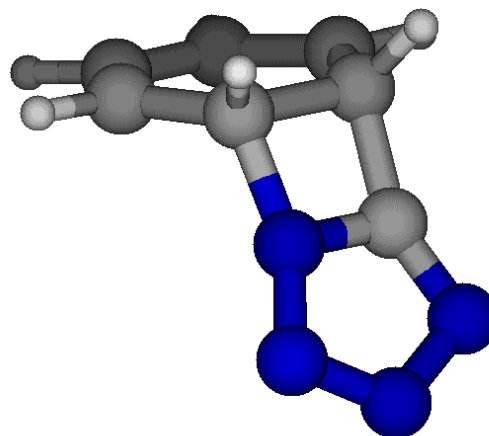
Compound **61S** - B3LYP/6-311G(d,p) - E=-489.327553 u.a.

C	-0.554392	-0.873787	0.776331
C	-0.446752	0.704111	0.989587
C	-1.456062	1.525132	0.246175
C	-2.369066	0.961771	-0.554167
C	-2.466932	-0.487323	-0.731030
C	-1.647290	-1.352592	-0.118965
C	0.933225	0.567772	0.330833
N	2.103877	0.989415	-0.082768
N	2.697334	-0.168537	-0.549884
N	1.948583	-1.223565	-0.420963
N	0.814067	-0.741312	0.134424
H	-1.409654	2.600915	0.374672
H	-3.078912	1.585866	-1.085090
H	-1.759534	-2.423077	-0.248391
H	-0.473456	-1.457597	1.694087
H	-3.254765	-0.864101	-1.374361
H	-0.380328	0.996324	2.040175



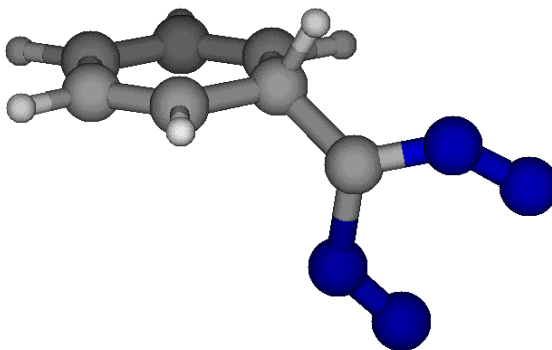
Compound **61T** - B3LYP/6-311G(d,p) - E=-489.246426 u.a.

C	-0.555389	-0.867968	0.784683
C	-0.433675	0.697356	0.991038
C	-1.467981	1.511775	0.304415
C	-2.431039	0.914491	-0.595582
C	-2.523236	-0.428383	-0.772153
C	-1.662118	-1.351450	-0.054480
C	0.946722	0.564022	0.314398
N	2.126011	0.989023	-0.076548
N	2.726120	-0.164264	-0.542266
N	1.975071	-1.219953	-0.427906
N	0.828906	-0.738838	0.107459
H	-1.430723	2.587817	0.418618
H	-3.094109	1.577054	-1.139753
H	-1.777453	-2.419490	-0.190857
H	-0.435711	-1.440492	1.705930
H	-3.258666	-0.839642	-1.452765
H	-0.332789	0.968356	2.046433



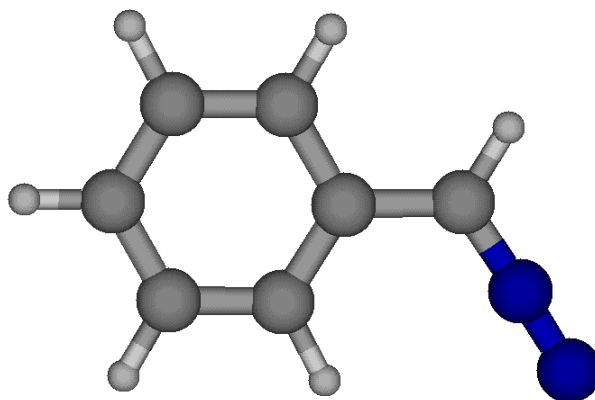
Compound TS **15S** – **11S** - B3LYP/6-311G(d,p) - E=-489.275075 u.a.

C	-1.162744	-1.260855	0.621477
C	-0.347747	-0.031510	0.718307
C	-1.002906	1.167827	0.133860
C	-2.276863	1.131697	-0.361078
C	-3.012231	-0.071877	-0.372234
C	-2.437017	-1.256847	0.107977
C	1.089124	-0.275331	0.334544
N	2.103627	0.450957	0.829289
N	3.153595	0.828152	0.512542
N	2.263288	-0.143561	-1.782460
N	1.287107	-0.400090	-1.246366
H	-0.437922	2.093442	0.135551
H	-2.721411	2.031920	-0.770534
H	-2.999652	-2.182321	0.061605
H	-0.710073	-2.176979	0.980960
H	-4.019301	-0.083000	-0.771395
H	-0.150308	0.179681	1.801943



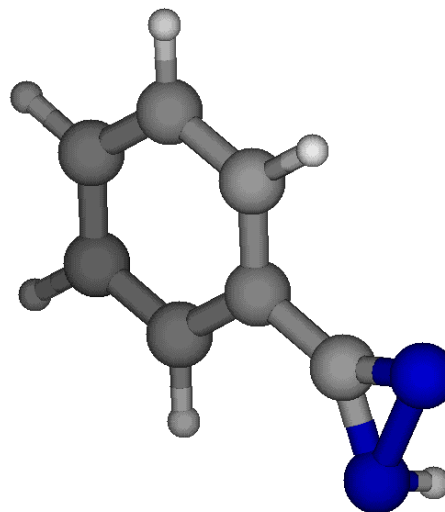
Compound **11S** - B3LYP/6-311G(d,p) - E=-379.896745 u.a.

C	-2.820706	-0.020025	-0.690273
C	-2.617607	-1.159991	0.086699
C	-1.418176	-1.304609	0.781833
C	-0.434905	-0.325799	0.703112
C	-0.630204	0.826665	-0.077348
C	-1.842984	0.963619	-0.774675
C	0.428380	1.825190	-0.129339
N	0.314338	2.914351	-0.831665
N	0.190523	3.859524	-1.453587
H	-2.021913	1.842287	-1.384891
H	-3.749150	0.105499	-1.236335
H	-1.245809	-2.185632	1.390175
H	0.494579	-0.449628	1.248738
H	-3.383368	-1.924104	0.149085
H	1.359481	1.716682	0.408191



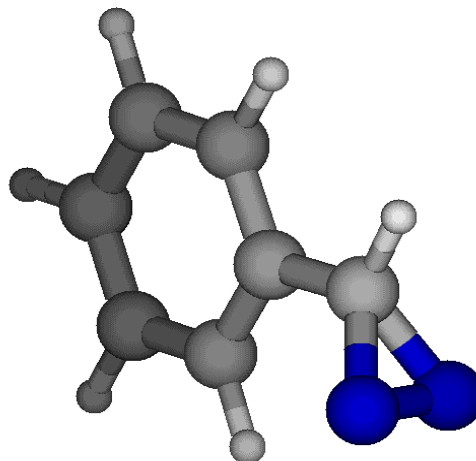
Compound **5aS** - B3LYP/6-311G(d,p) - E=-379.849101 u.a.

C	-0.176977	0.175140	-0.026081
C	0.462884	1.397598	-0.275434
C	1.849247	1.463334	-0.256507
C	2.600493	0.315744	0.007638
C	1.965416	-0.900732	0.251888
C	0.576550	-0.974382	0.235855
C	-1.619732	0.085070	-0.042007
N	-2.620635	-0.897111	0.147812
N	-2.673128	0.715155	-0.255250
H	-0.132624	2.279846	-0.479303
H	2.348319	2.406139	-0.447467
H	2.552025	-1.789587	0.452151
H	0.065570	-1.913567	0.413333
H	3.683031	0.371757	0.021048
H	-2.851664	-0.907674	1.147457



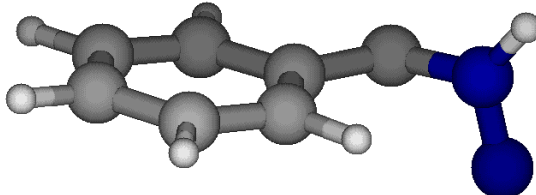
Compound **64S** - B3LYP/6-311G(d,p) - E=-379.872297 u.a.

C	2.779499	-0.290421	-0.343198
C	1.623496	-1.064168	-0.302104
C	0.382669	-0.493802	-0.578387
C	0.303301	0.860791	-0.897359
C	1.456365	1.637237	-0.939406
C	2.707891	1.071938	-0.663122
C	3.908993	1.924172	-0.716869
N	5.226830	1.325635	-1.054979
N	5.087772	1.596156	0.126846
H	3.737625	-0.746997	-0.126240
H	1.693157	-2.117083	-0.053182
H	-0.657934	1.313124	-1.113720
H	1.388984	2.691342	-1.188350
H	-0.515525	-1.099605	-0.545419
H	3.792019	2.970147	-0.970140



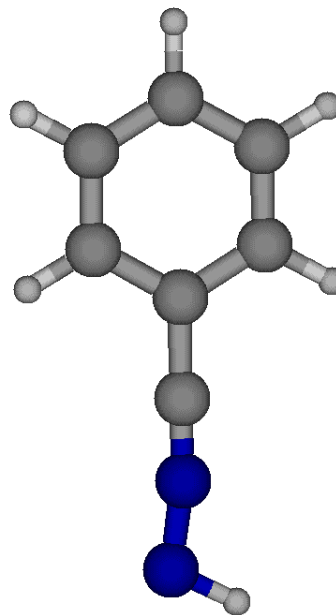
Compound **65S** - B3LYP/6-311G(d,p) - E=-379.752078 u.a.

C	0.112726	0.913830	0.079711
C	1.417007	1.378532	0.154871
C	2.486343	0.479605	0.108631
C	2.246632	-0.887247	-0.026275
C	0.941584	-1.354713	-0.116595
C	-0.151484	-0.468283	-0.049704
C	-1.468156	-1.092846	-0.055214
N	-2.519856	-0.180921	0.120573
N	-2.836187	0.082422	-1.030186
H	-0.706974	1.623049	0.090818
H	1.608671	2.441476	0.250661
H	3.076924	-1.582590	-0.071677
H	0.729134	-2.410674	-0.232116
H	3.504122	0.848520	0.169744
H	-2.977690	0.161289	0.993796



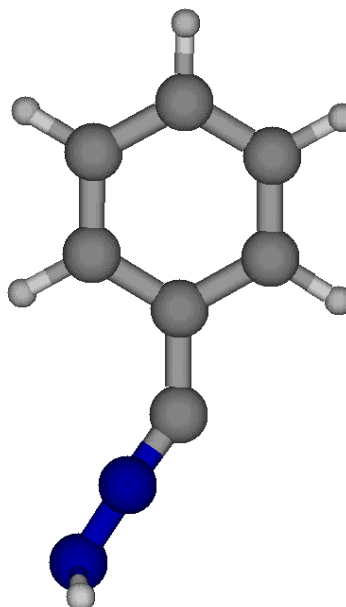
Compound **4aS** - B3LYP/6-311G(d,p) - E=-379.860106 u.a.

C	0.888784	-0.484565	0.002538
N	0.206544	0.458417	-0.115007
N	-0.371595	1.569745	-0.248835
C	1.719746	-1.620404	0.143527
H	-1.380659	1.412565	-0.256783
C	1.161989	-2.908231	0.268796
C	1.989643	-4.014489	0.406568
C	3.376224	-3.866778	0.422699
C	3.933354	-2.594278	0.299036
C	3.121671	-1.476422	0.160411
H	3.557935	-0.489803	0.064610
H	5.010206	-2.469694	0.310495
H	4.016128	-4.734452	0.530532
H	1.547467	-4.999705	0.502054
H	0.085523	-3.027776	0.256788



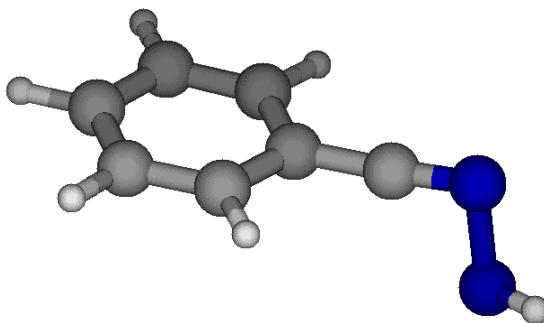
Compound **4aS** - B3LYP/6-311G(d,p) - E=-379.859609 u.a.

C	-1.452782	-0.567768	-0.119531
N	-2.540575	-0.118052	0.025029
N	-3.718343	0.300147	-0.042600
C	-0.047280	-0.258446	-0.052763
H	-4.178513	0.162209	0.861148
C	0.898687	-1.294076	-0.014355
C	2.257261	-1.000726	0.046393
C	2.687661	0.325455	0.051136
C	1.754083	1.362131	0.001010
C	0.394618	1.077669	-0.045328
H	-0.332790	1.880178	-0.080235
H	2.087244	2.393778	0.002519
H	3.747024	0.552003	0.091108
H	2.980729	-1.807051	0.081759
H	0.555245	-2.321215	-0.032672



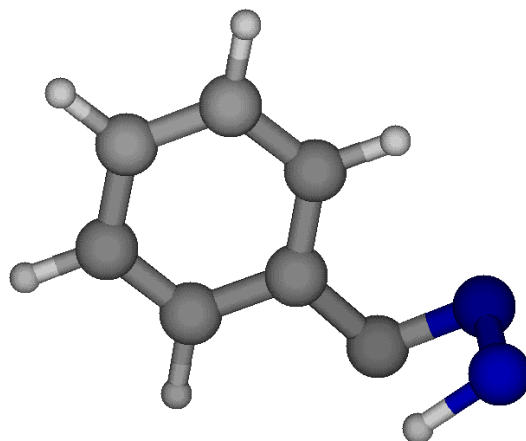
Compound TS **4aS** – **5aS** - B3LYP/6-311G(d,p) - E=-379.859609 u.a.

C	-1.449477	-0.222137	0.482149
N	-3.257725	0.130472	-0.507288
N	-2.621437	-0.390689	0.725299
H	-4.051622	0.623570	-0.076979
C	-0.086525	-0.063488	0.257290
C	0.725324	-1.194687	0.000011
C	0.501980	1.224790	0.299285
C	2.091347	-1.034524	-0.170880
H	0.268577	-2.174745	-0.050525
C	1.859248	1.365378	0.072729
H	-0.125663	2.086494	0.486459
C	2.660179	0.240061	-0.148111
H	2.713997	-1.903480	-0.347955
H	2.304751	2.353076	0.085108
H	3.725575	0.358902	-0.306251



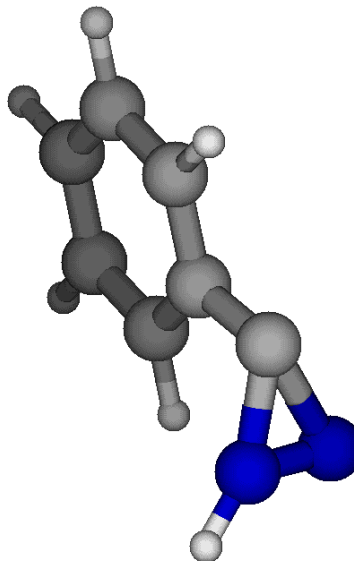
Compound TS **4aS** – **6aS** - B3LYP/6-311G(d,p) - E=-379.765562 u.a.

C	2.714161	1.072287	-0.511443
C	2.762733	-0.302294	-0.205510
C	1.608797	-1.072355	-0.261177
C	0.397014	-0.490394	-0.638500
C	0.335516	0.866915	-0.955735
C	1.485016	1.643091	-0.889628
C	3.837682	2.004286	-0.345625
N	5.085857	1.316199	-0.098420
N	5.465518	1.578374	-1.241989
H	3.707877	-0.754313	0.069015
H	1.649960	-2.128077	-0.018684
H	-0.607000	1.314444	-1.249024
H	1.455829	2.703007	-1.114208
H	-0.500013	-1.097590	-0.687964
H	4.556286	2.373119	-1.549650



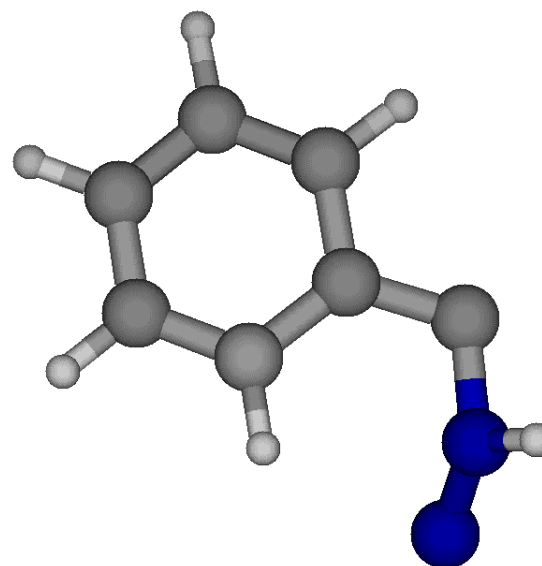
Compound TS **5aS** – **65S** - B3LYP/6-311G(d,p) - **E=-379.739895 u.a.**

C	-0.000968	-0.000422	0.000460
C	-0.000531	0.000480	1.405915
C	1.196344	0.000341	2.116849
C	2.414026	-0.006530	1.438938
C	2.429799	-0.007670	0.044323
C	1.233541	-0.002929	-0.664518
C	-1.192826	0.031410	-0.920187
N	-2.407621	-0.519868	-0.111853
N	-2.440337	0.688015	-0.013034
H	-0.933995	0.014936	1.957882
H	1.179981	0.006169	3.201378
H	3.374534	-0.010244	-0.487900
H	1.225634	0.001423	-1.748618
H	3.345095	-0.009517	1.994636
H	-2.998240	-1.200548	0.394775



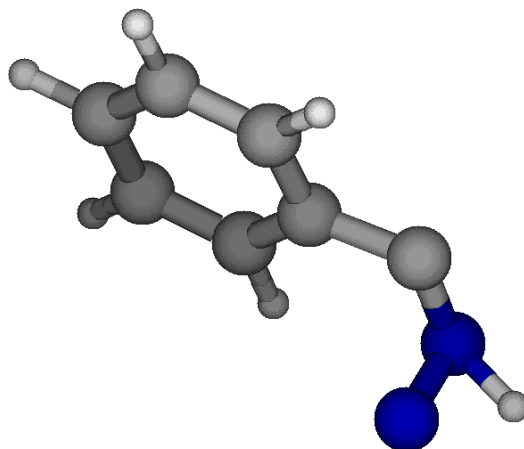
Compound TS **11S** – **65S** - B3LYP/6-311G(d,p) - **E=-379.738928 u.a.**

C	-0.000490	-0.026358	-0.001281
C	-0.002637	-0.021555	1.419209
C	1.194242	0.001343	2.117937
C	2.407707	0.004056	1.425356
C	2.436004	-0.017886	0.026558
C	1.246752	-0.046169	-0.679207
C	-1.151186	0.147527	-0.833659
N	-2.359789	0.248514	-0.059725
N	-2.884033	0.923112	0.795193
H	-0.942406	-0.042321	1.955555
H	1.191454	0.009539	3.201701
H	3.384889	-0.018910	-0.496675
H	1.228628	-0.057517	-1.762249
H	3.339818	0.013004	1.979854
H	-2.869102	-0.588624	-0.513076



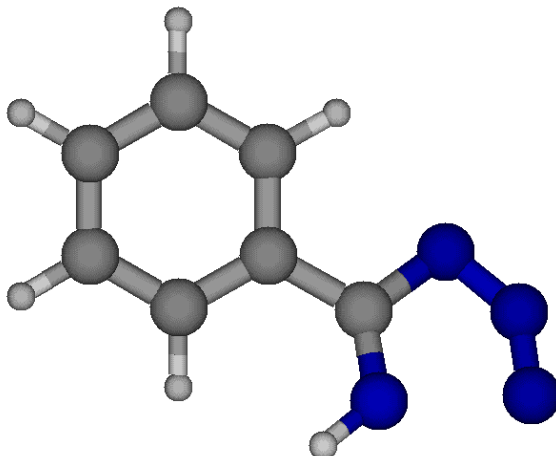
Compound TS **4aS** – **65S** - B3LYP/6-311G(d,p) - **E=-379.670754 u.a.**

C	-0.176688	-0.401130	-0.058124
C	0.127463	0.962755	-0.267277
C	1.443973	1.398741	-0.236179
C	2.478143	0.493742	0.012455
C	2.193005	-0.855304	0.223149
C	0.878351	-1.300508	0.182391
C	-1.515003	-0.942245	-0.169738
N	-2.557203	-0.090863	-0.232948
N	-2.654829	0.022685	1.117924
H	-0.673582	1.668153	-0.450292
H	1.669752	2.445309	-0.407097
H	2.996831	-1.556970	0.413750
H	0.637824	-2.345967	0.331398
H	3.504905	0.841002	0.038313
H	-3.577515	-0.361753	0.179986



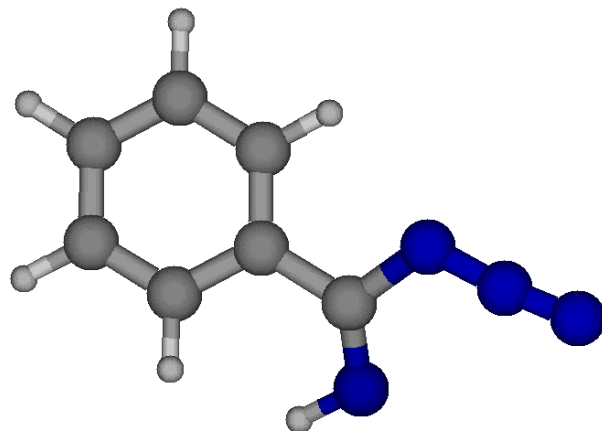
Compound TS **2aS** – **3aS** - B3LYP/6-311G(d,p) - **E=-489.389445 u.a.**

C	-1.058897	-1.171830	-0.017794
C	-0.433658	0.080285	0.033513
C	-1.223017	1.236652	0.074142
C	-2.609746	1.144140	0.054438
C	-3.225220	-0.105067	-0.007541
C	-2.446752	-1.260097	-0.042694
C	1.047318	0.173832	0.043157
N	1.770856	1.204472	-0.172055
N	3.604495	0.205410	0.072288
N	2.969166	-0.742803	0.273231
N	1.710685	-1.040046	0.323633
H	-0.445737	-2.062449	-0.038300
H	-2.921107	-2.233639	-0.087894
H	-3.209771	2.045953	0.091674
H	-0.757584	2.213424	0.141157
H	1.350102	2.090866	-0.414624
H	-4.306791	-0.176748	-0.024298



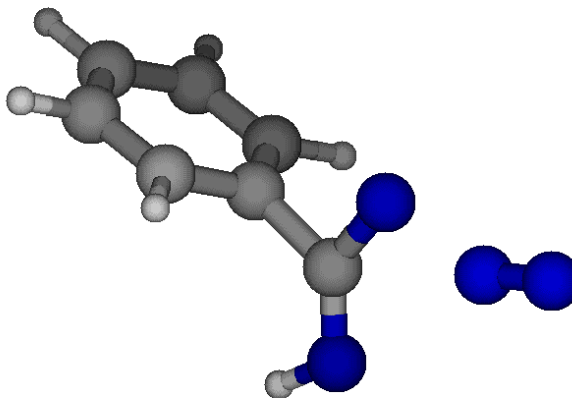
Compound **3aS** - B3LYP/6-311G(d,p) - **E=-489.415033 u.a.**

C	-2.378593	-1.278759	0.105774
C	-0.996154	-1.119053	0.112870
C	-0.428554	0.157465	0.014829
C	-1.276149	1.265918	-0.110737
C	-2.656164	1.104126	-0.124922
C	-3.212211	-0.169533	-0.012159
C	1.049012	0.345319	0.052423
N	1.745468	-0.873595	-0.187836
N	2.982307	-0.800323	-0.143662
N	4.106810	-0.854867	-0.133118
N	1.706436	1.413568	0.268716
H	-0.347162	-1.980459	0.197913
H	-2.804174	-2.272085	0.190305
H	-3.298116	1.971096	-0.230154
H	-0.859316	2.260821	-0.220269
H	1.089006	2.200158	0.455032
H	-4.288903	-0.295237	-0.022037



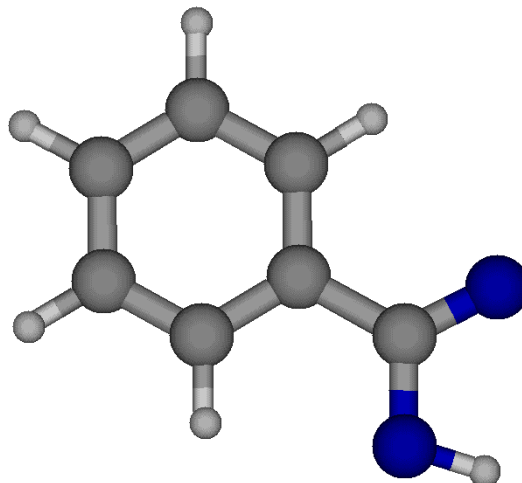
Compound TS **3aS** – **6aS** - B3LYP/6-311G(d,p) - **E=-489.361568 u.a.**

C	0.065089	-0.137811	-0.044030
C	0.009257	0.312116	1.275107
C	1.174066	0.401193	2.030619
C	2.399945	0.062253	1.450934
C	2.455162	-0.417794	0.139366
C	1.286202	-0.504177	-0.610013
C	3.706250	0.321489	2.223345
N	4.419145	1.383733	2.245995
N	3.776347	-0.864155	2.784348
N	5.271630	-0.814113	3.775148
N	5.979972	-1.296728	4.463867
H	1.143354	0.737128	3.060028
H	-0.942260	0.584063	1.717200
H	1.325767	-0.865749	-1.631036
H	3.408357	-0.710916	-0.283695
H	4.018617	2.110849	1.659709
H	-0.845025	-0.212225	-0.628298



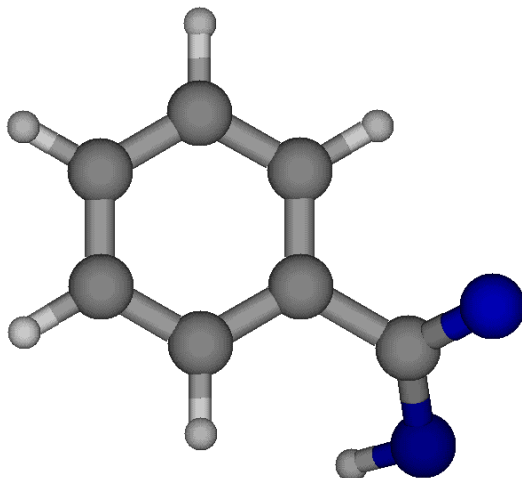
Compound **6aS** - B3LYP/6-311G(d,p) - E=-379.833658 u.a.

C	-0.118309	0.062899	-0.096664
N	-1.050144	-0.932300	-0.130099
N	-0.542986	1.284215	-0.019599
H	-1.976365	-0.491545	-0.085574
C	1.326450	-0.299251	-0.149288
C	2.305979	0.699600	-0.116828
C	1.706624	-1.641897	-0.231481
C	3.652347	0.356688	-0.166203
H	2.007713	1.739529	-0.053092
C	3.055920	-1.979735	-0.280644
H	0.940813	-2.406541	-0.255953
C	4.029772	-0.983447	-0.248188
H	4.407626	1.133745	-0.140804
H	3.346842	-3.022027	-0.344346
H	5.080057	-1.249637	-0.286633



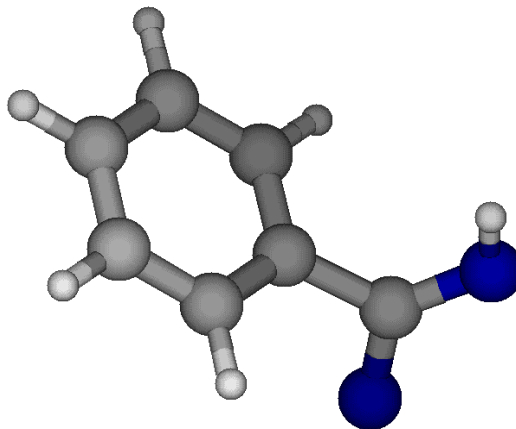
Compound **6aS** - B3LYP/6-311G(d,p) - E=-379.824642 u.a.

C	1.761353	0.009643	0.200353
N	2.565339	-0.942750	-0.321336
N	2.321016	1.005595	0.826534
H	1.983761	-1.617533	-0.829504
C	0.261926	-0.006440	0.107507
C	-0.447372	1.185657	-0.076783
C	-0.436948	-1.213726	0.217144
C	-1.835474	1.165316	-0.168700
H	0.094900	2.120002	-0.155850
C	-1.825689	-1.229117	0.130046
H	0.101267	-2.139571	0.390633
C	-2.526637	-0.040557	-0.066304
H	-2.377642	2.091255	-0.322016
H	-2.360170	-2.167677	0.221121
H	-3.608226	-0.054377	-0.136447



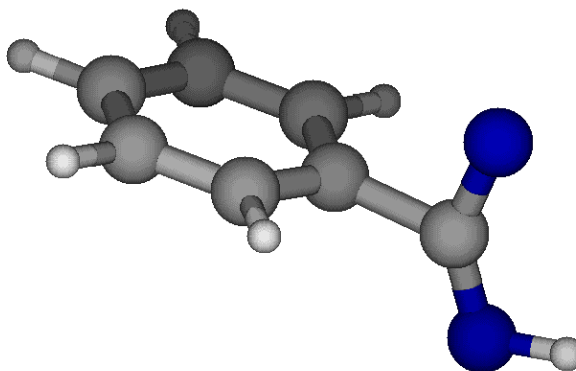
Compound TS **6aS** – **7aS** - B3LYP/6-311G(d,p) - **E=-379.791194 u.a.**

C	0.086923	-0.016428	-0.072438
N	-0.108451	0.454574	1.153546
N	1.203475	-0.504826	-0.455294
H	-1.113403	0.406338	1.344006
C	-0.874973	-0.060078	-1.239492
C	-1.241882	-1.263028	-1.855606
C	-1.400783	1.160806	-1.684441
C	-2.190154	-1.248025	-2.871670
H	-0.786624	-2.188135	-1.525306
C	-2.349437	1.164495	-2.700100
H	-1.075919	2.083875	-1.218414
C	-2.742844	-0.037486	-3.292236
H	-2.494269	-2.176118	-3.341217
H	-2.774347	2.102107	-3.039121
H	-3.473675	-0.028375	-4.092858



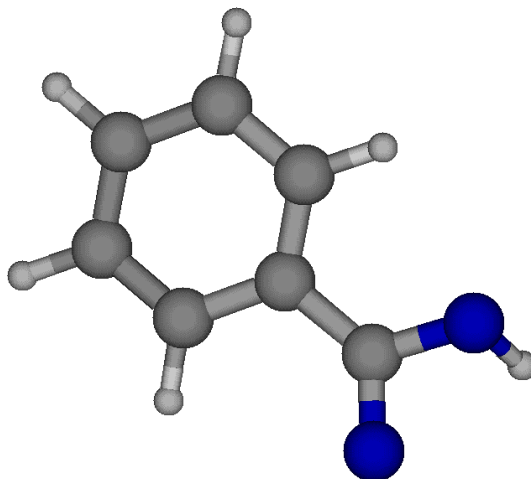
Compound TS **6aS**– **7aS** - B3LYP/6-311G(d,p) - **E=-379.813756 u.a.**

C	-1.843128	0.000007	0.009704
N	-2.553951	0.000177	-1.070228
C	-0.315960	-0.000004	0.041708
N	-1.978638	-0.000208	1.303521
H	-3.544707	0.000028	-0.809313
C	0.378342	-1.218444	0.035312
C	0.378336	1.218437	0.035402
C	1.763494	-1.213106	-0.060210
H	-0.174676	-2.148281	0.083508
C	1.763501	1.213123	-0.060028
H	-0.174691	2.148267	0.083647
C	2.453787	0.000014	-0.108539
H	2.307978	-2.149521	-0.089318
H	2.307985	2.149546	-0.088858
H	3.535994	0.000011	-0.172811



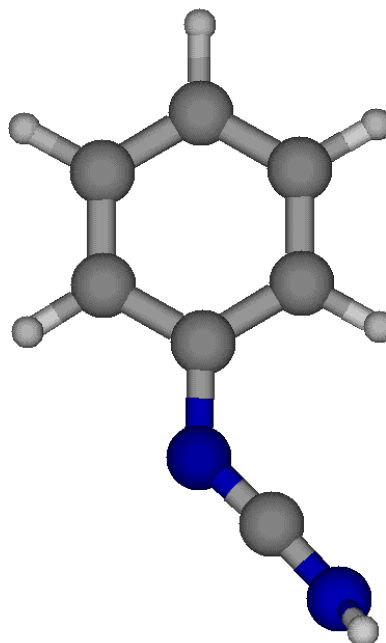
Compound TS **6aS** – **5aS** - B3LYP/6-311G(d,p) - **E=-379.830035 u.a.**

C	1.723450	0.122924	0.034428
N	2.539653	-1.003174	-0.059290
N	2.516254	1.099502	-0.078822
H	3.315347	-0.919474	0.601133
C	0.254188	0.060897	0.014715
C	-0.504910	1.236790	0.023956
C	-0.380347	-1.183638	-0.005327
C	-1.891908	1.163367	0.015735
H	-0.002562	2.197353	0.038217
C	-1.770268	-1.251507	-0.016563
H	0.221814	-2.084520	-0.021150
C	-2.525615	-0.080377	-0.005050
H	-2.481370	2.072821	0.024838
H	-2.263737	-2.216275	-0.035580
H	-3.608370	-0.134934	-0.012036



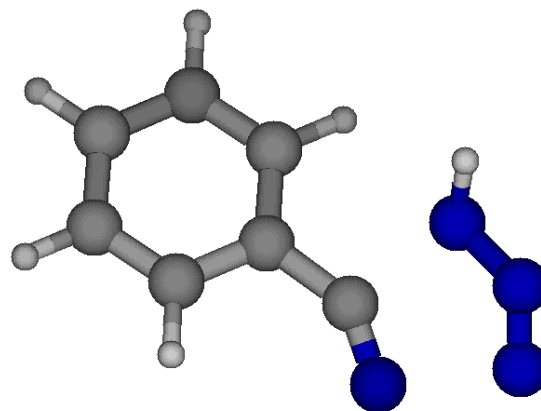
Compound **7aS** - B3LYP/6-311G(d,p) - E=-379.932741 u.a.

N	3.567107	0.387540	-0.072970
H	4.109240	0.569359	0.763104
C	2.469620	-0.143082	0.013910
N	1.425181	-0.764953	-0.051838
C	0.089049	-0.324858	-0.022162
C	-0.914836	-1.296716	0.003915
C	-0.259838	1.031908	-0.028797
C	-2.252820	-0.916195	0.028359
H	-0.626545	-2.340651	0.004130
C	-1.599486	1.403067	-0.005616
H	0.519078	1.786076	-0.056800
C	-2.601100	0.433008	0.023829
H	-3.024964	-1.676863	0.049034
H	-1.862206	2.455010	-0.012263
H	-3.643867	0.727722	0.041692



Compound TS **2aS** – **63S** - B3LYP/6-311G(d,p) - **E=-489.357839 u.a.**

C	-1.351060	-1.300547	0.164154
C	-0.496189	-0.217361	-0.086352
C	-1.036759	1.059682	-0.272377
C	-2.413235	1.250761	-0.204947
C	-3.258917	0.174602	0.055622
C	-2.724318	-1.099872	0.239714
C	0.935283	-0.479433	-0.179217
N	1.866396	1.119358	0.316707
N	3.066811	0.679454	0.291179
N	3.537510	-0.322619	-0.067140
N	1.753918	-1.306167	-0.454895
H	-0.926311	-2.287412	0.298334
H	-3.378516	-1.940656	0.439369
H	-2.825363	2.241424	-0.358447
H	-0.379094	1.890653	-0.493629
H	1.703077	1.838777	1.018897
H	-4.330585	0.327375	0.111694

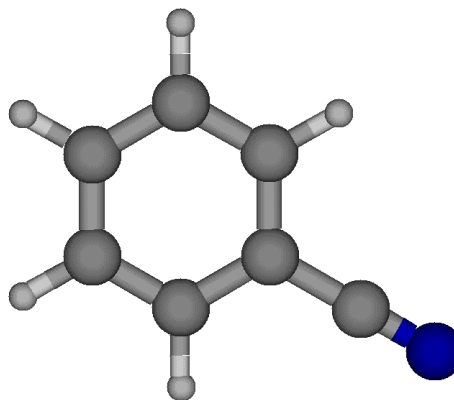


Compound NNNH - B3LYP/6-311G(d,p) - **E=-164.830536 u.a.**

N	1.884314	0.058255	1.067676
N	2.971194	0.284146	0.520087
N	3.873866	0.527762	-0.116422
H	2.031782	-0.230810	2.034139

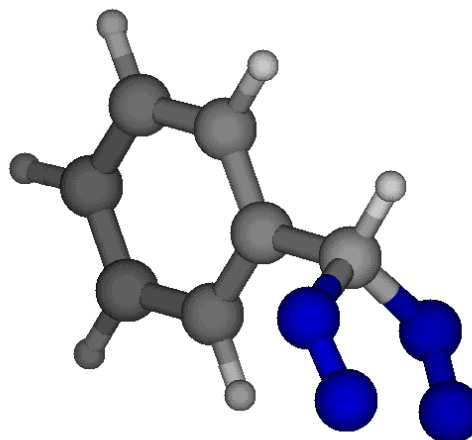
Compound **63S** - B3LYP/6-311G(d,p) - **E=-164.830536 u.a.**

C	1.394396	1.317529	0.211813
C	0.483551	0.314993	-0.098829
C	0.940826	-0.986614	-0.351128
C	2.312209	-1.272369	-0.289630
C	3.213669	-0.261417	0.022055
C	2.757729	1.031917	0.272704
C	0.007025	-2.023135	-0.671369
N	-0.746757	-2.859614	-0.929898
H	-0.577175	0.527339	-0.148458
H	1.040095	2.322867	0.406664
H	4.273238	-0.483420	0.069318
H	2.657470	-2.279808	-0.485903
H	3.464463	1.817042	0.515396



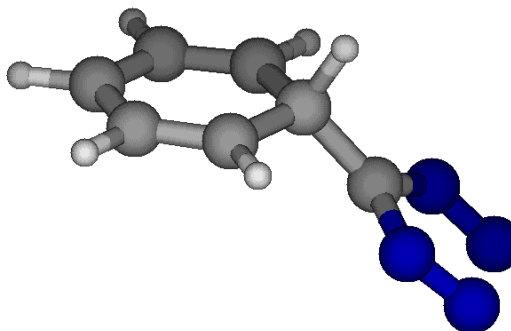
Compound TS **10aS** – **11S** - B3LYP/6-311G(d,p) - **E=-489.385625 u.a.**

C	2.603419	-1.012274	0.139172
C	1.226842	-1.211549	0.066177
C	0.364949	-0.123539	-0.082699
C	0.892525	1.169680	-0.159046
C	2.266706	1.366499	-0.093026
C	3.124086	0.276246	0.057447
C	-1.119704	-0.338001	-0.102901
N	-1.832490	0.426809	-1.124841
N	-2.674394	1.202265	-0.862544
N	-1.806486	0.139088	1.257058
N	-2.643028	0.947910	1.171007
H	0.228781	2.018698	-0.274790
H	2.670160	2.370255	-0.157389
H	3.266164	-1.861865	0.255271
H	0.821348	-2.215716	0.126300
H	4.195423	0.432744	0.109581
H	-1.383939	-1.391365	-0.211256



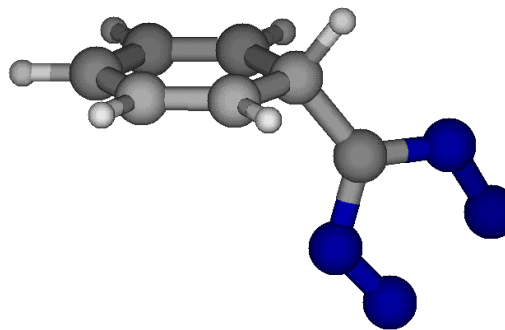
Compound TS **15T** – **16T**- B3LYP/6-311G(d,p) - E=-489.278960 u.a.

N	-1.819509	-1.125475	-0.023024
C	-1.032582	0.000006	0.144358
N	-1.819567	1.125465	-0.022919
N	-2.967457	1.014140	-0.324320
N	-2.967405	-1.014182	-0.324414
C	0.364334	0.000023	0.696469
C	1.107606	-1.261499	0.326050
C	2.362900	-1.223334	-0.199318
C	3.024992	-0.000007	-0.465394
C	2.362891	1.223335	-0.199405
C	1.107599	1.261527	0.325965
H	0.609067	2.204671	0.513146
H	2.866598	2.156895	-0.427330
H	2.866614	-2.156906	-0.427179
H	0.609081	-2.204635	0.513288
H	0.257231	0.000059	1.803919
H	4.022538	-0.000017	-0.885460



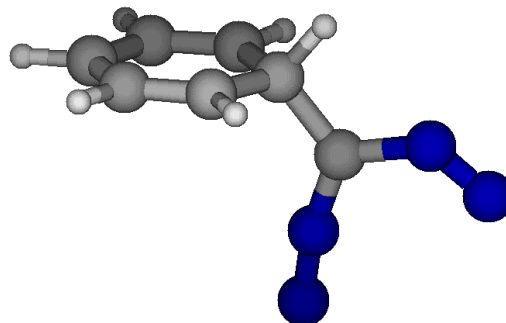
Compound TS **15T** – **16T**- B3LYP/6-311G(d,p) - E=-489.281010 u.a.

N	-2.179878	0.666974	-0.706162
C	-1.040541	-0.020179	-0.320497
N	-1.346198	-0.832435	0.765082
N	-2.470574	-0.873691	1.159177
N	-3.208911	0.455092	-0.134204
C	0.345220	0.282312	-0.808905
C	1.008043	1.343865	0.046803
C	2.200810	1.130109	0.671158
C	2.899314	-0.092100	0.539040
C	2.357765	-1.122787	-0.270602
C	1.167154	-0.979638	-0.913293
H	0.766488	-1.778869	-1.526020
H	2.910128	-2.049824	-0.382751
H	2.627449	1.920774	1.279626
H	0.481552	2.285656	0.151368
H	0.182632	0.699505	-1.818162
H	3.844086	-0.238317	1.046470



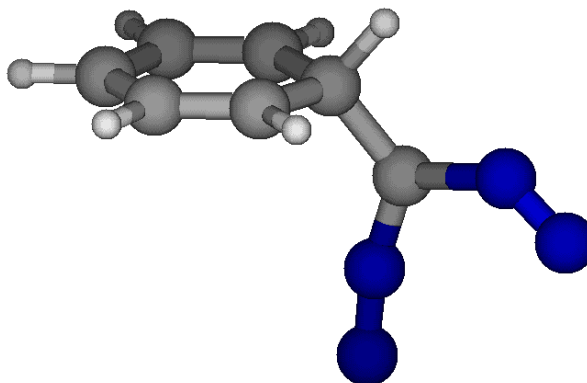
Compound **16T**- B3LYP/6-311G(d,p) - E=-489.296207 u.a.

N	-2.162929	-0.452382	1.085978
C	-1.055817	-0.138327	0.248154
N	-1.336924	0.278104	-0.957415
N	-1.775021	0.617137	-1.950192
N	-3.322754	-0.408672	0.898519
C	0.368022	-0.291358	0.763252
C	1.139032	-1.340129	-0.000323
C	2.326041	-1.069199	-0.612042
C	2.921242	0.214249	-0.538360
C	2.281421	1.241534	0.198020
C	1.093268	1.030355	0.830701
H	0.615012	1.823677	1.394624
H	2.751332	2.217529	0.261149
H	2.829966	-1.854233	-1.166252
H	0.695168	-2.327766	-0.060785
H	0.195808	-0.654968	1.790980
H	3.862928	0.407055	-1.036479



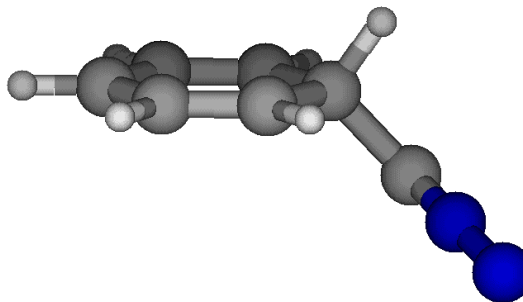
Compound TS **16T – 66T** - B3LYP/6-311G(d,p) - E=-489.288742 u.a.

N	-2.204722	0.056704	1.263318
C	-1.053086	-0.383741	0.098807
N	-1.371820	0.103675	-1.046403
N	-1.870555	0.503795	-1.999927
N	-3.290871	0.343270	1.110993
C	0.345430	-0.416441	0.694325
C	1.215870	-1.384017	-0.068204
C	2.394397	-1.004343	-0.633840
C	2.880426	0.323284	-0.522562
C	2.143027	1.278346	0.216627
C	0.962645	0.955029	0.818032
H	0.409757	1.692188	1.390167
H	2.529062	2.288203	0.309997
H	2.979371	-1.735895	-1.181526
H	0.850667	-2.399930	-0.163754
H	0.170421	-0.821801	1.705255
H	3.814855	0.601410	-0.993198



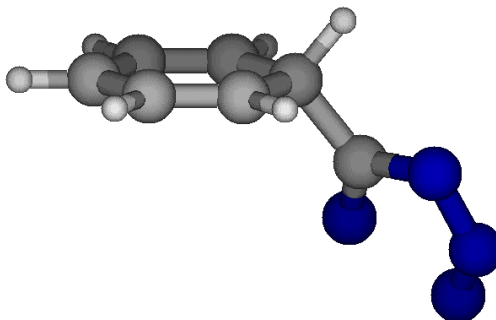
Compound **66T** - B3LYP/6-311G(d,p) - E=-379.770451 u.a.

C	-1.293945	-1.017141	0.535436
C	-0.433296	0.208336	0.373552
C	-1.181612	1.387918	-0.187548
C	-2.503966	1.320151	-0.504256
C	-3.249067	0.127512	-0.331172
C	-2.611822	-1.024996	0.185527
C	0.859951	-0.028007	-0.399296
N	1.474953	-1.132558	-0.355273
N	2.152307	-2.074246	-0.422750
H	-0.821341	-1.908793	0.932577
H	-3.186399	-1.937358	0.308533
H	-2.997197	2.197271	-0.909933
H	-0.611887	2.295655	-0.347298
H	-0.044639	0.498630	1.374988
H	-4.296875	0.095299	-0.601475



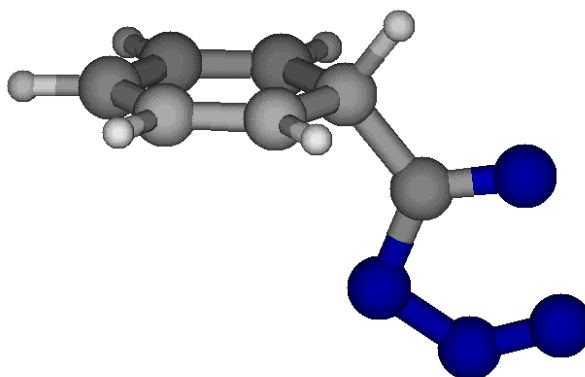
Compound TS **15T** – **17T** - B3LYP/6-311G(d,p) - E=-489.251320 u.a.

C	2.898369	-0.000374	-0.600744
C	2.287568	1.223642	-0.236493
C	1.114494	1.260179	0.453944
C	0.402184	0.000639	0.876117
C	1.114607	-1.259476	0.455883
C	2.287603	-1.223889	-0.234733
C	-1.041575	0.000243	0.360962
N	-2.034061	0.001399	1.172140
N	-1.270227	-0.001389	-1.001959
H	0.656547	2.203393	0.728090
H	2.766787	2.156896	-0.512853
H	2.766804	-2.157522	-0.509839
H	0.656794	-2.202316	0.731531
H	0.296604	0.001497	1.974386
H	3.827543	-0.000758	-1.155993
N	-2.614002	-0.001102	-1.056098
N	-3.417506	0.000095	-0.214788



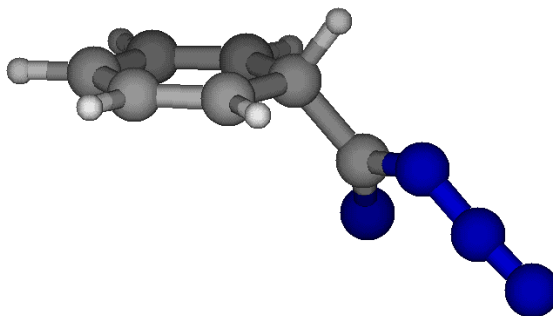
Compound TS **15T** – **17'T** - B3LYP/6-311G(d,p) - E=-489.252670 u.a.

C	-2.434732	-0.972619	0.604979
C	-1.122885	-0.917168	0.970442
C	-0.321939	0.353198	0.855166
C	-1.121578	1.520821	0.342033
C	-2.433187	1.396392	-0.005354
C	-3.118149	0.162173	0.106033
C	0.926038	0.096455	0.001619
N	1.103917	0.621508	-1.150482
N	1.888385	-0.754994	0.521695
N	2.809854	-0.775884	-0.456900
N	2.843244	-0.233676	-1.485359
H	-0.605404	-1.790454	1.347628
H	-2.970315	-1.910933	0.704533
H	-2.968134	2.266251	-0.371445
H	-0.611930	2.472793	0.252252
H	0.102181	0.597860	1.844902
H	-4.158919	0.088613	-0.181989



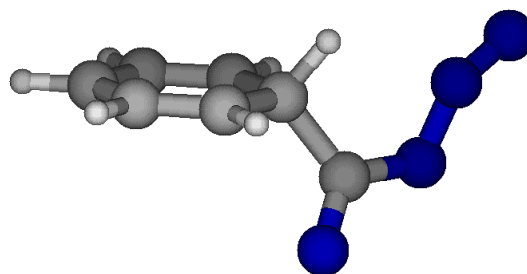
Compound **17T** - B3LYP/6-311G(d,p) - E=-489.292520 u.a.

C	-1.052994	-0.908912	0.816403
C	-0.309822	0.402235	0.727935
C	-1.186225	1.557365	0.322061
C	-2.522160	1.405360	0.099925
C	-3.156561	0.146806	0.219110
C	-2.389677	-0.991321	0.576534
C	0.902758	0.268578	-0.201725
N	1.880990	-0.639649	0.318912
N	2.878602	-0.863277	-0.387605
N	3.827725	-1.153427	-0.921911
N	1.025277	0.886428	-1.287165
H	-0.477698	-1.784934	1.090053
H	-2.882935	-1.954018	0.662982
H	-3.113379	2.270815	-0.180143
H	-0.712558	2.525702	0.215758
H	0.143092	0.613303	1.715641
H	-4.218647	0.050755	0.033306



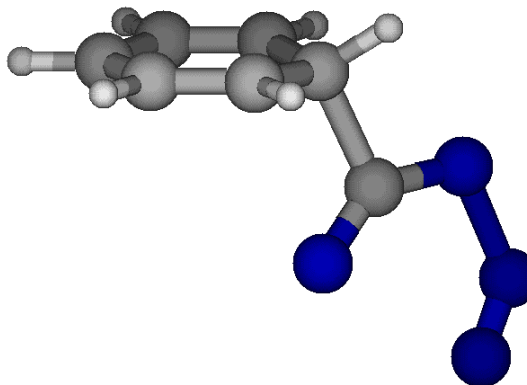
Compound **17'T** - B3LYP/6-311G(d,p) - E=-489.286094 u.a.

C	1.357172	-1.119109	0.513469
C	1.096497	-2.418511	0.833978
C	-0.225940	-2.881073	1.006082
C	-1.310641	-1.985267	0.842242
C	-1.109245	-0.676908	0.524734
C	0.268067	-0.113403	0.330241
C	0.380647	0.590877	-1.050615
N	-0.264559	1.840464	-1.193169
N	0.971371	0.004713	-2.002845
N	-0.734534	3.586006	0.376421
N	-0.365458	2.620917	-0.109740
H	-2.323954	-2.351709	0.967308
H	-1.948729	-0.004537	0.390980
H	-0.411861	-3.918319	1.253948
H	1.921145	-3.112826	0.952707
H	0.415946	0.724046	1.046359
H	2.374378	-0.776807	0.368575



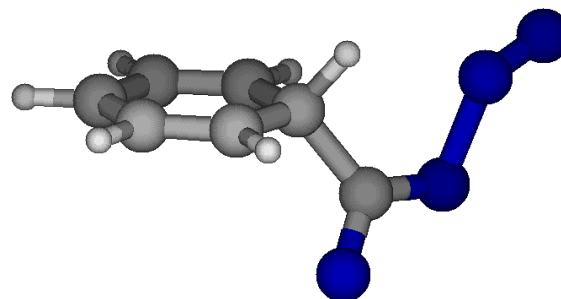
Compound TS **17T** – **67T** - B3LYP/6-311G(d,p) - E=-489.243715 u.a.

N	-0.955532	1.023990	-0.744720
C	-0.984577	0.161682	0.167653
N	-1.870764	-0.632843	0.760300
N	-3.256233	-0.325801	-0.020842
N	-3.516390	0.394365	-0.845181
C	0.529866	-0.178775	0.919621
C	1.067791	-1.342539	0.205317
C	2.155711	-1.224043	-0.616579
C	2.831728	0.007528	-0.738460
C	2.427897	1.123137	0.018973
C	1.349041	1.040930	0.859250
H	0.539030	-2.282030	0.307354
H	2.510562	-2.085434	-1.170557
H	2.988944	2.047797	-0.050455
H	1.040619	1.891601	1.454136
H	3.683118	0.089317	-1.403513
H	0.165415	-0.406752	1.921482



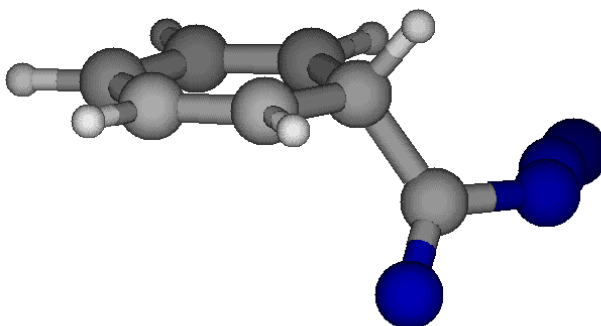
Compound TS **17'T** – **67T** - B3LYP/6-311G(d,p) - E=-489.240212 u.a.

C	-1.252911	-0.823573	0.955426
C	-2.568324	-0.524738	0.724380
C	-2.932411	0.569633	-0.083465
C	-1.933442	1.375369	-0.675065
C	-0.608869	1.117625	-0.470223
C	-0.150387	-0.014648	0.377890
C	0.857556	-0.923349	-0.430641
N	2.086144	-0.512923	-0.753546
N	0.435367	-2.051706	-0.888713
N	3.581792	1.093312	0.636944
N	2.666794	0.481090	0.462936
H	-2.225179	2.205906	-1.308220
H	0.151976	1.728416	-0.942175
H	-3.978275	0.787477	-0.261796
H	-3.342868	-1.142143	1.165437
H	0.517673	0.366908	1.183283
H	-0.981286	-1.672896	1.570314



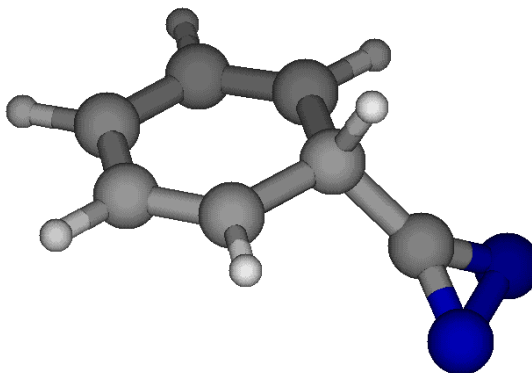
Compound TS **17T** – **17'T** - B3LYP/6-311G(d,p) - **E=-489.282536 u.a.**

C	0.291476	0.329523	0.691185
C	1.588444	1.078866	0.527293
C	2.698570	0.497847	-0.008143
C	2.703461	-0.857025	-0.413305
C	1.543291	-1.646464	-0.219157
C	0.401782	-1.127916	0.312521
C	-0.827275	1.037711	-0.111363
N	-0.593324	1.957746	-0.926176
N	-2.204333	0.732245	0.198772
N	-2.632616	-0.405794	-0.012511
N	-3.178207	-1.387380	-0.158519
H	1.570910	-2.698845	-0.481871
H	-0.451437	-1.770193	0.492321
H	3.594076	-1.295591	-0.844675
H	3.602386	1.087132	-0.120398
H	-0.053891	0.406372	1.737260
H	1.598825	2.118149	0.832225



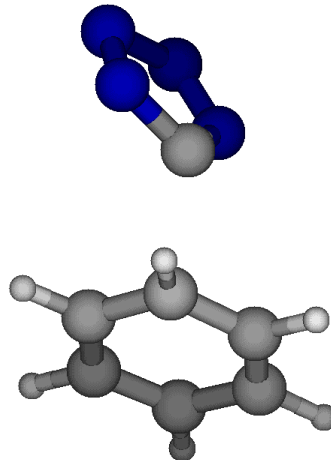
Compound **67T** - B3LYP/6-311G(d,p) - E=-379.762009 u.a.

C	-1.302071	-1.004850	0.611404
C	-0.504112	0.082759	0.429884
C	-1.061179	1.391306	-0.073352
C	-2.526835	1.334085	-0.426090
C	-3.262924	0.208211	-0.218386
C	-2.686367	-0.972840	0.311024
C	-0.249039	1.925861	-1.211292
N	0.946547	1.925211	-1.733438
H	0.557126	0.044263	0.644840
H	-0.864581	-1.923470	0.987637
H	-4.317306	0.212487	-0.473479
H	-2.971591	2.227218	-0.848487
H	-0.918299	2.160577	0.713696
H	-3.296304	-1.853643	0.464659
N	-0.302429	2.698265	-2.261597



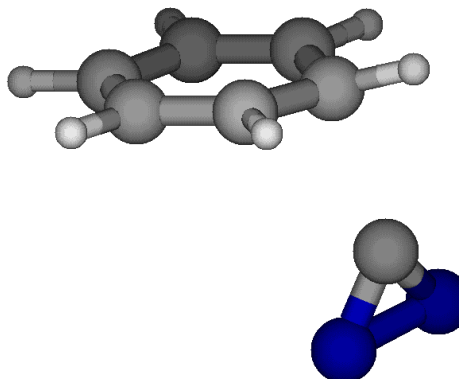
Compound TS **15T– NNC** (T) - B3LYP/6-311G(d,p) - **E=-489.243839 u.a.**

N	2.150876	0.699762	0.858118
C	1.203329	-0.244908	0.462031
N	1.452914	-0.688990	-0.832752
N	2.440170	-0.066248	-1.276067
N	2.924363	0.901847	-0.100143
C	-0.883655	0.006419	1.261243
C	-1.212812	1.185823	0.548854
C	-2.004588	1.110143	-0.586222
C	-2.521688	-0.121126	-1.000527
C	-2.261808	-1.280943	-0.262402
C	-1.471026	-1.221285	0.872756
H	-1.272061	-2.114767	1.452300
H	-2.686552	-2.226892	-0.577320
H	-2.233121	2.008627	-1.147551
H	-0.816205	2.137014	0.883238
H	-0.414303	0.091043	2.234083



Compound TS **67T** – **68T** - B3LYP/6-311G(d,p) - E=-379.725501 u.a.

C	-3.133525	0.384279	-0.313001
C	-2.562761	-0.873031	-0.084678
C	-1.264436	-0.974239	0.434721
C	-0.527248	0.164051	0.696724
C	-1.054687	1.446267	0.372421
C	-2.410154	1.535712	-0.057123
C	-0.111253	1.832199	-1.511355
N	-0.283868	2.576203	-2.571972
N	0.395594	1.136395	-2.483949
H	0.472757	0.090158	1.107065
H	-0.843820	-1.950877	0.644714
H	-4.151266	0.456287	-0.678777
H	-2.849814	2.511395	-0.225692
H	-0.581657	2.327275	0.789082
H	-3.133001	-1.771009	-0.291304



Compound **68T** - B3LYP/6-311G(d,p) - E=-147.422662 u.a.

C	0.058371	-0.138746	1.302928
C	-0.040187	0.095522	0.038065
N	-0.509507	1.211082	0.485101

Compound **68S** - B3LYP/6-311G(d,p) - E=-147.466517 u.a.

N	-0.031612	0.075141	1.288186
C	-0.001398	0.003324	-0.097099
N	-0.458313	1.089393	0.635007

Compound TS **68T – NCN** (T) - B3LYP/6-311G(d,p) - E=-147.418564 u.a.

N	0.905929	-0.242033	0.000000
C	0.053227	0.633551	0.000000
N	-0.959156	-0.300234	0.000000

Compound TS **68T – NNC** (T) - B3LYP/6-311G(d,p) - E=-147.405388 u.a.

N	0.078533	0.896108	0.000000
C	0.472144	-0.261173	0.000000
N	-1.113756	0.044356	0.000000

Compound **N₂** Σ_g (S) - B3LYP/6-311G(d.p) - **E=-109.555930 u.a.**

N	-2.990606	1.419437	0.000000
N	-4.086049	1.419437	0.000000

Compound **NCN** (S) - B3LYP/6-311G(d.p) - **E=-147.477276 u.a.**

C	-0.728291	0.266106	0.000000
N	0.495360	0.266106	0.000000
N	-1.951943	0.266106	0.000000

Compound **NCN** Σ_g (T) - B3LYP/6-311G(d.p) - **E=-147.530041 u.a.**

N	0.000000	0.000000	1.226180
C	0.000000	0.000000	0.000000
N	0.000000	0.000000	-1.226180

Compound **NNC** (S) - B3LYP/6-311G(d.p) - **E=-147.436460 u.a.**

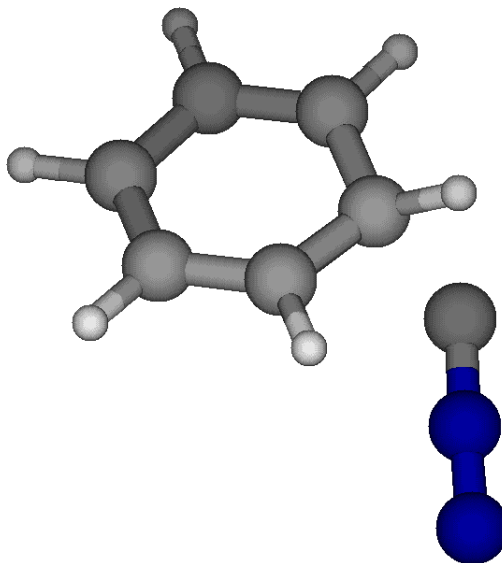
C	-0.812483	0.266106	0.322567
N	-2.024349	0.266106	-0.014894
N	-3.162553	0.266106	-0.331555

Compound **NNC** Σ_g (T) - B3LYP/6-311G(d.p) - **E=-147.482530 u.a.**

N	-1.946825	1.241622	0.000000
N	-3.146032	1.127455	0.000000
C	-0.716659	1.358737	0.000000

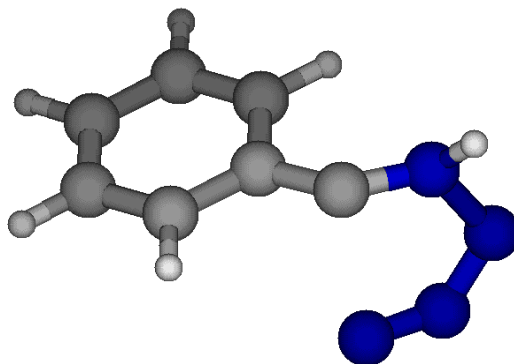
Compound TS **66T** – **NCN** (T) - B3LYP/6-311G(d,p) - E=-379.759089 u.a.

C	1.173967	1.472137	0.082864
C	2.184117	0.708834	-0.520639
C	2.161549	-0.694922	-0.410921
C	1.131992	-1.330317	0.237372
C	0.003604	-0.580438	0.751851
C	0.138795	0.858229	0.755571
C	-1.465702	-1.054675	-0.349132
N	-2.361490	-0.164426	-0.317627
N	-3.231743	0.624736	-0.343113
H	-0.626105	1.454301	1.240209
H	1.221920	2.554718	0.043299
H	2.973991	-1.277507	-0.830845
H	1.111200	-2.410556	0.316601
H	2.996005	1.199006	-1.044461
H	-0.494315	-1.015218	1.618580



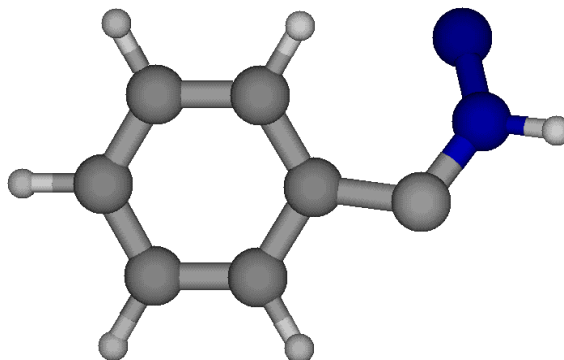
Compound TS **10aT- 77T** B3LYP/6-311G(d,p) - E=-489.253382 u.a.

C	4.590424	2.630605	0.219242
C	4.334783	1.376842	-0.387365
C	5.110614	0.990894	-1.511047
C	6.095931	1.832042	-1.999704
C	6.334776	3.067026	-1.389265
C	5.576976	3.461194	-0.281234
C	3.362681	0.499795	0.161570
N	2.817957	-0.582417	-0.377230
N	1.614942	-0.489853	-1.236389
N	1.188320	0.727789	-1.124523
N	1.541882	1.714919	-0.586626
H	3.988686	2.927143	1.069133
H	5.761478	4.421814	0.185431
H	6.682817	1.531302	-2.860192
H	4.915379	0.032175	-1.975548
H	2.715678	-1.410862	0.201270
H	7.107867	3.720787	-1.776313



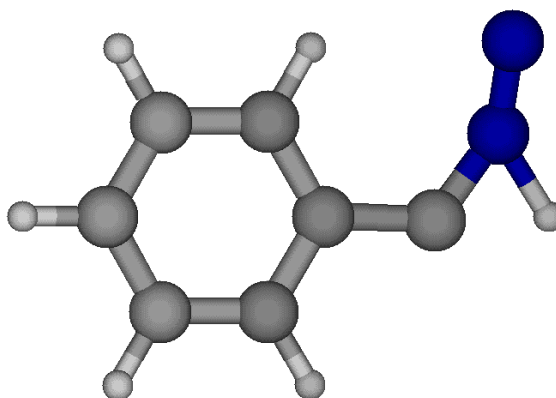
Compound **77T** B3LYP/6-311G(d,p) - E=-379.761882 u.a.

C	4.605898	2.612795	0.204889
C	4.412453	1.346606	-0.329947
C	5.116308	0.921000	-1.477671
C	6.068160	1.806047	-2.035729
C	6.282731	3.058994	-1.479316
C	5.545503	3.470739	-0.366810
C	4.824089	-0.439822	-1.903346
N	5.147826	-0.795517	-3.176468
N	5.416933	-0.022870	-4.204407
H	3.710098	0.653015	0.116536
H	4.040296	2.927504	1.074463
H	7.020966	3.723033	-1.914795
H	6.644115	1.499961	-2.900262
H	5.051657	-1.787644	-3.402533
H	5.712335	4.454303	0.05825



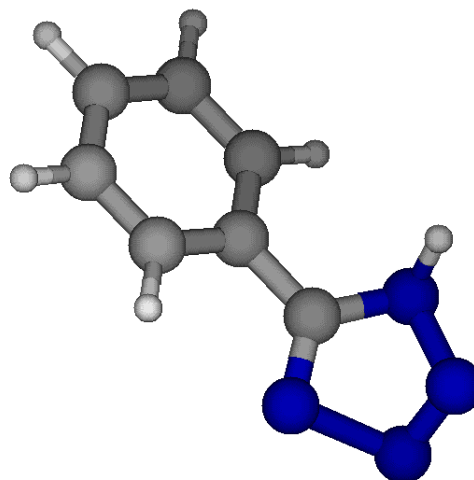
Compound TS **77T – 11T** B3LYP/6-311G(d,p) - E=-379.715784 u.a.

C	5.592604	3.484034	-0.293920
C	4.697577	2.607039	0.322923
C	4.408291	1.384519	-0.264823
C	5.014261	1.017856	-1.483500
C	5.918252	1.912541	-2.098275
C	6.199607	3.133593	-1.502825
C	4.679475	-0.263317	-2.064251
N	5.229571	-0.743334	-3.215878
N	6.077401	-0.698193	-4.081229
H	3.715039	0.691828	0.197206
H	4.228731	2.882085	1.260745
H	6.894524	3.816966	-1.977531
H	6.391807	1.637675	-3.033425
H	4.460975	-1.568347	-2.689400
H	5.817913	4.439466	0.166198



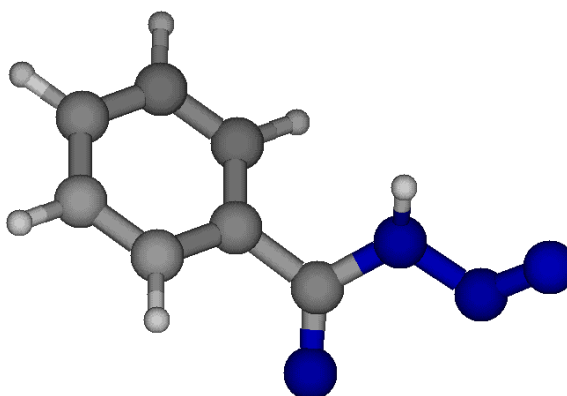
Compound TS **2aT** – **69T** - B3LYP/6-311G(d,p) - E=-489.275195 u.a.

C	0.035139	-0.000396	-0.027171
N	0.092340	-0.289092	1.352181
N	1.408905	0.325904	1.654448
N	1.404056	1.441930	1.089164
H	0.134901	-1.281731	1.566548
N	0.815297	0.943280	-0.449960
C	-0.910534	-0.700630	-0.901998
C	-2.118871	-1.193612	-0.386907
C	-3.012969	-1.850733	-1.224209
C	-2.713165	-2.014193	-2.576237
C	-1.516251	-1.517905	-3.093743
C	-0.615308	-0.863538	-2.263651
H	0.320099	-0.477936	-2.649137
H	-1.284704	-1.645789	-4.144610
H	-3.947250	-2.227779	-0.824996
H	-2.359376	-1.039535	0.658508
H	-3.412835	-2.526234	-3.226885



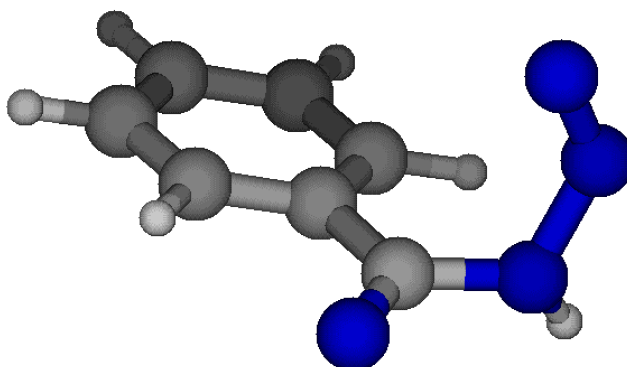
Compound **69T** - B3LYP/6-311G(d,p) - E=-489.332057 u.a.

C	0.741755	0.055632	0.055780
C	1.709801	-0.296227	-0.892652
C	2.701864	0.624804	-1.249107
C	2.718910	1.886987	-0.666437
C	1.749942	2.238499	0.272735
C	0.763971	1.322058	0.633008
C	1.716003	-1.655278	-1.511519
N	2.792346	-2.262437	-1.768637
N	0.432551	-2.200590	-1.734234
N	0.366433	-3.509688	-2.289236
N	-0.587824	-3.894262	-2.851342
H	-0.010728	-0.665690	0.351368
H	0.015438	1.589810	1.369767
H	3.486234	2.598698	-0.948046
H	3.446103	0.342140	-1.983126
H	1.764481	3.223949	0.724073
H	-0.272580	-1.566370	-2.103998



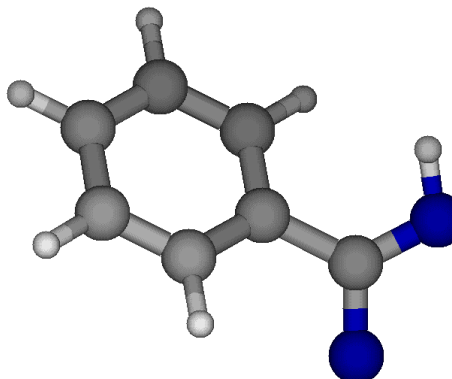
Compound TS **6aT** – **69T** - B3LYP/6-311G(d,p) - E=-489.320683 u.a.

C	0.549373	1.360151	0.020408
C	0.702097	0.028479	-0.356087
C	1.933951	-0.432886	-0.831237
C	3.009999	0.461395	-0.929454
C	2.853652	1.787729	-0.550918
C	1.623039	2.241011	-0.073835
C	2.130246	-1.861647	-1.206830
N	1.003622	-2.754461	-1.352637
N	0.027159	-2.441602	-2.374751
N	0.284237	-1.858314	-3.356224
N	3.267468	-2.370869	-1.405901
H	-0.145019	-0.642906	-0.287065
H	-0.410624	1.707872	0.383749
H	3.689944	2.472183	-0.633303
H	3.960561	0.107266	-1.309187
H	1.501585	3.278136	0.216861
H	0.496063	-2.950801	-0.499815



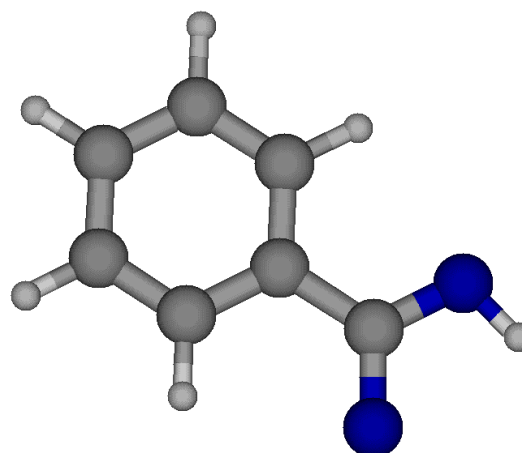
Compound **6aT** B3LYP/6-311G(d,p) - E=-379.837688 u.a.

C	1.749282	2.211654	0.297560
C	0.620586	1.435481	0.553441
C	0.481358	0.186428	-0.043374
C	1.479203	-0.302739	-0.894718
C	2.606357	0.484937	-1.153810
C	2.739910	1.735885	-0.559811
C	1.335333	-1.655129	-1.525815
N	2.324241	-2.487467	-1.804179
N	0.102845	-2.054852	-1.846134
H	-0.395056	-0.419023	0.154113
H	-0.151883	1.802284	1.219420
H	3.613336	2.341796	-0.771577
H	3.370639	0.131363	-1.837670
H	3.212109	-2.078366	-1.498871
H	1.855334	3.185725	0.761130



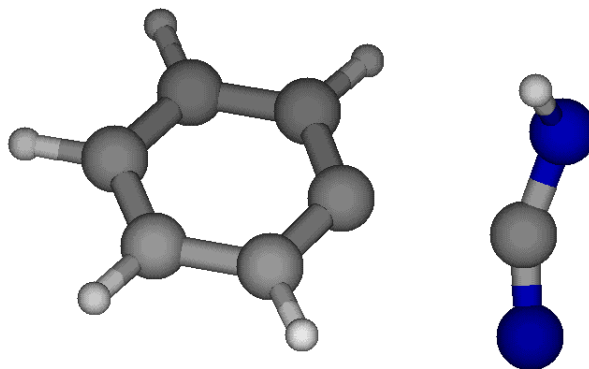
Compound **6aT** B3LYP/6-311G(d,p) - E=-379.846431 u.a.

C	2.809820	1.652457	-0.397984
C	1.732899	2.233253	0.271195
C	0.534602	1.533146	0.401039
C	0.412267	0.255968	-0.136201
C	1.491421	-0.329027	-0.808112
C	2.692406	0.375803	-0.936901
C	1.365592	-1.695014	-1.384538
N	0.253795	-2.403171	-1.290051
N	2.397221	-2.251831	-2.026245
H	-0.517913	-0.291349	-0.037116
H	-0.304200	1.981924	0.920524
H	3.742423	2.195580	-0.499750
H	3.520377	-0.086989	-1.458931
H	2.115720	-3.185367	-2.346561
H	1.827595	3.228702	0.690197



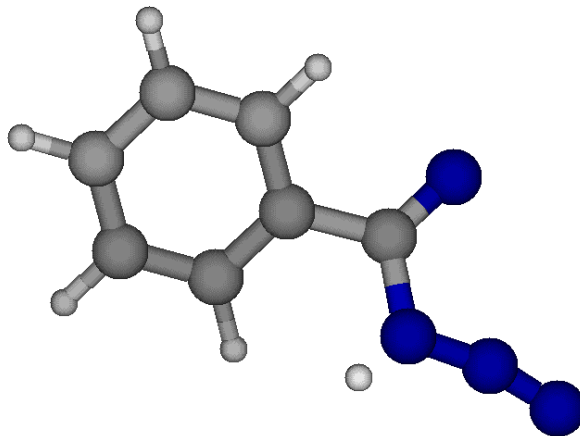
Compound TS **6aT – 56D** B3LYP/6-311G(d,p) - E=-379.784075 u.a.

C	2.590742	0.490483	-1.304541
C	2.714986	1.740343	-0.685407
C	1.765019	2.158088	0.246213
C	0.680388	1.342402	0.570521
C	0.535259	0.089688	-0.036224
C	1.506001	-0.278349	-0.941820
C	1.227947	-2.253794	-1.904325
N	2.462237	-2.661070	-1.908127
N	0.056254	-2.293727	-2.178023
H	-0.308354	-0.552770	0.185847
H	-0.058318	1.678184	1.290434
H	3.551574	2.383146	-0.937702
H	3.316430	0.150362	-2.034125
H	2.807722	-2.799036	-0.954612
H	1.867279	3.128177	0.718915



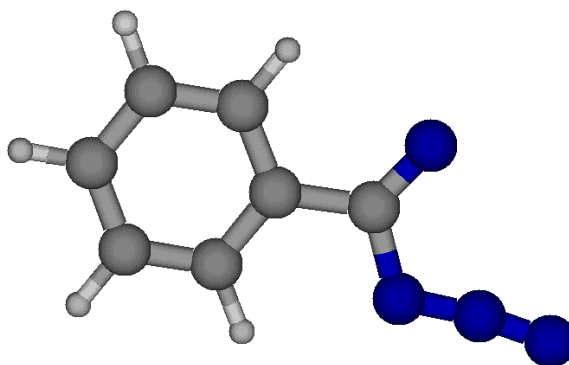
Compound TS **69T** – **62T** - B3LYP/6-311G(d,p) - **E=-489.2493905 u.a.**

C	0.625760	0.231819	-0.290453
C	1.668953	-0.183680	-1.124698
C	2.830554	0.592250	-1.228402
C	2.943061	1.772646	-0.504604
C	1.902163	2.185945	0.326850
C	0.746653	1.414961	0.432256
C	1.552627	-1.423987	-1.931257
N	2.181344	-1.623030	-3.005584
N	0.638048	-2.394563	-1.387501
N	0.349667	-3.385821	-2.091510
N	-0.004454	-4.390338	-2.479451
H	-0.272005	-0.367510	-0.212159
H	-0.063159	1.733760	1.078109
H	3.845392	2.367708	-0.583379
H	3.637101	0.258044	-1.869183
H	1.993821	3.105261	0.893947
H	1.014006	-2.708973	0.256537



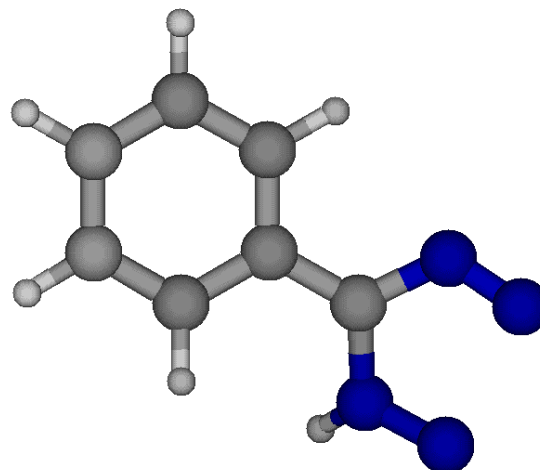
Compound **62D** - B3LYP/6-311G(d,p) - **E=-488.752923 u.a.**

C	1.161783	-0.075047	-1.054948
C	2.529621	0.138223	-0.836747
C	2.951106	1.276233	-0.142667
C	2.012187	2.190746	0.327815
C	0.653961	1.976389	0.109686
C	0.231294	0.840962	-0.583002
C	3.511305	-0.853109	-1.349140
N	3.202506	-1.900866	-1.982386
N	4.874409	-0.517127	-1.059901
N	5.748635	-1.302399	-1.459591
N	6.642775	-1.919756	-1.759755
H	0.839760	-0.958167	-1.593284
H	-0.825216	0.670726	-0.754733
H	2.344697	3.071287	0.865316
H	4.007383	1.440166	0.025346
H	-0.074504	2.690169	0.477207



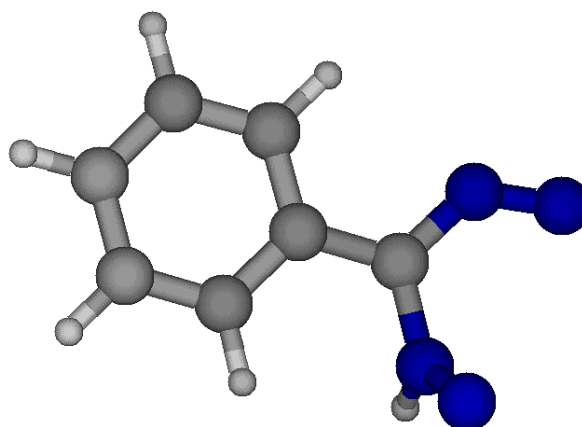
Compound TS **2aT** – **70T** B3LYP/6-311G(d,p) - E=-489.294767 u.a.

C	0.004521	-0.006933	-0.001061
C	0.001721	-0.009788	1.412736
C	1.241565	-0.008159	2.095264
C	2.428558	-0.030536	1.384100
C	2.418532	-0.046187	-0.014409
C	1.202909	-0.030715	-0.699419
C	-1.223839	-0.038047	2.141241
N	-1.307625	0.110744	3.524607
N	-2.375945	0.298209	4.045954
N	-2.483826	-0.286154	1.567420
N	-3.526251	0.131813	2.198493
H	-2.556662	-1.075008	0.912348
H	-0.933189	0.046308	-0.541006
H	1.191428	-0.023986	-1.783162
H	3.371797	-0.033883	1.917967
H	1.242665	0.002327	3.177518
H	3.352049	-0.059376	-0.564547



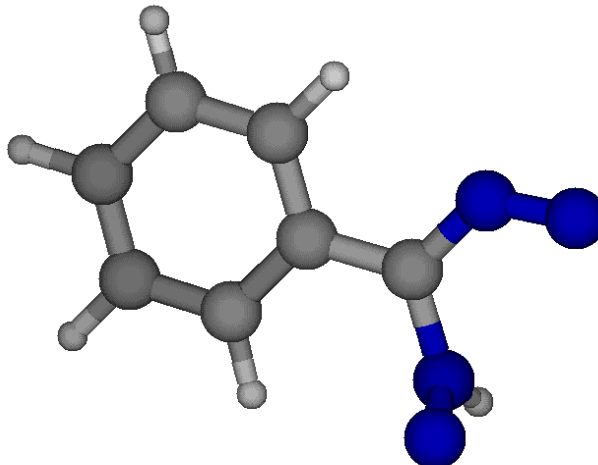
Compound **70T** B3LYP/6-311G(d,p) - E=-489.296924 u.a.

C	0.706012	-0.435019	0.683805
N	0.599973	-1.875120	0.884875
N	0.027300	-2.310050	1.875837
N	2.191328	-0.077844	2.438462
H	1.040987	-2.481895	0.157634
N	1.520905	0.302941	1.520599
C	-0.100595	0.191604	-0.315365
C	-0.030609	1.588306	-0.535999
C	-0.809943	2.181357	-1.513721
C	-1.675607	1.411679	-2.297130
C	-1.760299	0.034994	-2.086646
C	-0.991286	-0.572339	-1.106305
H	-1.099695	-1.634760	-0.929280
H	-2.440064	-0.564088	-2.681318
H	-0.748118	3.252150	-1.670056
H	0.640508	2.180722	0.072112
H	-2.284691	1.883962	-3.058885



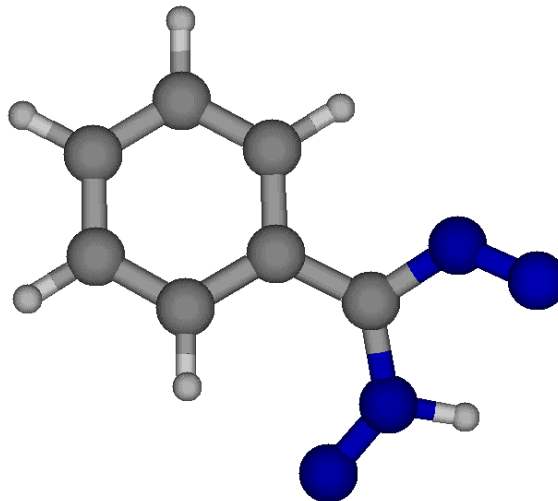
Compound TS **70T – 70'T** B3LYP/6-311G(d,p) - E=-489.288085 u.a.

C	0.101342	0.339704	0.211743
N	0.035202	-1.112001	0.458345
N	-0.755070	-1.554114	1.268900
N	1.622330	0.690088	1.917737
H	0.740380	-1.696249	-0.047945
N	0.920625	1.086389	1.021227
C	-0.729132	0.944797	-0.782950
C	-0.672628	2.342339	-1.004540
C	-1.447952	2.927812	-1.990294
C	-2.302505	2.149321	-2.776254
C	-2.375620	0.771836	-2.562896
C	-1.603947	0.170854	-1.580394
H	-1.687785	-0.895251	-1.413459
H	-3.043508	0.165140	-3.163279
H	-1.391833	3.998511	-2.149177
H	-0.011081	2.941836	-0.392984
H	-2.909501	2.613690	-3.544542



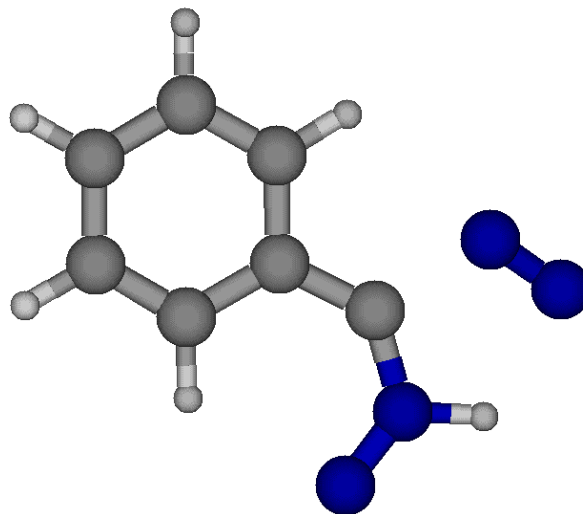
Compound **70'T** B3LYP/6-311G(d,p) - E=-489.302552 u.a.

C	0.721757	-0.419722	0.727052
N	0.821476	-1.801260	1.032848
N	0.166462	-2.751464	0.591115
N	2.130118	-0.014433	2.486927
H	1.553843	-1.931861	1.772029
N	1.557149	0.379791	1.506402
C	-0.142044	0.166100	-0.256542
C	0.015783	1.541980	-0.561031
C	-0.743165	2.132907	-1.554462
C	-1.685771	1.383084	-2.264900
C	-1.866185	0.034877	-1.961482
C	-1.120419	-0.573472	-0.960316
H	-1.278939	-1.611540	-0.707540
H	-2.608952	-0.546146	-2.495745
H	-0.603964	3.183879	-1.779864
H	0.750391	2.119525	-0.015666
H	-2.284141	1.852951	-3.036952



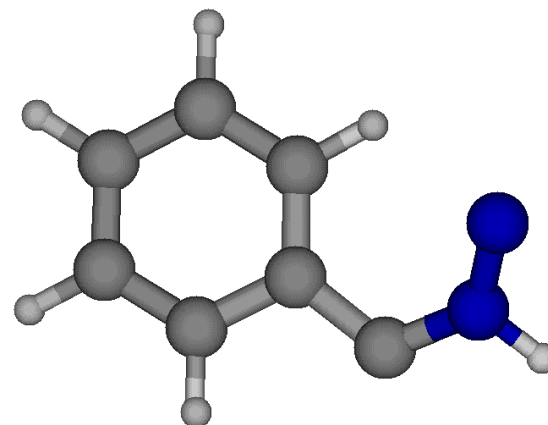
Compound TS **70'T – 71T** B3LYP/6-311G(d,p) - **E=-489.287232 u.a.**

C	-1.097267	-0.603933	-1.063273
C	-0.151313	0.131950	-0.298922
C	-0.012758	1.524165	-0.548580
C	-0.784322	2.143890	-1.515370
C	-1.710228	1.406568	-2.258623
C	-1.859309	0.037021	-2.026204
C	0.665691	-0.439397	0.701189
N	1.847058	0.530380	1.639413
N	2.435580	-0.076243	2.413626
N	0.778325	-1.727320	1.179816
N	0.137428	-2.713179	0.800023
H	1.519322	-1.760432	1.949343
H	-1.201664	-1.662627	-0.872507
H	-2.577640	-0.534153	-2.603112
H	-0.667761	3.206370	-1.694771
H	0.705154	2.090753	0.029162
H	-2.312167	1.897182	-3.014888



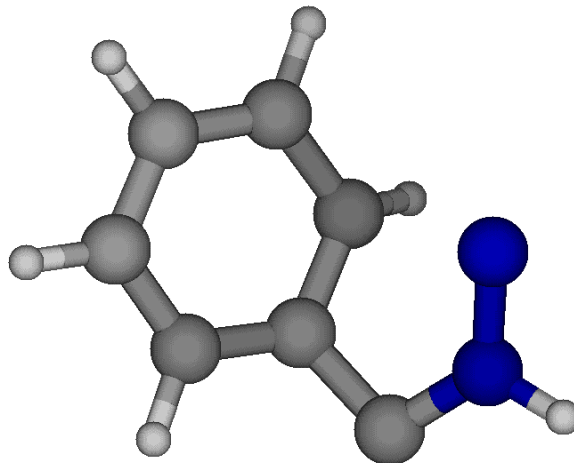
Compound **71T** B3LYP/6-311G(d,p) - **E=-379.761882 u.a.**

C	-1.124607	-0.567935	-0.959981
C	-0.223940	0.184159	-0.219030
C	-0.031167	1.557952	-0.494822
C	-0.797235	2.137562	-1.529786
C	-1.673255	1.375503	-2.290286
C	-1.841930	0.020804	-2.003830
C	0.822056	2.489749	0.228115
N	1.849841	1.980277	0.960400
N	2.397025	0.787837	0.894093
H	2.347295	2.644878	1.557205
H	0.328238	-0.285100	0.585745
H	-1.266451	-1.618295	-0.731470
H	-2.236766	1.835734	-3.093918
H	-0.673621	3.197864	-1.714722
H	-2.538010	-0.574559	-2.584261



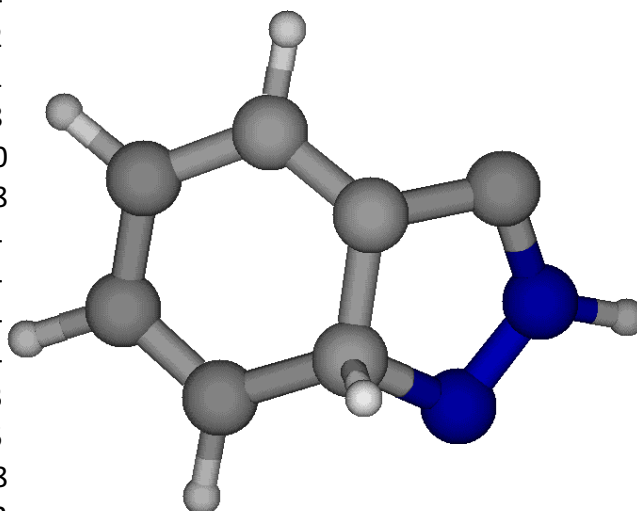
Compound TS **71T** – **72T** B3LYP/6-311G(d,p) - E=-379.727204 u.a.

N	0.028860	0.032416	-0.021765
C	-0.003750	0.008399	1.917915
C	1.446417	0.004151	2.000008
C	2.138259	-0.680920	0.903172
N	1.243442	-0.591917	-0.096800
C	2.107683	0.931851	2.784034
C	1.385086	1.914508	3.480038
C	-0.010158	1.971444	3.364701
C	-0.707076	1.028409	2.625649
H	1.482904	-0.912301	-1.031719
H	-0.511917	-0.948418	1.815197
H	-1.790802	1.033073	2.618592
H	1.908850	2.646479	4.083136
H	3.191508	0.931521	2.785197
H	-0.557746	2.739672	3.899756



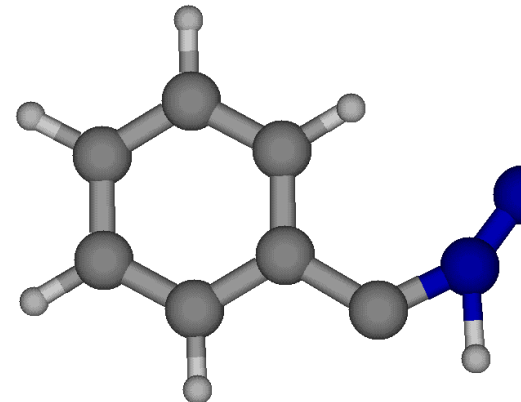
Compound **72T** B3LYP/6-311G(d,p) - E=-379.752655 u.a.

C	0.066669	-0.127024	0.116464
C	0.075443	-0.069949	1.481502
C	1.324926	0.349181	2.192091
C	2.572433	0.271481	1.335178
C	2.500175	0.209539	-0.031710
C	1.239164	0.083926	-0.659138
C	3.695979	-0.085477	2.176794
N	3.054042	-0.507064	3.284364
N	1.675249	-0.422792	3.393994
H	3.519745	-0.916200	4.083254
H	1.186182	1.396227	2.546163
H	-0.825401	-0.230348	2.062195
H	1.177180	0.035366	-1.739398
H	3.412949	0.145702	-0.613613
H	-0.860334	-0.353891	-0.399523

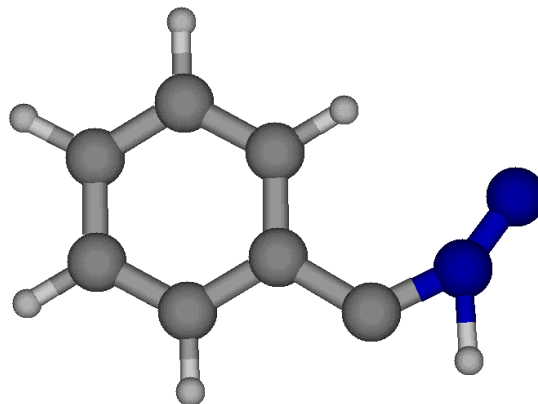


Compound TS **71T** – **11T** B3LYP/6-311G(d,p) - **E=-379.715784** u.a.

C	-1.928028	0.026359	-1.987923
C	-1.088184	-0.587381	-1.054828
C	-0.132473	0.156863	-0.378464
C	-0.004548	1.540643	-0.631999
C	-0.857570	2.146744	-1.576355
C	-1.810533	1.393885	-2.246251
C	0.979164	2.361432	0.038228
N	1.827007	1.898132	1.000566
N	2.143941	1.049045	1.806194
H	1.946427	3.124326	0.830152
H	0.516215	-0.316958	0.348878
H	-1.183798	-1.648887	-0.856546
H	-2.463877	1.866700	-2.970519
H	-0.749861	3.208296	-1.764498
H	-2.673197	-0.561259	-2.512093

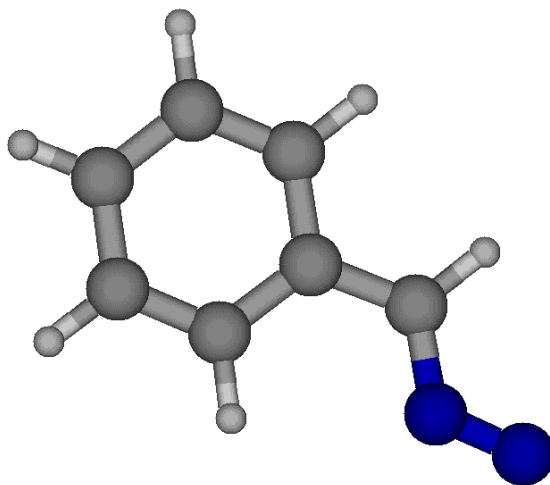
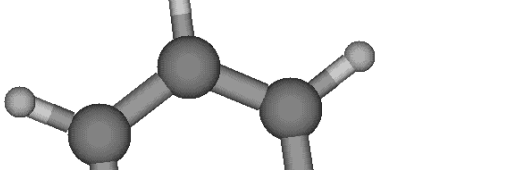


A 3D ball-and-stick model of a chemical structure. The structure features a central benzene ring (six carbon atoms in a hexagonal arrangement). Attached to one of the ring carbons is a side chain consisting of a nitrogen atom bonded to another nitrogen atom, which is in turn bonded to a hydrogen atom. The atoms are represented by spheres: carbon is grey, nitrogen is blue, and hydrogen is white. The bonds are shown as grey rods.



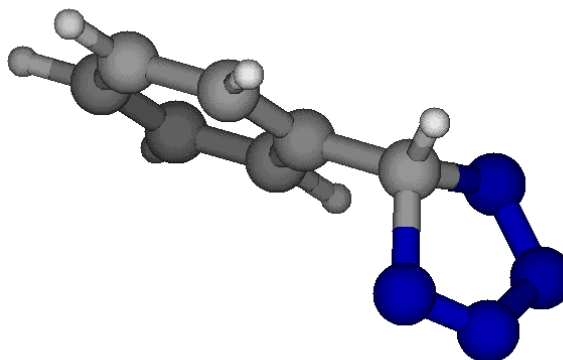
Compound **11T** B3LYP/6-311G(d,p) - E=-379.859418 u.a.

C	-0.349246	1.102936	-0.067381
C	-1.705560	1.361483	0.027247
C	-2.626653	0.309606	0.079174
C	-2.177157	-1.012638	0.035343
C	-0.821830	-1.284109	-0.059336
C	0.123272	-0.231741	-0.112812
C	1.509149	-0.540065	-0.209990
N	2.459504	0.453246	-0.264408
N	3.647645	0.257036	-0.347163
H	0.369251	1.911697	-0.108078
H	-2.055660	2.386859	0.061299
H	-2.889401	-1.828706	0.075427
H	-0.473142	-2.310689	-0.093310
H	-3.687291	0.519998	0.153241
H	1.849722	-1.573278	-0.243659



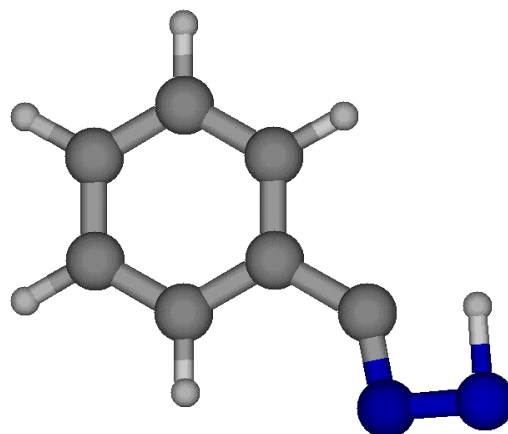
Compound TS **10aT– 11T** B3LYP/6-311G(d,p) - **E=-489.279250 u.a.**

N	5.215689	1.228546	-1.467961
C	4.001699	1.938290	-1.165391
N	4.468142	2.726306	0.236900
N	5.681152	2.525846	0.185461
N	6.190967	1.668602	-0.695907
C	2.802528	1.123420	-0.912182
C	2.926557	-0.218376	-0.510286
C	1.791760	-0.977319	-0.264596
C	0.524999	-0.405941	-0.403477
C	0.391942	0.929416	-0.796273
C	1.522874	1.689715	-1.049198
H	3.916664	-0.646289	-0.417335
H	1.888721	-2.013975	0.035438
H	-0.593198	1.367455	-0.904415
H	1.428144	2.726901	-1.351654
H	-0.360018	-1.000016	-0.205759
H	3.818048	2.778477	-1.848124



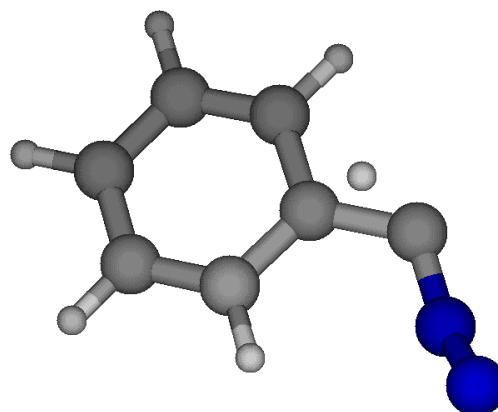
Compound TS **11T** – **4aT** - B3LYP/6-311G(d,p) - E=-370.755155 u.a.

C	-1.154592	-1.793899	0.696128
C	-2.350494	-1.075454	0.611381
C	-2.340124	0.256482	0.196036
C	-1.140801	0.872688	-0.135361
C	0.067658	0.157947	-0.054139
C	0.048997	-1.189393	0.367775
C	1.309718	0.792497	-0.395789
N	2.541952	0.337347	-0.395255
N	3.128564	1.459157	-0.813169
H	0.982682	-1.734685	0.430112
H	-1.166042	-2.828480	1.019588
H	-3.268551	0.811892	0.131640
H	-1.120369	1.906756	-0.458504
H	-3.288003	-1.554656	0.869199
H	1.990288	2.038110	-0.862675



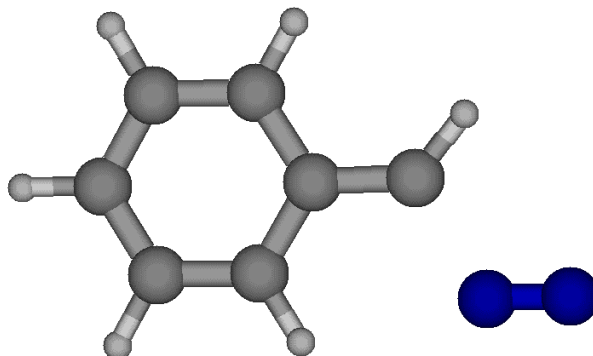
Compound TS **11T** – **66T** - B3LYP/6-311G(d,p) - E=-379.726849 u.a.

C	-2.899117	-0.215756	-0.173702
C	-1.810346	0.554925	-0.477194
C	-0.455993	0.013558	-0.360599
C	-0.339246	-1.384465	0.045101
C	-1.458873	-2.114135	0.357865
C	-2.745726	-1.550520	0.262090
C	0.632848	0.784646	-0.914198
N	1.802747	0.187870	-1.098823
N	2.914408	0.027501	-0.737867
H	0.649102	-1.822617	0.106969
H	-1.352335	-3.148189	0.667382
H	-3.894043	0.203265	-0.272424
H	-1.911769	1.578930	-0.815959
H	-3.617010	-2.142784	0.512697
H	0.146960	0.953326	0.394415



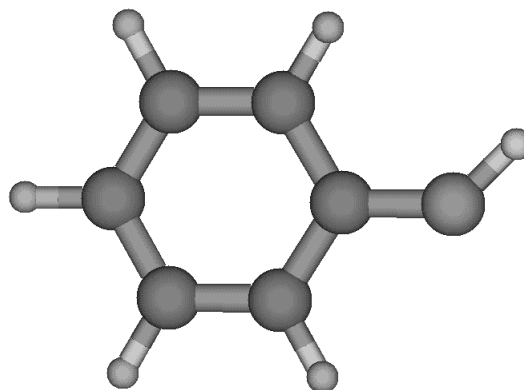
Compound TS **11T** – **12aT** - B3LYP/6-311G(d,p) - E=-379.834280 u.a.

C	-2.916791	-0.222666	-0.186000
C	-1.784781	0.511228	-0.491179
C	-0.484896	-0.067955	-0.375884
C	-0.400079	-1.420983	0.062428
C	-1.544145	-2.137506	0.362620
C	-2.808569	-1.550017	0.242571
C	0.645368	0.688404	-0.688325
N	2.341965	-0.134387	-0.514966
N	3.264371	0.461950	-0.761698
H	0.575709	-1.878611	0.156448
H	-1.457889	-3.166163	0.694616
H	-3.894430	0.236898	-0.280567
H	-1.874794	1.539447	-0.822816
H	-3.699097	-2.119893	0.480206
H	0.731577	1.712282	-1.028644



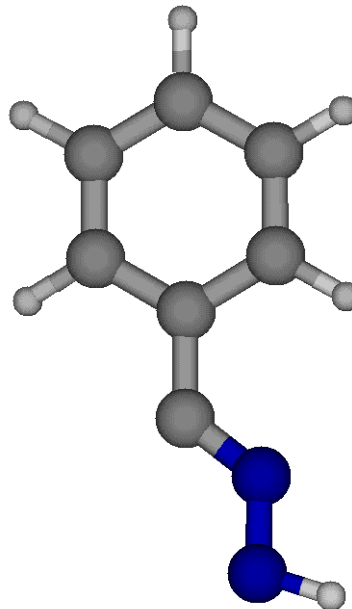
Compound **12aT** B3LYP/6-311G(d,p) - E=-270.296827 u.a.

C	0.126283	-0.278232	-0.113495
C	-0.319835	1.079958	-0.069702
C	-1.724581	1.307988	0.027979
C	-2.613183	0.249481	0.077807
C	-2.153379	-1.071589	0.033443
C	-0.779967	-1.322000	-0.062322
C	0.582666	2.134418	-0.120507
H	-2.083497	2.329745	0.062514
H	-3.676833	0.447547	0.152017
H	-0.418992	-2.344227	-0.096999
H	1.188699	-0.480371	-0.187657
H	-2.856030	-1.895553	0.072975
H	1.656919	2.226701	-0.192545



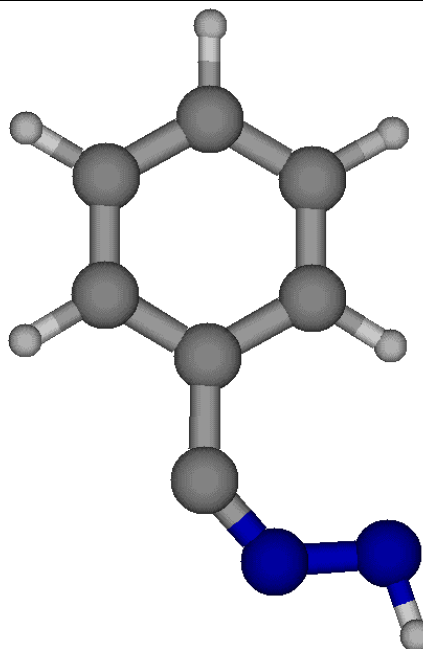
Compound **4aT** B3LYP/6-311G(d,p) - E=-379.807604 u.a.

C	0.242962	0.293898	0.256363
C	1.033050	-0.471406	-0.623905
C	2.220522	0.094602	-1.141688
C	2.594318	1.380425	-0.785013
C	1.799838	2.127585	0.089629
C	0.625343	1.581488	0.608195
C	0.604407	-1.799904	-0.964266
N	1.215769	-2.617973	-1.750980
H	-0.666616	-0.142562	0.651582
H	0.010315	2.161873	1.286181
H	3.506429	1.808097	-1.186049
H	2.825474	-0.496238	-1.818011
H	2.097421	3.133035	0.365097
N	0.805174	-3.819212	-2.043470
H	1.515574	-4.191834	-2.686547



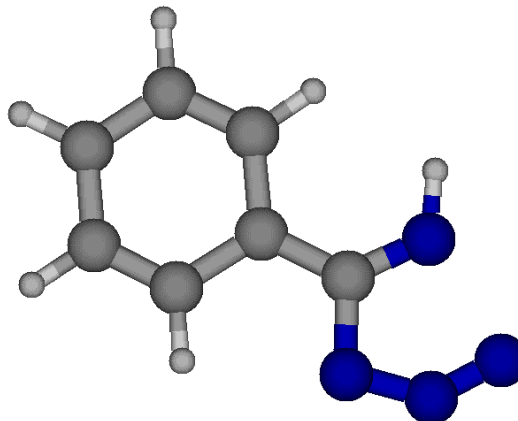
Compound **4aT** B3LYP/6-311G(d,p) - E=-379.799961 u.a.

C	0.990146	-0.389209	-0.784563
C	2.207058	0.172206	-1.232364
C	2.621997	1.402570	-0.741137
C	1.843070	2.088377	0.193226
C	0.639407	1.541999	0.641632
C	0.214306	0.312754	0.157852
C	0.531802	-1.661767	-1.273219
N	0.921578	-2.555828	-2.082515
N	2.038886	-2.527678	-2.796419
H	-0.717335	-0.125474	0.495472
H	0.037158	2.076870	1.366878
H	3.556084	1.831549	-1.085992
H	2.798688	-0.372011	-1.956662
H	2.174555	3.048856	0.571741
H	2.033698	-3.402409	-3.335806



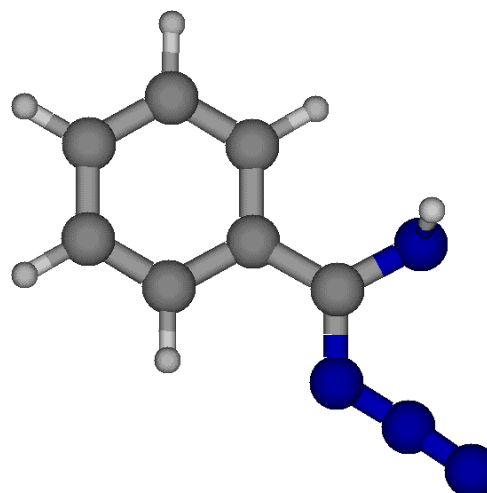
Compound TS **2aT** – **3aT** B3LYP/6-311G(d,p) - **E=-489.266649 u.a.**

C	-2.476572	-1.324564	0.000000
C	-1.131583	-1.236574	0.000000
C	-0.465630	0.084378	0.000000
C	-1.338464	1.288221	0.000000
C	-2.683864	1.160542	0.000000
C	-3.308807	-0.135472	0.000000
C	0.945463	0.194298	0.000000
N	1.664040	-1.041409	0.000000
N	2.902651	-0.700260	0.000000
N	3.504229	0.299510	0.000000
N	1.674699	1.280537	0.000000
H	-0.498295	-2.111953	0.000000
H	-2.956458	-2.296543	0.000000
H	-3.311063	2.044974	0.000000
H	-0.883015	2.270029	0.000000
H	1.245598	2.194903	0.000000
H	-4.386955	-0.222761	0.000000



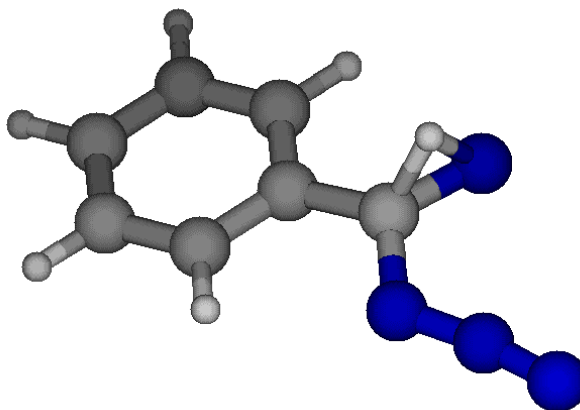
Compound **3aT** B3LYP/6-311G(d,p) - **E=-489.315834 u.a.**

C	2.732236	0.416328	-1.034271
C	2.819116	1.688033	-0.464048
C	1.735052	2.189199	0.263576
C	0.582969	1.437977	0.427919
C	0.485685	0.145846	-0.140476
C	1.585960	-0.348344	-0.881249
C	-0.686170	-0.660566	0.027670
N	-1.783042	-0.128003	0.670657
N	-2.831519	-0.786250	0.805516
N	-3.739004	-1.400945	1.120324
N	-0.786205	-1.941942	-0.529379
H	-0.251658	1.830802	0.994346
H	1.792490	3.177272	0.706729
H	3.563745	0.021612	-1.607554
H	1.518457	-1.325553	-1.346243
H	-0.155544	-2.599687	-0.045430
H	3.716825	2.282325	-0.587002



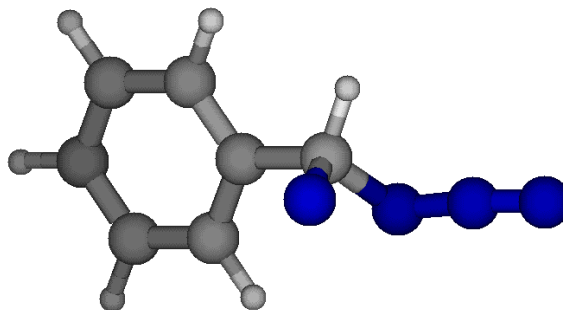
Compound TS **3aT** – **73T** B3LYP/6-311G(d,p) - **E=-489.244559 u.a.**

C	1.677964	-0.272161	-0.943050
C	2.769508	0.561377	-1.155708
C	2.829572	1.813812	-0.545917
C	1.783416	2.230397	0.277759
C	0.687440	1.405301	0.497277
C	0.625548	0.140770	-0.109411
C	-0.510006	-0.760957	0.142209
N	-0.655785	-1.990798	-0.594832
N	-1.676030	-0.152157	0.672899
N	-2.739838	-0.788138	0.665330
N	-3.775495	-1.243370	0.743069
H	-0.127587	1.733285	1.129724
H	1.819762	3.206017	0.749212
H	3.573380	0.234242	-1.805374
H	1.630735	-1.240074	-1.428487
H	-0.203209	-1.906361	0.629856
H	3.681992	2.461668	-0.714235



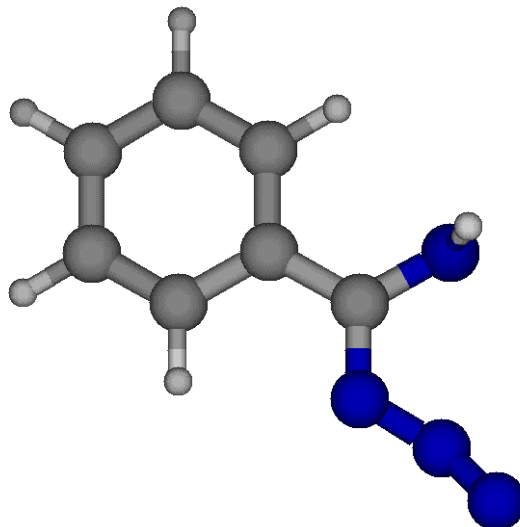
Compound **73T** B3LYP/6-311G(d,p) - E=-489.300493 u.a.

C	1.547738	1.626833	-1.161817
C	2.786457	1.025288	-0.936487
C	2.844347	-0.264481	-0.402107
C	1.668807	-0.949262	-0.112345
C	0.431421	-0.348614	-0.342912
C	0.372068	0.940097	-0.867545
C	4.063266	1.801481	-1.204021
N	4.596417	2.305886	0.019156
N	5.067479	0.898884	-1.852013
N	6.079260	1.458121	-2.286027
N	7.042518	1.847702	-2.737255
H	3.807973	-0.728896	-0.232853
H	1.717599	-1.952768	0.294645
H	-0.587184	1.409834	-1.052156
H	1.500287	2.630181	-1.571942
H	-0.482970	-0.884800	-0.115887
H	3.846189	2.652968	-1.870306



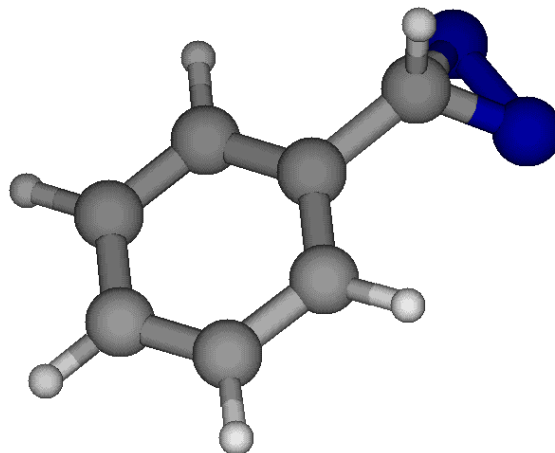
Compound TS **3aT** – **6aT** B3LYP/6-311G(d,p) - E=-489.312452 u.a.

C	-1.420213	1.192123	-0.010588
C	-2.787308	0.946458	-0.011373
C	-3.267579	-0.362382	0.000349
C	-2.364547	-1.429136	0.009020
C	-0.998138	-1.196596	0.010721
C	-0.503108	0.123066	0.002792
C	0.923549	0.387201	0.018211
N	1.408674	1.692840	-0.101205
N	1.788039	-0.628652	0.058959
N	3.044371	-0.424412	-0.194548
N	4.160377	-0.494469	0.093487
H	-0.298300	-2.022465	0.019147
H	-2.732352	-2.449008	0.014206
H	-3.481018	1.779423	-0.026135
H	-1.055820	2.212900	-0.038795
H	1.559797	2.114240	0.825108
H	-4.334680	-0.551603	0.000197



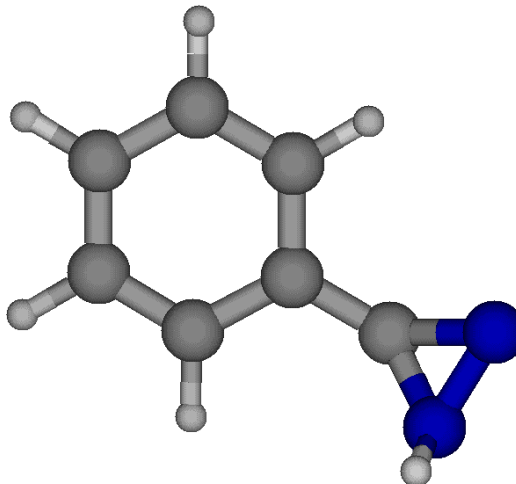
Compound TS **5aT** – **6aT** B3LYP/6-311G(d,p) - E=-379.751240 u.a.

C	-0.556520	1.184339	0.199712
C	0.288855	0.115208	-0.090938
C	-0.229114	-1.163318	-0.290967
C	-1.605584	-1.366134	-0.222767
C	-2.457617	-0.298308	0.053457
C	-1.932389	0.974624	0.266346
C	1.788416	0.348078	-0.209724
N	2.677620	-0.442141	0.553162
N	2.462635	1.076945	0.794957
H	0.440235	-1.991718	-0.491319
H	-2.010379	-2.359432	-0.379439
H	-2.591690	1.805206	0.491092
H	-0.139577	2.168339	0.378394
H	-3.528007	-0.459713	0.110566
H	2.123650	0.559750	-1.238954



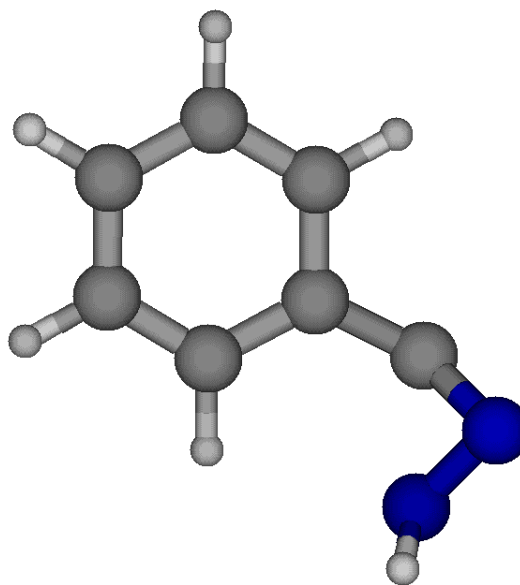
Compound **5aT** B3LYP/6-311G(d,p) - E=-379.780911 u.a.

C	2.737609	0.334382	-0.889006
C	2.812302	1.637436	-0.426326
C	1.714566	2.234559	0.202241
C	0.532133	1.505607	0.365944
C	0.439512	0.199726	-0.085050
C	1.542406	-0.413579	-0.732776
C	1.463646	-1.760348	-1.137169
N	1.916612	-2.607829	-2.113601
N	0.548582	-2.664096	-1.761652
H	-0.476001	-0.365400	0.043612
H	-0.322340	1.965044	0.850357
H	3.731438	2.198329	-0.555082
H	3.595744	-0.124930	-1.367129
H	1.781242	3.254237	0.562483
H	2.160438	-2.366167	-3.077119



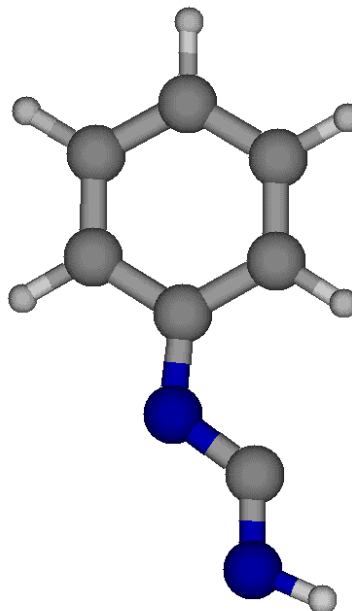
Compound TS **4aT – 5aT** B3LYP/6-311G(d,p) - E=-379.723922 u.a.

C	2.566571	0.242534	-0.926320
C	2.747323	1.555599	-0.517090
C	1.733236	2.230585	0.165283
C	0.536147	1.574651	0.458039
C	0.355058	0.251646	0.083773
C	1.356833	-0.429278	-0.647242
C	1.074332	-1.793427	-0.993419
N	2.256800	-2.465120	-2.151161
N	0.909879	-2.601249	-2.075817
H	-0.559768	-0.272255	0.333894
H	-0.250126	2.092271	0.995283
H	3.682053	2.060036	-0.734710
H	3.347510	-0.294814	-1.446748
H	1.879696	3.258146	0.477395
H	2.542344	-2.382354	-3.141433



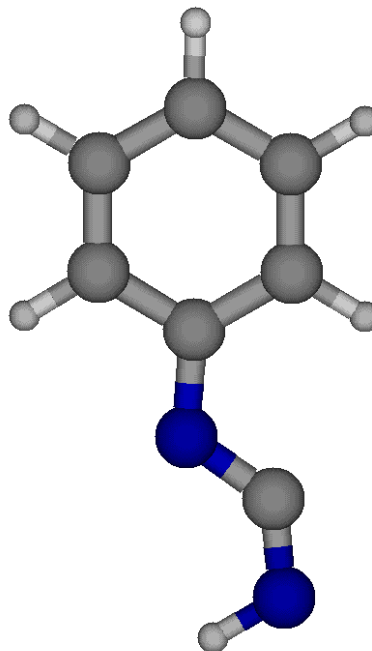
Compound **7aT** B3LYP/6-311G(d,p) - E=-379.842160 u.a.

C	0.610640	1.577616	0.591206
C	0.215394	0.300173	0.241671
C	1.011167	-0.493255	-0.630377
C	2.223763	0.062210	-1.132552
C	2.605037	1.340118	-0.773898
C	1.805400	2.105018	0.086854
N	0.544187	-1.732711	-0.917068
C	1.229869	-2.558226	-1.733410
N	0.878975	-3.730351	-2.061790
H	-0.702781	-0.136207	0.614698
H	-0.004612	2.172039	1.256541
H	3.528900	1.755641	-1.160213
H	2.829085	-0.542420	-1.795944
H	2.113671	3.107091	0.362005
H	1.541283	-4.184863	-2.690605



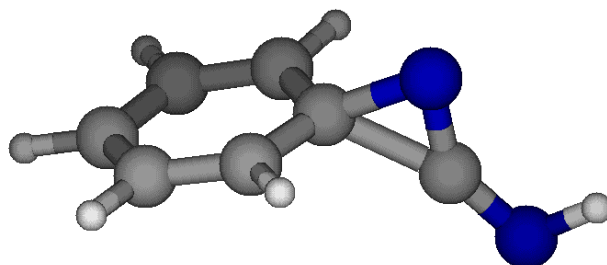
Compound **7aT** B3LYP/6-311G(d,p) - E=-379.836881 u.a.

C	1.816512	2.114950	0.084654
C	0.618358	1.604426	0.598869
C	0.207124	0.329321	0.260399
C	0.990659	-0.477674	-0.609996
C	2.206598	0.059681	-1.122832
C	2.603479	1.335729	-0.774911
N	0.512472	-1.715677	-0.889000
C	1.183139	-2.557994	-1.705024
N	0.933072	-3.723815	-2.093322
H	-0.714195	-0.093183	0.641783
H	0.013247	2.210438	1.263005
H	3.529755	1.738222	-1.168794
H	2.801232	-0.556886	-1.785341
H	2.136968	3.115379	0.351576
H	0.052911	-4.111789	-1.720890



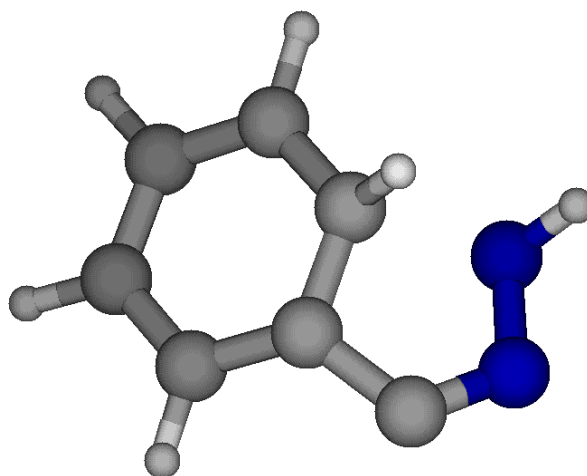
Compound TS **6aT** – **7aT** B3LYP/6-311G(d,p) - E=-379.770491 u.a.

C	0.062080	0.005449	-0.018155
C	0.014495	-0.022626	1.361139
C	1.187857	-0.004320	2.128165
C	2.429289	0.063877	1.480811
C	2.516635	0.078472	0.103667
C	1.326301	-0.023716	-0.688980
C	1.510982	-0.996113	-2.125535
N	1.592982	-2.015962	-2.902379
N	1.380963	0.307743	-2.148416
H	3.474531	0.145524	-0.397204
H	3.340863	0.113140	2.066290
H	-0.950899	-0.041960	1.855106
H	-0.843498	0.018209	-0.611776
H	1.675693	-1.704841	-3.886390
H	1.134785	-0.021132	3.209484



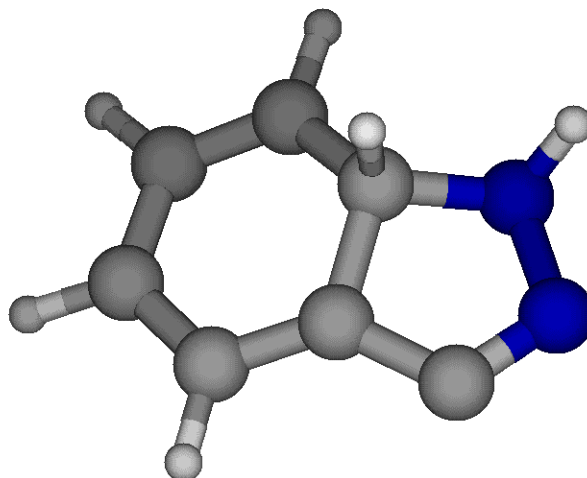
Compound TS **4aT** – **72'aT** B3LYP/6-311G(d,p) - E=-379.748653 u.a.

N	-0.014236	0.000222	0.014660
C	0.004673	-0.000337	1.924615
C	1.461779	-0.006532	1.989812
C	1.962410	0.579385	0.774591
N	1.209731	0.589695	-0.244329
C	-0.679492	-0.977799	2.721072
C	0.032781	-1.806357	3.559342
C	1.436851	-1.715746	3.679588
C	2.147535	-0.826907	2.878588
H	3.231429	-0.818680	2.884035
H	1.962130	-2.370066	4.364287
H	-1.762569	-1.015990	2.701618
H	-0.501822	-2.523819	4.172778
H	-0.746674	0.600438	-0.376700
H	-0.473245	0.979835	1.859957



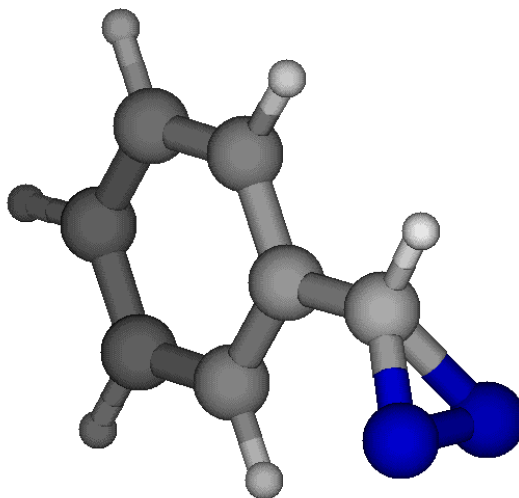
Compound **72'aT** B3LYP/6-311G(d,p) - **E=-379.768010 u.a.**

C	0.229169	0.239042	0.316620
C	0.955893	-0.510040	-0.590897
C	2.344637	-0.092157	-1.033156
C	2.590051	1.373974	-0.876235
C	1.830545	2.076753	0.004057
C	0.696431	1.504740	0.669146
C	0.681480	-1.606657	-1.452232
N	1.483673	-1.768014	-2.420922
N	2.426231	-0.709721	-2.387717
H	-0.728787	-0.117650	0.677176
H	0.134424	2.111911	1.367951
H	3.425009	1.829341	-1.396790
H	2.058811	3.121344	0.187669
H	3.339786	-1.058630	-2.656481
H	3.071572	-0.629578	-0.381769



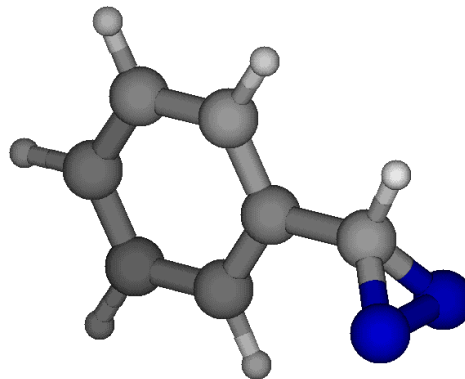
Compound **64T** B3LYP/6-311G(d,p) - E=-379.775878 u.a.

C	0.232930	0.298433	0.026812
C	-0.175593	-1.055352	0.037461
C	-1.520543	-1.372316	0.012698
C	-2.485611	-0.355647	-0.017860
C	-2.096714	0.985257	-0.024983
C	-0.749332	1.313185	-0.003885
C	1.619448	0.661645	0.060193
N	2.662181	-0.273135	0.505791
N	2.646515	-0.259711	-0.769181
H	0.584024	-1.825019	0.066582
H	-1.831723	-2.410316	0.019439
H	-2.845831	1.767871	-0.047714
H	-0.438580	2.352249	-0.011829
H	-3.538723	-0.612219	-0.034323
H	1.878737	1.715242	0.062457



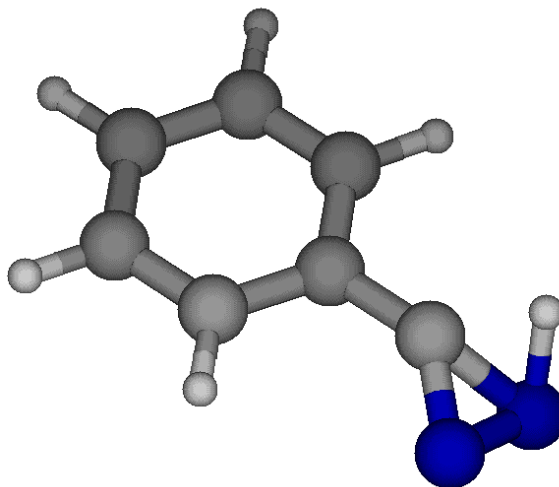
Compound **64T** B3LYP/6-311G(d,p) - E=-379.762289 u.a.

C	0.433335	-0.387026	-0.460631
C	0.391804	0.867378	-1.063297
C	1.566229	1.594635	-1.244903
C	2.786568	1.066332	-0.822677
C	2.829023	-0.193727	-0.217172
C	1.653483	-0.914600	-0.038779
C	4.058252	1.851543	-1.018120
N	5.070383	1.888719	-0.026244
N	5.266514	1.226075	-1.416305
H	3.777753	-0.601782	0.109781
H	1.689922	-1.890933	0.430849
H	-0.553435	1.282825	-1.393337
H	1.531409	2.571669	-1.714667
H	-0.480653	-0.952318	-0.319640
H	3.887324	2.825170	-1.506783



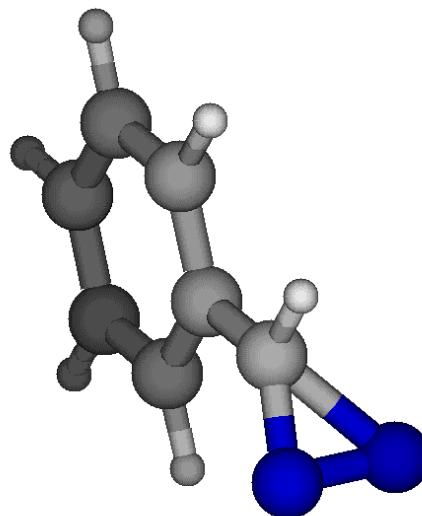
Compound TS **5aT** – **64T** B3LYP/6-311G(d,p) - E=-379.720759 u.a.

C	-0.664453	1.217393	0.121634
C	0.218579	0.166985	-0.184462
C	-0.287864	-1.128920	-0.376668
C	-1.647525	-1.372068	-0.239713
C	-2.520204	-0.327217	0.069895
C	-2.024748	0.964389	0.248279
C	1.624013	0.466075	-0.360360
N	2.916734	0.104013	0.422666
N	2.479305	1.408581	0.163386
H	0.388673	-1.938177	-0.628769
H	-2.030903	-2.376351	-0.378227
H	-2.700657	1.776107	0.491803
H	-0.269320	2.215024	0.269597
H	-3.582129	-0.519681	0.169547
H	2.575095	-0.463147	-0.579139



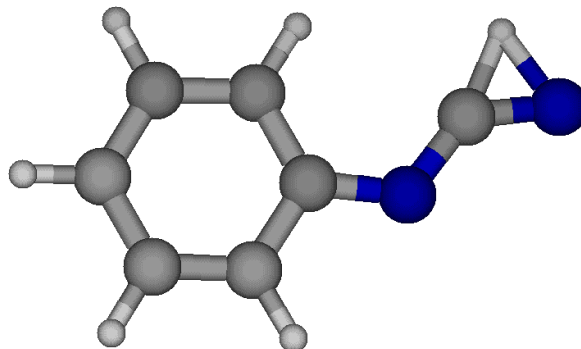
Compound TS **11T** – **64T** B3LYP/6-311G(d,p) - E=-379.774458 u.a.

C	1.628401	-1.063660	-0.277446
C	0.394228	-0.489308	-0.597409
C	0.310614	0.865757	-0.925850
C	1.457476	1.645036	-0.937436
C	2.706898	1.077948	-0.611724
C	2.778106	-0.290800	-0.280248
C	3.880159	1.904135	-0.607392
N	5.131352	1.453482	-0.125526
N	5.395507	1.373100	-1.371199
H	3.742870	-0.713790	-0.031234
H	1.684914	-2.116103	-0.025109
H	-0.648028	1.306219	-1.173432
H	1.402273	2.697044	-1.196261
H	-0.502303	-1.098805	-0.591407
H	3.781503	2.949782	-0.889981



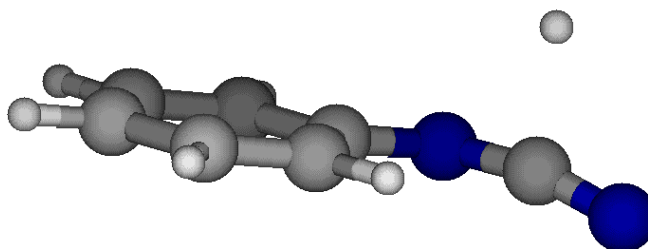
Compound TS **7aT** – **13T** B3LYP/6-311G(d,p) - E=-379.775271 u.a.

C	1.813296	2.097296	0.078227
C	0.616039	1.585494	0.591379
C	0.206651	0.309688	0.251662
C	0.990102	-0.497209	-0.618502
C	2.204862	0.042121	-1.129777
C	2.600664	1.318675	-0.781171
N	0.501338	-1.734223	-0.890162
C	1.162682	-2.585467	-1.704327
N	0.940789	-3.769905	-2.119149
H	-0.714079	-0.115096	0.631695
H	0.009581	2.190028	1.255562
H	3.526811	1.721793	-1.174753
H	2.806500	-0.566335	-1.792779
H	2.133377	3.097792	0.345245
H	1.991459	-3.136516	-2.483223



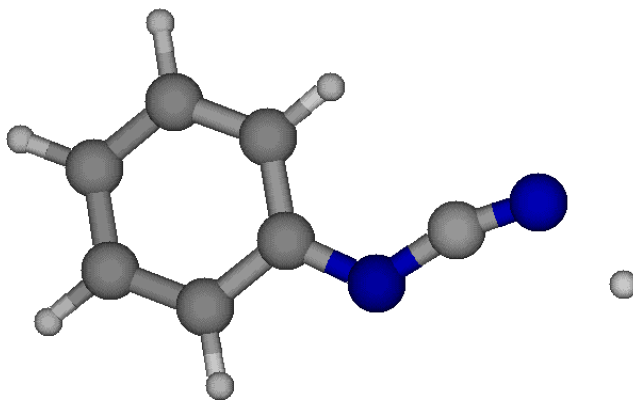
Compound TS **13T** – **76T** B3LYP/6-311G(d,p) - E=-379.790041 u.a.

C	2.568715	1.252689	-0.815996
C	1.826674	2.065455	0.052016
C	0.631567	1.596737	0.610115
C	0.176805	0.327628	0.305718
C	0.916655	-0.508469	-0.571201
C	2.128335	-0.018423	-1.130042
N	0.402411	-1.744116	-0.809979
C	0.998597	-2.599742	-1.610493
N	1.539678	-3.572939	-2.017878
H	-0.743567	-0.064985	0.719468
H	0.062345	2.229796	1.280326
H	3.493180	1.623427	-1.242995
H	2.697288	-0.655481	-1.796924
H	2.180777	3.061393	0.291247
H	0.507557	-1.830226	-3.207119



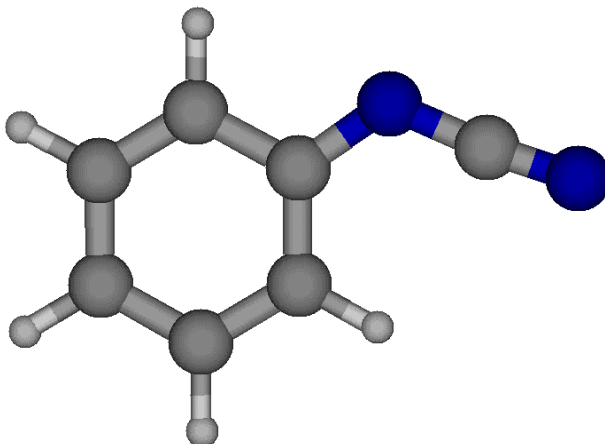
Compound TS **7aT – 76D** B3LYP/6-311G(d,p) - E=-379.789992 u.a.

C	2.614047	1.323993	-0.787050
C	1.910483	2.191269	0.061332
C	0.697856	1.790076	0.635823
C	0.187703	0.534391	0.368598
C	0.887562	-0.356559	-0.488562
C	2.118224	0.065905	-1.064413
N	0.319298	-1.572116	-0.700434
C	0.870046	-2.473226	-1.468690
N	1.124320	-3.452028	-2.086520
H	-0.746573	0.192280	0.795767
H	0.159896	2.465469	1.290261
H	3.551540	1.643683	-1.226719
H	2.650388	-0.615669	-1.718073
H	2.308211	3.176956	0.272825
H	0.083018	-4.685953	-2.008111



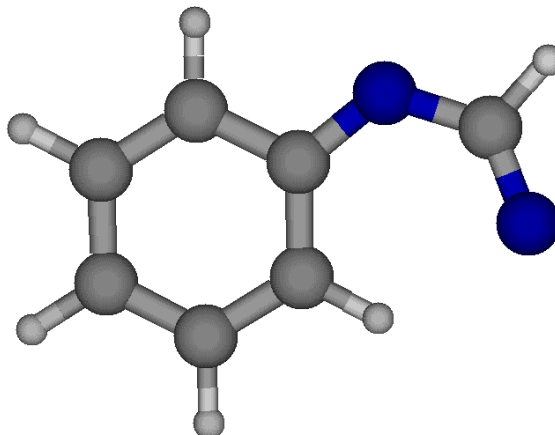
Compound **76D** B3LYP/6-311G(d,p) - E=-379.294436 u.a.

C	2.613644	1.239567	-0.826133
C	1.872641	2.044878	0.016439
C	0.665569	1.581989	0.558704
C	0.199273	0.298080	0.251196
C	0.928700	-0.520228	-0.590176
C	2.152999	-0.066660	-1.147646
N	2.810253	-0.932751	-1.965990
C	3.941688	-0.611218	-2.526825
N	4.958707	-0.417629	-3.075590
H	0.596657	-1.518028	-0.848231
H	-0.734426	-0.053837	0.673526
H	2.226233	3.039990	0.259694
H	3.548371	1.586850	-1.251274
H	0.091552	2.221685	1.218824



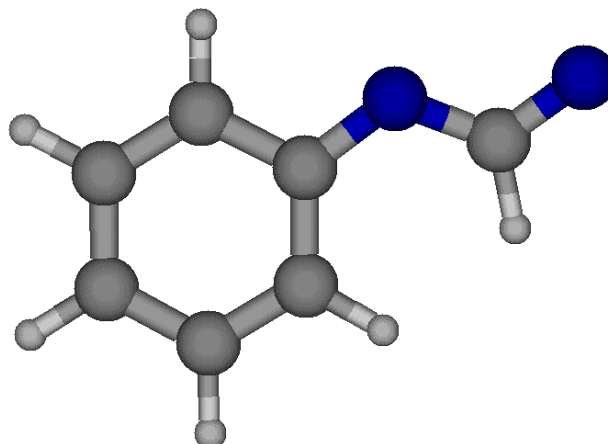
Compound **13T** B3LYP/6-311G(d,p) - E=-379.845664 u.a.

C	1.071825	-0.487296	-0.497537
C	2.107297	0.132337	-1.253114
C	2.420463	1.463404	-1.045045
C	1.727662	2.220686	-0.092144
C	0.706911	1.633201	0.661627
C	0.383106	0.303666	0.464325
N	0.642723	-1.778208	-0.579180
C	1.181290	-2.697023	-1.446212
N	2.124363	-2.560887	-2.297271
H	-0.401673	-0.181471	1.031096
H	0.170354	2.218614	1.399190
H	3.210938	1.923819	-1.626667
H	2.645023	-0.450124	-1.990740
H	1.984193	3.262864	0.059896
H	0.712573	-3.688023	-1.376029



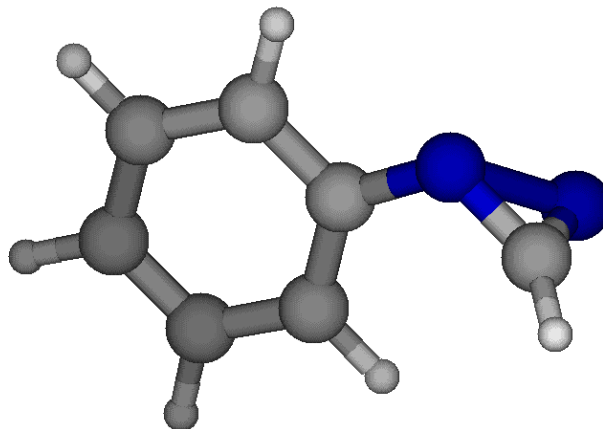
Compound **13T** B3LYP/6-311G(d,p) - E=-379.843450 u.a.

C	-0.329085	0.947473	0.340307
C	-1.658336	1.275696	0.140283
C	-2.610467	0.279397	-0.104896
C	-2.218375	-1.061003	-0.156459
C	-0.891062	-1.401123	0.036301
C	0.091078	-0.410261	0.297957
N	1.362785	-0.883550	0.470471
C	2.371233	-0.051744	0.822925
N	3.584023	-0.460157	0.947917
H	-0.555028	-2.429835	-0.000496
H	-2.952528	-1.834380	-0.350256
H	-1.963693	2.315459	0.170798
H	0.385982	1.740858	0.515309
H	-3.648660	0.549584	-0.259060
H	2.208955	1.017352	1.034151



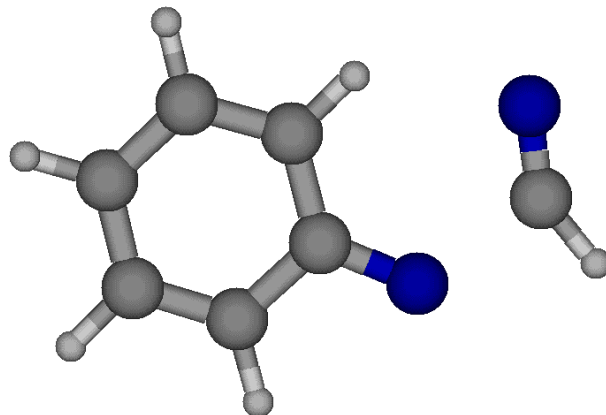
Compound **13S** B3LYP/6-311G(d,p) - **E=-379.830655 u.a.**

C	-0.292241	0.919568	0.410609
C	-1.630896	1.261356	0.249547
C	-2.581613	0.278848	-0.023810
C	-2.188852	-1.055331	-0.128025
C	-0.854603	-1.405058	0.040317
C	0.106896	-0.420016	0.298386
N	1.446275	-0.885810	0.371175
C	2.432319	0.084829	0.551505
N	2.332966	-0.239116	1.743706
H	-0.524102	-2.433998	-0.031481
H	-2.924873	-1.824367	-0.332921
H	-1.933586	2.298585	0.339372
H	0.433420	1.687603	0.650442
H	-3.623396	0.551044	-0.148003
H	2.979108	0.775630	-0.085567



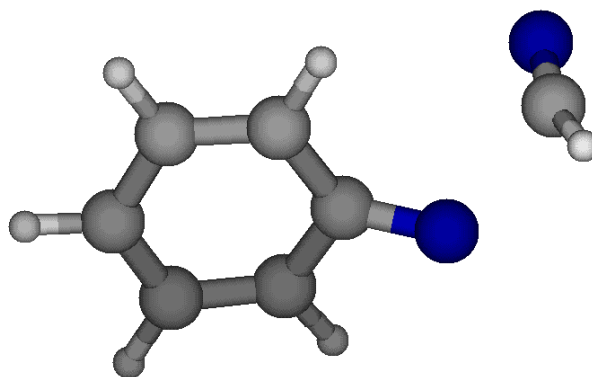
Compound TS **13T** – **14T** B3LYP/6-311G(d,p) - E=-379.812791 u.a.

C	2.119316	0.102950	-1.290249
C	2.420323	1.431119	-1.064510
C	1.725409	2.177282	-0.103547
C	0.706196	1.575655	0.646539
C	0.381737	0.250754	0.444727
C	1.080597	-0.537362	-0.536353
N	0.673964	-1.800704	-0.634857
C	1.447470	-3.041104	-1.863821
N	2.319053	-2.642624	-2.551019
H	-0.402423	-0.232305	1.013988
H	0.168199	2.152563	1.390204
H	3.208110	1.901274	-1.642286
H	2.649352	-0.481048	-2.029015
H	1.975953	3.218890	0.059503
H	0.819518	-3.863739	-1.576689



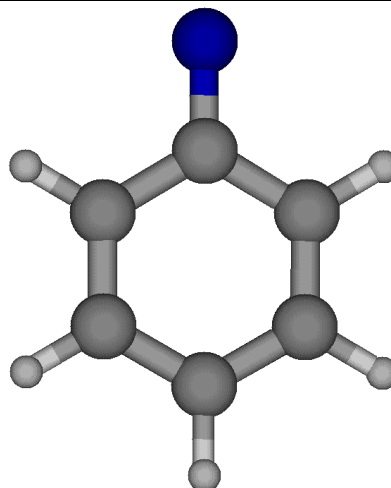
Compound TS **13S** – **14S** B3LYP/6-311G(d,p) - E=-379.780020 u.a.

C	2.203912	0.116399	-1.218581
C	2.483730	1.426519	-0.930287
C	1.729301	2.131380	0.036225
C	0.624759	1.542614	0.641428
C	0.226886	0.268354	0.251391
C	1.079448	-0.538313	-0.586364
N	0.829088	-1.818386	-0.483752
C	1.542472	-3.093874	-2.019966
N	0.981148	-2.650023	-2.937221
H	-0.668774	-0.201183	0.635228
H	0.030985	2.103606	1.354435
H	3.312424	1.924389	-1.421459
H	2.780557	-0.434177	-1.951274
H	2.000511	3.151770	0.281948
H	2.136326	-3.717474	-1.389137



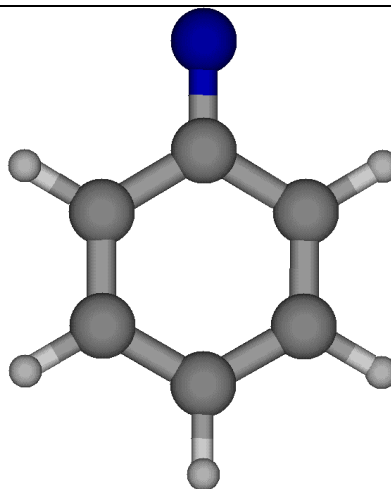
Compound **14T** A'' (Cs) B3LYP/6-311G(d,p) - E=-286.377175 u.a.

C	0.00000000	1.23070673	-0.29006464
C	0.00000000	1.21447972	1.09039967
C	0.00000000	0.00018683	1.78999903
C	0.00000000	-1.21450092	1.09024905
C	0.00000000	-1.23099976	-0.28984534
C	0.00000000	0.00001990	-1.02607575
N	0.00000000	0.00009117	-2.34858023
H	0.00000000	-2.16093865	-0.84464404
H	0.00000000	-2.15050221	1.63745123
H	0.00000000	2.15076105	1.63709355
H	0.00000000	2.16072720	-0.84473868
H	0.00000000	-0.00003333	2.87351755



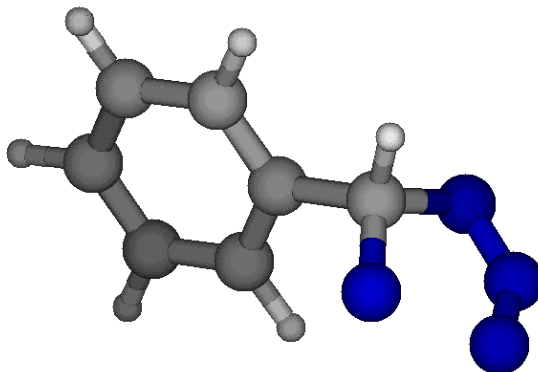
Compound **14S** A' (Cs) B3LYP/6-311G(d,p) - E=-286.325246 u.a.

C	0.00000000	1.22772834	-0.28309946
C	0.00000000	1.22705442	1.09908377
C	0.00000000	0.00106307	1.77885035
C	0.00000000	-1.22610679	1.10110102
C	0.00000000	-1.22860436	-0.28073166
C	0.00000000	-0.00089175	-1.03979571
N	0.00000000	-0.00044509	-2.35887597
H	0.00000000	-2.14596902	-0.85813254
H	0.00000000	-2.15199063	1.66511286
H	0.00000000	2.15336384	1.66248526
H	0.00000000	2.14518471	-0.86020251
H	0.00000000	0.00270158	2.86443355



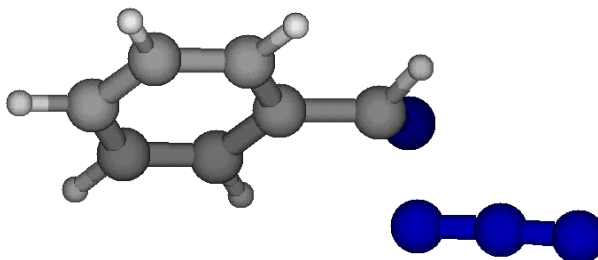
Compound TS **10aT** – **73T** B3LYP/6-311G(d,p) - E=-489.246419 u.a.

N	4.963789	1.489351	-1.964904
C	3.963163	2.097600	-0.990508
N	4.568554	2.328098	0.295971
N	6.360048	2.008421	-0.238146
N	6.051115	1.637713	-1.320061
C	2.759056	1.217999	-0.817734
C	2.917384	-0.067038	-0.276288
C	1.813438	-0.891677	-0.105286
C	0.543251	-0.442622	-0.469273
C	0.378777	0.835221	-1.005593
C	1.481673	1.663048	-1.177658
H	3.906297	-0.409218	0.004559
H	1.939480	-1.883836	0.312041
H	-0.608073	1.182873	-1.288057
H	1.357240	2.656953	-1.593362
H	-0.317809	-1.087143	-0.334155
H	3.669135	3.079968	-1.399396



Compound TS **73T** – **29T** B3LYP/6-311G(d,p) - E=-489.286530 u.a.

C	0.615426	1.750622	0.068621
C	0.397812	0.660289	-0.764645
C	1.481740	-0.107006	-1.205604
C	2.778303	0.225526	-0.805231
C	2.992015	1.319364	0.027973
C	1.911347	2.082418	0.465293
C	1.268379	-1.272392	-2.108139
N	0.825045	-2.669362	-0.872916
N	0.880130	-3.760652	-1.409931
N	0.929215	-4.811990	-1.867573
N	0.231463	-1.322977	-2.922498
H	-0.605570	0.393793	-1.073513
H	-0.225271	2.342764	0.411070
H	3.999149	1.574163	0.336809
H	3.617661	-0.372816	-1.142974
H	2.077547	2.933576	1.115681
H	2.188536	-1.736255	-2.485850

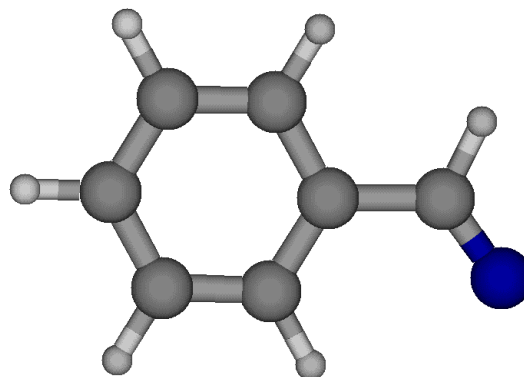


Compound **N₃ A'** (Cs) (T) B3LYP/6-311G(d,p) - **E=-164.180985 u.a.**

N	0.115603	0.000000	-0.011933
N	1.300175	0.000000	0.032732
N	2.484221	0.000000	0.079200

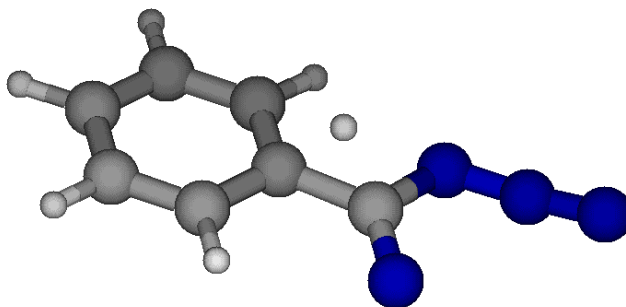
Compound **74D** B3LYP/6-311G(d,p) - **E=-325.124973 u.a.**

C	0.608641	1.732377	0.102016
C	0.392151	0.667195	-0.774676
C	1.465695	-0.063570	-1.265610
C	2.773221	0.265973	-0.882376
C	2.984299	1.333430	-0.004102
C	1.905185	2.064214	0.486249
C	3.938103	-0.498774	-1.392678
N	3.907836	-1.470772	-2.179336
H	1.306073	-0.891378	-1.946135
H	-0.617080	0.408500	-1.074100
H	2.076909	2.890431	1.166587
H	3.995094	1.590970	0.294647
H	-0.232304	2.300482	0.483149
H	4.924755	-0.162325	-1.032273



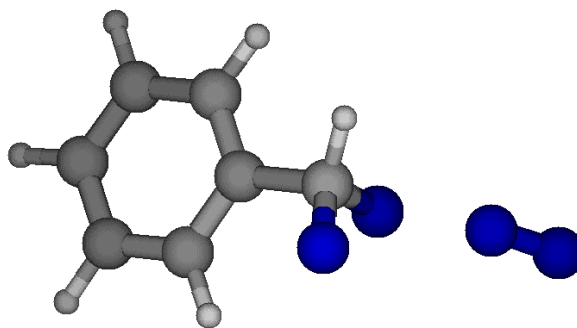
Compound TS **73T** – **17T** B3LYP/6-311G(d,p) - E=-489.238038 u.a.

C	0.404734	1.014107	-0.543032
C	1.547147	1.675172	-0.947621
C	2.778175	0.960466	-1.064982
C	2.814906	-0.411878	-0.678468
C	1.649876	-1.043590	-0.284083
C	0.436942	-0.348610	-0.219638
C	4.026057	1.711583	-1.426023
N	5.216111	0.899758	-1.389258
N	6.275468	1.444037	-1.731401
N	7.309621	1.806949	-2.001474
N	4.098388	3.006294	-1.546314
H	3.755626	-0.944690	-0.707430
H	1.686747	-2.090294	-0.003596
H	-0.525629	1.565226	-0.464763
H	1.525655	2.730152	-1.191093
H	-0.467230	-0.856609	0.092612
H	3.225809	1.090367	-2.430611



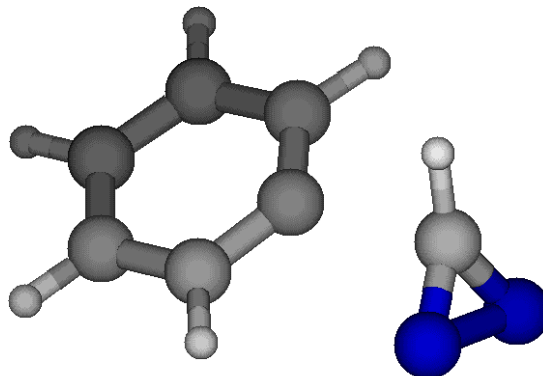
Compound TS **73T** – **64T** B3LYP/6-311G(d,p) - E=-489.241639 u.a.

C	0.473920	0.858744	-1.145449
C	1.654483	1.577117	-1.296383
C	2.847452	1.069385	-0.773775
C	2.864737	-0.175714	-0.137662
C	1.680453	-0.889746	0.010661
C	0.486191	-0.372991	-0.489955
C	4.154983	1.875758	-0.924400
N	4.533366	1.185689	-2.105024
N	6.138138	1.853831	-2.638946
N	6.950889	1.765458	-3.378549
N	5.039788	1.730011	0.181097
H	3.801438	-0.566563	0.239028
H	1.689876	-1.851078	0.510929
H	-0.453933	1.255250	-1.541099
H	1.656789	2.529192	-1.814349
H	-0.435307	-0.932451	-0.375128
H	3.913363	2.949451	-1.042818



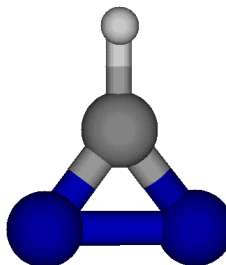
Compound TS **64T – 75T** B3LYP/6-311G(d,p) - **E=-379.720320 u.a.**

C	1.552891	-1.036949	-0.915497
C	0.392204	-0.401099	-0.474764
C	0.396652	0.959536	-0.169235
C	1.575472	1.707361	-0.299750
C	2.684098	1.018957	-0.728373
C	2.744687	-0.313112	-1.055288
C	4.802413	2.137639	-0.862562
N	4.871900	2.681410	-2.058254
N	5.530110	1.342409	-1.615132
H	3.658591	-0.777074	-1.406566
H	1.538820	-2.094359	-1.156832
H	-0.511768	1.447997	0.166590
H	1.593255	2.768074	-0.076458
H	-0.524961	-0.969585	-0.373008
H	4.591357	2.372682	0.171389



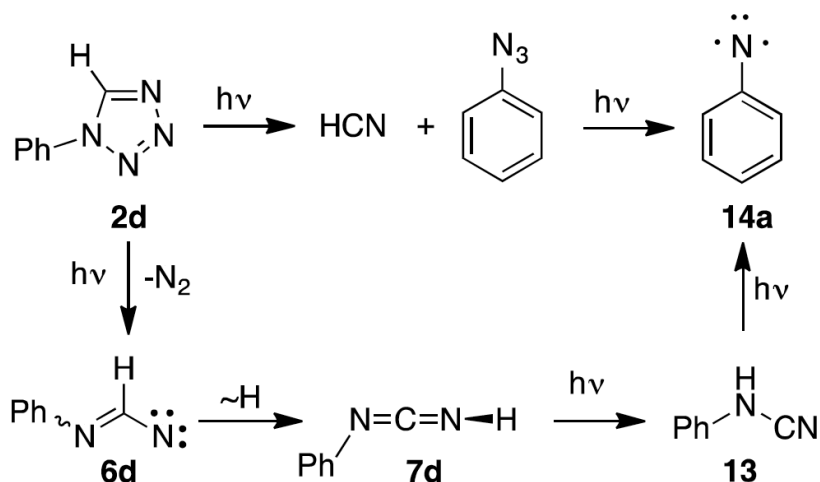
Compound **75T** B3LYP/6-311G(d,p) - **E=-148.099792 u.a.**

C	4.876313	2.174574	-0.858864
N	5.514774	1.325471	-1.609654
N	4.847049	2.680473	-2.057046
H	4.557644	2.353623	0.161005



numbering summary:

the numbering used in the paper is recalled below. This numbering is identical to the one used in the SI.



Scheme S4. Photochemistry of 1-phenyltetrazole **2d**

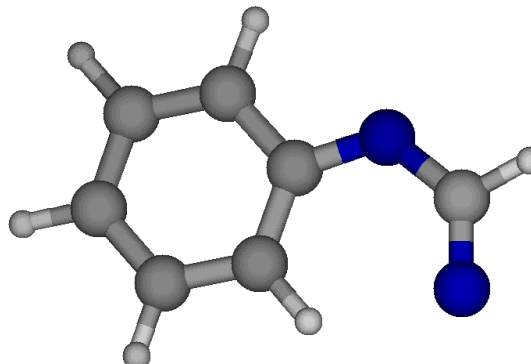
Table S23. Absolute and relative energies for **6d**, **7d**, and transition states calculated at the U-B3LYP/6-311G(d,p) level of theory.

Reference energy = **6d (Z)** T

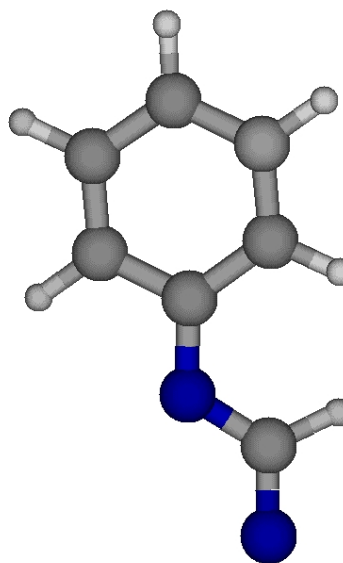
state	Compound	energy (u.a.)	(kcal/mol)
T	6d (Z)	-379.845664	0.0
T	6d (E)	-379.843461	1.4
T	TS 6d-7d	-379.768127	48.7
T	7d	-379.842160	2.2
S	6d (Z)	-379.836116	6.0
S	6d (E)	-379.839347	4.0
S	TS 6d-7d	-379.814430	19.6
S	7d	-379.932741	-54.6

Table S24. Cartesian coordinates related to the photochemistry of 1-phenyltetrazole **2d**Compound **6d** Z (T) B3LYP/6-311G(d,p) - E=-379.845664 u.a.

	X	Y	Z
N	0.828275	1.542061	0.000000
C	2.197942	1.441599	0.000000
H	2.705479	2.415823	0.000000
C	0.000000	0.459812	0.000000
C	-1.386970	0.778343	0.000000
C	0.368992	-0.915274	0.000000
C	-2.349233	-0.214391	0.000000
H	-1.651945	1.828222	0.000000
C	-0.604541	-1.897790	0.000000
H	1.418599	-1.181413	0.000000
C	-1.963323	-1.558372	0.000000
H	-3.400518	0.049050	0.000000
H	-0.310883	-2.941285	0.000000
H	-2.715055	-2.339370	0.000000
N	2.939884	0.401570	0.000000

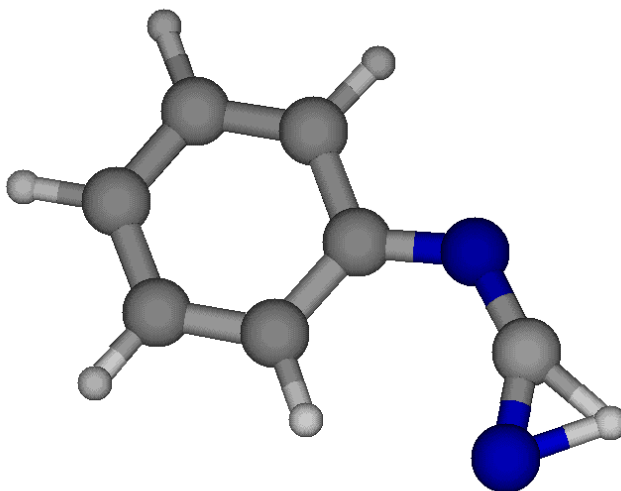
Compound **6d** E (T) B3LYP/6-311G(d,p) - E=-379.845664 u.a.

	X	Y	Z
C	2.614936	0.267396	0.015289
C	2.143725	-1.048286	0.018104
C	0.782420	-1.295300	-0.002707
C	-0.157458	-0.231680	-0.017077
C	0.344171	1.098771	-0.025378
C	1.707804	1.333108	-0.010189
N	-1.470072	-0.616000	-0.035238
C	-2.463042	0.300544	0.048681
N	-3.704851	-0.027514	-0.010968
H	0.385826	-2.302888	-0.004189
H	-0.332305	1.943017	-0.057548
H	2.843650	-1.875639	0.033621
H	2.076174	2.352648	-0.021380
H	3.680608	0.464363	0.027880
H	-2.264817	1.375776	0.184707



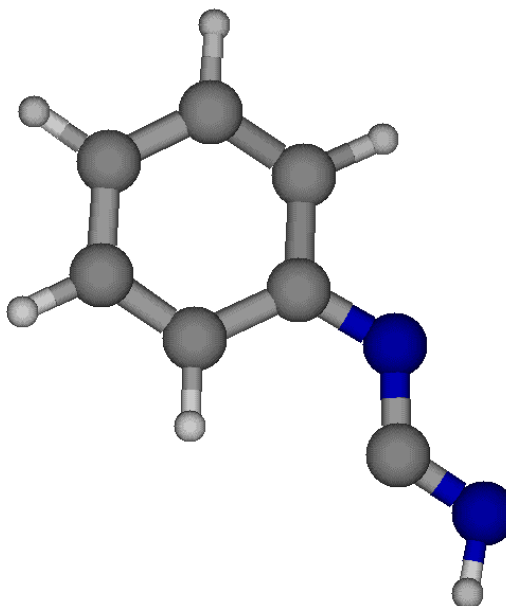
Compound TS **6d-7d** (T) B3LYP/6-311G(d,p) - E=-379.768127 u.a.

	X	Y	Z
C	1.432183	-0.004087	-1.439646
C	0.127467	-0.000874	-0.982447
C	-0.134963	0.001567	0.417850
C	0.968406	0.000629	1.314916
C	2.266509	-0.002610	0.840836
C	2.505056	-0.004982	-0.538125
N	-1.370756	0.004764	0.998447
C	-2.493982	0.005947	0.265045
N	-2.927366	0.005674	-0.939257
H	0.745990	0.002535	2.374711
H	3.098747	-0.003308	1.535070
H	3.522749	-0.007515	-0.911350
H	1.626414	-0.005922	-2.506054
H	-0.701403	-0.000164	-1.677953
H	-3.742558	0.008348	0.020477



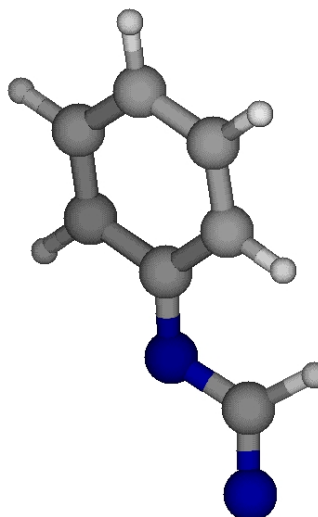
Compound **7d** (T) B3LYP/6-311G(d,p) - E=-379.842160 u.a.

	X	Y	Z
C	-0.011505	0.018547	0.010104
C	0.042386	-0.212583	1.415620
C	1.314518	-0.205811	2.052083
C	2.467145	0.019546	1.323475
C	2.392522	0.244120	-0.056311
C	1.149010	0.241887	-0.703962
N	-1.031472	-0.441404	2.209739
C	-2.278264	-0.465488	1.696739
N	-3.342396	-0.669423	2.353354
H	1.339126	-0.382821	3.120132
H	3.430181	0.022419	1.820591
H	3.297613	0.420762	-0.625948
H	1.099456	0.416693	-1.772788
H	-0.980176	0.013415	-0.473440
H	-4.181088	-0.646012	1.773238



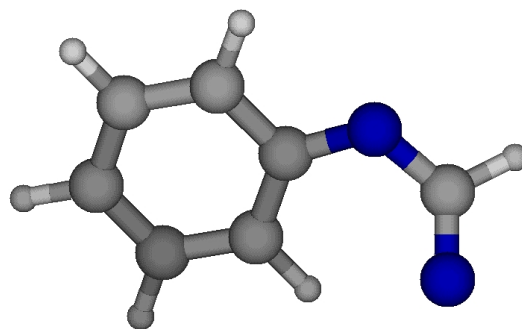
Compound **6d Z** (S) B3LYP/6-311G(d,p) - E=-379.83611§ u.a.

	X	Y	Z
N	-1.450713	-0.677889	-0.004027
C	-2.461279	0.247744	0.183129
C	1.653827	1.357777	-0.035898
C	-0.163858	-0.269421	-0.006971
C	0.816772	-1.306989	0.000252
C	0.299831	1.082099	-0.040531
C	2.165485	-1.013823	0.014451
H	0.452722	-2.326745	0.007170
N	-3.657911	0.049938	-0.174462
H	-0.409056	1.897759	-0.101823
C	2.594190	0.319592	-0.000743
H	2.893888	-1.816170	0.031868
H	1.992029	2.387228	-0.069379
H	3.653169	0.549827	0.002980
H	-2.252202	1.201885	0.696482



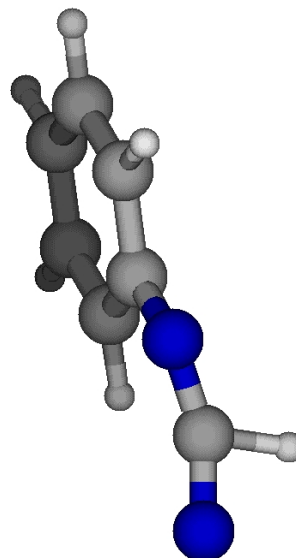
Compound **6d E** (S) B3LYP/6-311G(d,p) - E=-379.839347 u.a.

	X	Y	Z
N	1.429487	-0.993439	0.120422
C	2.595240	-0.230203	0.128650
H	3.445031	-0.742337	0.602477
C	0.209786	-0.422275	0.073398
C	-0.889350	-1.326735	-0.058961
C	-0.080918	0.974802	0.164585
C	-2.186964	-0.863742	-0.122584
H	-0.655419	-2.382474	-0.116023
C	-1.387115	1.419142	0.099446
H	0.734235	1.676609	0.282440
C	-2.445500	0.511881	-0.045877
H	-3.007749	-1.563101	-0.231786
H	-1.595529	2.480821	0.166694
H	-3.465642	0.875028	-0.092640
N	2.806798	0.890328	-0.412295



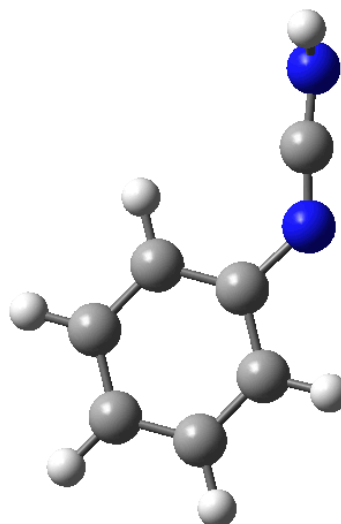
Compound TS **6d-7d** (S) B3LYP/6-311G(d,p) - E=-379.814430 u.a.

	X	Y	Z
N	1.414054	-0.833973	-0.074195
C	2.478081	-0.101384	0.108091
C	0.126833	-0.355558	-0.014767
C	-0.917153	-1.306160	-0.004501
C	-0.205381	1.018715	-0.008181
C	-2.240803	-0.895324	-0.003211
H	-0.650274	-2.355780	-0.007005
C	-1.533261	1.415738	0.003078
H	0.588613	1.757641	-0.016785
C	-2.557853	0.465143	0.003336
H	-3.032482	-1.635827	-0.002664
H	-1.776047	2.472390	0.008304
H	-3.593713	0.783227	0.011136
N	3.549890	0.470555	-0.168074
H	2.813516	0.075247	1.199828



Compound **7d** (S) B3LYP/6-311G(d,p) - E=-379.932741 u.a.

	X	Y	Z
N	3.567065	0.387434	-0.073538
H	4.109112	0.569537	0.762606
C	2.469553	-0.143138	0.014156
N	1.425129	-0.765075	-0.051371
C	0.089071	-0.324846	-0.021654
C	-0.914827	-1.296732	0.004004
C	-0.259793	1.031916	-0.028509
C	-2.252807	-0.916191	0.028195
H	-0.626469	-2.340635	0.004157
C	-1.599467	1.403065	-0.005567
H	0.519075	1.786098	-0.056486
C	-2.601087	0.433023	0.023758
H	-3.024923	-1.676875	0.048656
H	-1.862190	2.455001	-0.012302
H	-3.643826	0.727789	0.041423



References

- (1) Abe. M.; Bégué. D.; Santos-Silva. H.; Dargelos. A.; Wentrup. C. Direct Observation of an Imidoylnitrene: Photochemical Formation of PhC(=NMe)-N and Me-N from 1-Methyl-5-phenyltetrazole. *Angew. Chem. Int. Ed.* **2018**, 57, 3212–3216.
- (2) Bégué, D.; Qiao, G. G.; Wentrup, C. Nitrile Imines: Matrix Isolation, IR Spectra, Structures, and Rearrangement to Carbodiimides. *J. Am. Chem. Soc.* **2011**, 134, 5339-5350.
- (3) Frisch. M. J.; Trucks. G. W.; Schlegel. H. B.; Scuseria. G. E.; Robb. M. A.; Cheeseman. J. R.; Scalmani. G.; Barone. V.; Mennucci. B.; Petersson. G. A. et al. Gaussian 09. Revision A.2; Gaussian. Inc.: Wallingford. CT. 2009.
- (4) Werner. H.-J.; Knowles. P. J.; Knizia. G.; Manby. F. R.; Schütz. M.; Celani. P.; Korona. T.; Lindh. R.; Mitrushenkov. A.; Rauhut. G. et al. MOLPRO. Version 2012.1. A Package of Ab Initio Programs. 2012. <http://www.molpro.net>. Accessed 20 July 2018.
- (5) Neese. F. The ORCA Program System. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, 2, 73–78.