Supporting Information

Nitrenes, Diradicals and Ylides. Ring Expansion and Ring Opening in 2-Quinazolylnitrenes.

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All calculated IR spectra shown are at the B3LYP/6-31G** level, with wavenumbers scaled by 0.9613.

Content:

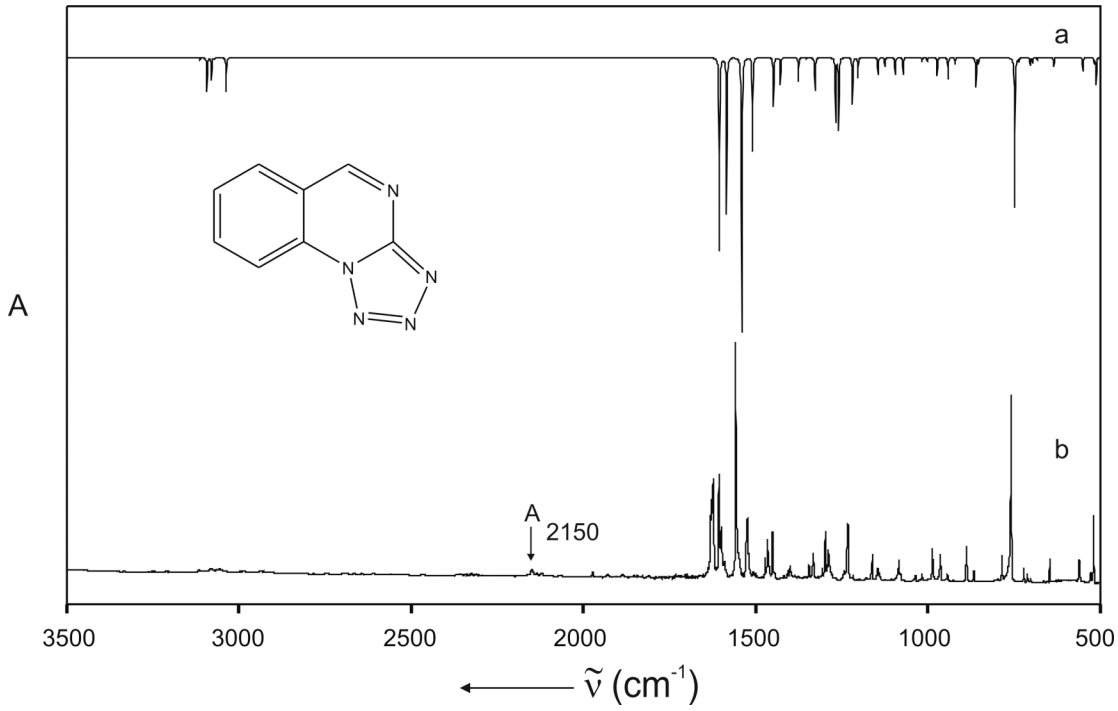


Figure S1. Calculated (a; B3LYP/6-31G**) and experimental (b) IR spectra of tetrazole **9** in Ar matrix. A = azide **10**

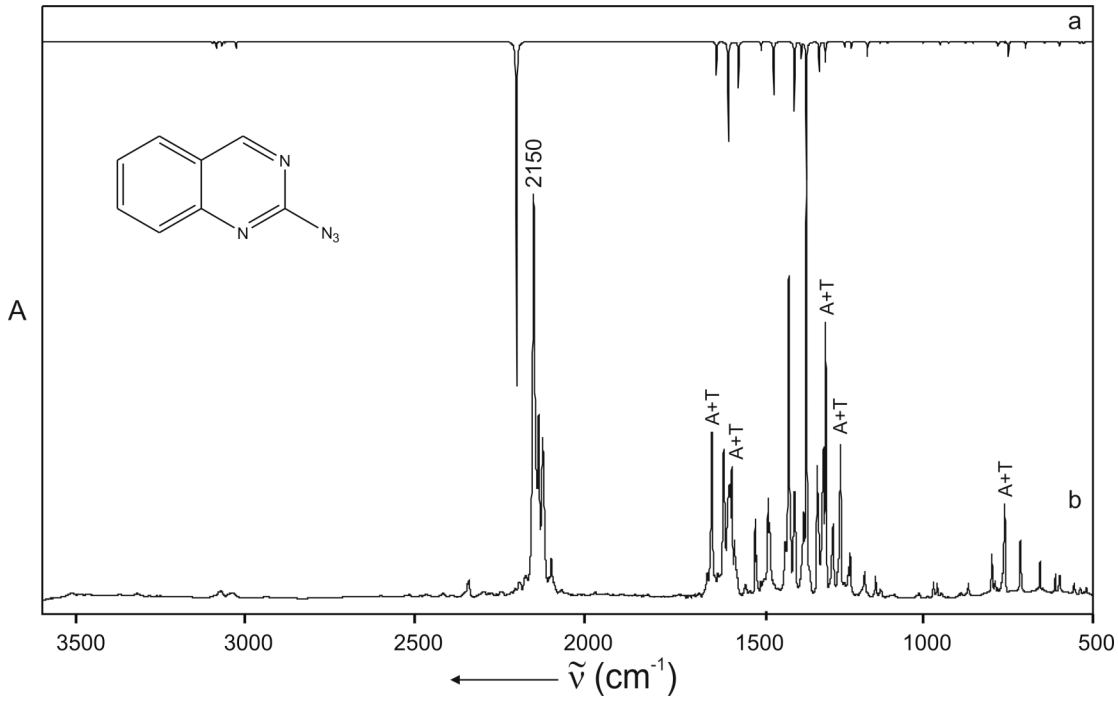
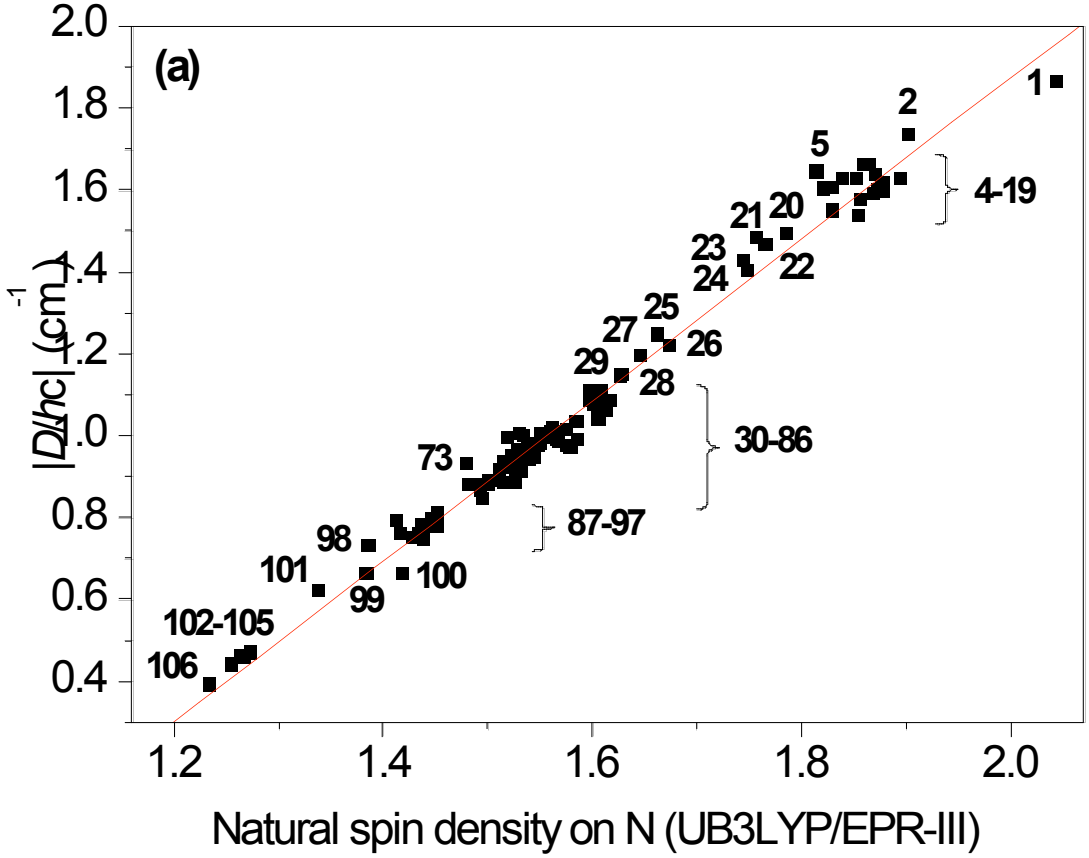
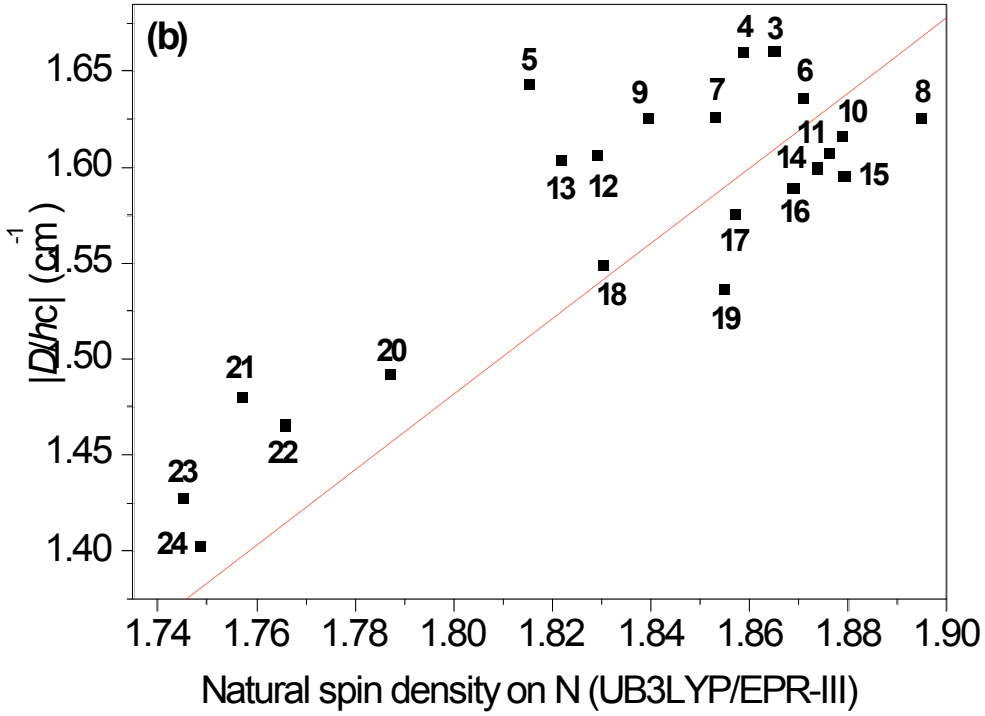
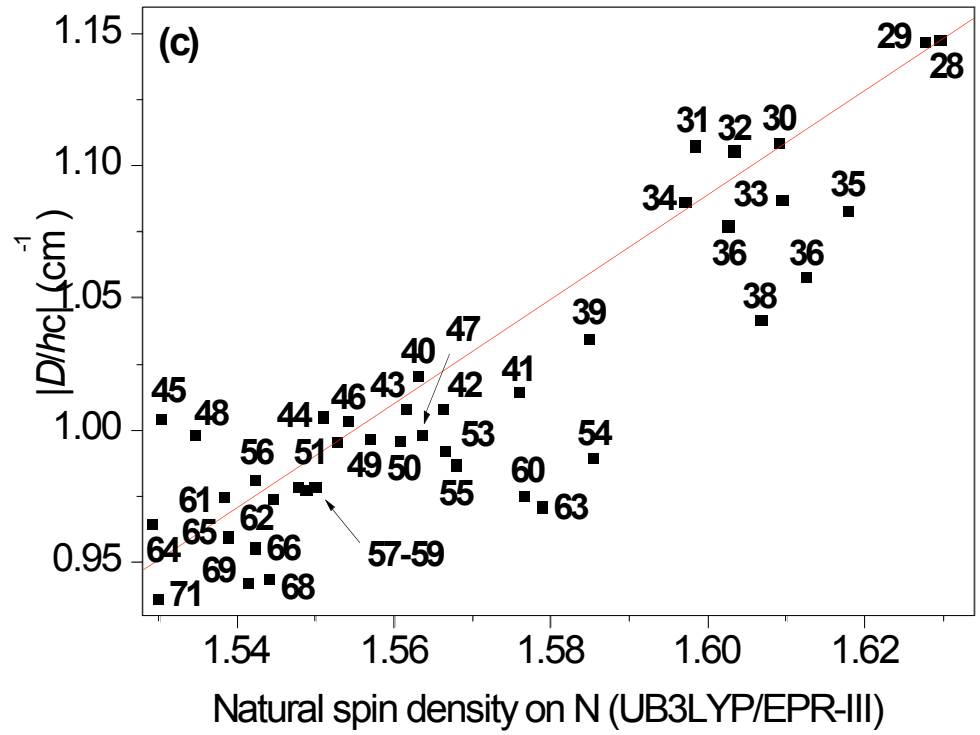


Figure S2. Calculated (a; B3LYP/6-31G**) and experimental (b) IR spectra of azide **10** in Ar matrix. A = azide **10.** T = tetrazole **9**.

Correlation of the |*D/hc*| zfs values of nitrenes with calculated natural spin densities at the UB3LYP/EPR-III level and table of the corresponding data and literature references.




(b)
|D/hc| (cm-1)
Natural spin density on N (UB3LYP/EPR-III)
1.40
1.45
1.50
1.55
1.60
1.65
1.74
1.76
1.78
1.80
1.82
1.84
1.86
1.88
1.90
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24


(c)
|D/hc|⊥ (cm-1)
Natural spin density on N (UB3LYP/EPR-III)
0.95
1.00
1.05
1.10
1.15
1.54
1.56
1.58
1.60
1.62
28 29 30 31 32 33 34 35 36 36 38 39 40 41 42 43 44 45 46 47 48 49 50 51 53 54 55 56 57-59 60 61 62 63 64 65 66 68 69 71

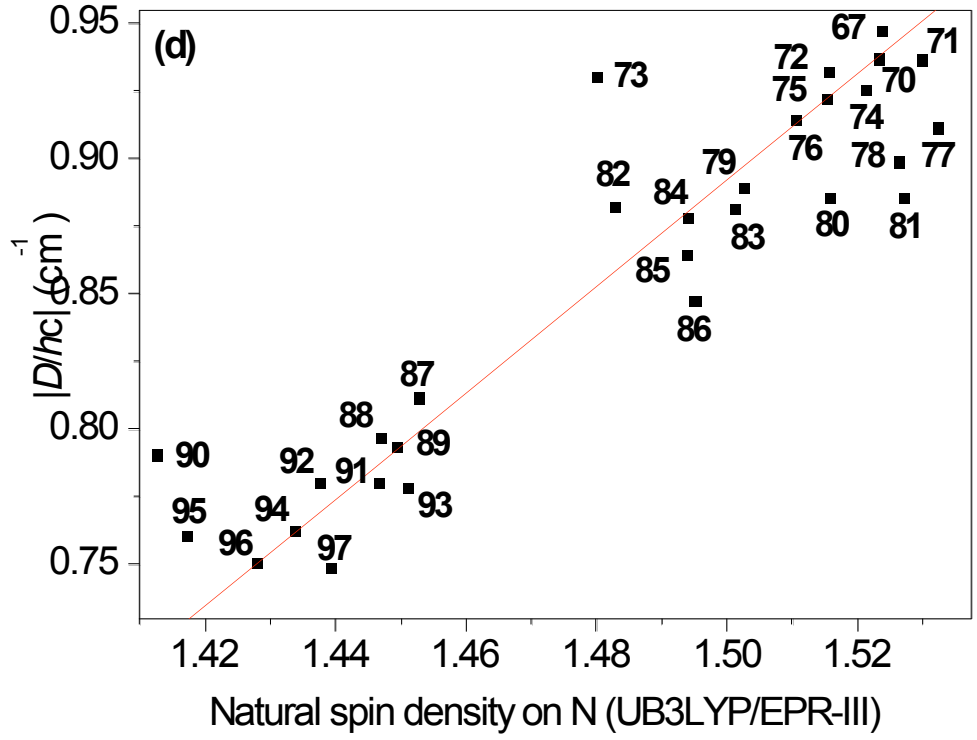


Figure S3. *D*-ρ correlation for nitrenes. Top graph (a): all nitrenes correlated here. Bottom graphs: details showing (b) alkyl- and (c)-(d) (hetero)aryl-nitrenes. R^2 for all data: 0.993.[§]

	nitrene[£]	PG	|*D*/*hc*| (cm^{-1})	|*E*/*hc*| (cm^{-1})	ρ [†] (Natural)	S^{2} [‡]	ref
1	imidogen	$C_{\infty v}$	1.8630	0	2.04402	2.0058	1
2	trifluoromethyl-	C_{3v}	1.7360	n/a	1.90305	2.0059	2
3	triphenylmethyl-	C_3	1.6600	< 0.002	1.86520	2.0080	3
4	*alpha*-carbethoxybenzyl-	C_1	1.6590	< 0.002	1.85903	2.0086	4
5	2-methyl-*o*-carboran-1-yl-	C_s	1.6430	0.0037	1.81535	2.0091	5
6	diphenylmethyl-	C_1	1.6360	< 0.002	1.87105	2.0080	3
7	*C*-azido-*C*-phenyl-methyl-	C_1	1.6260	< 0.002	1.85335	2.0087	3
8	*tert*-butyl-	C_{3v}	1.6250	< 0.002	1.89500	2.0074	4
9	*C*-azido-*C*,*C*-diphenyl-methyl-	C_1	1.6250	< 0.002	1.83976	2.0090	3
10	2-octyl-	C_1	1.6160	0.0019	1.87900	2.0078	4
11	*n*-propyl-	C_s	1.6070	0.0034	1.87641	2.0079	4
12	9-azido-9*H*-fluoren-9-yl-	C_s	1.6060	0.0030	1.82947	2.0088	3
13	*o*-carboran-1-yl-	C_s	1.6030	0.0029	1.82177	2.0089	5
14	(*equatorial*)-cyclohexyl-	C_s	1.5990	< 0.002	1.87386	2.0078	4
15	methyl-	C_{3v}	1.5950	< 0.003	1.87949	2.0079	6
16	adamantyl-	C_{3v}	1.5890*	0	1.86914	2.0078	7
17	cyclopentyl-	C_1	1.5750	< 0.002	1.85728	2.0083	4

18	norbornyl-	C_s	1.5490*	0	1.83045	2.0086	8
19	*o*-carboran-9-yl-	C_s	1.5360	< 0.002	1.85512	2.0075	5
20	(*o*-phenylenedioxy)boranyl-	C_s	1.4920	0.0040	1.78737	2.0108	9
21	4-azido-6-dimethylamino-*s*-triazin-2-yl-	C_s	1.4800	0.0031	1.75728	2.0218	10
22	4,6-bis(dimethylamino)-*s*-triazin-2-yl-	C_{2v}	1.4650	0.011	1.76586	2.0189	11
23	4,6-dimethoxy-*s*-triazin-2-yl-	C_s	1.4270	0.013	1.74537	2.0236	11
24	4,6-diazido-*s*-triazin-2-yl-	C_{2v}	1.4020	0.011	1.74873	2.0252	12
25	4,6-dimethyl-pyrimid-2-yl-	C_{2v}	1.2451*	0.0054*	1.66306	2.0429	13
26	2-pyrimidyl-	C_{2v}	1.2170*	0.0052*	1.67473	2.0416	14
27	4-pyrimidyl-	C_s	1.1937*	0.0012*	1.64774	2.0410	13
28	4-phenyl-2-quinazolinyl-	C_1	1.1470*	0.0060*	1.62974	2.0526	15
29	2-quinazolyl-	C_s	1.1465*	0.0064*	1.62788	2.0521	15
30	3,5-bis(trifluoromethyl)-2-pyridyl-	C_s	1.1080*	0	1.60927	2.0488	16
31	4-pyridyl-	C_{2v}	1.1070*	0	1.59853	2.0471	17
32	3-pyridazinyl-	C_s	1.1050*	0.0030*	1.60341	2.0468	13
33	5-trifluoromethyl-2-pyridyl-	C_s	1.0865*	0	1.60958	2.0468	16
34	2,3,5,6-tetrafluoro-4-pyridyl-	C_s	1.0860*	0	1.59722	2.0446	18
35	4-trifluoromethyl-2-pyridyl-	C_s	1.0826*	0	1.61786	2.0467	16
36	3-trifluoromethyl-2-pyridyl-	C_s	1.0768*	0	1.60271	2.0483	16
37	6-trifluoromethyl-2-pyridyl-	C_s	1.0575*	0	1.61275	2.0462	16
38	2-pyridyl-	C_s	1.0414*	0.0015*	1.60682	2.0458	14
39	2-quinolyl-	C_s	1.0340*	0.0039*	1.58493	2.0553	14
40	4,6-dimethyl-pyridazin-3-yl-	C_s	1.0200*	0.0023*	1.56326	2.0466	13
41	2-pyrazinyl-	C_s	1.0140*	0	1.57605	2.0478	14
42	3-biphenylyl-	C_1	1.0080	< 0.002	1.56639	2.0502	6
43	4-fluorophenyl-	C_{2v}	1.0080	< 0.002	1.56156	2.0473	19
44	3-pyridyl-	C_s	1.0048	< 0.003	1.55104	2.0478	6
45	4-(N-methylacetamido)phenyl-	C_1	1.0040	0.0008	1.53049	2.0482	20
46	2-(trifluoromethyl)phenyl-	C_s	1.0030	< 0.002	1.55418	2.0500	6
47	phenyl-	C_{2v}	0.9978	< 0.002	1.56372	2.0487	6
48	4-methoxyphenyl-	C_s	0.9978	0.0039	1.53484	2.0440	6
49	3-tolyl-	C_s	0.9966	< 0.003	1.55696	2.0497	6
50	3-aminophenyl-	C_s	0.9957	< 0.003	1.56100	2.0484	6
51	4-quinazolyl-	C_s	0.9953*	0.0035*	1.55295	2.0581	21
52	2-biphenylyl-	C_1	0.9940	0.0008	1.51880	2.0490	20
53	3-dimethylaminophenyl-	C_s	0.9919	< 0.003	1.56668	2.0473	6
54	3-nitrophenyl-	C_s	0.9890	< 0.002	1.58541	2.0500	6
55	4-azido-biphenyl-3'-yl	C_1	0.9866*	0	1.56797	2.0506	22
56	4-carboxyphenyl-	C_s	0.9810	0.0006	1.54230	2.0521	20
57	4-tolyl-	C_s	0.9780	< 0.002	1.55005	2.0485	19
58	4-nitrophenyl-	C_{2v}	0.9780	0.0015	1.54779	2.0520	20
59	4-ethylphenyl-	C_s	0.9770	< 0.002	1.54889	2.0482	19
60	3-carboxyphenyl-	C_s	0.9750	0.0008	1.57666	2.0501	20
61	4-hydroxyphenyl-	C_s	0.9740	< 0.002	1.53839	2.0450	19

62	3,5-diazido-2,4,6-tricyanobenzen-1-yl-	C_s	0.9735	0	1.54470	2.0617	23
63	3-methoxyphenyl-	C_s	0.9705	< 0.003	1.57903	2.0469	6
64	2-(*n*-butyl)phenyl-	C_s	0.9640	< 0.002	1.52939	2.0491	6
65	4-cyanophenyl-	C_{2v}	0.9590	0.001	1.53889	2.0553	20
66	2-quinoxalyl-	C_s	0.9550*	0.0030*	1.54235	2.0573	14
67	4-(acetylamino)phenyl-	C_1	0.9470	0.0004	1.52389	2.0470	20
68	3-isoquinolyl-	C_s	0.9430*	0.0049*	1.54421	2.0543	14
69	4-carbethoxyphenyl-	C_s	0.9420	< 0.002	1.54143	2.0517	19
70	4-biphenylyl-	C_1	0.9367	< 0.003	1.52350	2.0517	6
71	7-azido-2-phenanthrenyl-	C_s	0.9360	0	1.52996	2.0557	24
72	4-azidophenyl-	C_s	0.9320	0	1.51572	2.0513	25
73	4-(phenylethynyl)phenyl-	C_{2v}	0.9300	n/a	1.48023	2.0604	26
74	2-naphthyl-	C_s	0.9250	0.0023	1.52139	2.0573	14
75	6-phenanthridinyl-	C_s	0.9220*	0.0071*	1.51544	2.0578	17
76	7-azido-3-dibenzofuranyl-	C_s	0.9140	0	1.51069	2.0508	24
77	4-acetylphenyl-	C_s	0.9110	< 0.002	1.53256	2.0541	19
78	3-azido-biphenyl-4'-yl	C_1	0.8986*	0	1.52656	2.0521	22
79	2-fluorenyl-	C_s	0.8890	0	1.50267	2.0532	24
80	4'-azido[1,1'-biphenyl]-4-yl-	C_1	0.8853*	0	1.51601	2.0527	27
81	2'-cyano-biphenyl-2-yl-	C_1	0.8852*	0.0040*	1.52729	2.0490	17
82	4-quinolyl-	C_s	0.8820*	0.0020*	1.48290	2.0602	14
83	9-oxo-9*H*-fluoren-2-yl-	C_s	0.8810	0	1.50138	2.0611	24
84	7-azido-9H-fluoren-2-yl-	C_s	0.8780	0	1.49429	2.0542	24
85	7-azido-9-oxo-9H-fluoren-2-yl-	C_s	0.8640	0	1.49397	2.0626	24
86	1-isoquinolyl-	C_s	0.8470*	0.0042*	1.49521	2.0610	14
87	9-phenanthryl-	C_s	0.8110*	0.0023*	1.45290	2.0547	28
88	*E*-[4-[2-(4-azido-phenyl)-vinyl]-phenyl]-	C_s	0.7960	n/a	1.44712	2.0734	29
89	1-naphthyl-	C_s	0.7930*	0.0025*	1.44961	2.0592	14
90	8-methyl-1-naphthalenyl-	C_s	0.7900	< 0.003	1.41268	2.0597	30
91	8-nitro-1-naphthalenyl-	C_s	0.7800	< 0.003	1.44684	2.0614	31
92	8-carboxy-1-naphthalenyl-	C_1	0.7800	< 0.003	1.43776	2.0602	31
93	2-anthryl-	C_s	0.7779	0.003	1.45123	2.0026	6
94	*E*-4-[2-(4-amino-phenyl)-vinyl]-phenyl-	C_s	0.7620	n/a	1.43396	2.0707	29
95	8-azido-1-naphthalenyl-	C_s	0.7600	< 0.003	1.41726	2.0626	31
96	8-hydroxy-1-naphthalenyl-	C_s	0.7500	< 0.003	1.42807	2.0618	31
97	*E*-[4-[(4-azidophenyl)azo]phenyl]-	C_s	0.7480	n/a	1.43934	2.0827	32
98	1-pyrenyl-	C_s	0.7300	n/a	1.38633	2.0772	33
99	1-anthryl-	C_s	0.6625	0.003	1.38455	2.0724	6
100	*E,E*-[4-[4-(4-azidophenyl)-1,3-butadienyl]phenyl]-	C_s	0.6610	0	1.41880	2.0911	34
101	8-amino-1-naphthalenyl-	C_s	0.6200	< 0.003	1.33819	2.0585	31
102	9-anthryl-	C_{2v}	0.4700	< 0.001	1.27317	2.0711	35
103	10-methoxy-9-anthryl-	C_s	0.4600	< 0.001	1.26325	2.0688	35
104	10-phenyl-9-anthryl-	C_{2v}	0.4600	< 0.001	1.26713	2.0707	35

105	10-nitro-9-anthryl-	C_2	0.4400	< 0.001	1.25635	2.0717	35
106	10-cyano-9-anthryl-	C_{2v}	0.3900	< 0.001	1.23484	2.0692	35

†: Natural spin density at the UB3LYP/EPR-III level of theory (Gaussian 03 revision B.05)

‡: The degree of spin contamination can be assessed by inspection of $<S^2>$, which should be 2.00 for a triplet (within 5%).[36]

*: $|D/hc|$ and $|E/hc|$ (cm^{-1}) computed with an iterative computer program (FORTRAN)[14] based on Wasserman's equations[37] and using the experimental resonance fields and microwave frequency given in the reference.

§: The correlation fits the equation $|D| = (1.96673 \times \rho) - 2.05772$ with standard deviation on $D = \pm 0.04$ cm^{-1}. Carbonylnitrenes and cyanonitrene do not fit this correlation. A large $|D|$ value may occur even though there is extensive delocalization.[6] Overdelocalization is a known problem for DFT methods, including the B3LYP functional.[36]

£: When several literature ESR data are available for the same nitrene, the $|D|$ value offering the best fit was kept in the correlation. The other values will be found in the references (below).

n/a: not reported.

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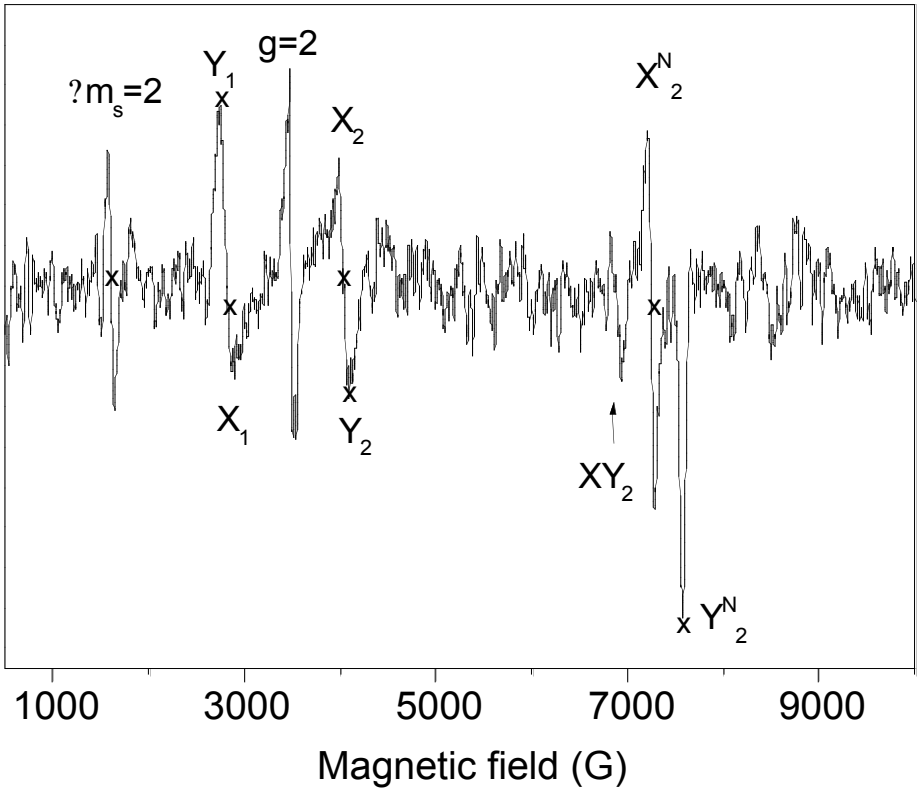


Figure S4: ESR spectrum of diradical **19** and 2-quinazolinylnitrene **11**, and the minor nitrene (XY_2 transition) obtained by FVT of tetrazole/azide **9/10** at 200°C with Ar matrix isolation at 15 K followed by photolysis at 254 nm (27 min); 40 scans (500-10,000 G), gain 1.6×10^6, microwave freq. = 9.72768 GHz (Ho = 3471.1 G)

Resonance fields of diradical **19** (marked with x on the spectrum):
(Δm_s=2) = 1597.3 G; Y_1 = 2740.2 G; X_1 = 2815.9 G; X_2 = 4014.9 G; Y_2 = 4085.7 G;
Zero-field splitting parameters of **19**: D= 0.1169 cm^{-1}; E= 0.0023 cm^{-1}

Resonance fields of nitrene **11** (marked with x on the spectrum):
X^N_1= 7240.8 G; Y^N_2= 7570.4 G
Zero-field splitting parameters of **3**: D= 1.1530 cm^{-1}; E= 0.0065

Resonance fields of the minor nitrene:
X_1= 6881.8 G; Y_2= 6928.2 G; zero-field splitting parameters: D = 0.9596 cm^{-1}; E ≤ 0.0010 cm^{-1}

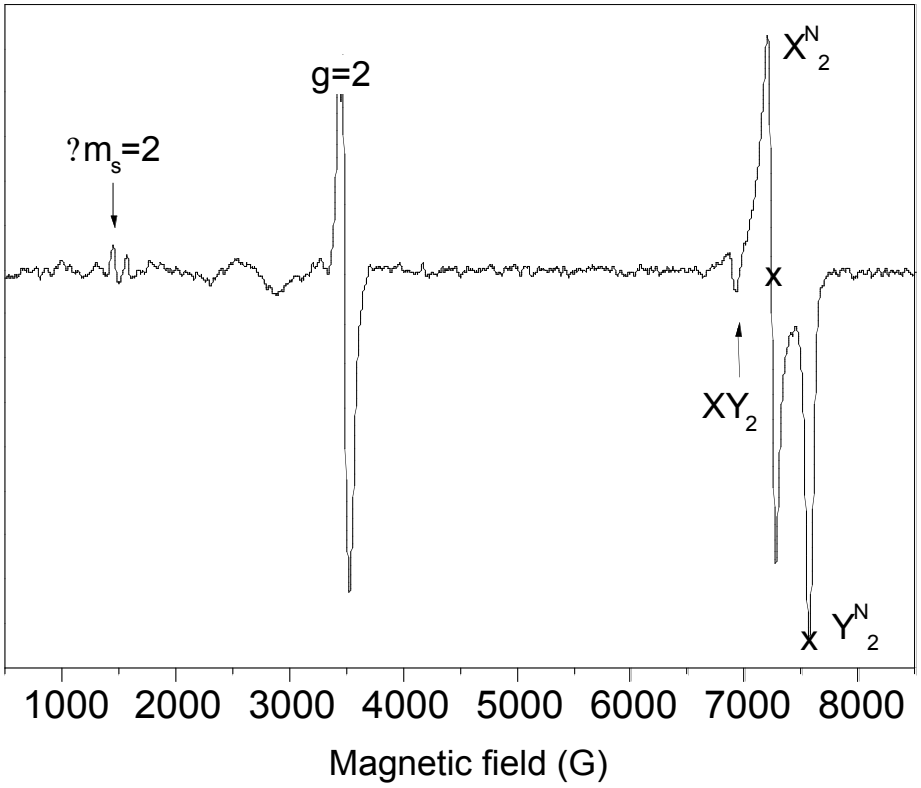


Figure S5: ESR spectrum of 2-quinazolinylnitrene **11** and the minor nitrene (XY_2 transition) obtained by FVT of tetrazole/azide **9/10** at 230°C with Ar matrix isolation at 15 K followed by photolysis at 308nm (10 min); 322 scans (500-8,500 G), gain $8.0x10^5$, microwave frequency= 9.72745 GHz (Ho = 3471.0 G)

Resonance fields of nitrene **11** (marked with x on the spectrum):
($\Delta m_s=2$) = 1468 G ; X^N_1 = 7231 G; Y^N_2 = 7563 G
Zero-field splitting parameters of **11**: D = 1.1496 cm^{-1}; E = 0.0066 cm^{-1}

Resonance fields of the minor nitrene:
X_1= 6884 G; Y_2= 6921 G; zero-field splitting parameters: D = 0.9587 cm^{-1}; E ≤ 0.0008 cm^{-1}.
Signal at g = 2 due to adventitious doublet radical formation.

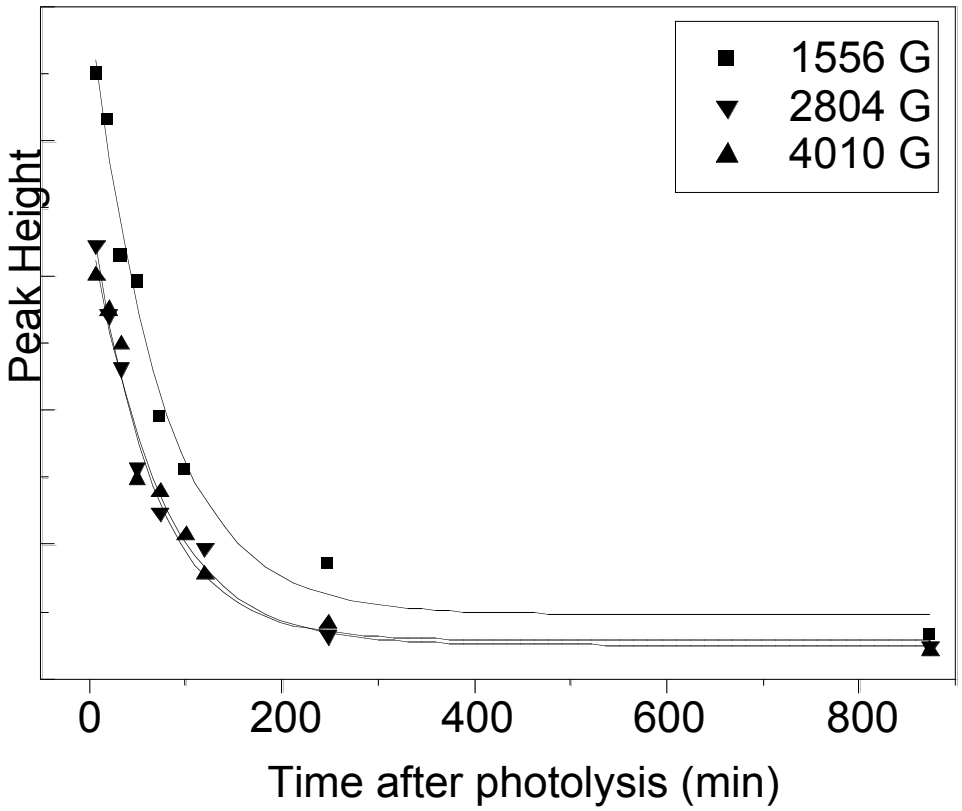


Figure S6. First order rate of disappearance of ESR signals of diradical **19** in Ar matrix at 15 K. $t_{1/2} \sim 47$ min

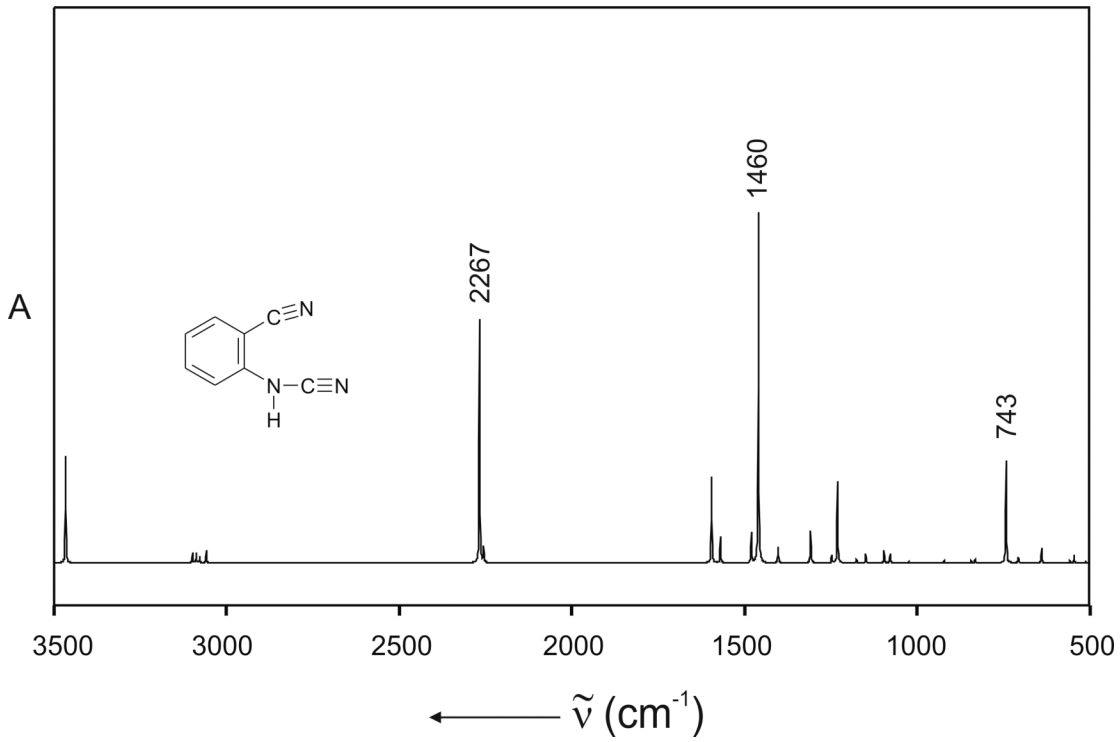


Figure S7. Calculated IR spectrum of *syn*-*N*-cyanoanthranilonitrile, *syn*-**22** (B3LYP/6-31G**) (fits experimental spectrum less well than that of *anti*-**22** (see Figure 5).

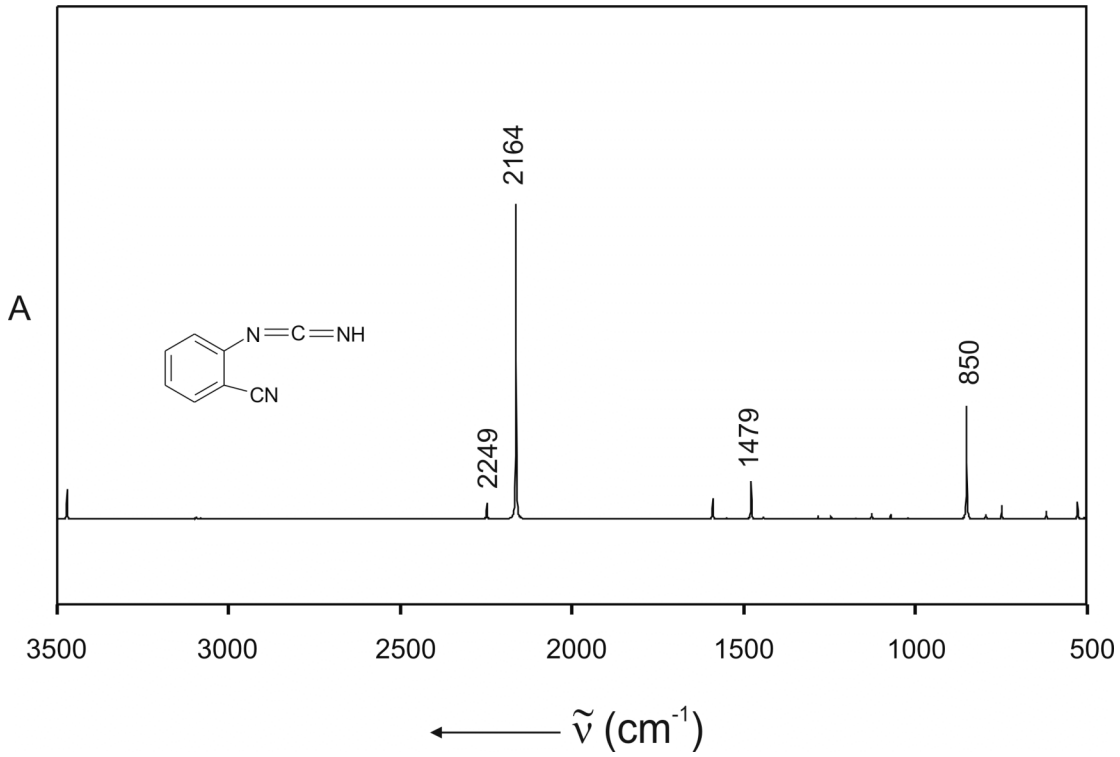


Figure S8. Calculated IR spectrum of *N*-(2-cyanophenyl)carbodiimide (2-NC-C_6H_4-N=C=NH).

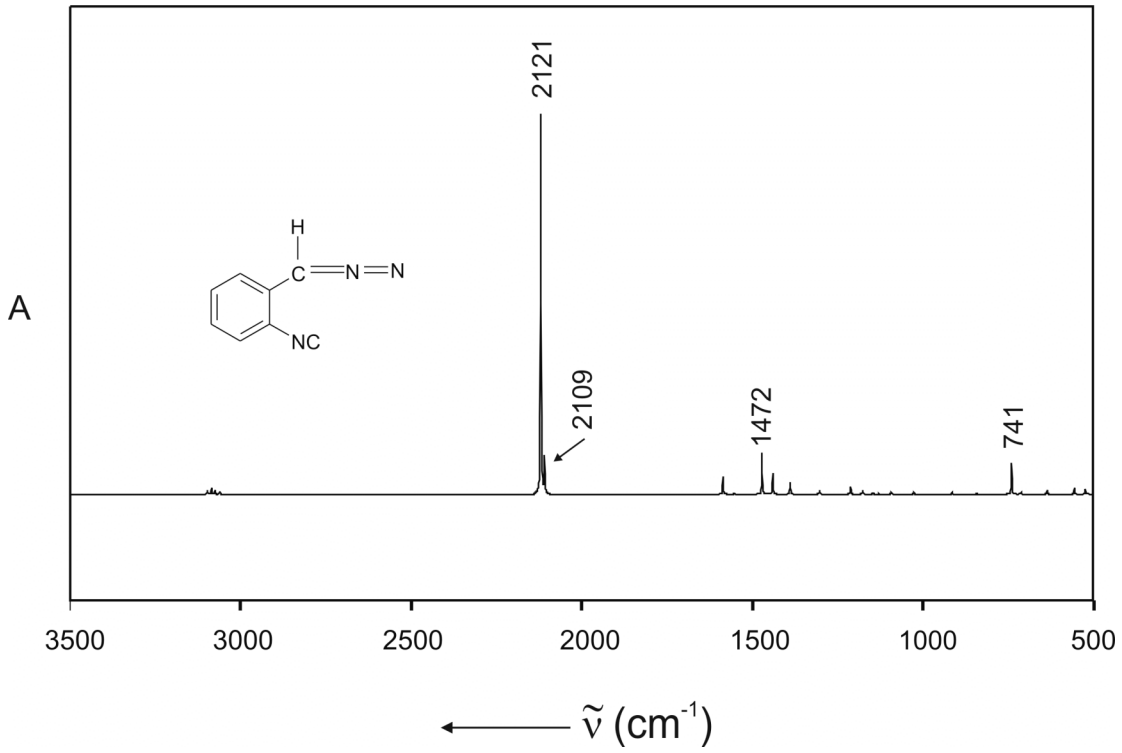


Figure S9. Calculated IR spectrum of (2-isocyanophenyl)diazomethane (2-CN-C_6H_4-CH=N_2) (B3LYP/6-31G**)

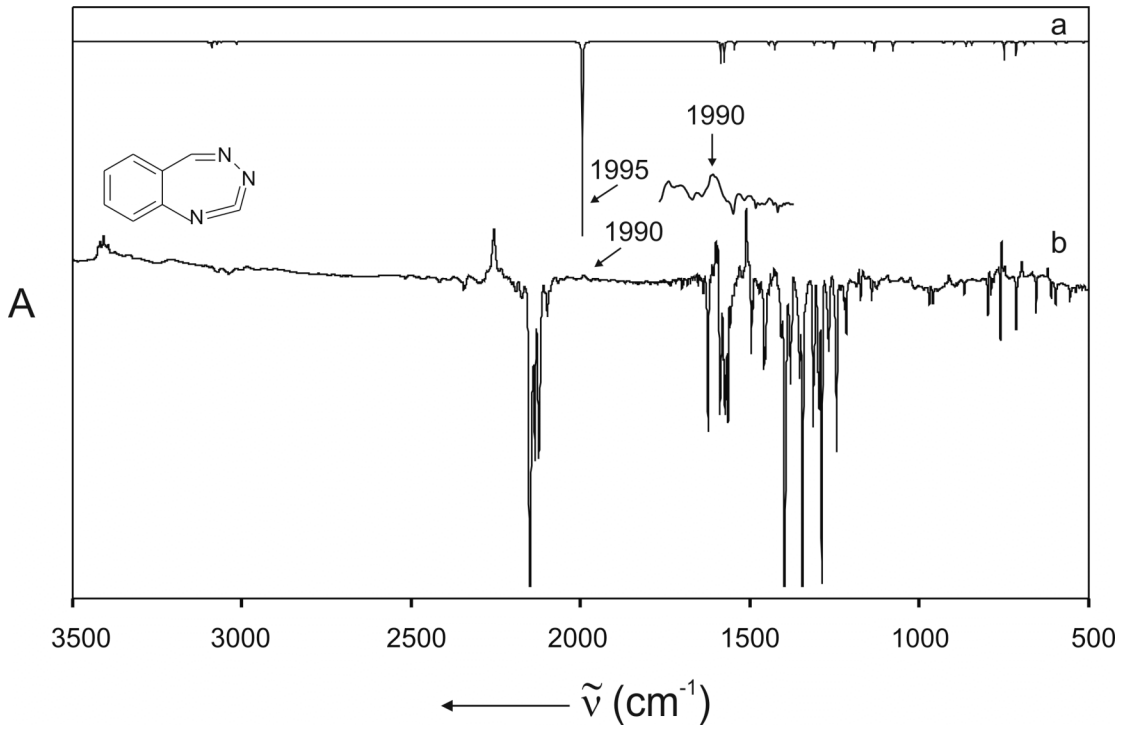


Figure S10. (a) Calculated IR spectrum of benzotriazacycloheptatetraene **14** (B3LYP/6-31G**). (b) Trace of species absorbing at 1990 cm^{-1} formed during early stages of photolysis of **9**/**10** in Ar matrix at 308 nm.

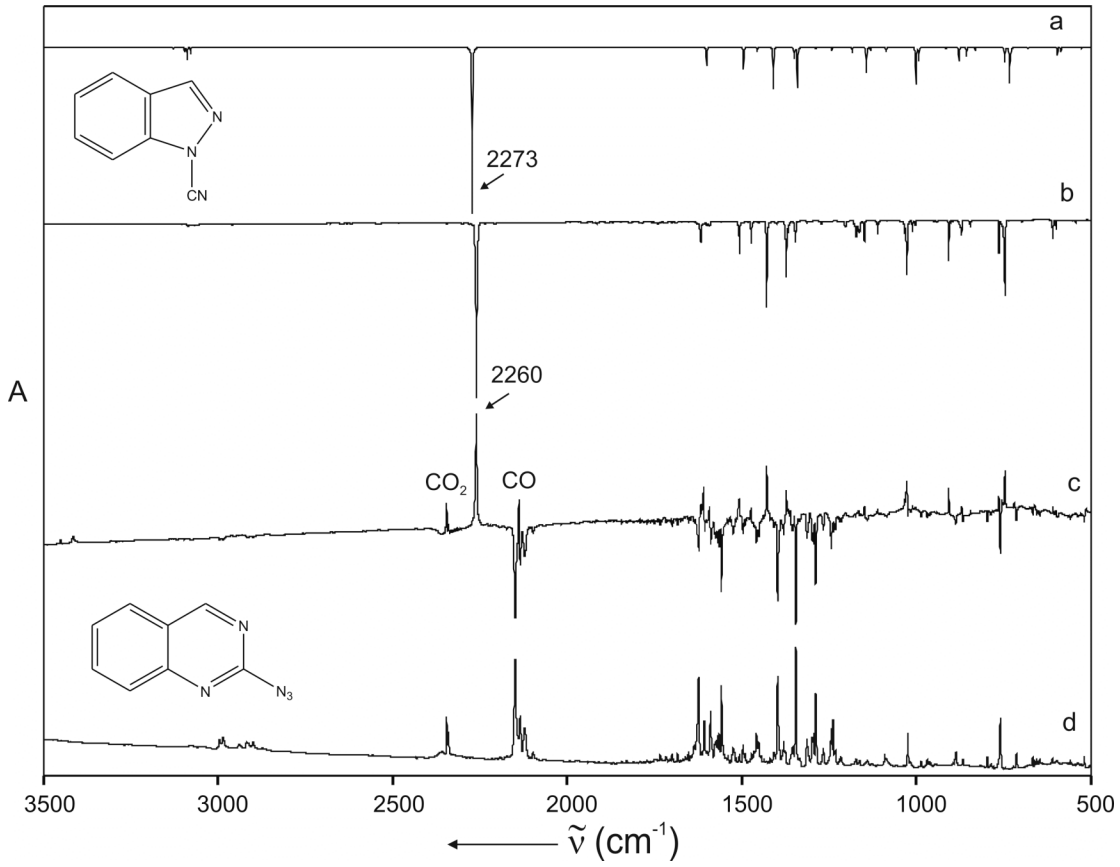


Figure S11. (a) Calculated (B3LYP/6-31G**) IR spectrum of 1-cyanoindazole **21**. (b) Experimental spectrum of the synthesized compound **21** in Ar at 10 K. (c) Positive spectrum showing the IR spectrum of compound **21** obtained by FVT of **9/10** at 500 ^{o}C with Ar matrix isolation at 10 K. (d) IR spectrum of the starting tetrazole/azide **9/10** in Ar matrix at 10 K.

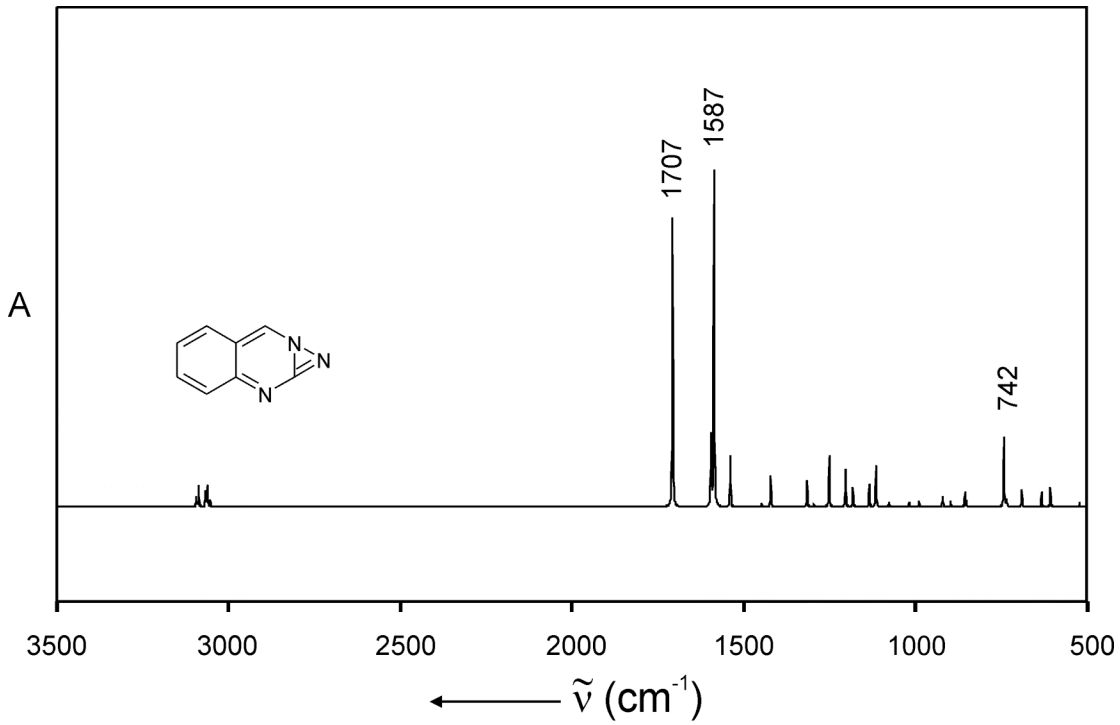


Figure S12. Calculated IR spectrum of diazirene **12** (B3LYP/6-31G**)

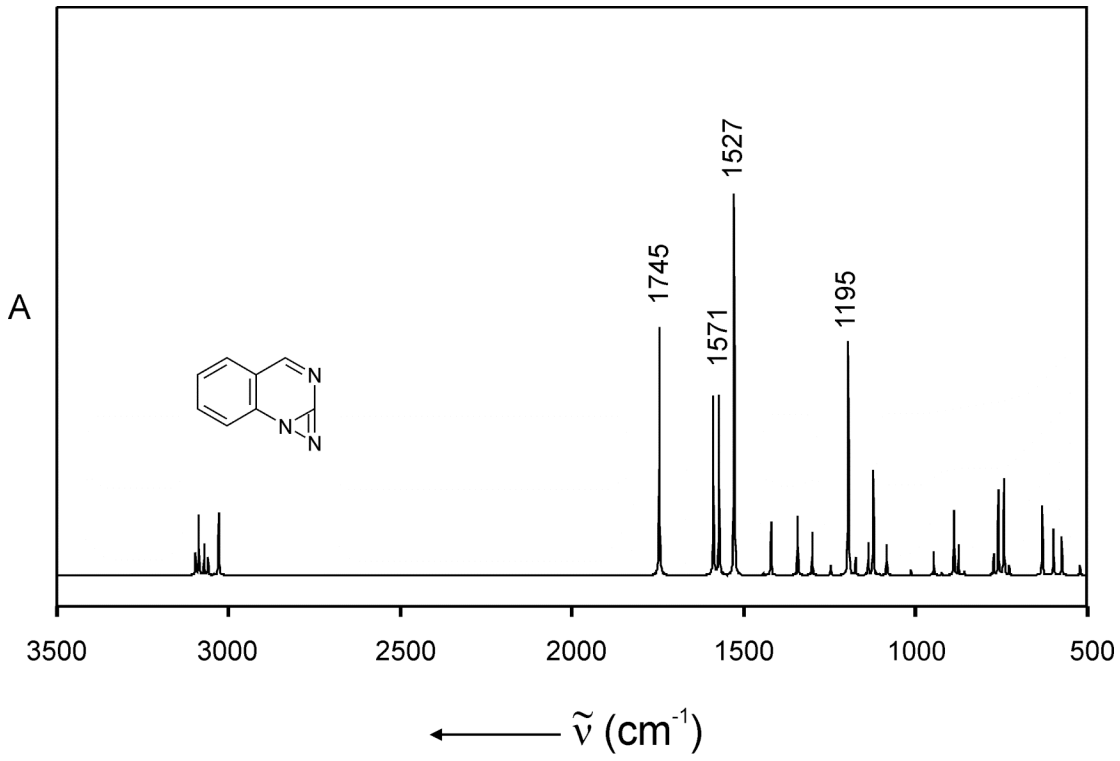


Figure S13. Calculated IR spectrum of diazirene **13** (B3LYP/6-31G**).

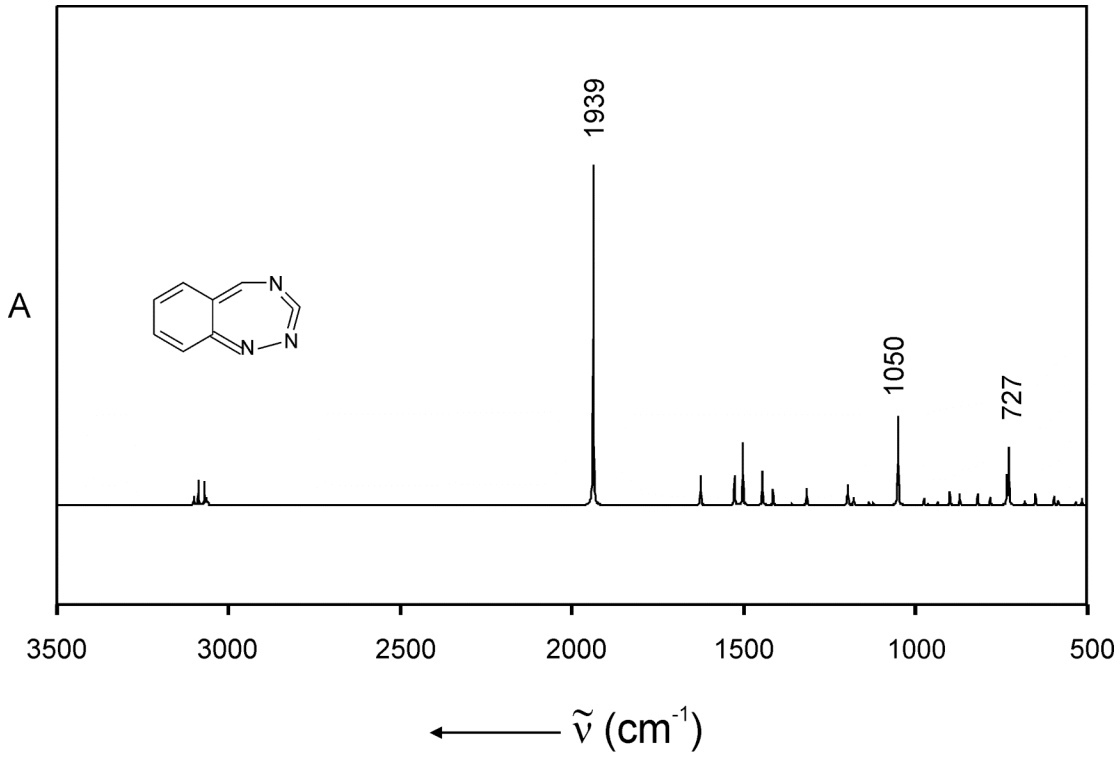


Figure S14. Calculated IR spectrum of cyclic carbodimide **16** (B3LYP/6-31G**)..

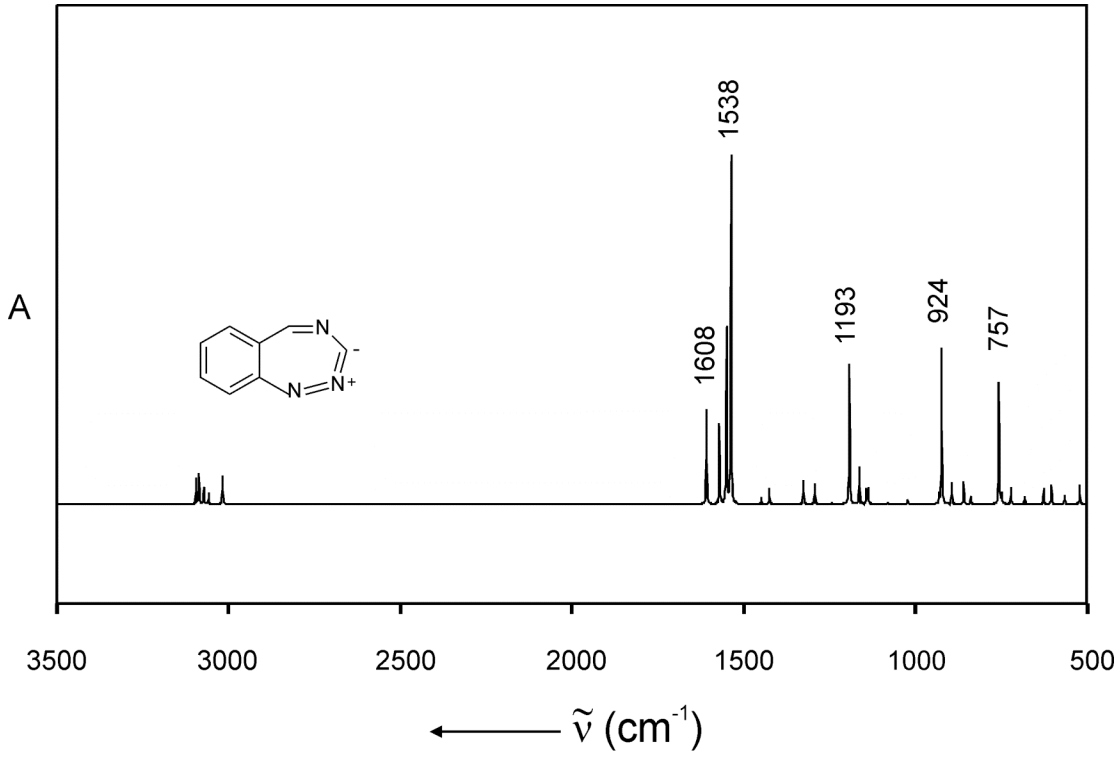


Figure S15. Calculated IR spectrum of cyclic nitrilimine **17** (B3LYP/6-31G**).

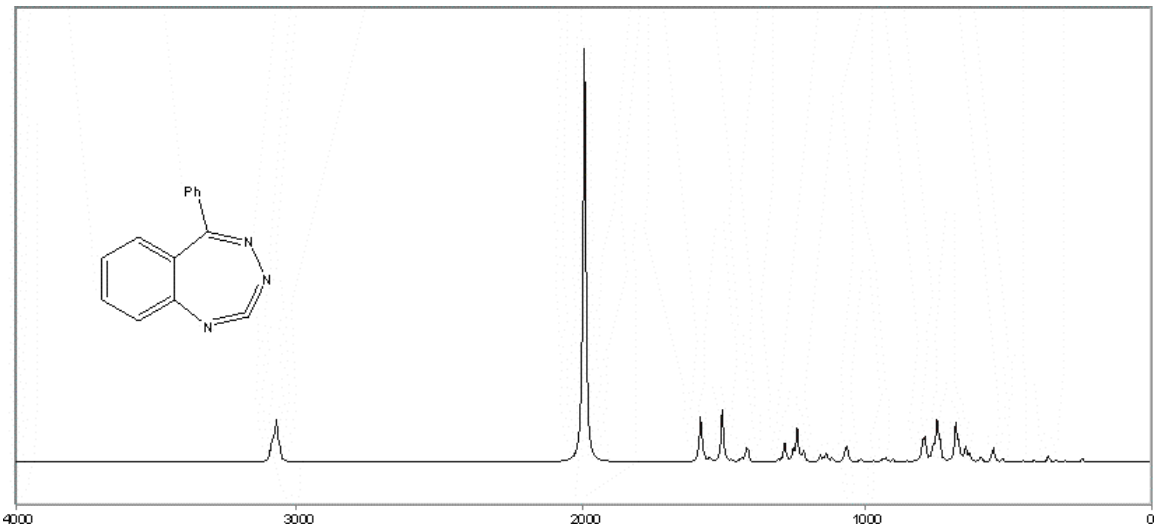


Figure S16. Calculated IR spectrum of **29** (B3LYP/6-31G*).

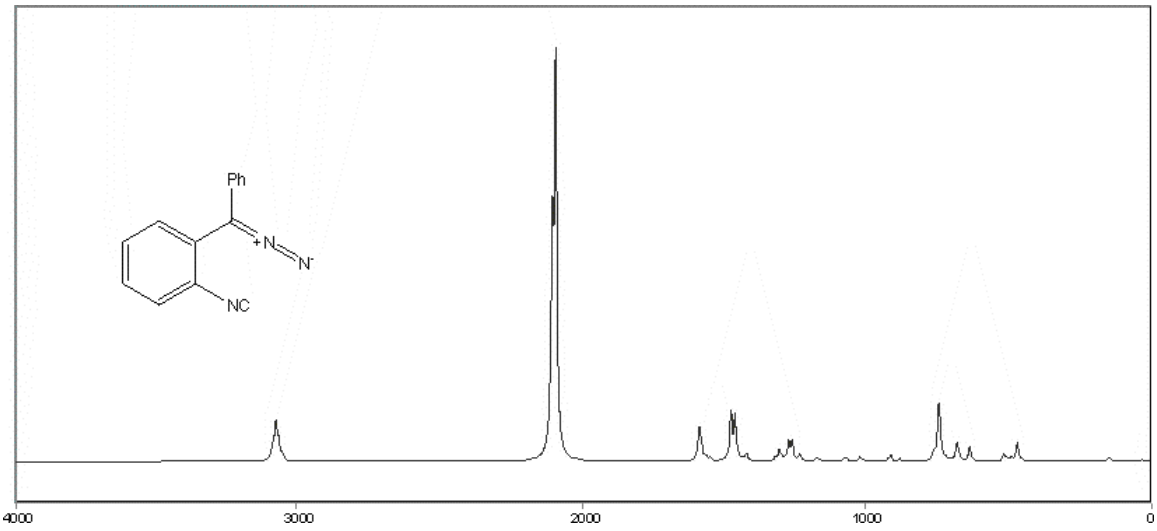


Figure S17. Calculated IR spectrum of **33** (B3LYP/6-31G*).

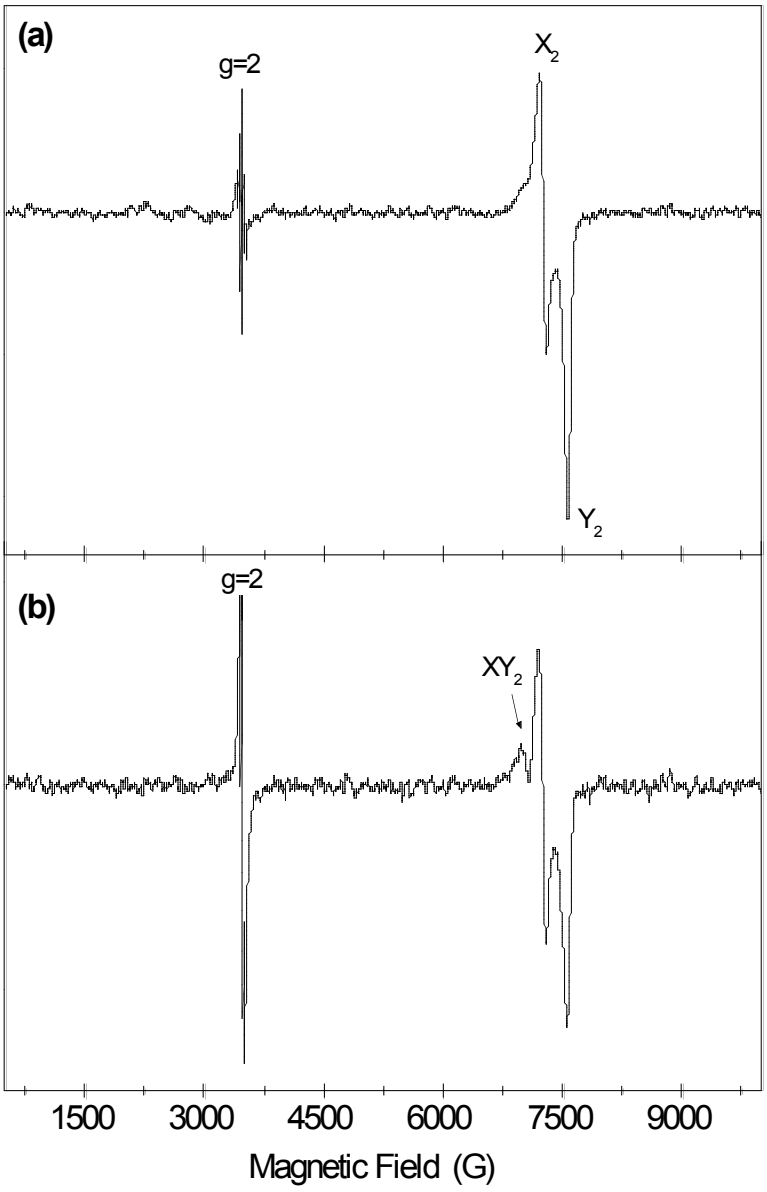


Figure S18. (a) ESR spectrum of nitrene **27** formed by Ar matrix photolysis of azide **26** at 308 nm (2 min). The azide was obtained by FVT of the tetrazole **25** at 200 ^{o}C. D = 1.147; E = 0.0060 cm^{-1}. (b) ESR spectrum of nitrene **27** after further photolysis above 475nm (24 hours). A minor amount of another nitrene is formed with an XY_2 resonance around 7040 G (D = 1.016; E < 0.0010 cm^{-1}).

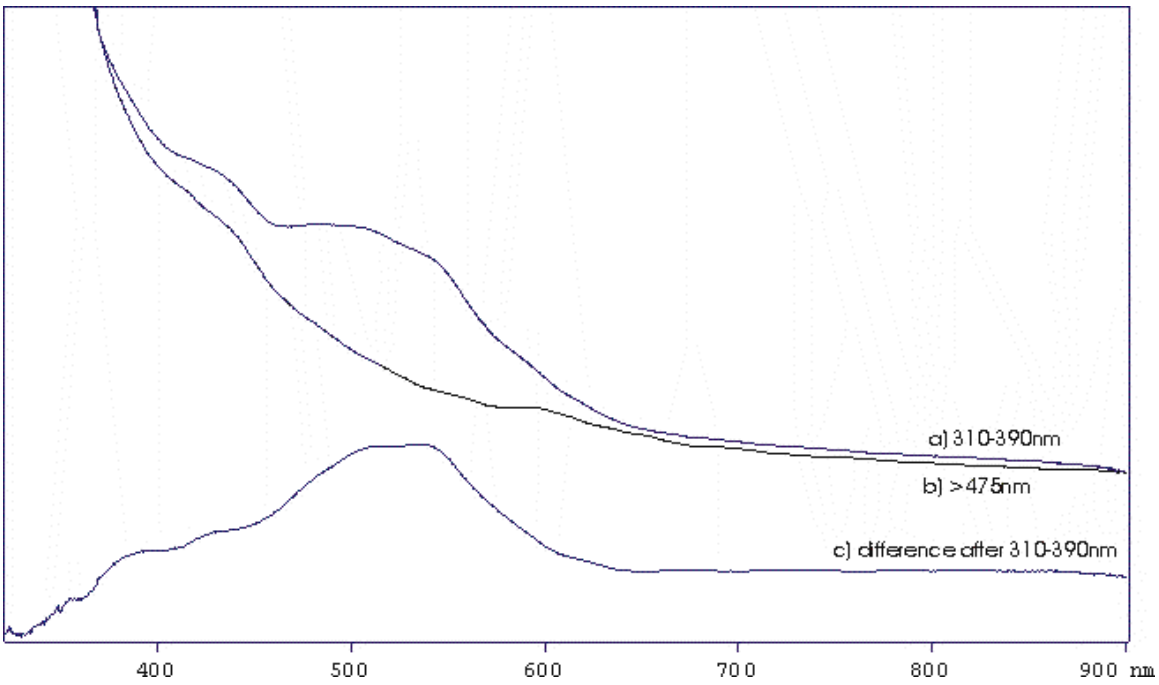


Figure S19. (a) 310-390 nm irradiation of azide **26** in Ar matrix at 10 K, (b) irradiation of the foregoing matrix at > 475nm, (c) difference spectrum after renewed irradiation at 310-390 nm. (The calculated λ_{max} for **33** is 513 nm, f = 0.0015 at the TDB3LYP/6-31G** level.)

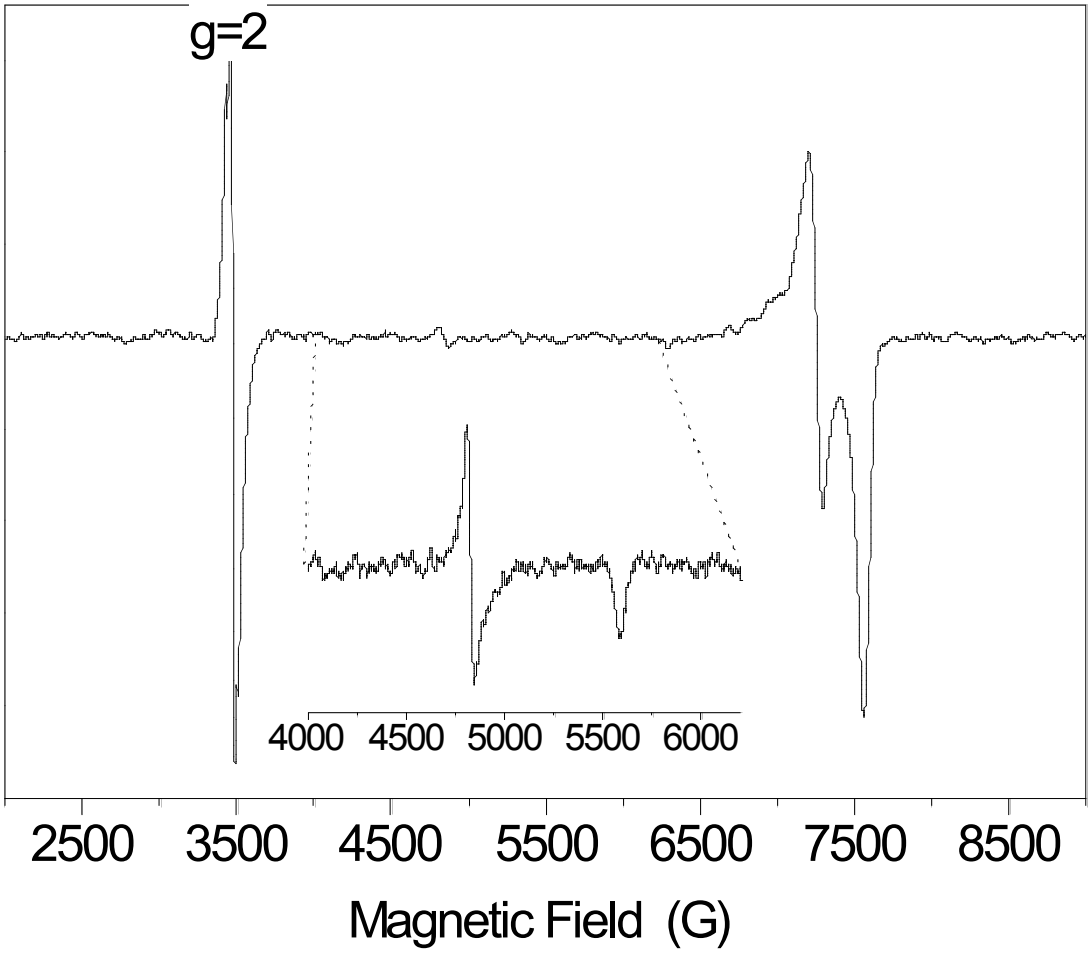


Figure S20. ESR spectrum ascribed to carbene **37** (insert) formed by Ar matrix photolysis of diazo compund **33** at 308 nm (from several minutes up to 3 hours). Resonance fields of **37** are: X_2 = 4824 G, Y_2 = 5577 G, microwave frequency 9.7280 GHz, H_0= 3471.2 G. ZFS parameters: D = 0.4053; E = 0.0192 cm^{-1}. Also on the spectrum, nitrene **27** (D = 1.1467; E = 0.0060 cm^{-1}) and g = 2 signal (doublet radicals).

Tables of Cartesian coordinates, energies and where relevant IR data for all calculated species. Calculations are at the B3LYP/6-31G level.**

A: Tetrazolo[1,5-*a*]quinazoline 9

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.664265	-1.366357	0.000017
2	6	-1.289792	-1.554888	0.000027
3	6	-0.468215	-0.422326	0.000018
4	6	-1.000888	0.888958	-0.000003
5	6	-2.402066	1.040808	-0.000010
6	6	-3.223007	-0.073976	-0.000001
7	1	-3.318776	-2.232248	0.000024
8	1	-0.843150	-2.541860	0.000040
9	6	-0.083032	2.004733	-0.000012
10	1	-2.824462	2.041353	-0.000024
11	1	-4.301390	0.045091	-0.000008
12	6	1.714548	0.638209	-0.000030
13	1	-0.499509	3.011816	-0.000030
14	7	1.217444	1.906346	-0.000008
15	7	0.916002	-0.480841	0.000016
16	7	2.932037	-1.116039	-0.000001
17	7	2.979173	0.231241	0.000088
18	7	1.710712	-1.577152	-0.000099

Energy = -581.5767511
E+ZPVE = -581.447833

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	111.4	1.6	2
2	A	137.0	0.0	0
3	A	246.7	1.7	2
4	A	262.6	0.4	0
5	A	277.1	0.2	0
6	A	417.8	0.0	0
7	A	432.2	0.7	1
8	A	471.2	0.8	1
9	A	512.0	8.7	10
10	A	518.7	1.9	2
11	A	550.1	4.4	5
12	A	635.9	3.0	3
13	A	683.2	0.7	1

14	A	696.8	1.8	2
15	A	704.0	2.6	3
16	A	736.7	1.3	1
17	A	748.7	47.8	54
18	A	755.8	0.2	0
19	A	854.8	1.9	2
20	A	861.9	9.3	11
21	A	921.2	2.1	2
22	A	942.7	6.8	8
23	A	969.0	0.1	0
24	A	973.2	5.6	6
25	A	1002.1	1.2	1
26	A	1017.5	1.4	2
27	A	1072.5	5.3	6
28	A	1095.9	5.5	6
29	A	1125.5	2.8	3
30	A	1145.1	5.6	6
31	A	1203.9	6.6	7
32	A	1219.8	14.8	17
33	A	1259.9	23.0	26
34	A	1268.3	20.4	23
35	A	1328.4	10.7	12
36	A	1352.4	0.3	0
37	A	1376.4	7.5	9
38	A	1428.5	8.7	10
39	A	1448.4	15.8	18
40	A	1509.7	30.0	34
41	A	1540.8	87.5	99
42	A	1584.9	50.1	57
43	A	1606.0	61.5	70
44	A	3036.9	11.0	13
45	A	3070.4	0.7	1
46	A	3079.1	7.2	8
47	A	3092.8	10.8	12
48	A	3112.1	0.7	1

B: 2-Azidoquinazoline 10

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.349780	-0.903697	-0.000026
2	6	-2.093144	-1.468407	-0.000080
3	6	-0.945746	-0.634311	-0.000082
4	6	-1.124076	0.782151	-0.000023
5	6	-2.427158	1.336610	0.000094
6	6	-3.523778	0.504023	0.000068
7	1	-4.226669	-1.544534	-0.000048
8	1	-1.944997	-2.542787	-0.000135
9	6	0.068724	1.548248	-0.000146
10	1	-2.545207	2.417048	0.000159
11	1	-4.526483	0.919538	0.000125
12	6	1.308933	-0.354634	0.000015
13	1	0.016931	2.637557	0.000103

14	7	1.268936	1.011624	0.000021
15	7	0.296289	-1.192192	-0.000062
16	7	2.579420	-0.960793	0.000344
17	7	3.558062	-0.190774	-0.000076
18	7	4.546233	0.368317	-0.000103

Energy = -581.5745544
E+ZPVE = -581.447561

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	59.7	0.5	0
2	A	121.6	0.7	0
3	A	126.6	0.0	0
4	A	172.9	0.1	0
5	A	283.1	1.9	0
6	A	291.8	0.5	0
7	A	401.9	0.2	0
8	A	403.4	0.0	0
9	A	459.2	5.1	1
10	A	461.8	1.4	0
11	A	510.9	0.0	0
12	A	527.6	6.1	1
13	A	538.6	5.2	1
14	A	598.7	11.6	1
15	A	642.2	2.2	0
16	A	699.0	16.3	2
17	A	749.0	35.3	4
18	A	760.0	2.6	0
19	A	776.4	5.7	1
20	A	780.2	10.5	1
21	A	855.0	3.7	0
22	A	876.0	2.5	0
23	A	925.9	4.1	0
24	A	926.2	0.5	0
25	A	950.2	7.1	1
26	A	969.7	0.2	0
27	A	1000.6	2.1	0
28	A	1106.5	2.7	0
29	A	1127.3	4.7	1
30	A	1166.0	35.8	4
31	A	1212.4	17.0	2
32	A	1232.6	12.6	1
33	A	1289.2	50.8	6
34	A	1307.8	74.6	9
35	A	1345.0	341.8	40
36	A	1360.8	40.4	5
37	A	1380.9	170.2	20
38	A	1441.8	131.6	16
39	A	1478.5	21.1	2
40	A	1545.6	113.5	13
41	A	1575.8	245.1	29
42	A	1610.4	83.5	10
43	A	2200.0	848.9	100

44	A	3027.3	16.8	2
45	A	3059.2	3.1	0
46	A	3068.5	10.3	1
47	A	3085.1	17.9	2
48	A	3097.2	6.6	1

C: Triplet 2-quinazolylnitrene 11 (UB3LYP/6-31G**)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.563946	-0.967472	0.000098
2	6	1.292589	-1.499405	0.000060
3	6	0.164788	-0.634029	-0.000027
4	6	0.376414	0.781577	-0.000070
5	6	1.686574	1.298347	-0.000023
6	6	2.766434	0.434339	0.000049
7	1	3.425724	-1.627943	0.000177
8	1	1.114191	-2.569164	0.000093
9	6	-0.803027	1.589570	-0.000041
10	1	1.835929	2.374779	-0.000023
11	1	3.777778	0.828558	0.000095
12	6	-2.104986	-0.284016	-0.000684
13	1	-0.706101	2.676569	0.000033
14	7	-2.012955	1.099874	-0.000096
15	7	-1.082148	-1.161290	-0.000116
16	7	-3.348315	-0.795192	0.000705

Energy = -472.0291853
E+ZPVE = -471.914576

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	106.0	0.4	1
2	A	165.5	0.0	0
3	A	273.0	0.0	0
4	A	286.6	1.1	3
5	A	392.2	0.0	0
6	A	424.0	1.8	5
7	A	457.1	0.7	2
8	A	474.9	0.2	1
9	A	502.1	2.0	6
10	A	512.0	2.4	7
11	A	610.3	7.8	24
12	A	685.0	19.5	59
13	A	726.1	4.5	13
14	A	748.2	31.1	94
15	A	749.8	5.2	16
16	A	776.5	14.1	43
17	A	855.0	2.4	7
18	A	890.3	9.3	28

19	A	909.1	5.8	18
20	A	927.1	0.6	2
21	A	950.0	7.9	24
22	A	969.9	0.0	0
23	A	1000.8	1.1	3
24	A	1107.5	1.5	5
25	A	1130.0	0.8	3
26	A	1178.1	17.1	52
27	A	1203.7	2.2	7
28	A	1235.2	24.2	73
29	A	1259.6	7.7	23
30	A	1293.5	10.9	33
31	A	1344.4	15.8	48
32	A	1361.5	14.1	43
33	A	1403.0	16.4	50
34	A	1463.0	8.9	27
35	A	1507.3	33.0	100
36	A	1556.0	10.9	33
37	A	1588.7	8.1	25
38	A	3018.2	20.0	61
39	A	3061.8	2.5	8
40	A	3072.3	8.1	25
41	A	3086.5	14.7	45
42	A	3099.0	5.3	16

D: 1-Cyanoindazole 21:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.941522	-1.583198	0.000083
2	6	2.746273	-0.422947	-0.000008
3	6	2.181323	0.844247	-0.000047
4	6	0.780646	0.945154	0.000000
5	6	0.001423	-0.228680	0.000084
6	6	0.553993	-1.511265	0.000126
7	6	-2.423217	-0.562507	-0.000153
8	1	2.419624	-2.557764	0.000095
9	1	3.826198	-0.530174	-0.000050
10	1	2.803016	1.733930	-0.000117
11	1	-0.068217	-2.399592	0.000156
12	7	-1.322574	0.203224	0.000002
13	7	-3.350931	-1.266673	-0.000316
14	7	-1.416281	1.590008	0.000243
15	6	-0.176217	2.016766	-0.000015
16	1	0.013390	3.082273	-0.000002

Energy = -472.0730766
E+ZPVE = -471.956676

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	88.7	0.8	0
2	A	126.9	4.2	2
3	A	206.6	0.0	0
4	A	251.1	0.0	0
5	A	367.2	1.1	1
6	A	418.0	1.2	1
7	A	464.7	9.5	5
8	A	490.3	0.1	0
9	A	530.6	1.3	1
10	A	545.2	0.2	0
11	A	590.6	4.5	3
12	A	600.9	8.4	5
13	A	684.6	1.8	1
14	A	734.6	11.4	6
15	A	737.5	37.4	21
16	A	751.5	15.6	9
17	A	835.2	3.8	2
18	A	860.9	10.2	6
19	A	881.8	15.5	9
20	A	918.1	1.7	1
21	A	956.0	0.0	0
22	A	996.7	13.7	8
23	A	1004.6	38.6	22
24	A	1090.2	5.7	3
25	A	1134.2	3.5	2
26	A	1146.9	27.7	16
27	A	1187.3	6.5	4
28	A	1245.0	3.6	2
29	A	1291.2	2.0	1
30	A	1343.9	43.4	25
31	A	1352.5	11.5	7
32	A	1412.5	44.2	25
33	A	1458.8	5.0	3
34	A	1497.9	23.4	13
35	A	1577.5	0.5	0
36	A	1603.2	20.4	12
37	A	2273.4	175.9	100
38	A	3069.6	0.3	0
39	A	3078.4	7.2	4
40	A	3088.9	13.2	7
41	A	3095.8	5.0	3
42	A	3127.6	2.4	1

E: N-Cyanoanthranilonitrile,anti- 22

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.000738	-2.203545	0.000083
2	6	-2.212583	-1.505134	0.000150
3	6	-2.199885	-0.116374	0.000029
4	6	-0.981014	0.581519	-0.000135
5	6	0.239468	-0.132758	-0.000232

6	6	0.217554	-1.530925	-0.000109
7	1	-1.001478	-3.289035	0.000125
8	1	-3.155599	-2.040428	0.000285
9	1	-3.124961	0.449677	0.000105
10	1	1.153427	-2.079485	-0.000148
11	6	-0.947019	2.010307	-0.000085
12	7	-0.842392	3.170469	0.000342
13	6	2.651784	0.005289	-0.000051
14	7	3.698871	-0.508820	0.000467
15	7	1.446348	0.583096	-0.000530
16	1	1.403415	1.595785	-0.000216

Energy = -472.0867471
E+ZPVE = -471.972281

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	67.2	3.5	2
2	A	104.7	10.9	6
3	A	127.6	4.0	2
4	A	147.2	2.8	2
5	A	225.0	1.0	1
6	A	339.2	1.1	1
7	A	377.1	42.6	23
8	A	390.3	70.0	38
9	A	406.5	0.3	0
10	A	474.6	5.8	3
11	A	487.0	0.6	0
12	A	488.0	2.0	1
13	A	557.9	3.5	2
14	A	578.5	0.2	0
15	A	622.9	3.6	2
16	A	714.8	3.1	2
17	A	744.8	49.3	27
18	A	753.6	0.6	0
19	A	812.4	4.1	2
20	A	849.5	1.3	1
21	A	923.5	1.5	1
22	A	960.4	0.2	0
23	A	1028.4	3.2	2
24	A	1054.0	0.1	0
25	A	1112.3	3.7	2
26	A	1149.5	7.8	4
27	A	1170.5	1.1	1
28	A	1233.6	23.0	13
29	A	1281.2	53.6	29
30	A	1292.9	31.2	17
31	A	1419.1	31.1	17
32	A	1439.7	48.9	27
33	A	1491.2	156.6	85
34	A	1571.7	69.6	38
35	A	1596.4	43.3	24
36	A	2242.8	45.2	25
37	A	2267.2	184.2	100

38	A	3075.1	2.3	1
39	A	3086.5	3.0	2
40	A	3092.3	2.0	1
41	A	3100.8	6.0	3
42	A	3442.2	75.0	41

F: N-Cyanoanthranilonitrile,syn-22

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.585934	-0.875673	0.061936
2	6	2.699954	0.507764	0.220509
3	6	1.556456	1.293787	0.174577
4	6	0.286495	0.720518	-0.027634
5	6	0.176845	-0.681470	-0.155223
6	6	1.338355	-1.462784	-0.116482
7	1	3.470143	-1.504516	0.090652
8	1	3.670346	0.967852	0.371269
9	1	1.621387	2.371451	0.277412
10	1	1.254226	-2.541819	-0.212998
11	6	-0.836135	1.600553	-0.153208
12	7	-1.698211	2.371762	-0.277330
13	6	-2.245349	-0.970433	0.131093
14	7	-3.306830	-0.713190	0.538720
15	7	-1.052581	-1.340605	-0.361915
16	1	-0.988080	-2.312301	-0.636063

Energy = -472.0759979
E+ZPVE = -471.961800

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	36.9	2.6	1
2	A	112.3	2.5	1
3	A	132.1	1.7	1
4	A	150.5	12.6	7
5	A	224.8	2.1	1
6	A	321.4	9.1	5
7	A	369.7	65.8	34
8	A	382.0	6.9	4
9	A	402.2	8.6	4
10	A	469.8	22.6	12
11	A	483.4	1.4	1
12	A	511.5	1.1	1
13	A	545.1	4.2	2
14	A	557.9	1.1	1
15	A	639.2	8.1	4
16	A	706.1	3.2	2
17	A	714.3	0.5	0
18	A	742.6	56.3	29

19	A	831.5	2.3	1
20	A	843.5	0.9	0
21	A	921.8	1.4	1
22	A	954.5	0.0	0
23	A	1024.2	0.7	0
24	A	1078.4	5.0	3
25	A	1095.4	6.8	4
26	A	1149.0	4.8	3
27	A	1175.0	2.2	1
28	A	1231.0	45.0	23
29	A	1247.9	4.6	2
30	A	1308.2	17.9	9
31	A	1402.8	8.7	5
32	A	1459.9	192.8	100
33	A	1480.9	17.2	9
34	A	1569.3	14.3	7
35	A	1595.5	47.7	25
36	A	2255.7	8.7	5
37	A	2267.3	134.3	70
38	A	3059.9	7.1	4
39	A	3078.5	4.1	2
40	A	3088.4	5.6	3
41	A	3100.0	5.6	3
42	A	3466.6	59.2	31

G: N-(2-Cyanophenyl)carbodiimide:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.596267	-0.960856	0.056894
2	6	2.775465	0.420380	0.180155
3	6	1.670870	1.262414	0.132054
4	6	0.379355	0.732940	-0.028111
5	6	0.196381	-0.668611	-0.140223
6	6	1.323975	-1.498747	-0.110018
7	1	3.455153	-1.624215	0.087107
8	1	3.769160	0.837098	0.305319
9	1	1.789043	2.337569	0.214542
10	1	1.175200	-2.567829	-0.212539
11	6	-0.747278	1.611362	-0.104179
12	7	-1.673438	2.312915	-0.178343
13	7	-1.049257	-1.261963	-0.333292
14	6	-2.177641	-0.935631	0.026569
15	7	-3.323738	-0.848242	0.439776
16	1	-3.967877	-0.181106	0.029743

Energy = -472.0857384
E+ZPVE = -471.972516

Vibrational Frequencies

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	63.3	7.4	1
2	A	93.4	2.3	0
3	A	129.0	1.9	0
4	A	148.9	6.2	1
5	A	233.7	11.1	1
6	A	327.8	15.3	1
7	A	385.1	0.5	0
8	A	399.5	33.9	3
9	A	427.3	20.5	2
10	A	483.2	17.5	2
11	A	507.4	7.3	1
12	A	527.7	60.7	5
13	A	558.1	1.8	0
14	A	571.2	1.0	0
15	A	618.3	29.7	3
16	A	700.0	1.2	0
17	A	716.5	1.4	0
18	A	748.0	49.9	4
19	A	794.6	16.9	2
20	A	850.3	401.6	36
21	A	856.4	4.0	0
22	A	925.8	1.8	0
23	A	959.8	0.2	0
24	A	1021.7	5.3	0
25	A	1071.6	16.2	1
26	A	1126.4	21.2	2
27	A	1143.8	1.1	0
28	A	1173.9	3.9	0
29	A	1245.4	7.4	1
30	A	1283.1	11.4	1
31	A	1390.0	0.2	0
32	A	1442.6	7.5	1
33	A	1478.5	133.5	12
34	A	1550.7	5.9	1
35	A	1590.0	76.1	7
36	A	2163.7	1119.2	100
37	A	2248.9	57.8	5
38	A	3071.6	2.5	0
39	A	3083.0	5.3	0
40	A	3094.3	8.6	1
41	A	3099.3	4.9	0
42	A	3471.6	107.9	10

H: (2-Isocyanophenyl)diazomethane:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.743523	0.476594	0.000163
2	6	1.610191	1.279873	0.000176
3	6	0.330100	0.709441	0.000014
4	6	0.156134	-0.696188	-0.000093
5	6	1.328052	-1.482323	-0.000193

6	6	2.594181	-0.913503	-0.000057
7	1	3.729668	0.928344	0.000325
8	1	1.688120	2.361593	0.000286
9	1	1.225256	-2.563554	-0.000374
10	1	3.468513	-1.557028	-0.000145
11	6	-1.108069	-1.406463	0.000071
12	1	-1.114997	-2.489604	-0.000012
13	7	-2.301667	-0.876957	0.000044
14	7	-3.374002	-0.482745	0.000201
15	7	-0.761968	1.561787	-0.000079
16	6	-1.642961	2.350180	-0.000289

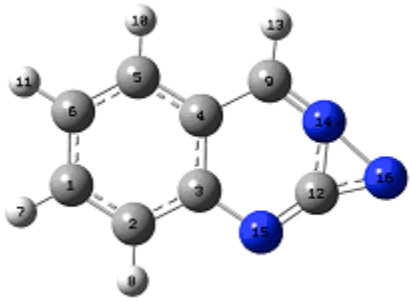
Energy = -472.014852
E+ZPVE = -471.902273

Vibrational Frequencies

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	17.1	0.0	0
2	A	134.2	0.6	0
3	A	139.8	2.0	0
4	A	161.7	4.3	1
5	A	209.1	1.0	0
6	A	303.5	2.0	0
7	A	339.7	1.2	0
8	A	391.6	0.5	0
9	A	440.5	14.4	2
10	A	491.8	3.2	0
11	A	498.4	1.4	0
12	A	516.9	1.7	0
13	A	524.8	8.9	1
14	A	556.7	12.8	2
15	A	636.1	7.8	1
16	A	712.2	3.4	0
17	A	716.9	2.3	0
18	A	740.7	59.7	8
19	A	842.9	0.3	0
20	A	842.9	1.1	0
21	A	915.3	2.5	0
22	A	946.0	0.0	0
23	A	1026.9	3.6	0
24	A	1092.2	4.2	1
25	A	1129.2	1.4	0
26	A	1146.5	2.6	0
27	A	1176.3	7.9	1
28	A	1212.2	13.4	2
29	A	1248.4	0.1	0
30	A	1304.0	7.8	1
31	A	1389.2	23.5	3
32	A	1440.7	40.4	6
33	A	1471.9	79.0	11
34	A	1553.8	2.3	0
35	A	1586.8	32.8	5
36	A	2109.0	67.9	9
37	A	2120.7	719.0	100

38	A	3061.6	5.5	1
39	A	3075.8	8.4	1
40	A	3086.0	11.5	2
41	A	3096.2	2.7	0
42	A	3098.1	6.8	1

I: Diazirene 12



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.646197	-0.757681	0.000154
2	6	1.425573	-1.425737	-0.000105
3	6	0.219649	-0.711759	-0.000137
4	6	0.285751	0.720831	-0.000044
5	6	1.526012	1.374713	0.000052
6	6	2.706778	0.642840	0.000226
7	1	3.566765	-1.334185	0.000284
8	1	1.374639	-2.509174	-0.000179
9	6	-0.966939	1.459962	0.000198
10	1	1.551243	2.461766	0.000052
11	1	3.665527	1.150523	0.000396
12	6	-1.995992	-0.616567	-0.000550
13	1	-1.014938	2.546424	0.000935
14	7	-2.045859	0.753754	-0.001354
15	7	-0.992458	-1.428566	-0.000085
16	7	-3.279599	-0.244468	0.001403

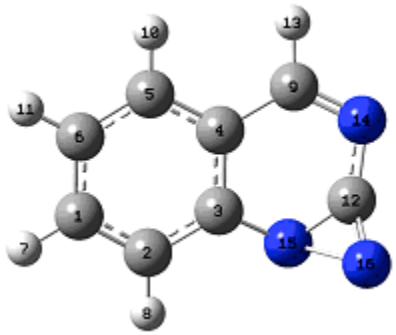
Energy = -471.9761685
E+ZPVE = -471.861704

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	133.7	0.0	0
2	A	163.4	2.4	1
3	A	236.3	0.0	0
4	A	250.1	6.2	3
5	A	336.8	0.0	0
6	A	375.8	9.9	4
7	A	450.7	0.7	0

8	A	471.0	0.8	0
9	A	490.6	5.8	3
10	A	522.7	3.1	1
11	A	606.2	13.1	6
12	A	633.0	9.7	4
13	A	691.0	11.3	5
14	A	732.9	0.4	0
15	A	735.0	4.6	2
16	A	742.1	47.0	21
17	A	851.2	4.4	2
18	A	855.5	10.2	5
19	A	896.1	4.2	2
20	A	920.8	7.4	3
21	A	957.9	0.3	0
22	A	989.9	3.7	2
23	A	1018.2	3.5	2
24	A	1077.7	3.4	2
25	A	1114.7	28.0	12
26	A	1134.8	15.7	7
27	A	1181.4	13.4	6
28	A	1203.9	25.3	11
29	A	1251.2	34.6	15
30	A	1294.9	2.1	1
31	A	1315.9	17.7	8
32	A	1421.7	20.8	9
33	A	1447.2	2.6	1
34	A	1539.3	34.4	15
35	A	1586.7	225.4	100
36	A	1595.9	47.1	21
37	A	1707.3	193.5	86
38	A	3053.7	4.8	2
39	A	3062.4	14.7	7
40	A	3067.3	10.4	5
41	A	3087.6	14.9	7
42	A	3094.9	6.8	3

J: Diazirene 13



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-2.495854	-0.872461	0.027434
2	6	-1.241033	-1.441279	-0.183131
3	6	-0.106049	-0.627465	-0.178305
4	6	-0.243817	0.781569	-0.017091
5	6	-1.518005	1.335957	0.164144
6	6	-2.637637	0.510303	0.205784
7	1	-3.374947	-1.509391	0.052350
8	1	-1.117803	-2.507675	-0.338486
9	6	0.955211	1.605355	-0.157849
10	1	-1.623779	2.411783	0.277296
11	1	-3.622216	0.938175	0.364308
12	6	2.108414	-0.235093	-0.005251
13	1	0.838982	2.683446	-0.276044
14	7	2.165070	1.131023	-0.150476
15	7	1.170386	-1.143280	-0.515128
16	7	2.374884	-1.181693	0.777914

Energy = -471.9953323
E+ZPVE = -471.880165

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	125.7	1.5	2
2	A	140.1	0.7	1
3	A	252.5	3.8	5
4	A	331.6	1.5	2
5	A	360.8	0.1	0
6	A	413.6	0.6	1
7	A	457.4	1.8	2
8	A	482.7	1.3	2
9	A	520.6	2.2	3
10	A	573.8	8.3	10
11	A	597.4	10.1	12
12	A	630.2	14.9	18
13	A	727.0	2.2	3
14	A	742.9	20.9	26
15	A	758.5	18.2	22
16	A	772.1	4.6	6
17	A	857.7	0.9	1
18	A	874.9	6.6	8
19	A	887.0	14.0	17
20	A	923.1	0.6	1
21	A	946.0	5.1	6
22	A	965.6	0.0	0
23	A	1012.7	1.1	1
24	A	1083.1	6.5	8
25	A	1122.3	22.6	28
26	A	1137.4	7.1	9
27	A	1174.4	3.8	5
28	A	1195.0	50.4	62
29	A	1246.0	2.2	3
30	A	1300.7	9.2	11
31	A	1342.1	12.8	16
32	A	1420.4	11.4	14

33	A	1443.6	0.5	1
34	A	1527.2	82.3	100
35	A	1571.4	38.7	47
36	A	1588.0	38.5	47
37	A	1745.2	53.4	65
38	A	3029.6	13.6	17
39	A	3060.1	4.0	5
40	A	3071.4	6.8	8
41	A	3087.3	12.9	16
42	A	3096.8	4.8	6

K: Cyclic carbodiimide 14

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.668786	-0.508532	0.138357
2	6	-1.565062	-1.339143	-0.049098
3	6	-0.294120	-0.780778	-0.165694
4	6	-0.105516	0.626776	-0.112939
5	6	-1.241648	1.436075	0.046888
6	6	-2.508942	0.878780	0.192910
7	1	-3.658967	-0.945126	0.226147
8	1	-1.670678	-2.416025	-0.121574
9	1	-1.119021	2.515789	0.066550
10	1	-3.370920	1.522870	0.332698
11	6	1.200155	1.313317	-0.336257
12	1	1.118990	2.297658	-0.801778
13	7	2.424666	0.993713	-0.088520
14	7	2.576589	-0.270840	0.678296
15	7	0.849447	-1.616508	-0.428602
16	6	1.808199	-1.079784	0.147458

Energy = -472.0118932
E+ZPVE = -471.896710

Vibrational Frequencies

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	129.0	0.2	0
2	A	153.6	0.8	0
3	A	293.5	1.9	0
4	A	306.7	4.0	1
5	A	363.9	6.1	2
6	A	411.8	0.2	0
7	A	457.8	1.4	0
8	A	479.6	9.7	2
9	A	516.7	5.0	1
10	A	566.4	5.1	1
11	A	597.9	3.5	1
12	A	663.3	2.2	1
13	A	688.2	7.5	2

14	A	714.5	29.6	8
15	A	728.0	1.6	0
16	A	749.9	38.0	10
17	A	779.0	3.0	1
18	A	845.8	8.8	2
19	A	862.7	12.0	3
20	A	897.8	4.3	1
21	A	928.9	3.8	1
22	A	958.8	0.0	0
23	A	1020.1	1.4	0
24	A	1077.3	20.7	5
25	A	1133.8	20.2	5
26	A	1139.5	0.9	0
27	A	1161.7	2.1	1
28	A	1226.7	0.2	0
29	A	1252.3	14.9	4
30	A	1280.4	4.0	1
31	A	1310.2	8.1	2
32	A	1426.7	18.4	5
33	A	1444.8	6.7	2
34	A	1545.3	18.5	5
35	A	1576.8	42.5	11
36	A	1586.0	44.7	11
37	A	1994.9	390.0	100
38	A	3015.2	6.4	2
39	A	3060.4	3.0	1
40	A	3072.3	6.2	2
41	A	3088.0	12.8	3
42	A	3097.1	5.0	1

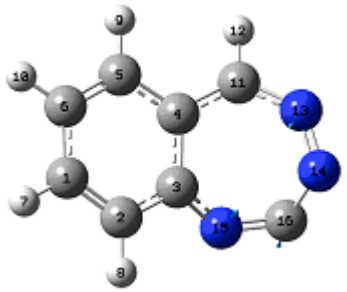
L: Transition state connecting 12 and 14:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.681447	-0.705615	0.000007
2	6	-1.477362	-1.416403	0.000030
3	6	-0.267409	-0.726658	0.000008
4	6	-0.272648	0.685790	-0.000025
5	6	-1.481736	1.383975	-0.000035
6	6	-2.692966	0.690870	-0.000029
7	1	-3.619913	-1.252222	0.000020
8	1	-1.460797	-2.500927	0.000060
9	6	1.009654	1.398392	0.000028
10	1	-1.469345	2.471456	-0.000051
11	1	-3.632801	1.232665	-0.000047
12	6	1.992297	-0.719494	0.000001
13	1	0.983826	2.490913	0.000108
14	7	2.190606	0.888918	0.000091
15	7	0.954031	-1.435055	0.000008
16	7	3.202324	-0.309152	-0.000100

Energy = -471.9676715

E+ZPVE = -471.855032
Imaginary Frequency = -589.6 cm^{-1}

M: Transition state connecting 14 and (2-isocyanophenyl)diazomethane 38:



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.536468	-0.770010	0.239285
2	6	-1.329743	-1.427017	0.162432
3	6	-0.136031	-0.701914	-0.097588
4	6	-0.212544	0.739142	-0.167503
5	6	-1.483250	1.376219	-0.149886
6	6	-2.623693	0.635708	0.051885
7	1	-3.445005	-1.337121	0.419069
8	1	-1.262642	-2.506760	0.244363
9	1	-1.532775	2.455286	-0.268445
10	1	-3.593980	1.120892	0.077486
11	6	1.000211	1.472902	-0.215785
12	1	1.026494	2.511398	-0.532422
13	7	2.127372	1.020445	0.331427
14	7	2.488866	-0.147475	0.630839
15	7	0.981153	-1.378524	-0.485426
16	6	2.259212	-1.109167	-0.369161

Energy = -471.9358255
E+ZPVE = -471.823770
Imaginary Frequency = - 762.5 cm^{-1}

N: Cyclic carbodiimide 16

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.530006	-0.690834	-0.197717
2	6	-1.366001	-1.367935	-0.364071
3	6	-0.084968	-0.750458	-0.052245
4	6	-0.097252	0.740099	0.122539
5	6	-1.381488	1.374013	0.349378

6	6	-2.545850	0.693941	0.203124
7	1	-3.474388	-1.200982	-0.363084
8	1	-1.344006	-2.418753	-0.629172
9	1	-1.383812	2.433168	0.590917
10	1	-3.497156	1.194462	0.350798
11	6	0.981193	1.541809	-0.175503
12	1	0.888714	2.625326	-0.172701
13	7	2.216656	1.029578	-0.608435
14	7	0.901277	-1.611938	0.051033
15	6	2.360152	-0.054836	0.007594
16	7	2.138633	-1.067355	0.680923

Energy = -471.9751984
E+ZPVE = -471.861100

Vibrational Frequencies

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	147.0	0.6	0
2	A	159.0	0.4	0
3	A	265.9	0.3	0
4	A	302.9	2.2	1
5	A	352.9	3.8	2
6	A	389.7	5.8	3
7	A	427.2	12.7	7
8	A	438.8	4.1	2
9	A	515.7	4.0	2
10	A	532.1	1.7	1
11	A	583.6	2.8	1
12	A	595.5	5.1	3
13	A	650.8	6.3	3
14	A	681.9	2.5	1
15	A	727.4	32.2	17
16	A	733.3	16.1	8
17	A	781.5	4.1	2
18	A	818.3	6.3	3
19	A	870.6	6.0	3
20	A	899.5	7.4	4
21	A	935.6	1.8	1
22	A	963.8	1.3	1
23	A	975.1	3.9	2
24	A	1050.1	50.3	26
25	A	1122.6	1.2	1
26	A	1135.2	1.6	1
27	A	1179.5	4.7	2
28	A	1196.6	11.4	6
29	A	1199.7	3.8	2
30	A	1316.6	9.5	5
31	A	1358.7	0.7	0
32	A	1414.2	8.7	5
33	A	1445.5	19.4	10
34	A	1502.9	35.1	18
35	A	1526.5	16.8	9
36	A	1625.2	16.4	9

37	A	1938.8	191.0	100
38	A	3060.4	1.7	1
39	A	3064.3	4.3	2
40	A	3070.5	13.6	7
41	A	3088.2	14.2	7
42	A	3101.6	4.8	3

O: Cyclic nitrilimine 17

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.480968	-1.347745	-0.029858
2	6	-0.223901	-0.752658	-0.137182
3	6	-0.094972	0.668453	-0.114379
4	6	-1.266236	1.428889	0.012195
5	6	-2.514803	0.827037	0.161474
6	6	-2.621704	-0.564449	0.138628
7	1	-1.539885	-2.429384	-0.091571
8	1	-1.187621	2.512935	-0.004321
9	1	-3.401484	1.442331	0.275436
10	1	-3.593424	-1.039061	0.233074
11	7	0.888385	-1.624045	-0.394589
12	6	1.183841	1.406330	-0.330305
13	1	1.089670	2.384929	-0.803935
14	7	2.377724	1.053714	0.019566
15	6	2.357185	-0.144657	0.729661
16	7	1.962762	-1.143804	0.062153

Energy = -471.963636
E+ZPVE = -471.849677

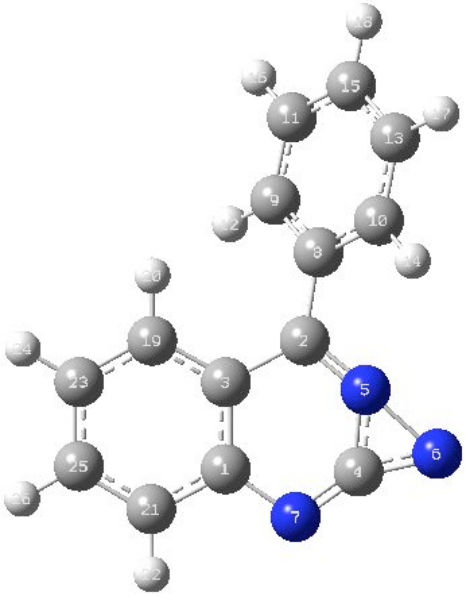
Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	127.0	3.1	3
2	A	145.3	0.9	1
3	A	208.7	15.7	14
4	A	290.4	17.3	15
5	A	343.4	0.2	0
6	A	380.4	7.8	7
7	A	433.2	1.2	1
8	A	454.4	5.5	5
9	A	521.1	6.4	6
10	A	565.5	2.9	3
11	A	603.5	6.5	6
12	A	626.3	5.2	4
13	A	681.7	2.7	2
14	A	721.3	5.8	5
15	A	748.0	3.3	3
16	A	756.8	40.6	35
17	A	838.1	2.5	2

18	A	859.8	7.6	7
19	A	893.7	7.1	6
20	A	923.8	51.9	45
21	A	931.0	3.0	3
22	A	962.3	0.1	0
23	A	1022.8	1.6	1
24	A	1080.8	0.7	1
25	A	1137.6	5.4	5
26	A	1142.3	5.2	5
27	A	1163.6	12.6	11
28	A	1192.5	46.8	40
29	A	1242.6	0.7	1
30	A	1292.3	6.8	6
31	A	1326.4	7.9	7
32	A	1425.1	5.1	4
33	A	1448.4	2.3	2
34	A	1538.0	115.8	100
35	A	1550.7	58.5	50
36	A	1570.3	26.9	23
37	A	1608.1	31.3	27
38	A	3017.7	9.6	8
39	A	3058.4	3.6	3
40	A	3072.7	5.6	5
41	A	3086.2	10.2	9
42	A	3094.2	8.5	7

P: 7-Phenyl-diazirino[1,3-b]quinazoline (28)

B3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0269648 Hartree
Zero-point correction (unscaled) = 0.195873 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.831092 Hartree
= -441033.187 Kcal/mol



	Coordinates (angstroms):		
Atom type	X	Y	Z
C	-2.346746	0.282383	0.065183
C	0.142738	0.492119	0.016777
C	-1.062126	-0.356717	-0.045742
C	-1.380794	2.264805	0.173463
N	-0.120937	1.764359	0.045580
N	-0.528069	3.291023	0.268146
N	-2.525205	1.667885	0.223839
C	1.548819	0.033216	0.004866
C	1.967473	-1.071113	0.764606
C	2.499922	0.758573	-0.731138
C	3.310268	-1.446503	0.775320
H	1.250275	-1.613990	1.371441
C	3.837826	0.373473	-0.724891
H	2.179156	1.620091	-1.309077
C	4.246108	-0.731430	0.026280
H	3.625366	-2.294923	1.376139
H	4.562655	0.937049	-1.305365
H	5.290797	-1.029668	0.032562
C	-1.001244	-1.741869	-0.276218
H	-0.036508	-2.214881	-0.422785
C	-3.497166	-0.518723	0.003544
H	-4.457964	-0.023387	0.099182
C	-2.157819	-2.509334	-0.340157
H	-2.090313	-3.578690	-0.515474
C	-3.405633	-1.891772	-0.187834
H	-4.313737	-2.487124	-0.233930

Vibrational Frequencies:

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	49.6	0.1	0
2	A	67.2	0.5	0
3	A	86.4	0.5	0
4	A	131.2	0.1	0
5	A	149.2	3.1	1
6	A	198.6	1.3	0
7	A	235.8	2.6	1
8	A	237.6	0.0	0
9	A	290.9	3.1	1
10	A	303.4	1.1	0
11	A	401.2	0.7	0
12	A	409.0	0.5	0
13	A	442.0	0.9	0
14	A	461.6	3.5	1
15	A	499.9	2.9	1
16	A	522.8	4.5	2
17	A	556.0	4.9	2
18	A	588.1	0.2	0
19	A	605.0	28.7	10
20	A	609.5	2.5	1
21	A	643.9	13.2	5
22	A	665.7	6.8	2
23	A	686.2	28.8	10

24	A	712.2	9.8	3
25	A	739.8	17.3	6
26	A	746.2	24.4	8
27	A	761.8	25.3	9
28	A	806.8	11.3	4
29	A	833.1	2.2	1
30	A	856.8	2.9	1
31	A	904.9	13.5	5
32	A	916.4	13.8	5
33	A	923.7	1.9	1
34	A	944.5	1.5	1
35	A	954.3	0.4	0
36	A	967.5	0.1	0
37	A	978.6	1.6	1
38	A	1012.7	2.2	1
39	A	1017.9	5.4	2
40	A	1040.9	3.1	1
41	A	1075.7	3.0	1
42	A	1085.8	7.9	3
43	A	1098.4	12.1	4
44	A	1142.9	42.0	15
45	A	1150.5	0.2	0
46	A	1170.3	6.8	2
47	A	1171.4	17.1	6
48	A	1204.0	31.6	11
49	A	1271.7	10.3	4
50	A	1280.7	38.2	13
51	A	1295.3	7.8	3
52	A	1307.7	84.7	29
53	A	1318.9	20.4	7
54	A	1417.6	30.2	10
55	A	1435.4	7.4	3
56	A	1447.8	2.2	1
57	A	1485.1	4.0	1
58	A	1539.1	64.7	22
59	A	1552.4	125.4	43
60	A	1576.5	16.1	6
61	A	1592.6	94.7	33
62	A	1597.9	4.9	2
63	A	1708.0	288.9	100
64	A	3067.2	0.1	0
65	A	3067.9	5.4	2
66	A	3076.3	5.3	2
67	A	3083.0	19.6	7
68	A	3084.8	18.0	6
69	A	3092.3	15.7	5
70	A	3095.5	0.9	0
71	A	3097.4	12.9	4
72	A	3102.0	11.9	4

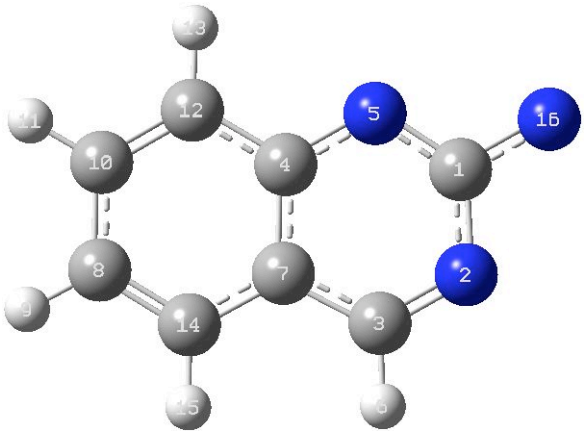
Calculations on Nitrenes and Diradicals.

Tables of energies at the UB3LYP/6-31G* level and Cartesian coordinates, energies and spin densities at the UB3LYP/EPR-III level on nitrenes and diradicals

Triplet 2-quinazolylnitrene (11)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: CS
HF = -472.0215467 Hartree
Zero-point correction (unscaled) = 0.114770 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.9067767 Hartree
= -296125.986 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: CS
State=3-A"
S^2 = 2.052088
HF = -472.2114249 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	2.103268	-0.254441	0.000000
N	1.662589	-1.562876	0.000000
C	0.375421	-1.735406	0.000000
C	0.000000	0.654582	0.000000
N	1.335075	0.843956	0.000000
H	0.009145	-2.759440	0.000000
C	-0.557594	-0.658068	0.000000
C	-2.776489	0.274476	0.000000
H	-3.850705	0.147710	0.000000
C	-2.230053	1.575980	0.000000
H	-2.896162	2.428685	0.000000

C	-0.871663	1.771564	0.000000
H	-0.434736	2.760428	0.000000
C	-1.951104	-0.828223	0.000000
H	-2.365164	-1.829037	0.000000
N	3.429037	-0.074098	0.000000

Mulliken spin densities:

1	C	-0.17030
2	N	0.12758
3	C	-0.08113
4	C	-0.05595
5	N	0.31545
6	H	0.00647
7	C	0.14156
8	C	0.14791
9	H	-0.00858
10	C	-0.06950
11	H	0.00369
12	C	0.11614
13	H	-0.00546
14	C	-0.08485
15	H	0.00369
16	N	1.61329

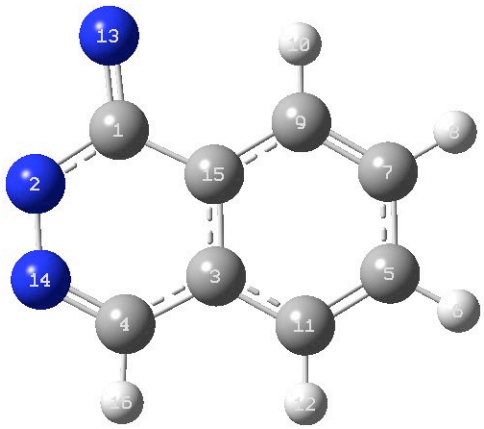
Natural spin densities:

1	C	-0.18763
2	N	0.13634
3	C	-0.08350
4	C	-0.07050
5	N	0.32896
6	H	0.00352
7	C	0.13261
8	C	0.13814
9	H	-0.00421
10	C	-0.06363
11	H	0.00195
12	C	0.11477
13	H	-0.00337
14	C	-0.07345
15	H	0.00213
16	N	1.62788

Triplet 1-phtalazinylnitrene (15)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: CS
HF = -471.9889757 Hartree
Zero-point correction (unscaled) = 0.113586 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.875390 Hartree
= -296106.29 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: CS
State=3-A"
S^2 = 2.058064
HF = -472.1785614 Hartree



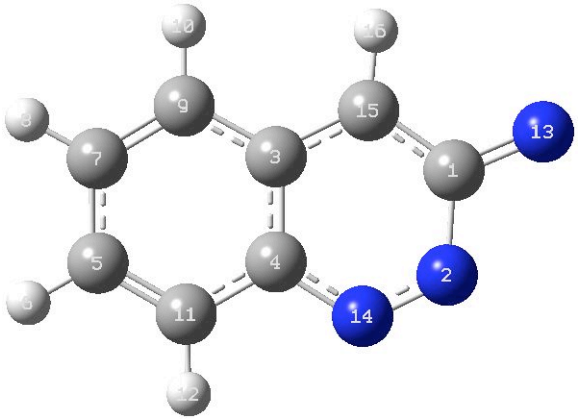
Atom type	Coordinates (angstroms): X	Y	Z
C	-1.418879	0.836861	0.000000
N	-2.394837	-0.133453	0.000000
C	0.315452	-0.863000	0.000000
C	-0.774500	-1.770340	0.000000
C	2.662918	-0.325518	0.000000
H	3.700503	-0.631575	0.000000
C	2.342638	1.044302	0.000000
H	3.138850	1.776776	0.000000
C	1.028517	1.463371	0.000000
H	0.783299	2.516103	0.000000
C	1.664940	-1.271491	0.000000
H	1.900074	-2.328114	0.000000
N	-1.823558	2.081933	0.000000
N	-2.046575	-1.411453	0.000000
C	0.000000	0.510330	0.000000
H	-0.594453	-2.839470	0.000000

Mulliken spin densities:			Natural spin densities:		
1	C	-0.21727	1	C	-0.21972
2	N	0.38157	2	N	0.39809
3	C	-0.05809	3	C	-0.06162
4	C	0.28030	4	C	0.27132
5	C	-0.06083	5	C	-0.05356
6	H	0.00307	6	H	0.00153
7	C	0.10314	7	C	0.07788
8	H	-0.00455	8	H	-0.00220
9	C	-0.05895	9	C	-0.05813
10	H	0.00488	10	H	0.00117
11	C	0.07246	11	C	0.06760
12	H	-0.00266	12	H	-0.00182
13	N	1.50007	13	N	1.51238
14	N	-0.08667	14	N	-0.08188
15	C	0.15796	15	C	0.15721
16	H	-0.01443	16	H	-0.00827

Triplet 3-cinnolinylnitrene (18)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: CS
HF = -471.9871294 Hartree
Zero-point correction (unscaled) = 0.113500 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.873630 Hartree
= -296105.186 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: CS
State=3-A"
S^2 = 2.055019
HF = -472.1773154 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	2.148682	-0.381036	0.000000
N	1.522180	-1.652917	0.000000
C	0.000000	0.708940	0.000000
C	-0.544860	-0.603815	0.000000
C	-2.772360	0.302158	0.000000
H	-3.844994	0.163235	0.000000
C	-2.241029	1.609688	0.000000
H	-2.914676	2.456335	0.000000
C	-0.884119	1.816464	0.000000
H	-0.474818	2.818665	0.000000
C	-1.935520	-0.791341	0.000000
H	-2.315527	-1.803756	0.000000
N	3.461650	-0.362014	0.000000
N	0.254380	-1.729749	0.000000
C	1.393603	0.807712	0.000000
H	1.896159	1.765665	0.000000

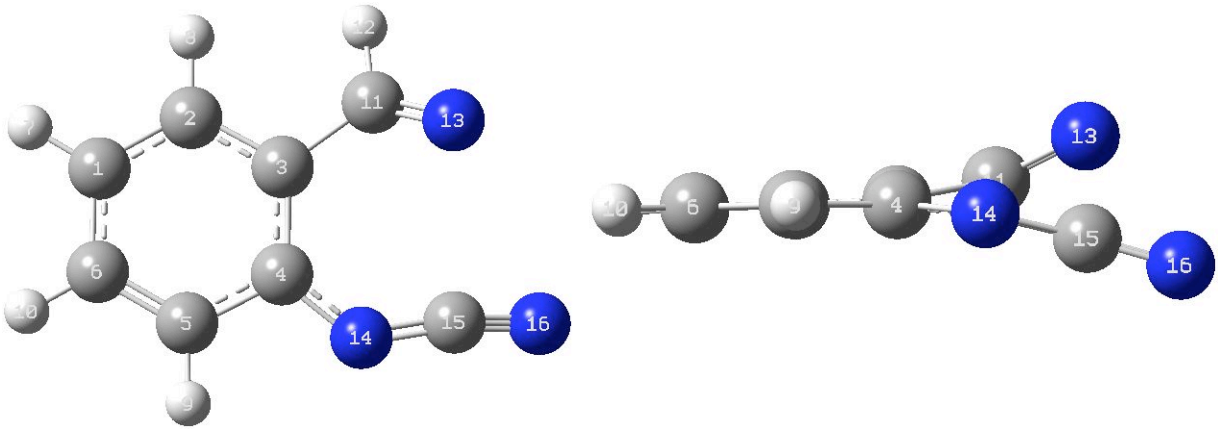
Mulliken spin densities:			Natural spin densities:		
1	C	-0.21073	1	C	-0.20572
2	N	0.17007	2	N	0.17881
3	C	-0.07422	3	C	-0.08554
4	C	0.12528	4	C	0.12529
5	C	0.15343	5	C	0.13914
6	H	-0.00870	6	H	-0.00425
7	C	-0.07969	7	C	-0.06970
8	H	0.00409	8	H	0.00219
9	C	0.12929	9	C	0.12516
10	H	-0.00577	10	H	-0.00391
11	C	-0.08470	11	C	-0.07298
12	H	0.00423	12	H	0.00207
13	N	1.52510	13	N	1.53946
14	N	-0.04953	14	N	-0.05528
15	C	0.42348	15	C	0.39738
16	H	-0.02163	16	H	-0.01212

Triplet 2-(iminylmethyl)phenylcyanamidyl diradical (19a)

UB3LYP/6-31G*; Gaussian 03, Revision B.05

Point group: C1
HF = -471.9829836 Hartree
Zero-point correction (unscaled) = 0.110425 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.872558 Hartree
= -296104.513 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.054859
HF = -472.1776176 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	-2.730629	0.365019	-0.199318
C	-1.634895	1.219002	-0.261173
C	-0.333289	0.763830	-0.071872
C	-0.119944	-0.642024	0.122962
C	-1.262726	-1.480315	0.230131
C	-2.539271	-0.991922	0.068059
H	-3.727456	0.759215	-0.342490
H	-1.794637	2.276121	-0.431552
H	-1.079332	-2.530679	0.406343
H	-3.387114	-1.659728	0.135527
C	0.716238	1.800309	0.013077
H	0.450866	2.765481	-0.444176
N	1.809463	1.732176	0.611852
N	1.052903	-1.308961	0.171917
C	2.238688	-0.914290	-0.155097
N	3.356583	-0.755797	-0.470093

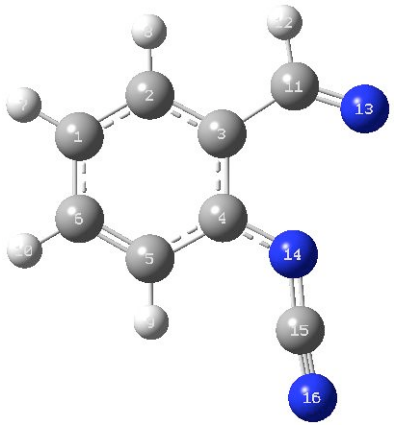
Mulliken spin densities:			Natural spin densities:		
1	C	0.22673	1	C	0.21705
2	C	-0.09881	2	C	-0.08867
3	C	0.23869	3	C	0.25284
4	C	-0.07676	4	C	-0.10318
5	C	0.19715	5	C	0.19021
6	C	-0.10882	6	C	-0.09927
7	H	-0.01223	7	H	-0.00588
8	H	0.00380	8	H	0.00343
9	H	-0.00804	9	H	-0.00543

10	H	0.00537	10	H	0.00295
11	C	-0.15294	11	C	-0.16099
12	H	0.11159	12	H	0.10358
13	N	1.01866	13	N	1.02319
14	N	0.42709	14	N	0.44859
15	C	-0.12752	15	C	-0.13559
16	N	0.35603	16	N	0.35719

Triplet 2-(iminylmethyl)phenylcyanamidyl diradical (19b)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: CS
HF = -471.9919402 Hartree
Zero-point correction (unscaled) = 0.110782 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.881158 Hartree
= -296109.91 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: CS
State=3-A"
S^2 = 2.056838
HF = -472.1866709 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	2.343398	-1.265812	0.000000
C	1.100852	-1.889900	0.000000
C	-0.078489	-1.153543	0.000000
C	0.000000	0.276820	0.000000
C	1.282010	0.891247	0.000000
C	2.428441	0.132025	0.000000
H	3.245017	-1.863057	0.000000
H	1.044253	-2.970839	0.000000
H	1.332578	1.972120	0.000000
H	3.396152	0.615037	0.000000
C	-1.360855	-1.880525	0.000000
H	-1.260131	-2.976957	0.000000
N	-2.523331	-1.418215	0.000000
N	-1.151510	0.973447	0.000000

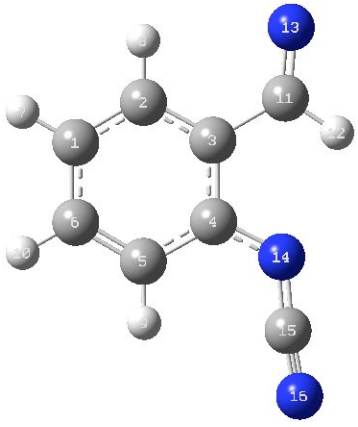
C	-1.183611	2.272825	0.000000
N	-1.317779	3.434037	0.000000

Mulliken spin densities:			Natural spin densities:		
1	C	0.25872	1	C	0.23813
2	C	-0.12400	2	C	-0.10378
3	C	0.26075	3	C	0.26393
4	C	-0.08293	4	C	-0.10027
5	C	0.20176	5	C	0.19559
6	C	-0.11472	6	C	-0.10093
7	H	-0.01334	7	H	-0.00651
8	H	0.00408	8	H	0.00410
9	H	-0.01090	9	H	-0.00563
10	H	0.00539	10	H	0.00283
11	C	-0.14983	11	C	-0.16613
12	H	0.11127	12	H	0.10168
13	N	1.00986	13	N	1.02676
14	N	0.44782	14	N	0.46147
15	C	-0.11365	15	C	-0.12489
16	N	0.30973	16	N	0.31369

Triplet 2-(iminylmethyl)phenylcyanamidyl diradical (19c)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: CS
HF = -471.9964702 Hartree
Zero-point correction (unscaled) = 0.110951 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.885519 Hartree
= -296112.646 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: CS
State=3-A"
S^2 = 2.054873
HF = -472.1910782 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	2.035790	-1.514816	0.000000

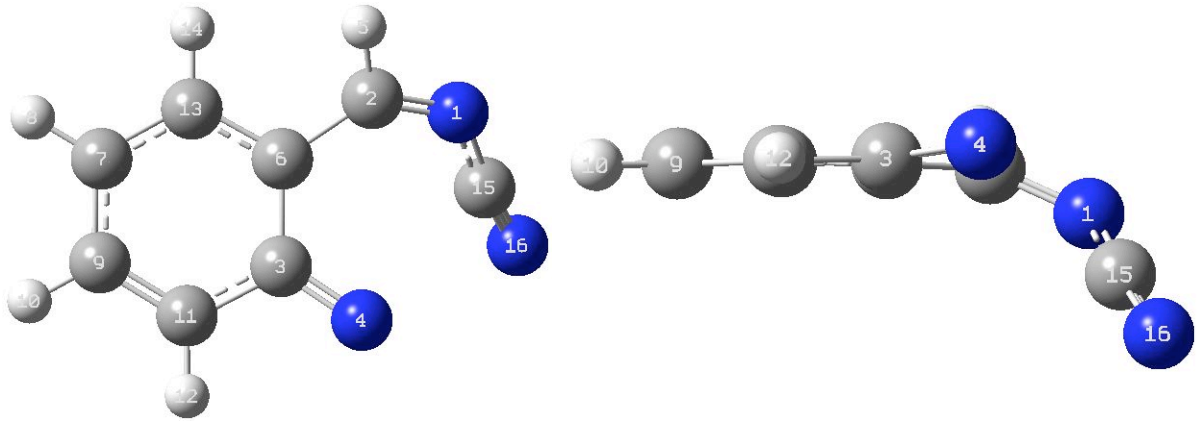
C	0.709754	-1.921805	0.000000
C	-0.322096	-0.987738	0.000000
C	0.000000	0.407695	0.000000
C	1.367771	0.797671	0.000000
C	2.361820	-0.148862	0.000000
H	2.823936	-2.255540	0.000000
H	0.461656	-2.974056	0.000000
H	1.603786	1.853565	0.000000
H	3.399205	0.157295	0.000000
C	-1.736456	-1.410634	0.000000
H	-2.480191	-0.604851	0.000000
N	-2.127514	-2.598200	0.000000
N	-1.022474	1.289366	0.000000
C	-0.827219	2.576489	0.000000
N	-0.756380	3.742488	0.000000

Mulliken spin densities:			Natural spin densities:		
1	C	0.27023	1	C	0.22952
2	C	-0.08007	2	C	-0.10498
3	C	0.25477	3	C	0.28057
4	C	-0.08244	4	C	-0.08352
5	C	0.17381	5	C	0.17750
6	C	-0.11051	6	C	-0.09354
7	H	-0.01300	7	H	-0.00632
8	H	0.00977	8	H	0.00304
9	H	-0.00960	9	H	-0.00483
10	H	0.00503	10	H	0.00257
11	C	-0.17005	11	C	-0.16447
12	H	0.09188	12	H	0.09084
13	N	1.04058	13	N	1.04691
14	N	0.43148	14	N	0.44633
15	C	-0.10939	15	C	-0.12165
16	N	0.29752	16	N	0.30202

Triplet *Z*-[2-[[(cyanimino)methyl]phenyl-nitrene] (*Z*-20)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -471.9780647 Hartree
Zero-point correction (unscaled) = 0.111805 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.866260 Hartree
= -296100.561 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State =3-A
S^2 = 2.053055
HF = -472.1724326 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
N	-2.205154	1.063079	-0.202434
C	-0.980101	1.380983	-0.411758
C	0.385069	-0.799917	-0.347690
N	-0.579546	-1.556400	-0.814028
H	-0.835572	2.404702	-0.753545
C	0.259306	0.636144	-0.213130
C	2.614220	0.760912	0.383107
H	3.470675	1.364188	0.650058
C	2.728726	-0.633846	0.318666
H	3.675888	-1.107622	0.539687
C	1.650733	-1.403708	-0.045707
H	1.727615	-2.477908	-0.134872
C	1.397335	1.372946	0.103328
H	1.319245	2.451803	0.158635
C	-2.648403	-0.063444	0.335733
N	-3.186609	-0.954619	0.845711

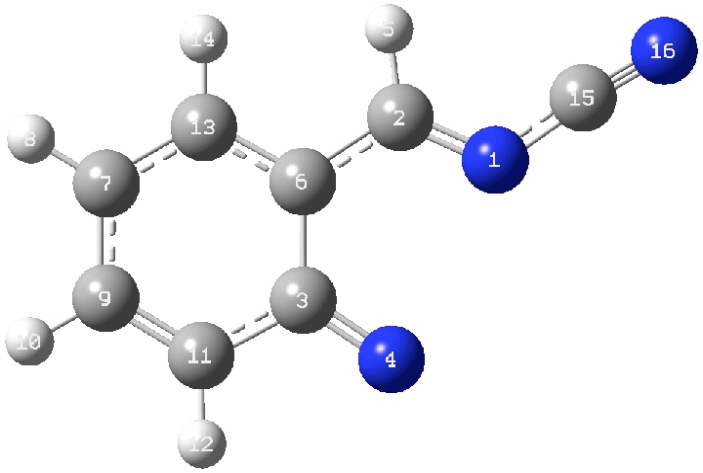
Mulliken spin densities:			Natural spin densities:		
1	N	0.08195	1	N	0.08115
2	C	-0.03027	2	C	-0.04237
3	C	-0.18788	3	C	-0.21024
4	N	1.48824	4	N	1.51519
5	H	0.00330	5	H	0.00429
6	C	0.27219	6	C	0.27261
7	C	0.27009	7	C	0.26750
8	H	-0.01666	8	H	-0.00825
9	C	-0.12109	9	C	-0.11597
10	H	0.01034	10	H	0.00625
11	C	0.31280	11	C	0.30532
12	H	-0.01597	12	H	-0.00948
13	C	-0.11038	13	C	-0.10052
14	H	0.00874	14	H	0.00573
15	C	-0.02201	15	C	-0.02549
16	N	0.05660	16	N	0.05428

Triplet *E*-[2-[[(cyanimino)methyl]phenyl-nitrene] (*E*-20)

UB3LYP/6-31G*; Gaussian 03, Revision B.05

Point group: CS
HF = -471.9871337 Hartree
Zero-point correction (unscaled) = 0.111729 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.875405 Hartree
= -296106.299 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: CS
State = 3-A"
S^2 = 2.057801
HF = -472.1818194 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
N	1.437538	-1.426354	0.000000
C	1.290316	-0.148584	0.000000
C	-1.248281	-0.248175	0.000000
N	-1.318695	-1.555041	0.000000
H	2.154472	0.519438	0.000000
C	0.000000	0.494805	0.000000
C	-1.254368	2.577891	0.000000
H	-1.255417	3.658968	0.000000
C	-2.466732	1.873702	0.000000
H	-3.403211	2.415546	0.000000
C	-2.475082	0.499800	0.000000
H	-3.400661	-0.058062	0.000000
C	-0.048584	1.886923	0.000000
H	0.882630	2.439806	0.000000
C	2.642949	-1.977354	0.000000
N	3.649854	-2.551425	0.000000

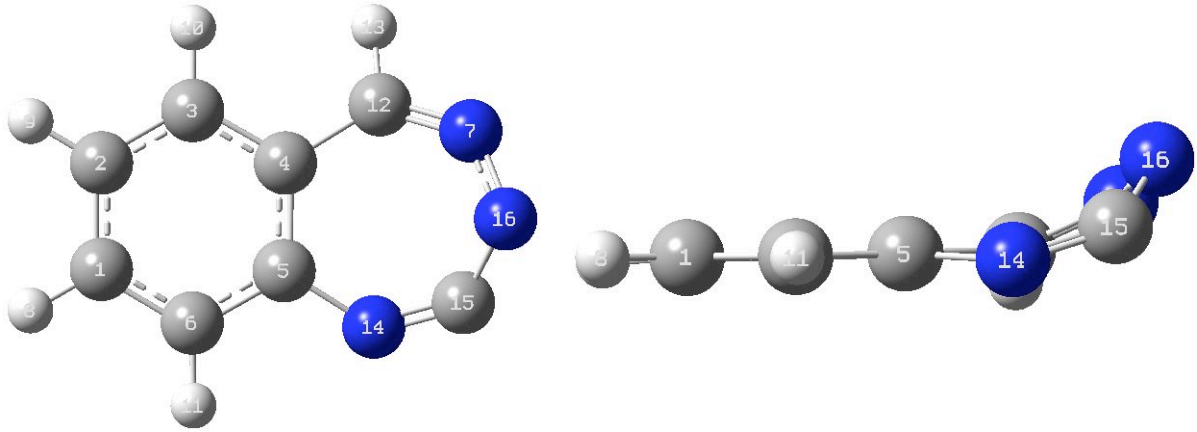
Mulliken spin densities:			Natural spin densities:		
1	N	0.11759	1	N	0.12356
2	C	-0.03326	2	C	-0.05329
3	C	-0.16020	3	C	-0.21392
4	N	1.44674	4	N	1.48043
5	H	0.00623	5	H	0.00480
6	C	0.27215	6	C	0.26134

7	C	0.28487	7	C	0.26966
8	H	-0.01679	8	H	-0.00825
9	C	-0.13181	9	C	-0.11979
10	H	0.01048	10	H	0.00632
11	C	0.30325	11	C	0.31290
12	H	-0.01659	12	H	-0.00969
13	C	-0.12981	13	C	-0.09883
14	H	0.00861	14	H	0.00591
15	C	-0.03131	15	C	-0.03180
16	N	0.06985	16	N	0.07063

Triplet 2H-1,3,4-benzotriazepin-2-ylidene

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -471.9489152 Hartree
Zero-point correction (unscaled) = 0.113479 (Hartree/Particle)
Sum of electronic and zero-point Energies = -471.835437 Hartree
= -296081.219 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.013977
HF = -472.1415836 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	-2.632640	-0.649373	0.163745
C	-2.595834	0.743153	0.126967
C	-1.383305	1.397234	-0.027611
C	-0.187161	0.678616	-0.131080
C	-0.241660	-0.729841	-0.118278
C	-1.462737	-1.382658	0.025973
N	2.251524	1.033802	0.107546
H	-3.577100	-1.163432	0.281594
H	-3.510857	1.313624	0.209817
H	-1.349754	2.479060	-0.065673
H	-1.474631	-2.463731	0.015511

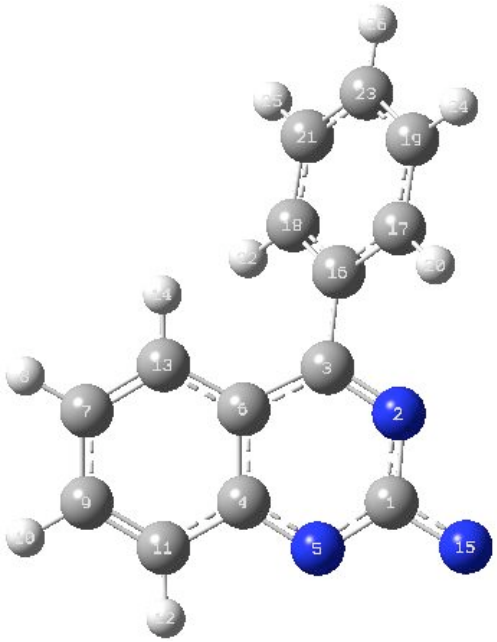
C	1.071544	1.408900	-0.264982
H	1.019823	2.426018	-0.638498
N	0.914596	-1.496662	-0.327230
C	2.095923	-1.208857	-0.117864
N	2.677841	-0.127793	0.541974

Mulliken spin densities:			Natural spin densities:		
1	C	0.02926	1	C	0.03167
2	C	0.01569	2	C	0.01052
3	C	0.00439	3	C	0.02726
4	C	0.03277	4	C	0.01670
5	C	0.11870	5	C	0.07958
6	C	-0.02047	6	C	-0.00017
7	N	0.15928	7	N	0.17863
8	H	-0.00189	8	H	-0.00085
9	H	-0.00083	9	H	-0.00019
10	H	-0.00023	10	H	-0.00041
11	H	0.00274	11	H	0.00114
12	C	0.16348	12	C	0.18438
13	H	-0.00993	13	H	-0.00465
14	N	0.21310	14	N	0.25616
15	C	0.72747	15	C	0.64840
16	N	0.56646	16	N	0.57151

Triplet 4-phenyl-2-quinazolylnitrene (27)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0784174 Hartree
Zero-point correction (unscaled) = 0.195882 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.882536 Hartree
= -441065.469 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.052576
HF = -703.3593401 Hartree



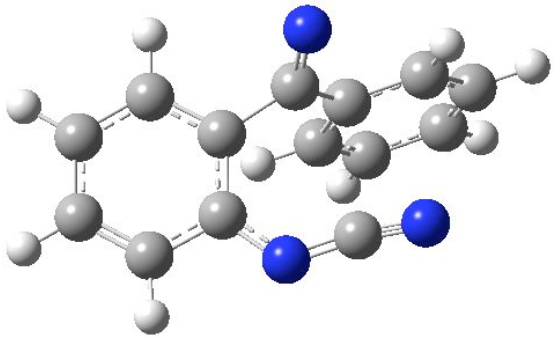
Atom type	Coordinates (angstroms): X	Y	Z
C	-1.421218	2.214685	0.165890
N	-0.112380	1.806099	0.105627
C	0.130048	0.523457	0.025537
C	-2.272644	0.100308	0.057872
N	-2.500434	1.422509	0.185854
C	-0.950107	-0.430927	-0.061781
C	-1.894347	-2.637668	-0.355420
H	-1.759484	-3.694949	-0.540550
C	-3.193756	-2.120829	-0.185494
H	-4.044077	-2.788513	-0.228812
C	-3.384443	-0.777973	0.013199
H	-4.370029	-0.347243	0.121439
C	-0.794389	-1.809254	-0.294909
H	0.193575	-2.218775	-0.442533
N	-1.630426	3.536026	0.226552
C	1.560789	0.122029	0.018525
C	2.464353	0.837643	-0.772172
C	2.040768	-0.910092	0.829777
C	3.812184	0.508230	-0.773895
H	2.098451	1.654263	-1.378569
C	3.393946	-1.225616	0.840600
H	1.363589	-1.445961	1.480827
C	4.280966	-0.524567	0.032051
H	4.499140	1.062849	-1.399347
H	3.755109	-2.015103	1.486390
H	5.333501	-0.775557	0.036259

Mulliken spin densities:			Natural spin densities:		
1	C	-0.15644	1	C	-0.18464
2	N	0.12581	2	N	0.13542
3	C	-0.07669	3	C	-0.07647
4	C	-0.05548	4	C	-0.06996

5	N	0.30830	5	N	0.32541
6	C	0.14135	6	C	0.13242
7	C	0.14781	7	C	0.13765
8	H	-0.00873	8	H	-0.00420
9	C	-0.06699	9	C	-0.06279
10	H	0.00367	10	H	0.00193
11	C	0.12069	11	C	0.11564
12	H	-0.00551	12	H	-0.00338
13	C	-0.08421	13	C	-0.07187
14	H	0.00376	14	H	0.00213
15	N	1.60892	15	N	1.62974
16	C	0.00723	16	C	0.00945
17	C	-0.00729	17	C	-0.00831
18	C	-0.01013	18	C	-0.00827
19	C	0.00887	19	C	0.00352
20	H	0.00027	20	H	0.00028
21	C	0.00271	21	C	0.00370
22	H	0.00040	22	H	0.00034
23	C	-0.00829	23	C	-0.00770
24	H	-0.00024	24	H	-0.00015
25	H	-0.00028	25	H	-0.00015
26	H	0.00050	26	H	0.00025

Triplet [2-(phenyliminylmethyl)phenyl]cyanamidyl diradical (30a)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.042319 Hartree
Zero-point correction (unscaled) = 0.192379 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.849940 Hartree
= -441045.014 Kcal/mol

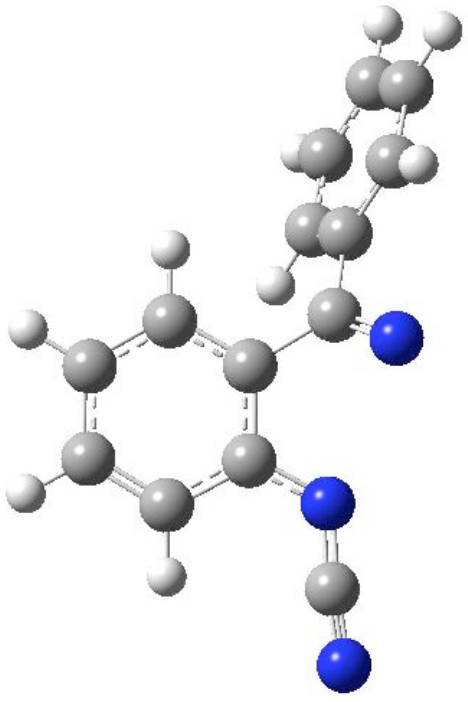


Atom type	Coordinates (angstroms): X	Y	Z
C	3.328428	-1.530972	0.234155
C	2.078703	-1.354669	0.842912
C	1.261261	-0.272761	0.527408
C	1.735302	0.702364	-0.413017
C	2.997589	0.485616	-1.035509
C	3.781932	-0.609373	-0.717238
H	3.939369	-2.387885	0.502160
H	1.724008	-2.077882	1.570344

H	3.324798	1.230758	-1.753008
H	4.746136	-0.746247	-1.197352
C	-0.086852	-0.195871	1.199804
N	-0.105188	-0.035632	2.454576
N	1.124301	1.862800	-0.773373
C	0.039852	2.359665	-0.255666
N	-0.908725	2.961106	0.115814
C	-1.335488	-0.413868	0.404452
C	-2.568331	0.026594	0.911918
C	-1.295114	-1.088806	-0.823186
C	-3.739889	-0.211761	0.201065
H	-2.591273	0.571203	1.849842
C	-2.473466	-1.324180	-1.532303
H	-0.347228	-1.438832	-1.220853
C	-3.696190	-0.887542	-1.022318
H	-4.688865	0.140251	0.595460
H	-2.433419	-1.848949	-2.482805
H	-4.612655	-1.066949	-1.577768

Triplet [2-(phenyliminylmethyl)phenyl]cyanamidyl diradical (30b)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0462115 Hartree
Zero-point correction (unscaled) = 0.192580 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.853631 Hartree
= -441047.331 Kcal/mol

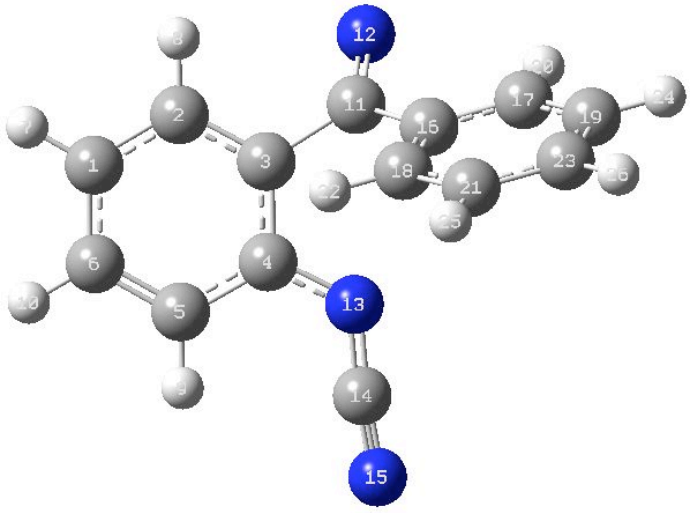


Atom type Coordinates (angstroms):
X Y Z

C	1.332064	2.700354	-0.447267
C	0.346367	1.718186	-0.560920
C	0.642967	0.368400	-0.358779
C	1.987086	-0.001039	-0.012940
C	2.975035	1.020494	0.097424
C	2.650660	2.345730	-0.116025
H	1.076187	3.741335	-0.621309
H	-0.667245	2.001035	-0.824970
H	3.987543	0.729147	0.361294
H	3.414918	3.112275	-0.027873
C	-0.417580	-0.664708	-0.573272
N	-0.143975	-1.762268	-1.146275
N	2.246674	-1.310654	0.232308
C	3.455780	-1.729872	0.495232
N	4.502808	-2.216058	0.742020
C	-1.831586	-0.385838	-0.152032
C	-2.893742	-0.865493	-0.933693
C	-2.109316	0.296517	1.041736
C	-4.210935	-0.658077	-0.530012
H	-2.675348	-1.393609	-1.856456
C	-3.429509	0.497592	1.443850
H	-1.293579	0.658521	1.660458
C	-4.482234	0.023540	0.658803
H	-5.026763	-1.027422	-1.145166
H	-3.634530	1.022060	2.373074
H	-5.510099	0.184794	0.971946

Triplet [2-(phenyliminylmethyl)phenyl]cyanamidyl diradical (30c)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0472573 Hartree
Zero-point correction (unscaled) = 0.192562 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.854695 Hartree
= -441047.998 Kcal/mol



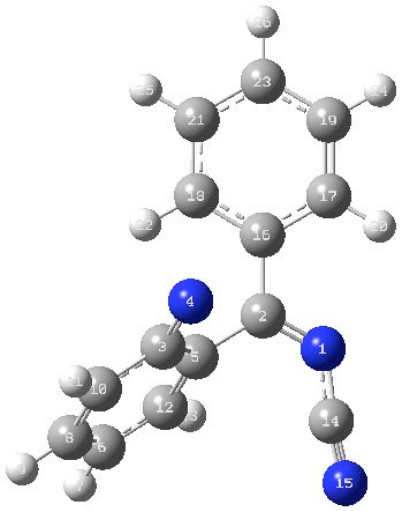
Atom type Coordinates (angstroms):

	X	Y	Z
C	3.131384	-1.758149	0.660402
C	1.845167	-1.981665	0.154211
C	1.035373	-0.918720	-0.235745
C	1.543965	0.417162	-0.144156
C	2.851983	0.622074	0.380656
C	3.629459	-0.451355	0.776265
H	3.743785	-2.602343	0.963119
H	1.460868	-2.992385	0.065500
H	3.226195	1.639352	0.452207
H	4.626710	-0.281593	1.171200
C	-0.331206	-1.204797	-0.795559
N	-0.406311	-2.026695	-1.755922
N	0.747551	1.424145	-0.593479
C	1.139096	2.670750	-0.553969
N	1.388504	3.824406	-0.564364
C	-1.559961	-0.601075	-0.192459
C	-2.714143	-0.451475	-0.975686
C	-1.592041	-0.236435	1.160226
C	-3.879398	0.061933	-0.412245
H	-2.682462	-0.727509	-2.024842
C	-2.762280	0.273286	1.720958
H	-0.705193	-0.355914	1.775625
C	-3.906969	0.425209	0.936675
H	-4.766176	0.184268	-1.027910
H	-2.778341	0.553552	2.770556
H	-4.816169	0.829133	1.373450

Triplet *Z*-[2-[(cyanimino)phenylmethyl]phenyl-nitrene] (*Z*-34)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0409216 Hartree
Zero-point correction (unscaled) = 0.192839 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.848083 Hartree
= -441043.849 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.049217
HF = -703.3286179 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
N	-0.030857	2.089188	0.058202
C	-0.129460	0.802724	-0.039182
C	1.279115	-1.102869	0.889522
N	0.432706	-1.297085	1.879334
C	1.069392	-0.078562	-0.104518
C	3.160130	-0.700490	-1.159085
H	3.880364	-0.540342	-1.949200
C	3.373755	-1.700584	-0.205588
H	4.263341	-2.314105	-0.257727
C	2.462943	-1.903722	0.804905
H	2.616179	-2.661257	1.560421
C	2.021115	0.102780	-1.093006
H	1.874176	0.877708	-1.833255
C	1.121625	2.733907	0.162074
N	2.058681	3.411329	0.246819
C	-1.480138	0.220569	-0.108965
C	-2.590597	0.979055	0.288232
C	-1.683324	-1.075607	-0.597902
C	-3.866304	0.449082	0.202885
H	-2.432603	1.977766	0.668240
C	-2.964787	-1.598876	-0.692480
H	-0.839845	-1.671694	-0.915800
C	-4.057486	-0.840542	-0.289077
H	-4.715489	1.038066	0.522681
H	-3.109636	-2.599093	-1.077896
H	-5.056064	-1.252265	-0.354844

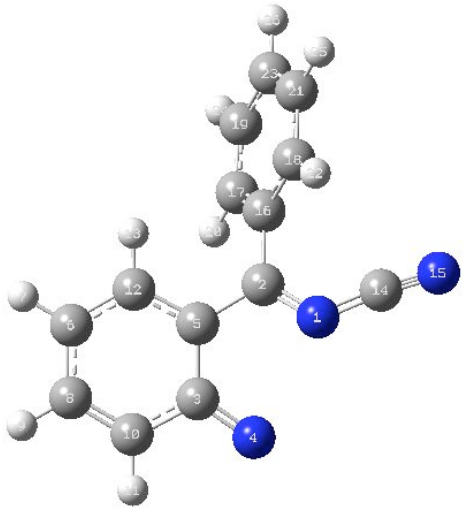
Mulliken spin densities:			Natural spin densities:		
1	N	0.02544	1	N	0.0218
2	C	-0.00528	2	C	-0.0149
3	C	-0.18495	3	C	-0.2018
4	N	1.50564	4	N	1.5434
5	C	0.29910	5	C	0.2842
6	C	0.28791	6	C	0.2791
7	H	-0.01715	7	H	-0.0086
8	C	-0.11390	8	C	-0.1153
9	H	0.01017	9	H	0.0061

10	C	0.31708	10	C	0.3016
11	H	-0.01694	11	H	-0.0094
12	C	-0.11401	12	C	-0.1070
13	H	0.00880	13	H	0.0059
14	C	-0.00109	14	C	-0.0029
15	N	0.00557	15	N	0.0051
16	C	0.00503	16	C	0.0052
17	C	-0.00841	17	C	0.0004
18	C	-0.00517	18	C	0.0030
19	C	0.00126	19	C	0.0017
20	H	-0.00024	20	H	-0.0000
21	C	-0.00098	21	C	-0.0004
22	H	-0.00048	22	H	-0.0000
23	C	0.00263	23	C	0.0029
24	H	-0.00004	24	H	-0.0000
25	H	0.00018	25	H	0.0000
26	H	-0.00018	26	H	-0.0001

Triplet *E*-[2-[(cyanimino)phenylmethyl]phenyl-nitrene] (*E*-34)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0408548 Hartree
Zero-point correction (unscaled) = 0.192986 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.847869 Hartree
= -441043.715 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.054416
HF = -703.3263395 Hartree



Atom type Coordinates (angstroms):
X Y Z

N	0.022457	1.910116	-0.098580
C	0.015614	0.616842	-0.061976
C	-2.502358	0.680999	0.254920
N	-2.523105	1.923419	0.676585
C	-1.293291	-0.045834	-0.092824
C	-2.650615	-2.006065	-0.582586
H	-2.701445	-3.033617	-0.915252
C	-3.822056	-1.316536	-0.249484
H	-4.780514	-1.814204	-0.316301
C	-3.758518	-0.007866	0.163916
H	-4.649157	0.542564	0.432136
C	-1.414187	-1.372856	-0.494246
H	-0.524114	-1.920937	-0.767049
C	1.107744	2.660686	-0.037791
N	1.975904	3.429237	0.003554
C	1.256141	-0.202567	0.004438
C	1.413019	-1.170883	1.001718
C	2.297921	0.018794	-0.900442
C	2.594490	-1.893263	1.097738
H	0.617746	-1.342586	1.714703
C	3.468492	-0.722503	-0.815420
H	2.190777	0.765797	-1.674600
C	3.621525	-1.675337	0.185454
H	2.713042	-2.625279	1.885484
H	4.264077	-0.548921	-1.527344
H	4.539256	-2.243896	0.256814

Mulliken spin densities:

1	N	0.08793
2	C	-0.00990
3	C	-0.17668
4	N	1.45453
5	C	0.27790
6	C	0.27976
7	H	-0.01725
8	C	-0.12982
9	H	0.01048
10	C	0.31217
11	H	-0.01683
12	C	-0.11856
13	H	0.00918
14	C	-0.02729
15	N	0.06035
16	C	0.00871
17	C	-0.00664
18	C	-0.00054
19	C	0.00312
20	H	-0.00050
21	C	0.00204
22	H	-0.00017
23	C	-0.00203
24	H	-0.00007
25	H	-0.00003
26	H	0.00013

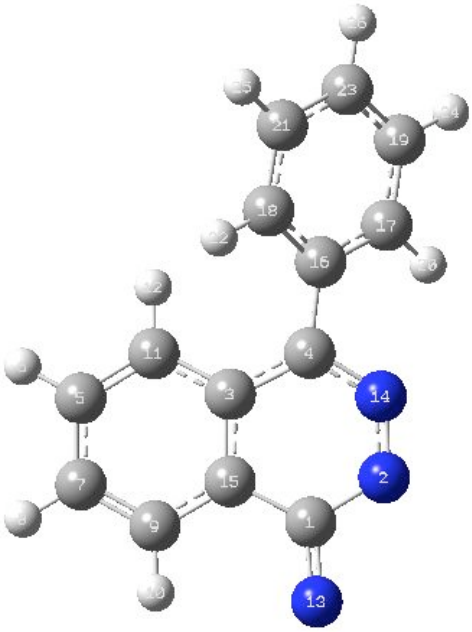
Natural spin densities:

1	N	0.10210
2	C	-0.03948
3	C	-0.21131
4	N	1.49072
5	C	0.26633
6	C	0.26951
7	H	-0.00823
8	C	-0.11644
9	H	0.00627
10	C	0.30782
11	H	-0.00957
12	C	-0.10015
13	H	0.00567
14	C	-0.02725
15	N	0.06162
16	C	0.00708
17	C	-0.00247
18	C	-0.00236
19	C	0.00107
20	H	0.00011
21	C	0.00077
22	H	0.00013
23	C	-0.00197
24	H	-0.00003
25	H	0.00000
26	H	0.00006

Triplet 4-phenyl-1-phtalazinylnitrene (35)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0474455 Hartree
Zero-point correction (unscaled) = 0.194773 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.852673 Hartree
= -441046.729 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.058982
HF = -703.3277787 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	-2.313186	-1.558769	0.203666
N	-1.224344	-2.402740	0.060735
C	-0.857504	0.382539	-0.109919
C	0.213976	-0.572582	-0.040843
C	-1.778178	2.600043	-0.406471
H	-1.638047	3.652858	-0.612550
C	-3.070871	2.099714	-0.188252
H	-3.918931	2.770924	-0.214364
C	-3.266079	0.753333	0.033299
H	-4.260511	0.352955	0.171593
C	-0.688292	1.760006	-0.371098
H	0.299517	2.150180	-0.562656
N	-3.469070	-2.107654	0.429071
N	-0.023942	-1.890277	-0.018426
C	-2.166997	-0.116574	0.058663

C	1.642039	-0.210513	0.001881
C	2.572604	-0.994690	-0.694518
C	2.111180	0.861476	0.773127
C	3.925162	-0.695354	-0.643857
H	2.218023	-1.836193	-1.271725
C	3.468198	1.147410	0.834250
H	1.417914	1.448416	1.359286
C	4.378565	0.376676	0.119375
H	4.629023	-1.302637	-1.197470
H	3.815371	1.967504	1.448811
H	5.435427	0.604406	0.163579

Mulliken spin densities:

1	C	-0.212230
2	N	0.375206
3	C	-0.048288
4	C	0.242622
5	C	-0.056861
6	H	0.003127
7	C	0.090213
8	H	-0.004202
9	C	-0.064058
10	H	0.005751
11	C	0.068616
12	H	-0.002727
13	N	1.430409
14	N	-0.078581
15	C	0.170214
16	C	-0.022181
17	C	0.051192
18	C	0.052732
19	C	-0.031580
20	H	-0.002622
21	C	-0.018145
22	H	-0.002406
23	C	0.054064
24	H	0.001417
25	H	0.001407
26	H	-0.003089

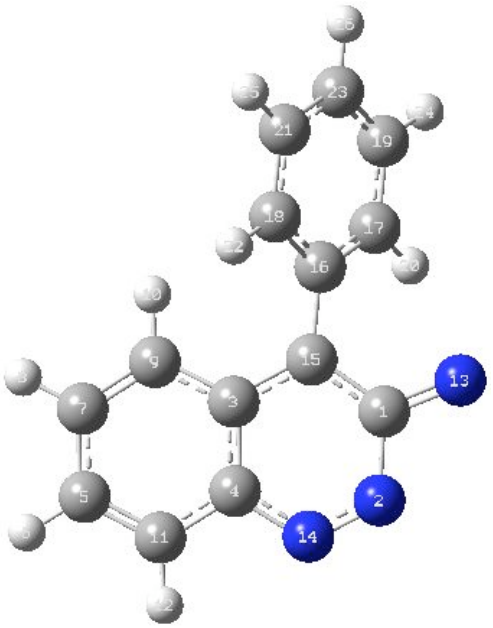
Natural spin densities:

1	C	-0.21428
2	N	0.38201
3	C	-0.06281
4	C	0.26308
5	C	-0.05257
6	H	0.00151
7	C	0.07355
8	H	-0.00198
9	C	-0.05503
10	H	0.00102
11	C	0.06672
12	H	-0.00176
13	N	1.44303
14	N	-0.06386
15	C	0.15495
16	C	-0.03255
17	C	0.04691
18	C	0.04618
19	C	-0.02083
20	H	-0.00149
21	C	-0.02037
22	H	-0.00152
23	C	0.05005
24	H	0.00078
25	H	0.00078
26	H	-0.00153

Triplet 4-phenyl-3-cinnolinylnitrene (36)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -703.0425582 Hartree
Zero-point correction (unscaled) = 0.194786 (Hartree/Particle)
Sum of electronic and zero-point Energies = -702.847772 Hartree
= -441043.654 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.053474
HF = -703.3232062 Hartree



Atom type	Coordinates (angstroms): X	Y	Z
C	0.180916	1.943803	0.153662
N	1.489923	2.482080	0.209090
C	1.075722	-0.287099	-0.045322
C	2.347595	0.343143	0.037585
C	3.462313	-1.777795	-0.196100
H	4.369604	-2.363987	-0.250886
C	2.210517	-2.412210	-0.313954
H	2.168518	-3.482039	-0.470737
C	1.042875	-1.691585	-0.243812
H	0.091944	-2.190148	-0.356355
C	3.527573	-0.413393	-0.029699
H	4.469968	0.111661	0.044329
N	-0.786553	2.823580	0.251742
N	2.495150	1.709940	0.165562
C	-0.065153	0.545248	0.037056
C	-1.451277	0.034177	0.015217
C	-2.386719	0.552302	-0.888576
C	-1.864543	-0.956905	0.913800
C	-3.690948	0.078029	-0.904170
H	-2.086621	1.322928	-1.584677
C	-3.174180	-1.418021	0.905847
H	-1.164332	-1.345770	1.640911
C	-4.089856	-0.906873	-0.007271
H	-4.398073	0.483200	-1.615732
H	-3.480378	-2.172753	1.618205
H	-5.109284	-1.269208	-0.015393

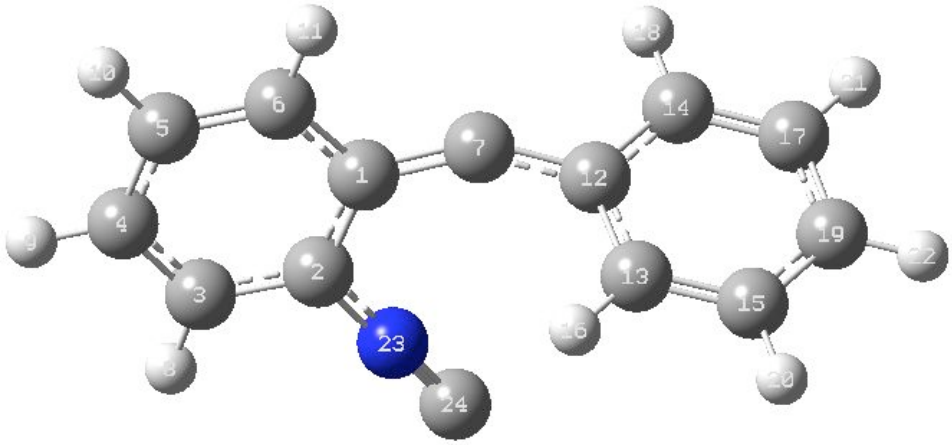
Mulliken spin densities:			Natural spin densities:		
1	C	-0.207801	1	C	-0.20209
2	N	0.159800	2	N	0.17377
3	C	-0.065897	3	C	-0.08300
4	C	0.107463	4	C	0.11727

5	C	0.145025	5	C	0.13122
6	H	-0.008189	6	H	-0.00400
7	C	-0.080081	7	C	-0.06598
8	H	0.003908	8	H	0.00207
9	C	0.121040	9	C	0.11978
10	H	-0.006323	10	H	-0.00365
11	C	-0.081565	11	C	-0.06919
12	H	0.003979	12	H	0.00198
13	N	1.486113	13	N	1.50911
14	N	-0.048408	14	N	-0.05082
15	C	0.423683	15	C	0.38107
16	C	-0.007599	16	C	-0.02203
17	C	0.021189	17	C	0.02757
18	C	0.023059	18	C	0.02616
19	C	-0.008199	19	C	-0.00766
20	H	-0.002127	20	H	-0.00092
21	C	-0.006949	21	C	-0.00580
22	H	-0.002143	22	H	-0.00093
23	C	0.029968	23	C	0.02572
24	H	0.000875	24	H	0.00061
25	H	0.000823	25	H	0.00051
26	H	-0.001645	26	H	-0.00077

Triplet *ortho*-(isocyanophenyl)phenylcarbene (37)

UB3LYP/6-31G*; Gaussian 03, Revision B.05
Point group: C1
HF = -593.5119722 Hartree
Zero-point correction (unscaled) = 0.181825 (Hartree/Particle)
Sum of electronic and zero-point Energies = -593.330147 Hartree
= -372320.304 Kcal/mol

UB3LYP/EPR-III; Gaussian 03, Revision B.05
Point group: C1
State=3-A
S^2 = 2.064087
HF = -593.7546447 Hartree



Atom type Coordinates (angstroms):

	X	Y	Z
C	1.247983	-0.585395	-0.045792
C	1.789423	0.740280	-0.163016
C	3.154600	0.973687	-0.054920
C	4.033996	-0.078404	0.163792
C	3.541807	-1.383427	0.275240
C	2.191976	-1.633199	0.172366
C	-0.095155	-0.867585	-0.177741
H	3.515257	1.988718	-0.147189
H	5.094358	0.115795	0.244437
H	4.225600	-2.204490	0.445010
H	1.812590	-2.641888	0.257549
C	-1.435870	-0.535801	-0.047997
C	-1.920694	0.141490	1.106885
C	-2.382337	-0.911409	-1.040445
C	-3.263718	0.432803	1.239403
H	-1.220180	0.430773	1.877896
C	-3.721052	-0.610352	-0.888686
H	-2.033466	-1.432586	-1.921356
C	-4.173087	0.062196	0.247830
H	-3.610568	0.956731	2.120624
H	-4.423554	-0.897719	-1.660147
H	-5.223287	0.295584	0.359484
N	0.945840	1.804242	-0.391833
C	0.239189	2.715013	-0.592497

Mulliken spin densities:

1	C	-0.173655
2	C	0.236982
3	C	-0.110426
4	C	0.242886
5	C	-0.118101
6	C	0.237653
7	C	1.381585
8	H	0.007640
9	H	-0.014827
10	H	0.006387
11	H	-0.011865
12	C	-0.177961
13	C	0.223882
14	C	0.229373
15	C	-0.108946
16	H	-0.013752
17	C	-0.106930
18	H	-0.012555
19	C	0.239098
20	H	0.007679
21	H	0.006005
22	H	-0.014061
23	N	-0.025111
24	C	0.069020

Natural spin densities:

1	C	-0.15750
2	C	0.23834
3	C	-0.09653
4	C	0.22651
5	C	-0.09599
6	C	0.22392
7	C	1.31133
8	H	0.00478
9	H	-0.00704
10	H	0.00349
11	H	-0.00706
12	C	-0.15371
13	C	0.22963
14	C	0.21712
15	C	-0.09034
16	H	-0.00680
17	C	-0.09172
18	H	-0.00674
19	C	0.21989
20	H	0.00443
21	H	0.00329
22	H	-0.00678
23	N	-0.02469
24	C	0.06221

CASSCF and CASPT2 Calculations on Nitrene 11
CASPT2 calculations on triplet nitrene 11

These were performed with the MOLCAS 5 suite of programs. CASPT2 excitations were obtained for the B3LYP/6-31G* optimized geometry. The active space consists of 12 electrons on 11 orbitals (1 occupied p type orbital on the nitrene nitrogen and 6 π-type occupied and 4 π* unoccupied orbitals). The ANO-S basis set was used for this calculation. All reference CASSCF weights of wave function were above 0.60.
Level shift of 0.1 Hartree was used.

		CAS	CASPT2	Ref. weight
CAS(12,11)	lvs=0.10	-469.313	-470.659	0.6905
CAS(12,11)	lvs=0.10	-469.207	-470.571	0.6795
CAS(12,11)	lvs=0.10	-469.186	-470.550	0.6782
CAS(12,11)	lvs=0.10	-469.160	-470.527	0.6729
CAS(12,11)	lvs=0.10	-469.148	-470.528	0.6620
CAS(12,11)	lvs=0.10	-469.123	-470.507	0.6339
CAS(12,11)	lvs=0.10	-469.118	-470.524	0.6556
CAS(12,11)	lvs=0.10	-469.114	-470.499	0.6216

XYZ coordinates (B3LYP/6-31G* optimized)

6	-2.787035	0.276227	0.000000
6	-2.238315	1.582061	0.000000
6	-0.873532	1.776614	0.000000
6	0.000000	0.655144	0.000000
6	-0.561180	-0.661843	0.000000
6	-1.959120	-0.832163	0.000000
7	1.339559	0.851230	0.000000
6	2.109091	-0.254944	0.000000
7	1.671525	-1.571126	0.000000
6	0.377573	-1.740536	0.000000
7	3.440757	-0.073374	0.000000
1	-3.865622	0.148902	0.000000
1	-2.906477	2.438640	0.000000
1	-0.431322	2.767482	0.000000
1	-2.375219	-1.836731	0.000000
1	0.010856	-2.768767	0.000000

Predicted UV-Vis excitation of triplet nitrene **11** by CASPT2

Wavelength (nm)	oscillator strength
517	0.013164
416	0.009554
346	0.016812
345	0.002519
336	0.021898
299	0.010211
285	0.009309

CASSCF(8,8)/6-31G* and CASPT2 calculations on Nitrenes 11, Diradicals 19 And Relevant Intermediates and Transition States

Summary: relative energies (kcal/mol)

	CAS	CASPT2
11T	-26.1	-14.3
11OSS	-6.5	7
12	13.5	42.6
13	10.4	6.7
14	0	0
14 ->19aOSS (TS5)	18.9	21.1
19aOSS	9.3	17.0

11 OSS
CAS(8,8)/6-31G*

N	-0.982995	-1.155989	0.004385
N	-1.947904	1.139805	0.008155
N	-3.231581	-0.748931	-0.006660
C	2.824311	0.434285	-0.006834
C	2.614900	-0.984294	-0.006198
C	1.374594	-1.502490	-0.001213
C	0.222025	-0.631438	0.001577
C	0.438314	0.786975	0.001304
C	1.737403	1.299535	-0.003471
C	-2.077360	-0.267975	0.002078
C	-0.760114	1.616989	0.006904
H	3.824942	0.822911	-0.010238
H	3.471509	-1.633327	-0.008855
H	1.195944	-2.560915	-0.000387
H	1.891270	2.363863	-0.004253
H	-0.655023	2.689236	0.011723

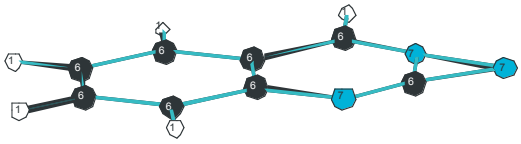
	CAS(8,8)/6-31G*	CASPT2	Ref. weight
11 OSS	-469.19186243	-470.56335193	0.6767

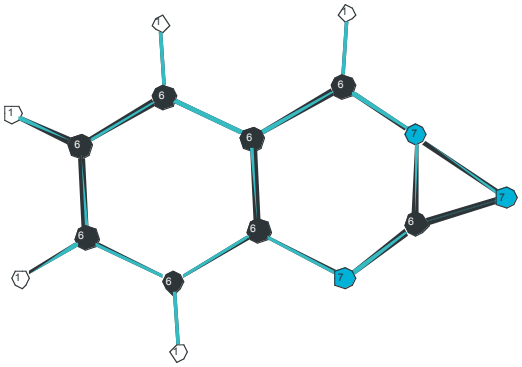
11T
CAS(8,8)/6-31G*

N	-1.023511	-1.125779	0.000472

N	-1.923003	1.101241	0.006098
N	-3.284237	-0.777526	0.000687
C	2.825574	0.439950	-0.006114
C	2.608623	-0.968529	-0.005616
C	1.356368	-1.481621	-0.002345
C	0.233549	-0.605428	-0.000479
C	0.439655	0.781800	0.001610
C	1.757767	1.303042	-0.002139
C	-2.021713	-0.267875	0.002206
C	-0.745230	1.592763	0.005459
H	3.830248	0.820131	-0.009489
H	3.458807	-1.626222	-0.007651
H	1.174286	-2.539669	-0.002072
H	1.908681	2.367766	-0.001914
H	-0.653554	2.666900	0.008609

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
11T	-469.22320463	-470.59722569	0.6794





12

CAS(8,8)/6-31G*

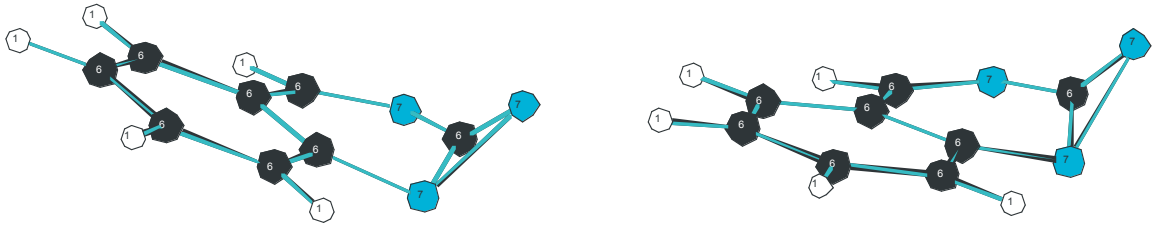
N	2.008991	0.944204	0.049975
N	0.949116	-1.209652	0.052556
N	3.231435	-0.933266	0.153687
C	0.849052	1.521406	-0.018922
C	1.967414	-0.419313	0.082833
C	-0.274828	-0.589421	0.008148
C	-0.380148	0.791969	-0.035403
C	-1.657604	1.413995	-0.100678
C	-2.790359	0.641160	-0.119955
C	-2.680969	-0.774801	-0.071926
C	-1.452164	-1.384201	-0.008311
H	-3.761112	1.099076	-0.167706
H	-3.573375	-1.373829	-0.083232
H	-1.348669	-2.451916	0.026849

H	-1.720808	2.487112	-0.133693
H	0.841502	2.597253	-0.056256

12 N-N bond is 1.78 A at CAS(8,8)/6-31G*

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
12	-469.16001393	-470.50653508	0.6899

13



CAS(8,8)/6-31G*

N	1.112490	-1.147054	-0.492927
N	2.142518	1.117574	-0.135307
N	2.084856	-1.190331	0.800767
C	-1.304101	-1.401239	-0.191540
C	-0.166651	-0.599357	-0.200321
C	-0.272284	0.780570	-0.039571
C	-1.529387	1.363910	0.155985
C	-2.662166	0.564250	0.200422
C	-2.547081	-0.819564	0.022780
C	2.057155	-0.253339	-0.006135
C	0.950224	1.602393	-0.151039
H	-3.627748	1.007108	0.361317
H	-3.426821	-1.436253	0.048571
H	-1.196849	-2.458443	-0.344538
H	-1.611814	2.429772	0.274306
H	0.850752	2.670123	-0.243365

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
13	-469.16498338	-470.56378940	0.6768

14
CAS(8,8)/6-31G*

N	0.799216	-1.577050	-0.459777
N	2.402903	-0.196649	0.721113

N	2.329268	0.989811	-0.062445
C	-1.604307	-1.313386	-0.058651
C	-0.338181	-0.751457	-0.188025
C	-0.158182	0.645130	-0.136614
C	-1.287551	1.448847	0.039517
C	-2.538407	0.896173	0.198661
C	-2.703324	-0.488539	0.147698
C	1.767901	-1.106577	0.161008
C	1.152098	1.329911	-0.367192
H	-1.171414	2.518165	0.058478
H	-3.390197	1.533744	0.348414
H	-3.682108	-0.918477	0.254850
H	-1.709555	-2.379697	-0.126328
H	1.085672	2.278161	-0.874647

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
14	-469.18157394	-470.57446350	0.6775

14 -> **19aOSS** (**TS5**)
CAS(8,8)/6-31G*

N	0.927332	-1.352409	-0.514304
N	2.898009	-0.706135	0.744553
N	2.119969	1.480005	-0.194913
C	-1.455095	-1.401186	-0.152298
C	-0.275636	-0.660741	-0.224625
C	-0.297258	0.734483	-0.076978
C	-1.534722	1.347375	0.165534
C	-2.692663	0.616128	0.281038
C	-2.659778	-0.767052	0.116634
C	1.918500	-1.042404	0.118440
C	0.863125	1.647827	-0.278601
H	-1.570611	2.417075	0.272133
H	-3.622791	1.114416	0.483679
H	-3.563304	-1.343620	0.190002
H	-1.404510	-2.462991	-0.302354
H	0.585859	2.664595	-0.528907

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
14 -> **19aOSS** (**TS5**)	-469.15154233	-470.54077913	0.6692
Freq -187 cm-1			

19aOSS
CAS(8,8)/6-31G*

N	1.201263	1.116944	0.000000
N	3.442010	0.098392	0.000000
N	1.428257	-2.162220	0.000000
C	-0.567982	-0.694830	0.000000
C	-1.945663	-0.862384	0.000000
C	-2.855204	0.211730	0.000000
C	-2.368533	1.521031	0.000000
C	-1.002849	1.735728	0.000000
C	-0.046956	0.663656	0.000000
C	2.364197	0.466726	0.000000
C	0.203449	-1.968437	0.000000
H	-2.339315	-1.862191	0.000000
H	-3.910460	0.014722	0.000000
H	-3.043789	2.356047	0.000000
H	-0.597076	2.728244	0.000000
H	-0.414286	-2.859141	0.000000

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
19aOSS	-469.16684429	-470.54737350	0.6727
19aCSS at **OSS** geom	-469.05653108	-470.44095470	0.6744

19aT

N	1.200056	1.116133	0.000000
N	3.441398	0.098084	0.000000
N	1.427232	-2.159198	0.000000
C	-0.565864	-0.696237	0.000000
C	-1.949680	-0.863335	0.000000
C	-2.853330	0.207070	0.000000
C	-2.364709	1.522291	0.000000
C	-1.004239	1.738214	0.000000
C	-0.044338	0.663949	0.000000
C	2.363711	0.466534	0.000000
C	0.202490	-1.967546	0.000000
H	-2.342936	-1.863238	0.000000
H	-3.908996	0.011977	0.000000
H	-3.041499	2.356107	0.000000
H	-0.598545	2.730758	0.000000
H	-0.416093	-2.857214	0.000000

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
19aT	-469.16901515	-470.55049432	0.672

19bOSS
CAS(8,8)/6-31G*

N	1.388970	0.444206	0.000000
N	3.508965	-0.833244	0.000000
N	0.041624	2.901556	0.000000
C	-2.210761	0.070603	0.000000
C	-2.362962	-1.337521	0.000000
C	-1.237702	-2.148942	0.000000
C	0.031599	-1.572650	0.000000
C	0.190317	-0.165202	0.000000
C	-0.988933	0.665218	0.000000
C	2.500660	-0.269242	0.000000
C	-0.947843	2.150386	0.000000
H	-3.094723	0.682510	0.000000
H	-3.347459	-1.765544	0.000000
H	-1.337569	-3.218226	0.000000
H	0.906924	-2.194376	0.000000
H	-1.919860	2.631113	0.000000

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
19bOSS	-469.18064354	-470.55782804	0.6720
19bCSS at **OSS** geom.	-469.07902624	-470.46545557	0.6740

19bT

N	1.379124	0.452925	0.000000
N	3.489327	-0.849123	0.000000
N	0.049934	2.903641	0.000000
C	-2.229767	0.063819	0.000000
C	-2.365853	-1.333181	0.000000
C	-1.219757	-2.148967	0.000000
C	0.037308	-1.581017	0.000000
C	0.202281	-0.152884	0.000000
C	-0.983578	0.675809	0.000000
C	2.501438	-0.283441	0.000000
C	-0.944164	2.159197	0.000000
H	-3.113292	0.675829	0.000000
H	-3.344368	-1.774754	0.000000
H	-1.321273	-3.218151	0.000000
H	0.914856	-2.198981	0.000000
H	-1.914599	2.642457	0.000000

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
19bT	-469.18426651	-470.56178236	0.6741

19cOSS
CAS(8,8)/6-31G*

N	-1.014072	1.239742	0.000000
N	-0.654958	3.692852	0.000000
N	-2.049750	-2.663637	0.000000
C	0.744489	-1.934017	0.000000
C	2.086152	-1.513403	0.000000
C	2.396352	-0.143365	0.000000
C	1.386928	0.799989	0.000000
C	0.012105	0.393478	0.000000
C	-0.292765	-1.015907	0.000000
C	-0.781078	2.561568	0.000000
C	-1.711841	-1.467159	0.000000
H	0.515154	-2.982597	0.000000
H	2.872653	-2.244186	0.000000
H	3.421942	0.175508	0.000000
H	1.617752	1.848286	0.000000
H	-2.483768	-0.712939	0.000000

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
19cOSS	-469.18746683	-470.56367704	0.6752
19cCSS at **OSS** geom.	-469.07283499	-470.45358049	0.6765

19cT

N	-1.013348	1.238825	0.000000
N	-0.654513	3.692506	0.000000
N	-2.046548	-2.662243	0.000000
C	0.747956	-1.937532	0.000000
C	2.082174	-1.516532	0.000000
C	2.393218	-0.140255	0.000000
C	1.388518	0.801277	0.000000
C	0.009698	0.394851	0.000000
C	-0.295260	-1.016289	0.000000
C	-0.780441	2.561263	0.000000
C	-1.710903	-1.465832	0.000000
H	0.518955	-2.985979	0.000000
H	2.870486	-2.245361	0.000000
H	3.419288	0.177106	0.000000
H	1.619428	1.849495	0.000000
H	-2.481075	-0.710220	0.000000

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
19cT	-469.18975321	-470.56697119	0.6747

Transition state for the Cyclization of 19b to 1-Cyanoindazole 21

19b → 21 (TS1, Scheme 2)

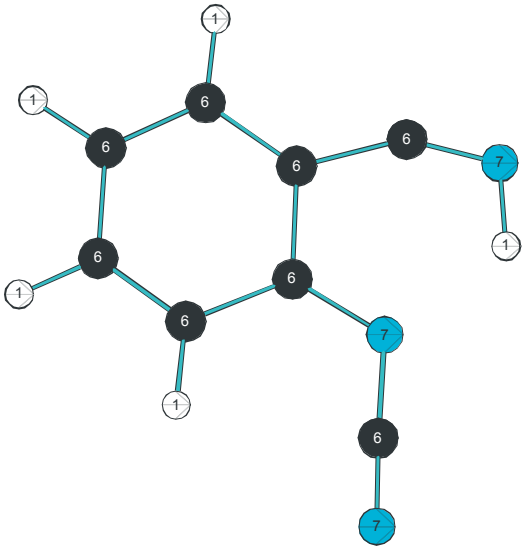
N	1.383114	0.180675	0.421255
N	3.263464	-1.278014	-0.265084
N	0.832293	2.527120	-0.212456
C	-0.871524	0.823010	0.059366
C	-2.200400	0.513435	-0.054828
C	-2.620167	-0.823184	-0.098624
C	-1.682331	-1.846540	-0.046754
C	-0.321788	-1.549814	0.065678
C	0.084311	-0.215362	0.155010
C	2.379619	-0.621783	0.028331
C	-0.381303	2.214836	-0.021003
H	-2.926538	1.301644	-0.142843
H	-3.664903	-1.050943	-0.198881
H	-1.998235	-2.872014	-0.094725
H	0.405957	-2.337299	0.124086
H	-1.101650	3.017311	0.056429

	CAS(8,8)/6-31G*
19b → 21 (TS1)	-469.17857089

Imaginary freq. -237.1770 cm-1

N-N distance 2.49Å compared to 2.8Å in **19b OSS**

The transition state for the H-shift reaction **19c → 22 (TS2**, Scheme 2) was not located. This energy surface is quite flat. The final structure of **19c** before the migration is shown below.



Transition State for the Triazacycloheptatetraene 14 (CSS) → 19a (OSS) Ring Opening (TS5)

14→19aOSS TS5
CAS(8,8)/6-31G*

N	0.927332	-1.352409	-0.514304
N	2.898009	-0.706135	0.744553
N	2.119969	1.480005	-0.194913
C	-1.455095	-1.401186	-0.152298
C	-0.275636	-0.660741	-0.224625
C	-0.297258	0.734483	-0.076978
C	-1.534722	1.347375	0.165534
C	-2.692663	0.616128	0.281038
C	-2.659778	-0.767052	0.116634
C	1.918500	-1.042404	0.118440
C	0.863125	1.647827	-0.278601
H	-1.570611	2.417075	0.272133
H	-3.622791	1.114416	0.483679
H	-3.563304	-1.343620	0.190002
H	-1.404510	-2.462991	-0.302354
H	0.585859	2.664595	-0.528907

	CAS(8,8)/6-31G*	CASPT2	Ref. weight
14→19aOSS TS5	-469.15154233	-470.54077913	0.6692

Freq -187 cm-1

UB3LYP/6-31G* Calculations on Diradicals 19a-c

In the case of **19a OSS** and **19 T the** planar structure - CS is not a minimum (very low imaginary frequency, -30cm-1). Fully optimized structure of **19T** in C1 differs only by 0.13 kcal/mol, which is negligible.

OSS states are contaminated with the triplet, and S^2=1 instead of 0. Cramer (ref 18) estimates the energies using Ziegler's "sum method" as 2 × E(OSS) – E(T). This give $S^2 = 2 \times 1 - 2 = 0$.

Summary:

19a CSS at **OSS** geometry	26.61 kcal/mol
19a OSS by Cramer's method	0 kcal/mol
19a T	-2.81 kcal/mol

19b CSS at **OSS** geometry 27.0 kcal/mol
19b OSS Cramer's method 0 kcal/mol
19b T -2.83 kcal/mol

19c CSS at **OSS** geometry 28.0 kcal/mol
19c OSS Cramer's method 0 kcal/mol
19c T -2.55 kcal/mol

19a OSS

6	-0.518780	-0.694569	0.000000
6	-1.905303	-0.868283	0.000000
6	-2.796799	0.207218	0.000000
6	-2.302545	1.515608	0.000000
6	-0.934764	1.724804	0.000000
6	0.000000	0.648760	0.000000
7	1.288634	1.074803	0.000000
6	2.416314	0.440692	0.000000
7	3.552913	0.100870	0.000000
6	0.280678	-1.941021	0.000000
7	1.525402	-2.114007	0.000000
1	-2.298966	-1.881344	0.000000
1	-3.866427	0.020711	0.000000
1	-2.982834	2.361704	0.000000
1	-0.516598	2.725550	0.000000
1	-0.336623	-2.857539	0.000000

State=1-A"\HF=-471.9806066\S2=1.034436

Sum of electronic and zero-point Energies= -471.870146
Sum of electronic and thermal Energies= -471.861761
Sum of electronic and thermal Enthalpies= -471.860817
Sum of electronic and thermal Free Energies= -471.903732

19a CSS at **19a OSS** geom.. State=1-A\HF=-471.9361034

19a T

6	0.352330	0.775406	-0.048324
6	1.669489	1.226538	-0.188231
6	2.760975	0.359027	-0.145630
6	2.552491	-1.013934	0.048284
6	1.263450	-1.497085	0.168030
6	0.124452	-0.641082	0.090875
7	-1.051638	-1.312453	0.125683
6	-2.259636	-0.901780	-0.112422
7	-3.413218	-0.765542	-0.343932
6	-0.688673	1.821930	0.016244
7	-1.874881	1.736206	0.430636
1	1.841818	2.292685	-0.310694
1	3.767316	0.753105	-0.250514
1	3.396167	-1.695622	0.095946

```
1                     1.064265   -2.555822    0.294374
1                    -0.340674    2.824057   -0.288778

State=3-A\HF=-471.9829835\S2=2.06169

Sum of electronic and zero-point Energies=           -471.872558
Sum of electronic and thermal Energies=              -471.863333
Sum of electronic and thermal Enthalpies=            -471.862389
Sum of electronic and thermal Free Energies=         -471.908753
```

19b OSS

```
6                     1.112790   -1.889609    0.000000
6                     2.360707   -1.256039    0.000000
6                     2.438723    0.144019    0.000000
6                     1.279440    0.900082    0.000000
6                     0.000000    0.275556    0.000000
6                    -0.071324   -1.156837    0.000000
7                    -1.167712    0.966104    0.000000
6                    -1.195189    2.271312    0.000000
7                    -1.334228    3.443893    0.000000
6                    -1.357592   -1.893071    0.000000
7                    -2.528944   -1.434830    0.000000
1                     1.061947   -2.975214    0.000000
1                     3.267893   -1.852795    0.000000
1                     3.406699    0.636011    0.000000
1                     1.321778    1.985461    0.000000
1                    -1.247463   -2.992098    0.000000

State=1-A"\HF= -471.9896563\S2=1.034859

Sum of electronic and zero-point Energies=           -471.879016
Sum of electronic and thermal Energies=              -471.869727
Sum of electronic and thermal Enthalpies=            -471.868782
Sum of electronic and thermal Free Energies=         -471.914457
```

19b CSS at **19b OSS** geom. State=1-A'\HF=-471.9443756\S2=0.

19b T

```
6                     1.108202   -1.898258    0.000000
6                     2.354223   -1.269345    0.000000
6                     2.437279    0.134493    0.000000
6                     1.284658    0.895425    0.000000
6                     0.000000    0.275456    0.000000
6                    -0.076591   -1.159509    0.000000
7                    -1.162253    0.966388    0.000000
6                    -1.187650    2.273684    0.000000
7                    -1.324618    3.445555    0.000000
6                    -1.363059   -1.883291    0.000000
7                    -2.531659   -1.409047    0.000000
1                     1.052610   -2.983564    0.000000
1                     3.260593   -1.867345    0.000000
1                     3.408098    0.620979    0.000000
1                     1.331233    1.980572    0.000000
```

```
1                    -1.265191   -2.982839    0.000000

State=3-A"\HF=-471.991948\S2=2.062507

Sum of electronic and zero-point Energies=           -471.881157
Sum of electronic and thermal Energies=              -471.872019
Sum of electronic and thermal Enthalpies=            -471.871075
Sum of electronic and thermal Free Energies=         -471.916959
```

19c OSS

```
6                     0.725453   -1.920559    0.000000
6                     2.058188   -1.503081    0.000000
6                     2.375078   -0.133400    0.000000
6                     1.365985    0.810802    0.000000
6                     0.000000    0.408059    0.000000
6                    -0.312826   -0.990759    0.000000
7                    -1.042820    1.282027    0.000000
6                    -0.850803    2.575380    0.000000
7                    -0.793039    3.753973    0.000000
6                    -1.731294   -1.427411    0.000000
7                    -2.112589   -2.625534    0.000000
1                     0.481422   -2.978156    0.000000
1                     2.853112   -2.242912    0.000000
1                     3.413575    0.183820    0.000000
1                     1.593174    1.872923    0.000000
1                    -2.480835   -0.623123    0.000000

State=1-A"\HF=-471.9944163\S2=1.033299

Sum of electronic and zero-point Energies=           -471.883451
Sum of electronic and thermal Energies=              -471.874266
Sum of electronic and thermal Enthalpies=            -471.873322
Sum of electronic and thermal Free Energies=         -471.918354
```

19c CSS at **19c OSS** geom. \State=1-A\HF=-471.947851\S2=0.

19c T

```
6                     0.714470   -1.928039    0.000000
6                     2.045649   -1.518439    0.000000
6                     2.371151   -0.146772    0.000000
6                     1.371579    0.803515    0.000000
6                     0.000000    0.410440    0.000000
6                    -0.321701   -0.989845    0.000000
7                    -1.033590    1.287964    0.000000
6                    -0.832987    2.582013    0.000000
7                    -0.767964    3.759328    0.000000
6                    -1.737335   -1.414988    0.000000
7                    -2.127456   -2.613408    0.000000
1                     0.463713   -2.983951    0.000000
1                     2.837642   -2.261378    0.000000
1                     3.412179    0.162286    0.000000
1                     1.605751    1.864048    0.000000
1                    -2.481171   -0.605502    0.000000
```

State=3-A"\HF=-471.9964825\S2=2.060447

Sum of electronic and zero-point Energies= -471.885540
Sum of electronic and thermal Energies= -471.876400
Sum of electronic and thermal Enthalpies= -471.875456
Sum of electronic and thermal Free Energies= -471.921344

B3LYP/6-31G* calculations on 27, 29, 33, and 34

Triplet nitrene 27 (UB3LYP/6-31G*)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.220901	-2.113464	-0.176913
2	6	-3.400163	-0.763172	0.024804
3	6	-2.278115	0.109677	0.062630
4	6	-0.955338	-0.433211	-0.064696
5	6	-0.810669	-1.817155	-0.304276
6	6	-1.921716	-2.640837	-0.357958
7	1	-4.080029	-2.777240	-0.215516
8	1	-4.384270	-0.320622	0.138913
9	6	0.133135	0.518333	0.022024
10	1	0.177068	-2.233173	-0.465292
11	1	-1.794643	-3.702849	-0.547332
12	6	-1.412701	2.224269	0.161106
13	7	-0.100344	1.810623	0.098386
14	7	-2.503894	1.437935	0.191392
15	7	-1.615294	3.554105	0.217210
16	6	1.565544	0.113053	0.018053
17	6	2.484211	0.874266	-0.722281
18	6	2.038142	-0.964418	0.784458
19	6	3.836962	0.544349	-0.723350
20	1	2.121259	1.724822	-1.289809
21	6	3.396165	-1.283375	0.793468
22	1	1.350268	-1.531874	1.403854
23	6	4.296885	-0.536936	0.032659
24	1	4.534881	1.135093	-1.310215
25	1	3.750007	-2.110759	1.402399
26	1	5.353537	-0.790319	0.035694

Energy = -703.0784174
E+ZPVE = -702.882537

Vibrational frequencies (unscaled)

ModeNr. Symmetry Wavenumber Abs.Int. Rel.Int.

1	A	52.1	0.4	0
2	A	74.1	0.2	0
3	A	89.2	1.2	1
4	A	123.7	0.2	0
5	A	182.1	0.4	0
6	A	241.6	0.2	0
7	A	251.0	0.5	0
8	A	290.4	1.0	1
9	A	313.7	0.8	1
10	A	336.2	0.4	0
11	A	418.8	0.6	0
12	A	445.0	0.4	0
13	A	462.9	1.3	1
14	A	498.9	0.6	0
15	A	507.2	4.0	3
16	A	530.2	3.6	3
17	A	592.3	2.1	2
18	A	631.8	3.6	3
19	A	633.0	18.5	13
20	A	669.9	5.0	4
21	A	688.3	0.1	0
22	A	713.7	44.0	31
23	A	715.4	4.4	3
24	A	759.9	3.0	2
25	A	783.2	15.7	11
26	A	793.4	52.9	38
27	A	823.1	1.0	1
28	A	852.5	7.6	5
29	A	866.0	2.3	2
30	A	898.7	1.2	1
31	A	944.2	2.9	2
32	A	961.4	4.5	3
33	A	973.7	1.8	1
34	A	982.8	1.4	1
35	A	1000.7	3.7	3
36	A	1005.1	4.1	3
37	A	1007.2	2.5	2
38	A	1018.2	2.1	1
39	A	1054.5	1.6	1
40	A	1059.4	2.4	2
41	A	1115.3	4.4	3
42	A	1151.2	1.4	1
43	A	1174.7	0.4	0
44	A	1195.3	0.0	0
45	A	1206.1	6.5	5
46	A	1216.4	6.1	4
47	A	1229.4	37.5	27
48	A	1294.0	10.8	8
49	A	1309.0	6.8	5
50	A	1336.1	20.9	15
51	A	1347.0	3.8	3
52	A	1367.8	1.2	1
53	A	1388.7	31.6	23
54	A	1406.3	140.0	100
55	A	1449.1	0.6	0
56	A	1491.7	12.1	9
57	A	1519.9	27.5	20

58	A	1543.5	4.0	3
59	A	1555.1	44.7	32
60	A	1596.5	55.8	40
61	A	1637.6	1.5	1
62	A	1652.5	9.7	7
63	A	1661.2	2.4	2
64	A	3186.9	0.4	0
65	A	3195.7	2.0	1
66	A	3196.5	8.7	6
67	A	3205.7	32.0	23
68	A	3209.4	12.9	9
69	A	3213.8	14.8	11
70	A	3225.0	5.4	4
71	A	3226.8	7.7	6
72	A	3231.8	7.9	6

Benzotriazacycloheptatetraene 29

XYZ coordinates

6	1.862398	-2.338691	-0.869200
6	3.073684	-2.081444	-0.223433
6	3.277940	-0.860696	0.415114
6	2.270868	0.102536	0.404526
6	1.011921	-0.146659	-0.209833
6	0.843410	-1.389658	-0.845353
7	2.488968	1.376412	1.047129
6	1.910253	2.195393	0.315949
7	1.139858	2.720169	-0.495343
7	-0.172471	2.103236	-0.242122
6	-0.162491	0.804641	-0.162651
6	-1.529038	0.216420	-0.012577
6	-2.617718	0.806314	-0.675693
6	-3.904323	0.301055	-0.507735
6	-4.126223	-0.793690	0.330756
6	-3.052116	-1.382056	0.999734
6	-1.761028	-0.885380	0.826891
1	1.705746	-3.282425	-1.381596
1	3.860046	-2.830103	-0.218289
1	4.209004	-0.631663	0.921872
1	-0.100605	-1.606101	-1.332677
1	-2.437971	1.660108	-1.319101
1	-4.735245	0.761291	-1.033976
1	-5.130283	-1.186574	0.460729
1	-3.217846	-2.228075	1.660001
1	-0.932544	-1.343676	1.356425

Energy = -703.0740667
E+ZPVE = -702.877843

Wavenumber	Abs.Int. (unscaled)
3224.62	3.3324
3222.40	5.8242
3218.60	7.9724

3213.25	9.9987
3206.02	10.1293
3204.21	28.4431
3193.71	9.4484
3192.50	2.2286
3183.50	0.1168
2074.78	429.6475
1656.54	0.5510
1648.04	45.8025
1635.19	2.0441
1615.63	3.6800
1569.11	54.4731
1534.45	1.9890
1499.65	3.7752
1484.01	6.3024
1476.52	12.4080
1363.42	1.8916
1340.53	18.9619
1338.66	0.1845
1309.15	10.6926
1293.72	33.2506
1270.99	10.7733
1210.94	6.0834
1196.09	3.1094
1189.24	0.2138
1187.18	7.3756
1167.14	4.4482
1116.36	11.0074
1111.32	9.9844
1064.61	1.9682
1057.65	2.3972
1016.11	1.6447
1004.54	0.1272
997.01	0.0330
982.39	2.0310
976.49	1.6002
967.69	3.9742
943.64	3.1789
891.80	1.5770
863.99	0.8102
834.66	17.9873
825.78	20.3072
795.64	12.6035
781.57	38.3700
771.48	15.1485
719.76	3.0304
712.46	36.2270
701.25	15.2680
677.19	13.6348
661.89	7.5402
631.95	0.1218
620.36	5.1408
575.38	15.2687
540.84	3.7058
504.72	0.2384
486.74	0.4019
464.62	2.2508

```
  425.16    2.8678
  417.83    0.1004
  373.57    6.5176
  344.84    2.0334
  310.09    1.5434
  260.20    0.0780
  248.40    4.2583
  179.50    0.1330
  137.96    0.1545
   83.64    0.9618
   78.49    0.0340
   53.05    0.3878
-----------------------------------------------------------------
```

Diazo compound 33

B3LYP/6-31G*

```
XYZ coordinates

6         2.159191   -2.356292   -0.763161
6         3.361717   -1.867749   -0.243386
6         3.409964   -0.583121    0.283095
6         2.257495    0.215153    0.298282
6         1.036858   -0.251128   -0.245482
6         1.021593   -1.556934   -0.769612
6        -0.183992    0.576255   -0.292763
7         2.331957    1.469004    0.879517
6         2.416022    2.527643    1.399877
6        -1.558316    0.091287   -0.050360
7        -0.046368    1.832930   -0.644540
7         0.057022    2.928679   -0.955598
6        -2.673346    0.744165   -0.607279
6        -3.964700    0.292960   -0.348142
6        -4.175251   -0.825453    0.460460
6        -3.075974   -1.481825    1.016025
6        -1.781649   -1.027972    0.772273
1         2.112075   -3.357532   -1.180005
1         4.254241   -2.484805   -0.245155
1         4.324679   -0.180684    0.704117
1         0.098323   -1.933494   -1.196009
1        -2.529830    1.607198   -1.250907
1        -4.809504    0.813823   -0.789205
1        -5.182672   -1.179019    0.656576
1        -3.224205   -2.347190    1.655515
1        -0.939049   -1.534516    1.230453

Energy = -703.0767737
E+ZPVE = -702.882746

Wavenumber  Abs.Int. (unscaled)

3222.77    6.8395
 3216.63    8.7239
 3213.45    6.9363
 3207.35   14.3867
```

3206.37	22.0700
3197.09	16.2037
3193.44	1.5964
3187.22	1.6920
3181.14	4.5600
2194.01	230.2885
2181.65	428.2321
1656.09	34.3340
1647.10	15.4599
1629.96	4.2278
1614.92	3.0213
1539.15	52.6376
1523.19	48.9886
1496.16	1.4685
1481.66	7.9691
1376.35	3.9213
1360.59	10.5369
1352.91	3.1929
1328.04	20.5825
1314.07	21.9195
1286.82	6.6244
1224.75	3.3371
1216.39	1.4784
1191.27	0.4795
1189.31	0.2247
1156.01	0.4042
1124.26	3.0488
1114.39	3.1869
1066.97	4.5924
1057.40	1.4569
1012.62	0.0614
997.24	0.0936
992.80	0.3720
973.30	0.2159
964.93	1.4369
952.84	6.3754
920.82	2.4705
888.68	0.1254
854.35	0.2123
795.49	7.9733
777.60	50.9002
771.79	26.8114
750.66	3.3248
710.06	18.9056
702.00	5.0600
662.79	16.2936
633.90	0.1537
585.15	0.5071
559.07	0.8380
537.65	7.2339
526.33	2.2904
508.80	3.3102
488.77	19.5355
471.07	1.5169
416.04	0.5499
406.82	0.1798
379.31	0.1175

```
 352.71    0.2402
 281.41    0.1599
 237.83    0.1861
 220.17    0.1910
 153.89    3.9332
 145.60    0.9686
 127.03    0.0808
  97.66    0.2429
  75.59    0.5313
  53.63    0.2857
  33.09    1.9916
```

Triplet nitrene 34 (UB3LYP/6-31G*)

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.274978	-1.870621	-0.262003
2	6	-3.122473	-1.018789	0.816067
3	6	-1.971128	-0.169738	0.918781
4	6	-0.981839	-0.220813	-0.133932
5	6	-1.160572	-1.108496	-1.189608
6	6	-2.297637	-1.923563	-1.267809
7	1	-4.154976	-2.504010	-0.327721
8	1	-3.860678	-0.969592	1.609503
9	6	0.193495	0.703227	-0.112010
10	1	-0.411774	-1.153340	-1.975536
11	1	-2.420231	-2.594072	-2.112792
12	6	-1.108291	2.595936	-0.361533
13	7	0.070062	1.993395	-0.205504
14	7	-1.816743	0.611283	1.980295
15	7	-2.065665	3.248334	-0.523142
16	6	1.558121	0.147928	-0.019175
17	6	2.669713	0.979363	-0.259731
18	6	1.776997	-1.197048	0.328103
19	6	3.960007	0.473684	-0.162409
20	1	2.497051	2.016979	-0.523182
21	6	3.073566	-1.698382	0.428649
22	1	0.933373	-1.847184	0.533313
23	6	4.166461	-0.866998	0.181378
24	1	4.809247	1.122978	-0.355393
25	1	3.228924	-2.737494	0.704290
26	1	5.176850	-1.259473	0.257375

```
Energy = - 703.0409219
E+ZPVE = -702.848078
```

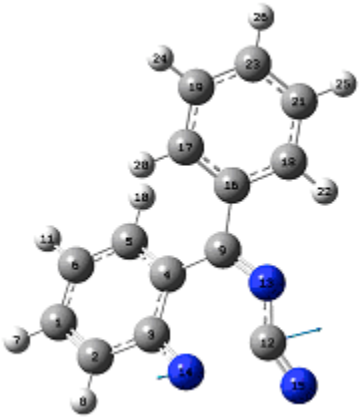
Vibrational frequencies (unscaled)

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	24.6	0.8	1
2	A	49.9	0.6	0
3	A	67.3	1.7	1
4	A	84.4	0.9	1

5	A	107.0	2.6	2
6	A	162.7	0.5	0
7	A	184.4	1.5	1
8	A	198.7	0.7	0
9	A	258.5	2.8	2
10	A	273.1	0.4	0
11	A	329.7	0.8	1
12	A	402.9	0.4	0
13	A	407.6	5.6	4
14	A	415.9	0.5	0
15	A	455.0	7.6	5
16	A	481.2	2.5	2
17	A	522.6	2.8	2
18	A	543.7	2.8	2
19	A	557.3	1.9	1
20	A	602.1	4.4	3
21	A	631.6	0.4	0
22	A	662.4	19.1	13
23	A	687.0	2.9	2
24	A	703.1	23.1	16
25	A	719.2	15.9	11
26	A	752.8	6.2	4
27	A	762.5	42.6	29
28	A	801.0	13.4	9
29	A	852.9	3.2	2
30	A	864.3	1.0	1
31	A	874.9	0.7	0
32	A	940.6	16.3	11
33	A	953.9	0.9	1
34	A	960.3	2.7	2
35	A	986.0	0.3	0
36	A	986.6	0.8	1
37	A	1011.4	0.0	0
38	A	1017.2	4.3	3
39	A	1033.3	13.0	9
40	A	1057.0	0.3	0
41	A	1060.6	9.6	7
42	A	1115.6	2.5	2
43	A	1124.5	1.9	1
44	A	1169.1	8.9	6
45	A	1191.0	1.0	1
46	A	1196.7	0.3	0
47	A	1216.1	27.3	19
48	A	1260.7	6.7	5
49	A	1308.0	60.9	42
50	A	1315.4	10.0	7
51	A	1333.9	112.3	77
52	A	1355.6	38.3	26
53	A	1372.4	3.9	3
54	A	1436.0	0.8	1
55	A	1470.1	4.4	3
56	A	1494.4	22.4	15
57	A	1540.4	1.6	1
58	A	1563.8	3.2	2
59	A	1603.9	24.8	17
60	A	1621.1	145.4	100
61	A	1641.6	60.3	42

62	A	1662.7	9.6	7
63	A	2298.3	72.1	50
64	A	3191.1	0.0	0
65	A	3196.6	0.2	0
66	A	3202.3	9.2	6
67	A	3203.1	10.0	7
68	A	3212.2	26.7	18
69	A	3218.8	9.9	7
70	A	3225.0	8.6	6
71	A	3227.9	6.6	5
72	A	3233.5	3.7	3

Transition state connecting 27 and 34 (UB3LYP/6-31G*)



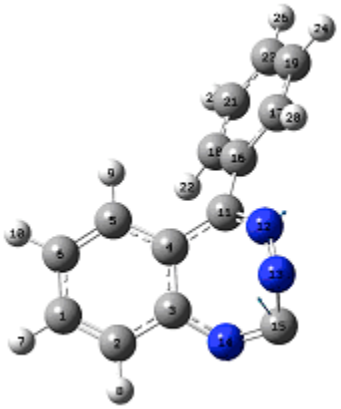
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.118816	-2.204888	-0.182297
2	6	3.332983	-0.936749	0.319753
3	6	2.280979	0.041012	0.316690
4	6	0.964001	-0.363491	-0.127395
5	6	0.795656	-1.654572	-0.637479
6	6	1.854106	-2.564045	-0.681007
7	1	3.933309	-2.923518	-0.200689
8	1	4.303856	-0.624326	0.689293
9	6	-0.137425	0.596378	-0.014811
10	1	-0.176668	-1.951264	-1.015515
11	1	1.692652	-3.555635	-1.092750
12	6	1.242038	2.495606	0.007264
13	7	0.036753	1.884599	0.058523
14	7	2.602826	1.264672	0.728651
15	7	1.828358	3.510774	-0.258523
16	6	-1.554001	0.142434	0.024226
17	6	-1.942021	-1.022222	0.707943
18	6	-2.542624	0.935823	-0.582452
19	6	-3.286203	-1.387273	0.774152
20	1	-1.196593	-1.625598	1.216108
21	6	-3.881636	0.560263	-0.526914

22	1	-2.242485	1.843543	-1.094964
23	6	-4.257620	-0.602558	0.151012
24	1	-3.573883	-2.282013	1.319139
25	1	-4.634208	1.176506	-1.010766
26	1	-5.303827	-0.892318	0.197471

Energy = - 703.0194109
E+ZPVE = -702.827372
Imaginary frequency = -619.4 cm^{-1}

Transition state connecting 29 and 33

B3LYP/6-31G*



Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.366464	-1.820828	-0.231469
2	6	-3.418090	-0.517175	0.209722
3	6	-2.236589	0.264147	0.296200
4	6	-0.993219	-0.321311	-0.139340
5	6	-0.971199	-1.681471	-0.550243
6	6	-2.134786	-2.416820	-0.599003
7	1	-4.280167	-2.406563	-0.287477
8	1	-4.349334	-0.061179	0.531004
9	1	-0.030234	-2.119976	-0.866973
10	1	-2.113415	-3.449292	-0.934693
11	6	0.163568	0.535019	-0.207731
12	7	-0.014350	1.811516	-0.587753
13	7	-0.975910	2.607708	-0.477670
14	7	-2.291094	1.457127	0.965473
15	6	-1.626762	2.566701	0.772200
16	6	1.555897	0.088062	-0.073158
17	6	2.593997	0.777387	-0.728942
18	6	1.882584	-0.991346	0.770301
19	6	3.919713	0.398903	-0.541492
20	1	2.342082	1.595754	-1.395257
21	6	3.211074	-1.365834	0.951908
22	1	1.095082	-1.509165	1.308142
23	6	4.233053	-0.674696	0.296223

24	1	4.710224	0.935737	-1.058215
25	1	3.450036	-2.192271	1.615218
26	1	5.268550	-0.971933	0.436833

Energy = - 702.9910226
E+ZPVE = -702.797519
Imaginary frequency = -721.3 cm^{-1}

Calculated electronic transitions in 33 and 29 at the TD-B3LYP/6-31G** level

Diazo compound 33

```
Excited State   1:   Singlet-A      2.4162 eV  513.15 nm  f=0.0015
      57 -> 58         0.66050
      57 -> 59         0.10519
      57 -> 60         0.12049

 Excited State   2:   Singlet-A      3.6199 eV  342.51 nm  f=0.0859
      57 -> 59         0.64621
      57 -> 60        -0.19700

 Excited State   3:   Singlet-A      4.0492 eV  306.19 nm  f=0.0846
      57 -> 60         0.47085
      57 -> 61         0.46795

 Excited State   4:   Singlet-A      4.4546 eV  278.33 nm  f=0.1355
      56 -> 58         0.22204
      56 -> 61         0.11676
      57 -> 60        -0.28208
      57 -> 61         0.37742
      57 -> 62         0.38647
 Excited State   5:   Singlet-A      4.6042 eV  269.28 nm  f=0.0829
      56 -> 58         0.52255
      57 -> 60         0.23128
      57 -> 61        -0.23979
      57 -> 62         0.22350

 Excited State   6:   Singlet-A      4.6347 eV  267.51 nm  f=0.0502
      55 -> 58         0.30803
      56 -> 58        -0.39004
      56 -> 61         0.12739
      57 -> 60         0.11949
      57 -> 61        -0.12190
      57 -> 62         0.41159

Excited State   7:   Singlet-A      4.6600 eV  266.06 nm  f=0.0291
```

```
      55 -> 58         0.61388
      56 -> 58         0.14121
      57 -> 62        -0.24528

 Excited State   8:   Singlet-A      4.9458 eV  250.69 nm  f=0.0175
      54 -> 58         0.68498

 Excited State   9:   Singlet-A      5.1639 eV  240.10 nm  f=0.0052
      55 -> 59         0.13364
      55 -> 60        -0.10123
      56 -> 59         0.66505
      56 -> 60         0.10212

 Excited State  10:   Singlet-A      5.2549 eV  235.94 nm  f=0.0143
      53 -> 59         0.11842
      54 -> 59         0.46455
      55 -> 59         0.20254
      55 -> 60         0.37546
      55 -> 61         0.19000
      56 -> 59         0.13294
      56 -> 60        -0.11058
```

Benzotriazacycloheptatetraene29

```
Excited State   1:   Singlet-A      3.5973 eV  344.66 nm  f=0.0088
      56 -> 58         0.14632
      57 -> 58         0.64116
      57 -> 59        -0.13040

 Excited State   2:   Singlet-A      3.8647 eV  320.81 nm  f=0.0095
      56 -> 58         0.15035
      57 -> 58         0.10061
      57 -> 59         0.64404

 Excited State   3:   Singlet-A      4.4636 eV  277.77 nm  f=0.0695
      54 -> 58        -0.11296
      55 -> 58        -0.17244
      56 -> 58         0.58729
      56 -> 59         0.12038
      57 -> 58        -0.13332
      57 -> 60        -0.10750

 Excited State   4:   Singlet-A      4.5464 eV  272.71 nm  f=0.0342
      55 -> 58         0.64189
      56 -> 58         0.13925
      56 -> 59        -0.10330
      57 -> 61         0.10220

 Excited State   5:   Singlet-A      4.6733 eV  265.30 nm  f=0.0072
      53 -> 58         0.29073
      53 -> 59         0.15436
      54 -> 58        -0.12938
      56 -> 58        -0.12048
      56 -> 59         0.54449
      57 -> 60        -0.12062
```

```
Excited State   6:   Singlet-A      4.7152 eV  262.95 nm  f=0.0103
     53 -> 58        -0.36203
     54 -> 58         0.41888
     55 -> 58         0.10057
     55 -> 59         0.10368
     56 -> 59         0.31788

Excited State   7:   Singlet-A      4.8757 eV  254.29 nm  f=0.0033
     53 -> 58         0.37357
     53 -> 59        -0.19301
     54 -> 58         0.22797
     55 -> 59         0.13367
     57 -> 60         0.45890

Excited State   8:   Singlet-A      5.0620 eV  244.93 nm  f=0.0077
     53 -> 59         0.11615
     54 -> 58        -0.17936
     55 -> 59         0.63018

Excited State   9:   Singlet-A      5.1112 eV  242.57 nm  f=0.0959
     53 -> 58        -0.10149
     53 -> 59         0.26428
     54 -> 58        -0.25118
     54 -> 59        -0.32505
     55 -> 59        -0.20926
     56 -> 60         0.10178
     57 -> 60         0.35913
     57 -> 61         0.10178

Excited State  10:   Singlet-A      5.1932 eV  238.74 nm  f=0.1178
     53 -> 58         0.17560
     53 -> 59         0.34115
     54 -> 58         0.22527
     54 -> 59        -0.17007
     56 -> 59        -0.12216
     57 -> 60        -0.22798
     57 -> 61         0.32054
     57 -> 62         0.16364
```