Supporting Information

2-Pyridylnitrene, 3-Pyridazylcarbene and their Relationship via Ring Expansion, Ring Opening, Ring Contraction, and Fragmentation

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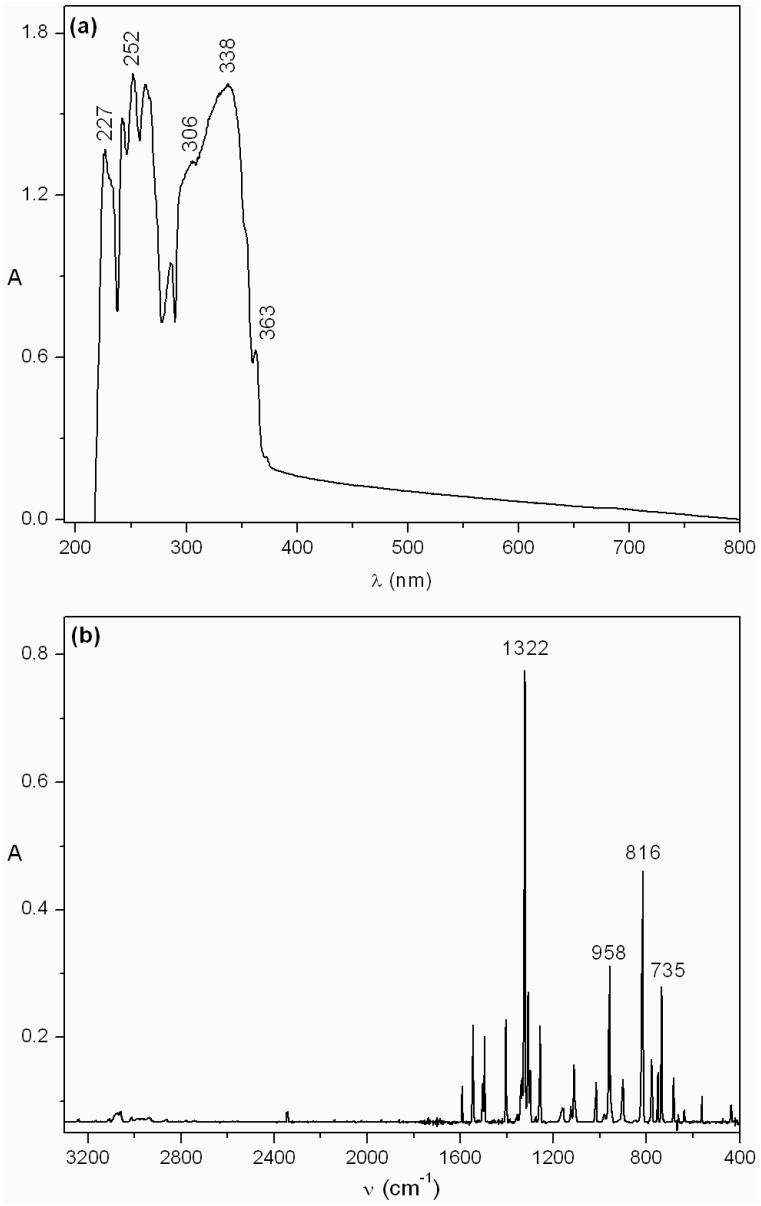


Figure S1. (a) UV spectrum of triazolo[1,5-*b*]pyridazine **8** in Ar matrix, and (b) the corresponding matrix IR spectrum, obtained by FVT of **8** at 200 ºC (8 x 10^{-6} mbar).

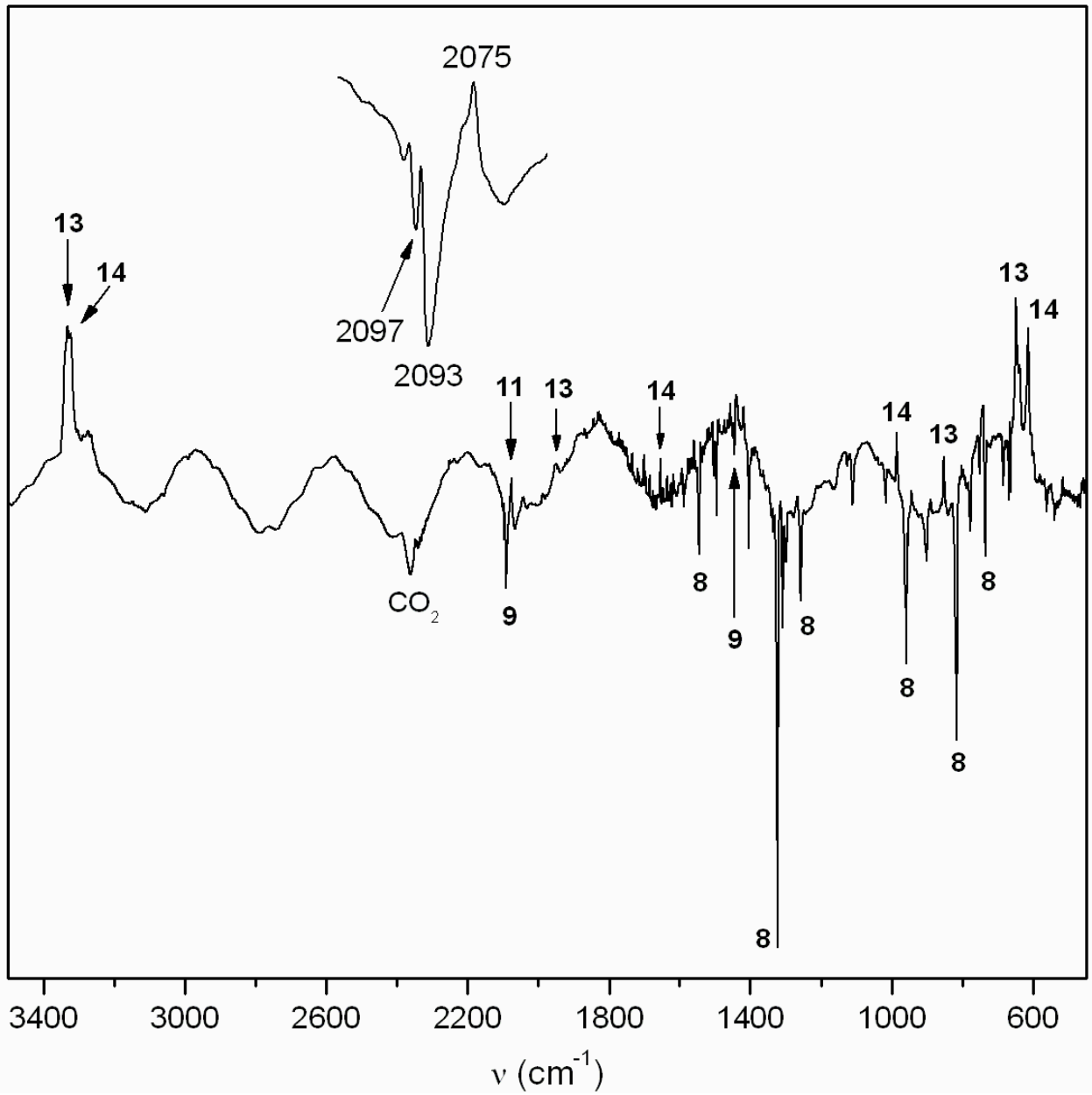


Figure S2. Difference IR spectrum showing a mixture of **11** as well as **13** and **14** (positive peaks), formed at the expense of triazole **8** and **9Z,E** (negative peaks), obtained by photolysis of **8** at 222 nm for 40 min. This spectrum is consistent with the order of photolysis **8** → **9** → **11** → **13**/**14**.

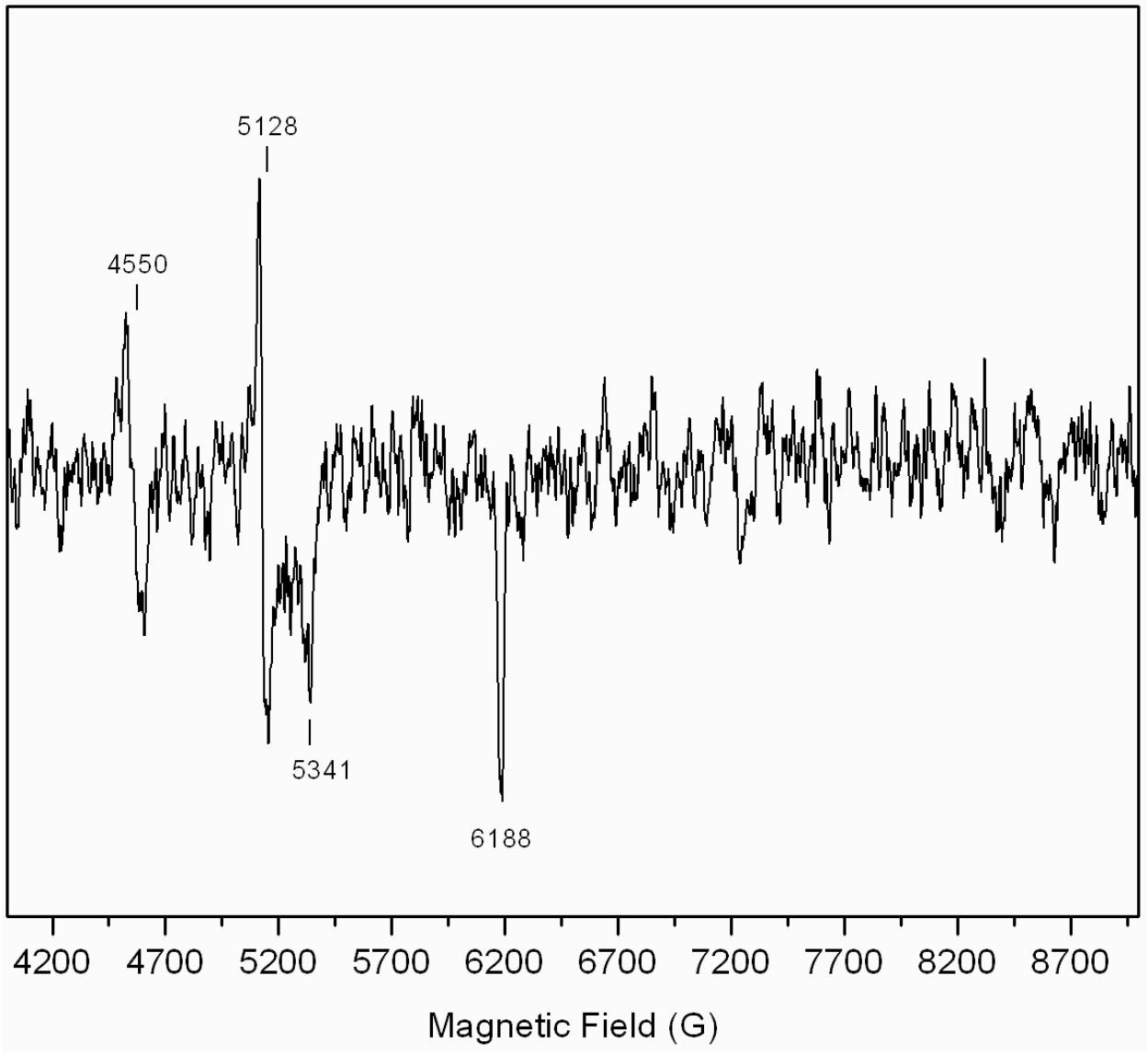


Figure S3. ESR spectrum obtained after 45 s of photolysis of **8** at 308 nm in Ar matrix (the spectrum is an early stage of the experiment described in Figure 3). The peaks are weak at short photolysis times, but the spectrum shows the presence of **10** (5128, 6188 G) and only one isomer of **12** (4550 ,5341 G)..

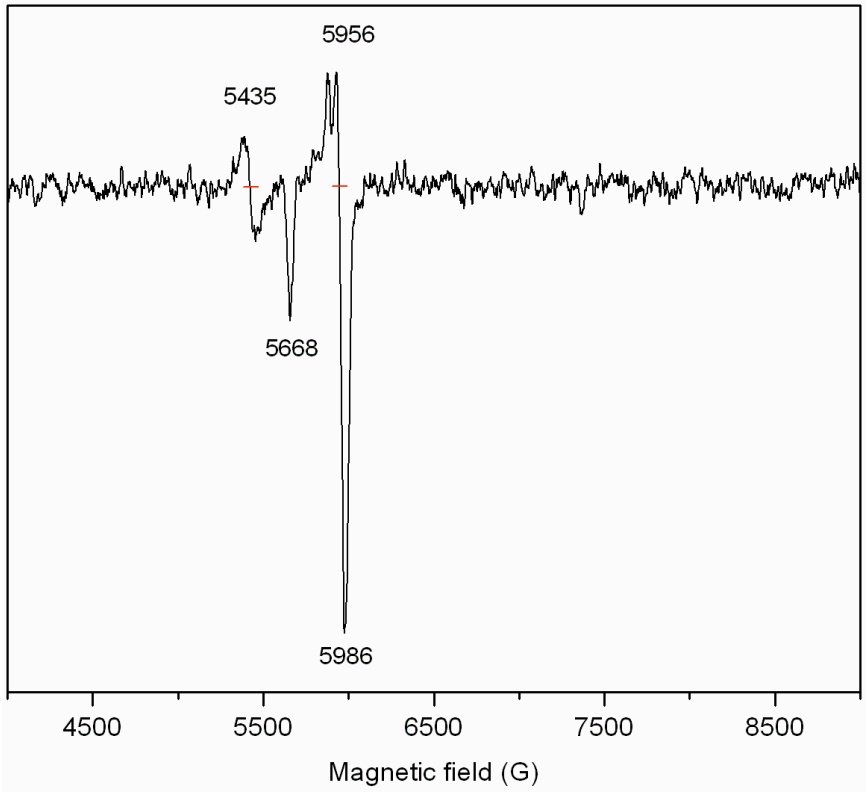
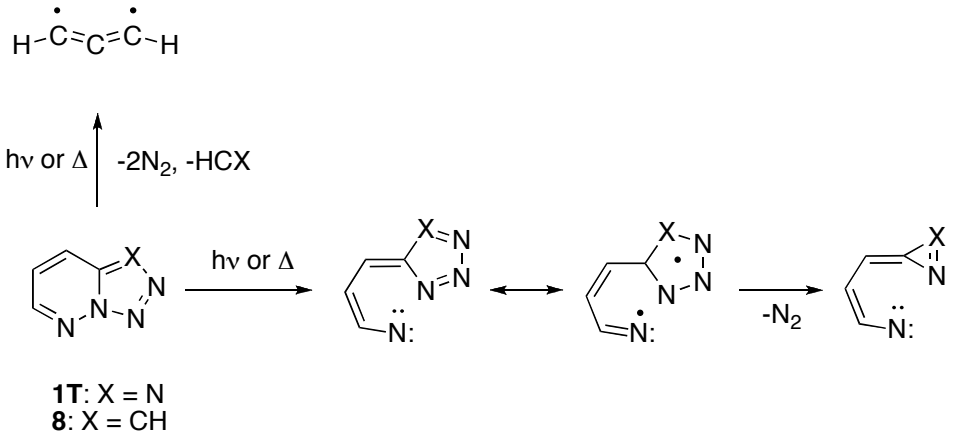


Figure S4. Difference ESR spectrum of unassigned triplet species after photolysis of **8** at 308 nm for 7 min (not shown) and 222 nm for 30 min. Ar matrix, 10-15 K.
Species **A**: D/hc = 0.5057 ; E/hc = 0.0057 cm^{-1} (**A**: X_2 = 5435; Y_2 = 5668 G).
Species **B**: D/hc = 0.6357; E/hc = 0.0007 cm^{-1} (**B**: X_2 = 5956; Y_2 = 5986 G). The apparent splitting of the X_2 signal is not always present.
Microwave frequency 9.7272 GHz, H_0= 3471 G.



Scheme S1. Potential carriers of the major triplet signal B (X_2= 5956; Y_2 = 5986 G) in Figure S4, which is formed on matrix photolysis of **8** and either FVT or photolysis of **1T**.

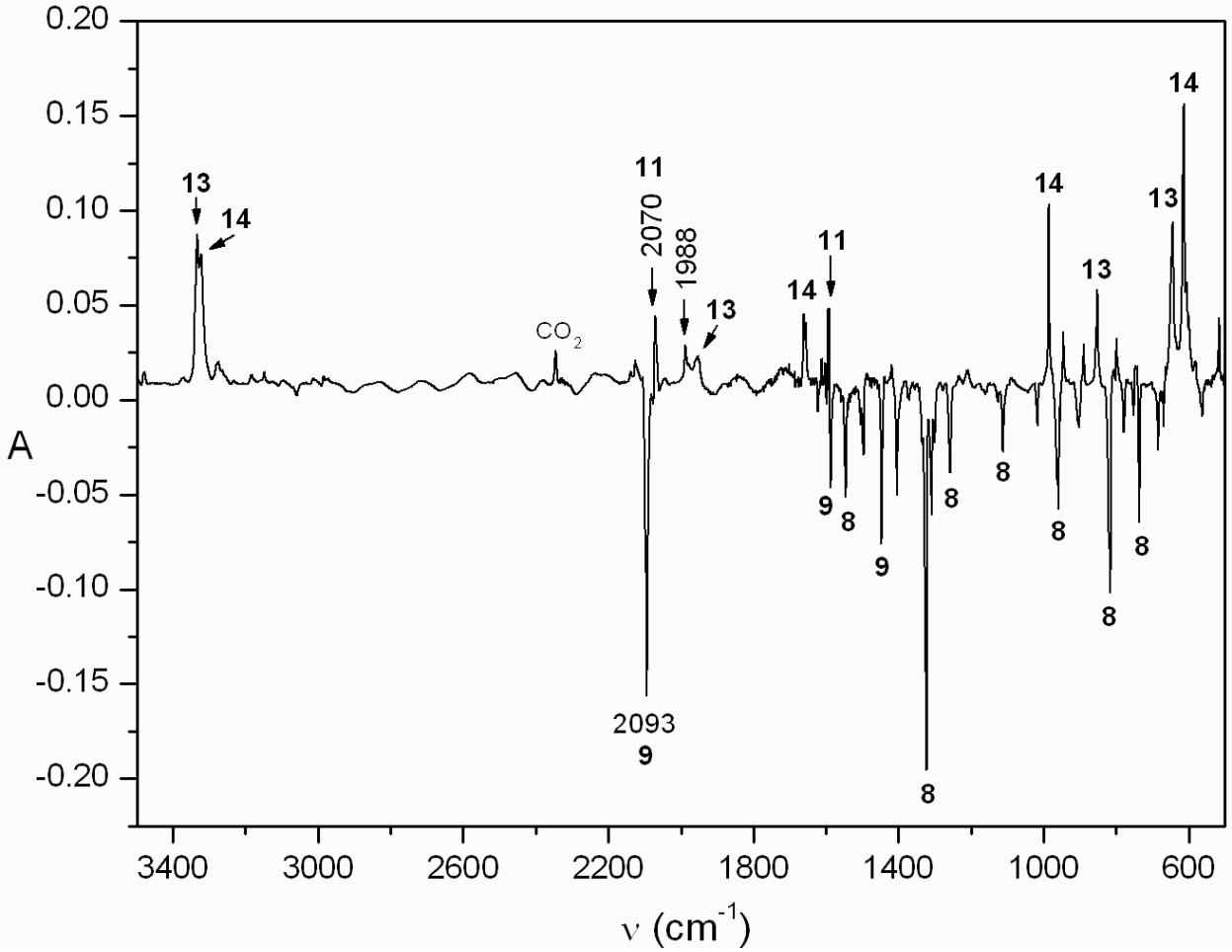


Figure S5. Ar matrix IR spectrum from prolonged photolysis of triazole **8** at 254 nm (low pressure Hg lamp). Positive peaks, a mixture of **11**, **13** and **14** after photolysis for 7 h. Negative peaks, a mixture of **9** and **8** after photoysis for 5 h. The positive peak at 1988 cm^{-1} is possibly due to cyclic carbodiimide **21** (see text).

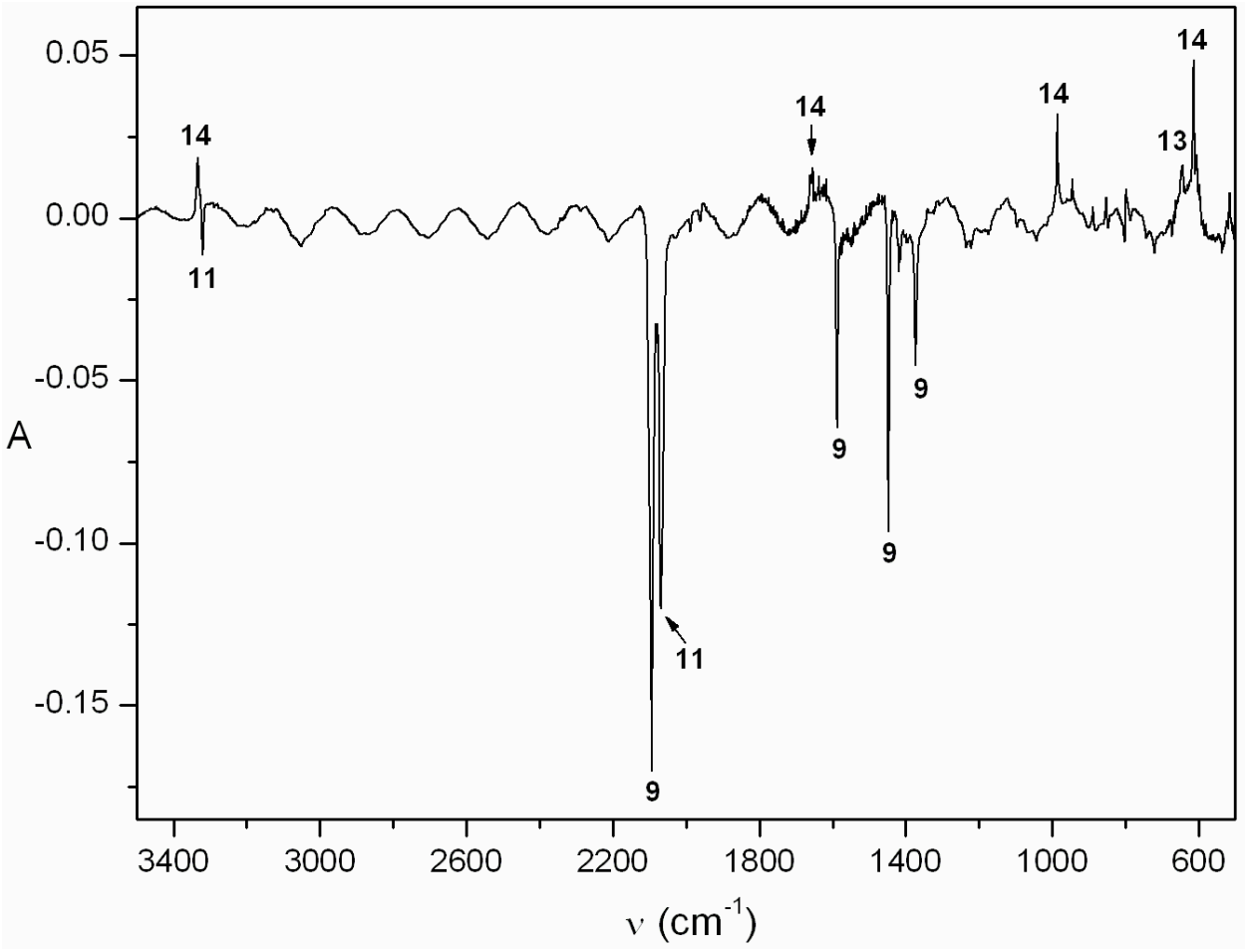


Figure S6. Matrix IR spectrum from photolysis of a mixture of diazo compounds **9** and **11** at 281 nm (interference filter) for 20 min (positive peaks, **14** and a trace of **13**), after initial photolysis of triazole **8** at 254 nm for 4 h (negative peaks, a mixture of **9** and **11**). The photolysis at 281 nm apparently does not touch the triazole **8** which has minimum absorption in the UV spectrum at 281 nm (Figure S1).

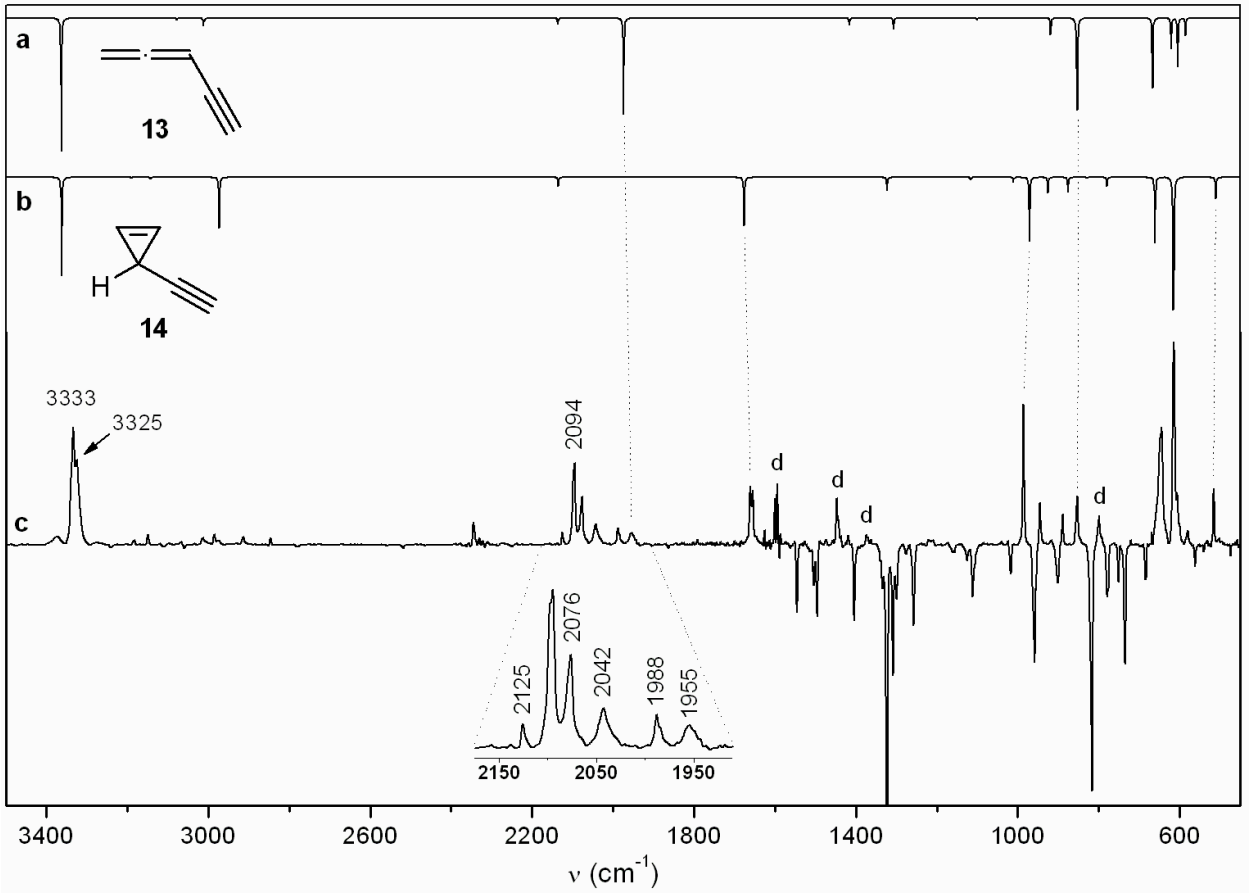


Figure S7. Matrix IR and calculated spectra of 1,2-pentadien-4-yne **13** and 3-ethynylcyclopropene **14**. (a) Calculated spectrum of **13**, and (b) calculated spectrum of **14** at the B3LYP/6-311G** level, wavenumbers scaled by 0.967. (c) Difference IR spectrum obtained after photolysis at 222 nm for 4 min, then > 405 nm for 45 min (not shown), and 308 nm for **13** min. The negative spectrum is due to triazole **8** before photolysis. Peaks belonging to the diazo compounds **9** (2094 cm^{-1}) are labeled "d". Diazo compound **11** appears at 2076 cm-1 (see also Figures 1 and 2). Allene **13** appears at 1955 cm^{-1}. The peak at 1988 $cm^{-1}$is possibly due to the cyclic carbodiimide **21**. The peak at 2042 cm^{-1} is assigned to a ketenimine (see paper proper).

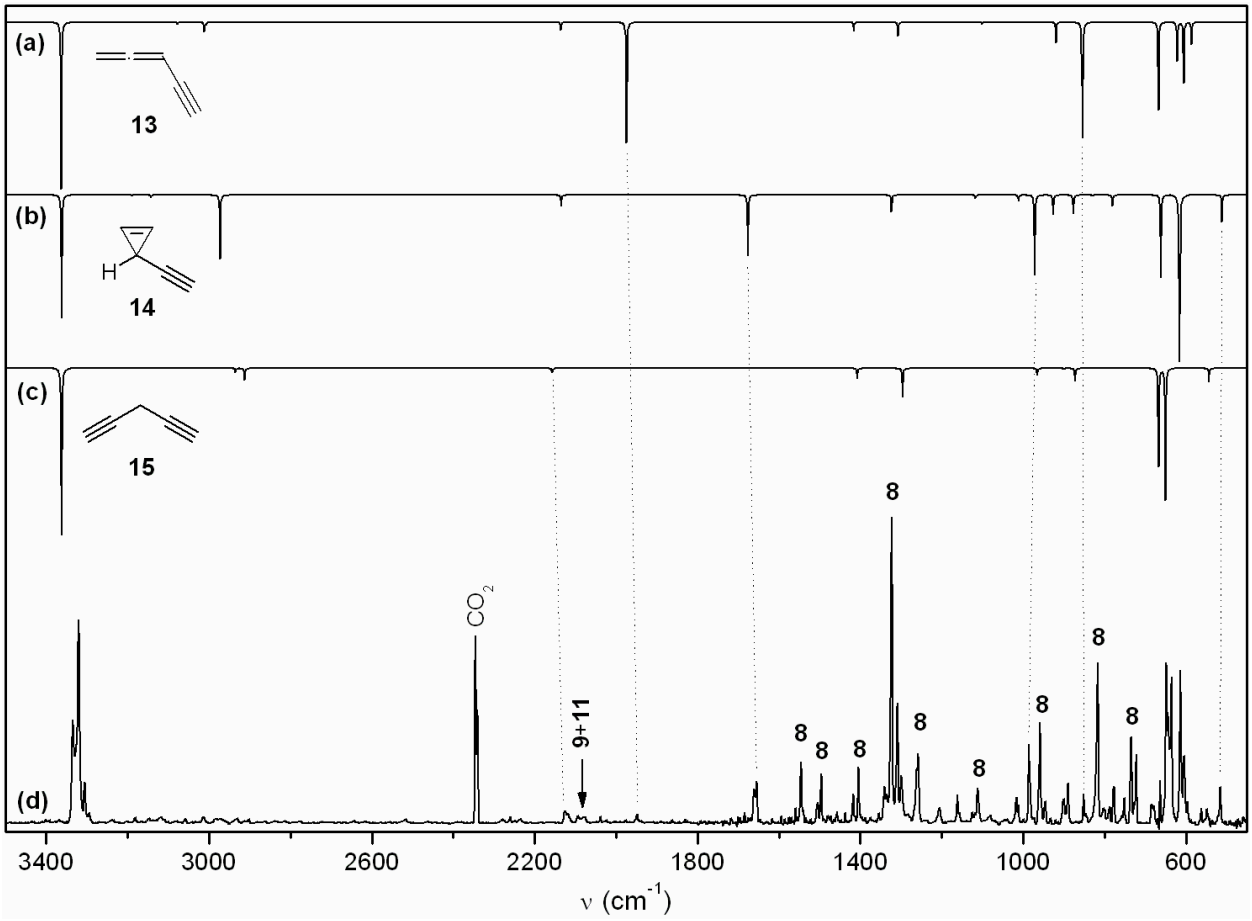


Figure S8. IR spectrum from the FVT of **8** at 600 °C, and calculated spectra showing absorptions of 1,4-pentadiyne **15**, 1,2-pentadien-4-yne **13**, and 3-ethynylcyclopropene **14**. (a) Calculated spectrum of **13**, (b) calculated spectrum of **14** and (c) calculated spectrum of 1,4-pentadiyne **15** at the B3LYP/6-311G** level, scaled by 0.967. (d) Product of FVT at 600 °C in Ar matrix, showing absorptions of **8**, **9**, **11**, **13**, **14**, and **15**. The presence of both diazo compounds, **9** and **11**, is indicated by the 2094-2071 bands.

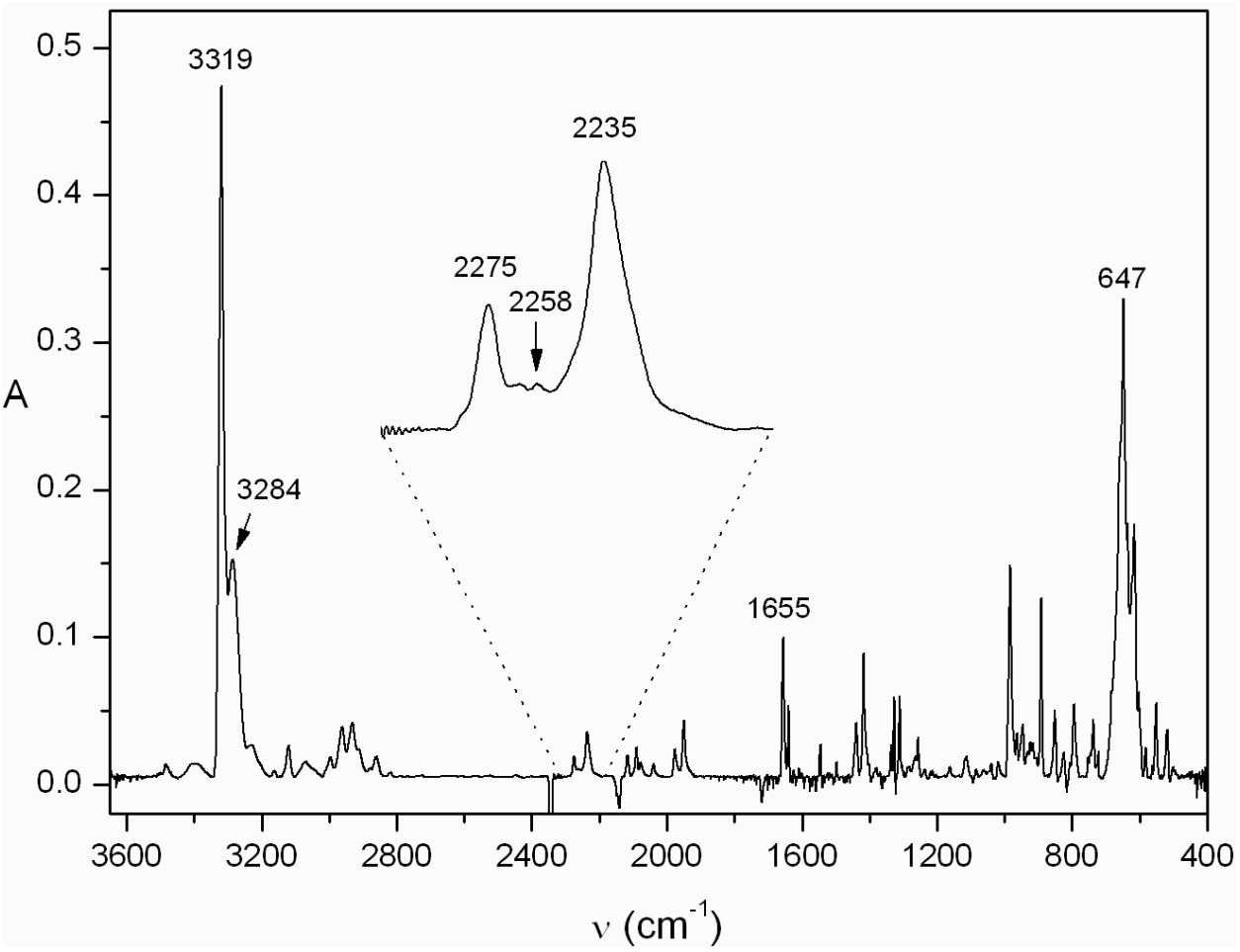


Figure S9. Ar matrix IR (difference) spectrum obtained from the FVT of **8** at 700 °C, showing CN peaks of glutacononitrile (2275 and 2235 cm^{-1}), 2-cyanopyrrole (2235 cm^{-1}), and 3-cyanopyrrole (2260 cm^{-1}). The absorption at 3284 cm^{-1} is probably due to NH stretches in cyanopyrroles. The strong band at 3319-3333 cm^{-1} is due to acetylenes **13-15**.

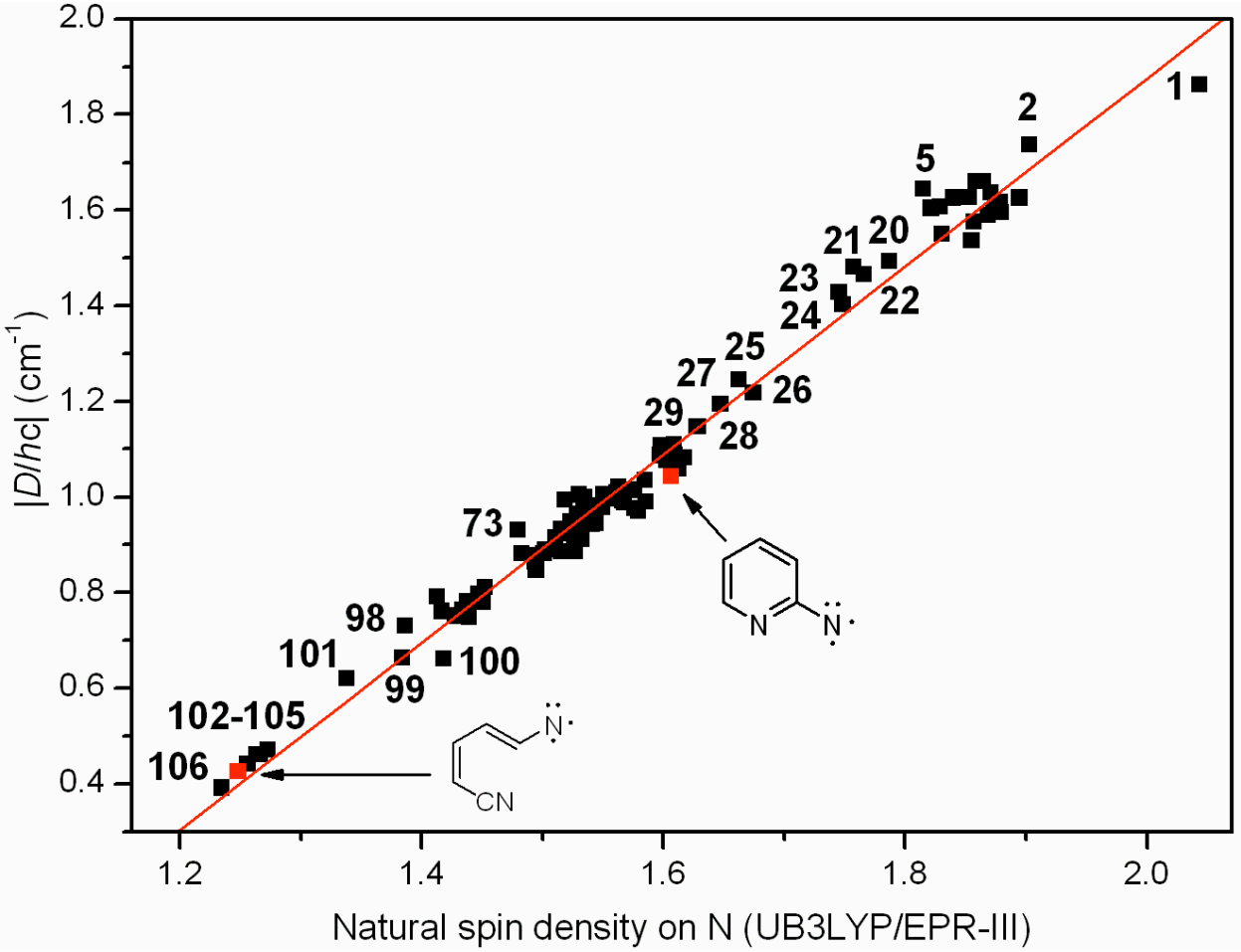


Figure S10. *D*-ρ correlation with data point for nitrene **19** (D = 1.0414 cm^{-1}, ρ = 1.6068), and nitrene **23** (D = 0.4253 cm^{-1}, ρ = 1.2486) added. For more details and complete list of nitrenes, see ref. 6.

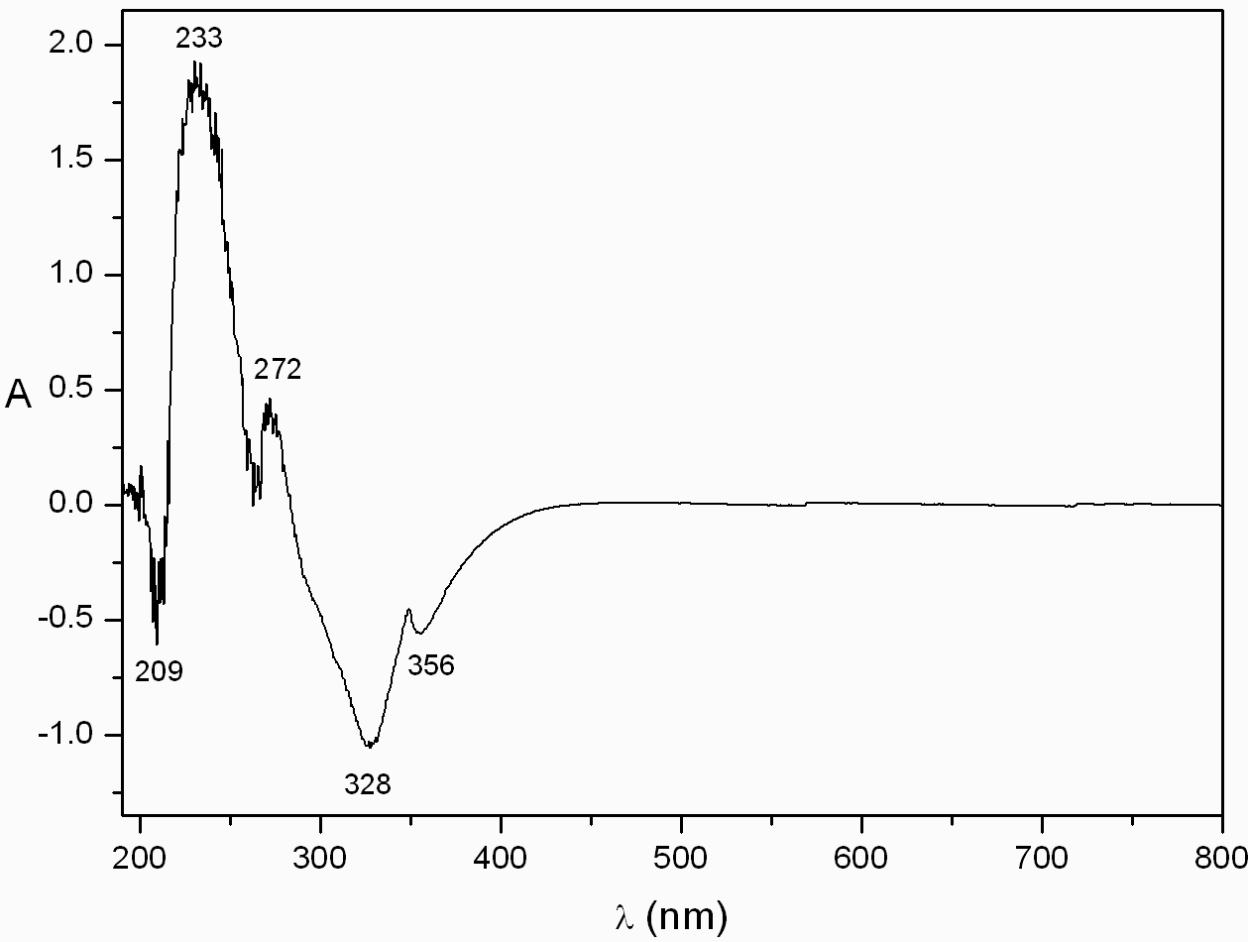


Figure S11. Difference UV spectrum obtained after photolysis of tetrazolopyridine **22T** in Ar matrix at 222 nm for 30 min (not shown), followed by 308 nm (30 min). Negative bands belong to diazacycloheptatetraene **21**. The product band at 233 and 272 nm are assigned to spiroazirene **25**, in relation to the corresponding matrix IR spectrum shown on Figure 7.

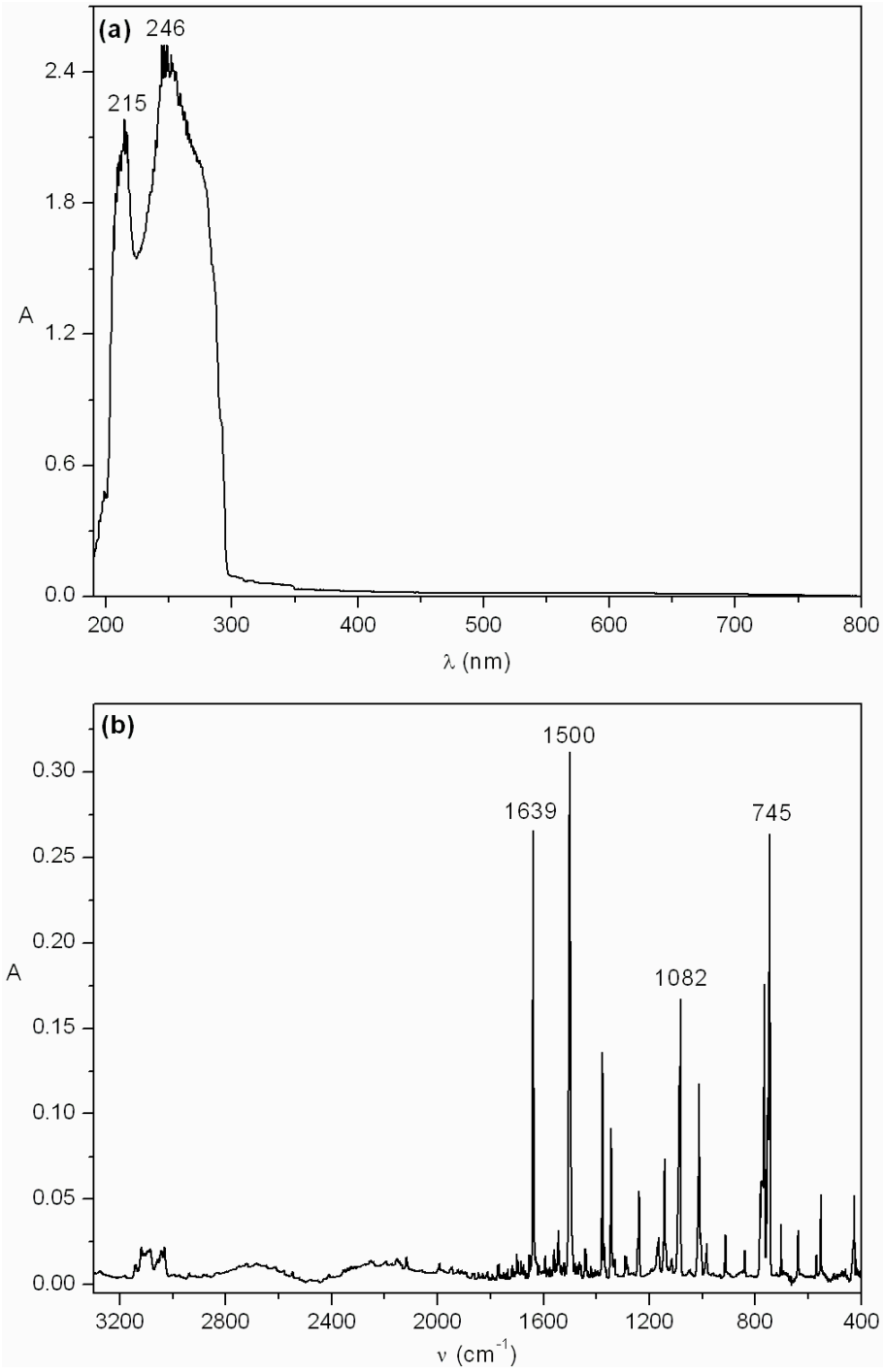


Figure S12. (a) Difference UV spectrum of tetrazolo[1,5-*a*]pyridine **22T** (Ar, 7K), and (b) its corresponding matrix IR spectrum, obtained from sublimation of **22T** at 80 ºC (8 x 10^{-6} mbar).

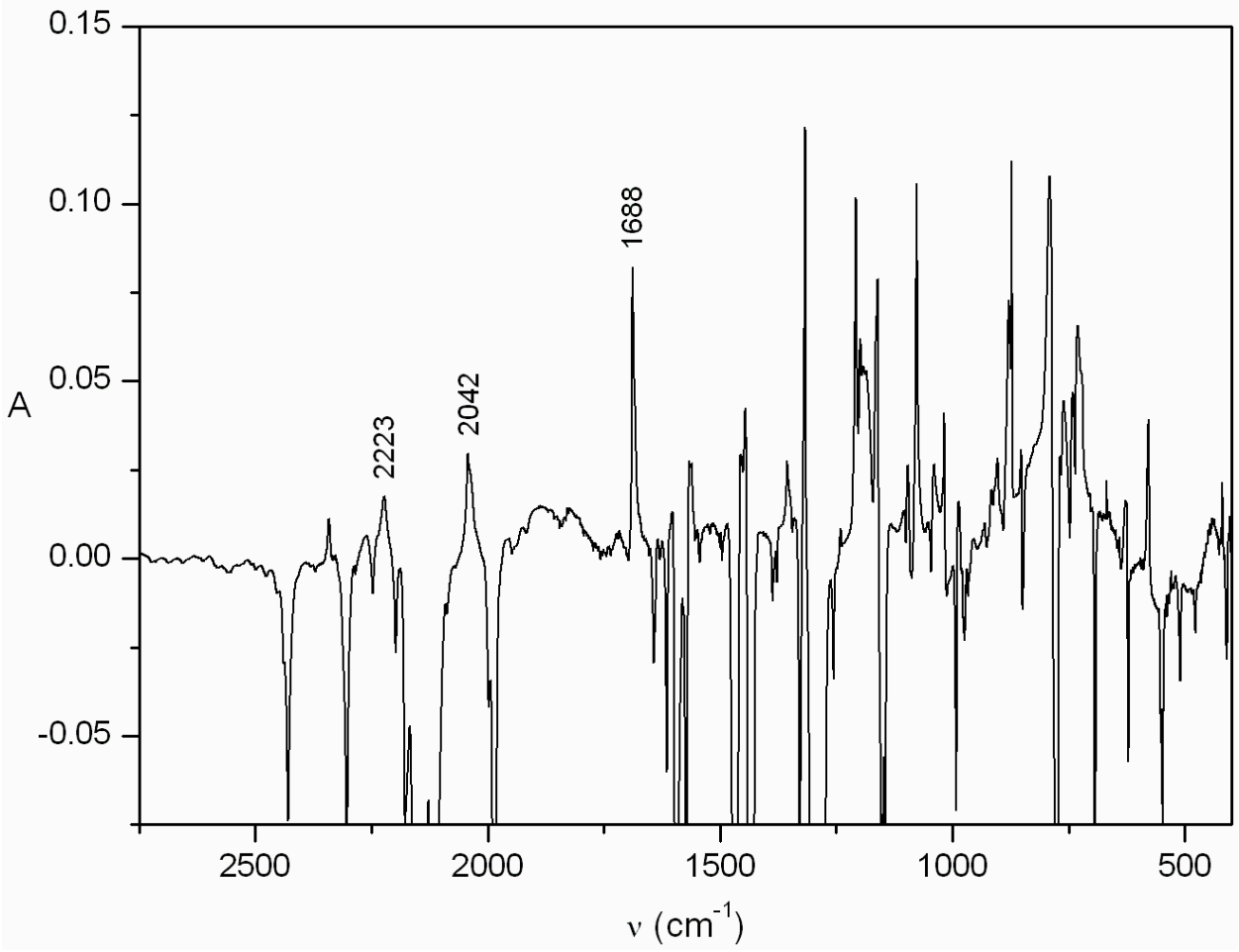


Figure S13. IR spectrum obtained after photolysis of 2-azidopyridine in Ar matrix at 254 nm (100 min), followed by 365 nm (310-390 nm interference filter) for 20 min. Negative bands are due to both 2-azidopyridine **22A** and diazacycloheptatetraene **21**. The same product bands are formed on photolysis of **21** at 308 nm (Figure 4). The product band at 2042 cm^{-1} is possibly due to ketenimine **26** or **39**. Other, unmarked bands are at 1316, 1207, 1200, 1077, 872, 787, and 577 cm^{-1}.

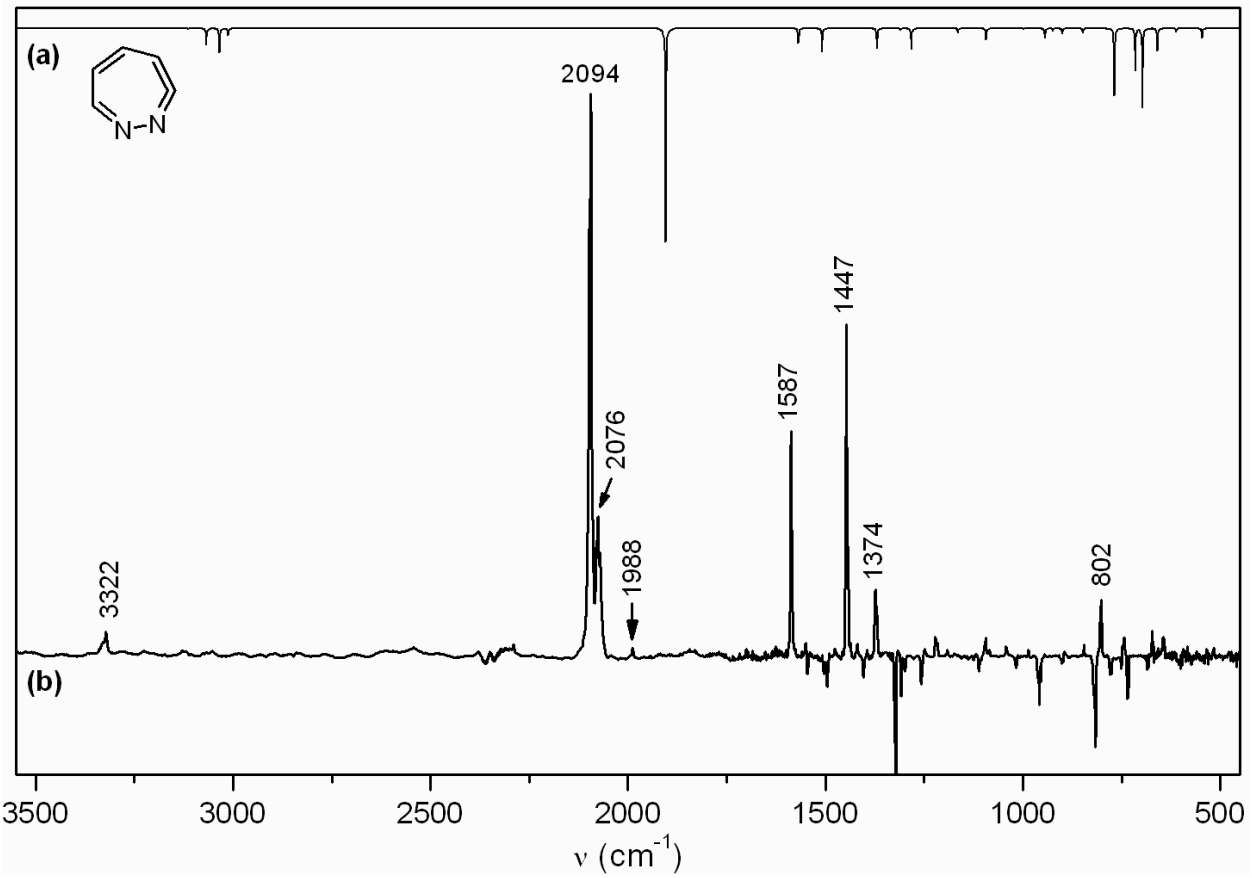


Figure S14. (a) Calculated spectrum of ketenimine **17** at the B3LYP/6-311G** level, wavenumbers scaled by 0.967. (b) Ar matrix IR spectrum resulting from photolysis of triazolopyridazine **8** at 222 nm for 2 min, showing prominent presence of diazo compounds and absence of **17**.

Complete citation for reference 32:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara,

A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. *Gaussian 03, Revision E.01*; Gaussian, Inc., Wallingford CT, 2004.

Complete citation for reference 36(b):

Andersson, K.; Barysz, M.; Bernhardsson, A.; Blomberg, M. R. A.; Carissan, Y.; Cooper,D. L.; Cossi, M.; Devarajan, A.; Fülscher, M. P.; Gaenko, A.; Gagliardi, L.; de Graaf, C.; Hess, B. A.; Hagberg, D.; Karlström, G.; Krogh, J. W.; Lindh, R.; Malmqvist, P.-Å.; Nakajima, T.; Neogrády, P.; Olsen, J.; Pedersen, T. B.; Raab, J.; Roos, B. O.; Ryde, U.; Schimmelpfennig, B.; Schütz, M.; Seijo, L.; Serrano-Andrés, L.; Siegbahn, P. E. M.; Stålring, J.; Thorsteinsson, T.; Veryazov, V.; Widmark, P.-O. *MOLCAS*, version 7.2, University of Lund: Sweden, 2008.

Computational Data

Table S1. Summary of the relative energies of species calculated at the B3LYP/6-31G*, CAS(8,8)/6-31G* and CASPT2//CAS(8,8)/6-31G* level

Energies relative to triplet 2-pyridylnitrene **19T$_0$** in kcal/mol (or kJ/mol).

§ Relative energy of open-shell species where triplet contamination is non-negligible, i.e. $\langle S^2 \rangle \neq 0$ (UB3LYP/6-31G* only). For cases where $\langle S^2 \rangle \cong 1$, the energies were corrected using the Ziegler-Cramer's method (ref. 24); see notes to Table S2.

Structure	Relative Energy (kcal/mol)#			Relative Energy (kJ/mol)#		
	B3LYP	CASSCF	CASPT2	B3LYP	CASSCF	CASPT2
10Z T_0	44.2	--	--	184.8	--	--
10Z S_1	55.0	58.9	64.4	230.2	246.4	269.4
10E T_0	45.6	--	--	191.0	--	--
10E S_1	59.0	62.4	68.1	246.7	261.1	284.9
10Z → 10E TS	61.8	--	--	258.5	--	--
10Z → 11Z TS	66.4	--	--	277.6	--	--
10Z → 16 TS	65.7	80.0	76.1	274.9	334.7	318.4
10E → 16 TS	69.0	82.9	76.6	288.9	346.9	320.5
10Z → 42 TS	68.6	--	--	287.0	--	--
10E → 42 TS	69.5	--	--	290.8	--	--
11Z	28.9	--	--	120.8	--	--
11E	26.5	--	--	111.0	--	--

11Z → 11E TS	37.5	--	--	157.1	--	--
11Z → 12E TS	65.5	--	--	273.9	--	--
12Z T_0 + N_2	47.7	--	--	199.4	--	--
12Z S_1 + N_2	62.8	--	--	262.8	--	--
12E T_0 + N_2	47.7	--	--	199.5	--	--
12E S_1 + N_2	64.0	--	--	267.8	--	--
12E → 13 TS + N_2	69.1	--	--	289.2	--	--
12E → 14 TS + N_2	66.4	--	--	278.0	--	--
12E → 15 TS + N_2	80.2	--	--	335.5	--	--
13 + N_2	4.4	--	--	18.2	--	--
14 + N_2	29.0	--	--	121.5	--	--
15 + N_2	15.1	--	--	63.2	--	--
16	51.2	66.6	50.7	214.3	278.6	212.2
16 → 17 TS	52.4	75.8	47.2	219.3	317.2	197.5
17	27.5	35.1	25.5	115.1	146.9	106.5
17 → 18 TS	40.9	--	--	171.3	--	--
17 → 19 S_1 TS	--	62.3	40.0	--	260.7	167.3
17 → 23 S_1 TS	39.6[§]	39.4	39.0	165.9[§]	164.8	163.0
17 → 17' TS	55.4	--	--	231.7	--	--
17'	47.1	--	--	196.9	--	--
18	34.3	--	--	143.4	--	--
18 → 19 TS	36.3	--	--	152.0	--	--
19 T_0	0	0	0	0	0	0
19 S_1	16.2[§]	18.6	19.7	67.8[§]	77.7	82.5
19 S_2	37.5	43.3	37.6	157.0	181.2	157.2
19 S_1 → 20 TS	22.5[§]	44.0	45.1	94.1[§]	184.1	188.7
19 T_0 → 23ZZ T_0 TS	29.0	31.8	36.5	121.3	133.1	152.7
19 S_1 → 23ZZ S_1 TS	24.2[§]	26.4	22.7	101.1[§]	110.5	95.0
19 → 32 TS	48.6	--	--	203.5	--	--
19 → 33 TS	52.3	67.7	47.3	218.8	283.3	197.8
20	13.1	18.1	10.1	55.0	75.6	42.2
20 → 21 TS	13.7	37.3	11.8	57.1	156.0	49.5

21	2.6	13.5	0.5	10.8	56.3	1.9
21 → 24 TS	49.0	70.4	46.7	205.0	294.6	195.4
23ZZ T_0	20.1	22.1	23.6	84.3	92.3	98.7
23ZZ S_1	16.3[§]	29.4	30.8	68.2[§]	122.9	128.9
23EZ T_0	15.7	16.3	18.1	65.8	68.1	75.8
23EZ S_1	11.9[§]	23.6	25.3	49.7[§]	98.6	106.1
23ZZ T_0 → 23EZ T_0 TS	24.8	--	--	104.0	--	--
23ZZ S_1 → 23EZ S_1 TS	24.6[§]	--	--	102.9[§]	--	--
23ZZ → 26Z TS	49.8	54.6	42.4	208.3	228.4	177.3
23ZZ → 27Z TS	49.0	--	--	205.1	--	--
23EZ → 27Z TS	45.5	--	--	190.3	--	--
23ZZ S_1 → 32 TS	29.1[§]	29.5	30.4	121.8[§]	123.3	127.1
24	20.8	25.0	12.7	87.0	104.7	53.3
24 → 25 TS	28.7	34.7	22.8	120.2	145.0	95.5
25	6.6	9.0	0.9	27.7	37.7	3.8
25 → 36 TS	43.7	51.5	42.0	183.0	215.5	175.8
25 → 38 S_1 TS	21.6[§]	--	--	90.4[§]	--	--
26Z	-12.6	-18.1	-10.1	-52.7	-75.9	-42.4
26Z → 27Z TS	30.7	--	--	128.4	--	--
27Z	-28.7	--	--	-120.3	--	--
27E	-29.3	--	--	-122.5	--	--
28	-45.0	--	--	-188.2	--	--
29	-45.7	--	--	-191.0	--	--
29 → 35 TS	1.5	--	--	6.3	--	--
30	9.9	-7.5	5.5	41.6	-31.5	22.9
32	-22.9	-42.9	-32.4	-96.0	-179.4	-135.5
32 → 28 TS	5.7	--	--	24.0	--	--
32 → 33 TS	17.9	30.0	10.3	74.8	125.4	43.0
32 → 34 TS	12.4	--	--	51.7	--	--
33	-30.7	-8.7	-38.2	-128.6	-36.4	-159.7
34	-21.1	--	--	-88.4	--	--
34 → 35 TS	-0.0	--	--	-0.1	--	--

35	-31.7	--	--	-132.5	--	--
36	4.1	20.9	1.9	17.2	87.3	8.1
36 → 40 TS	45.6	62.4	42.1	190.7	260.9	176.2
36 → 41 TS	50.4	--	--	211.0	--	--
37Z T_0	27.4	--	--	114.6	--	--
37E T_0	27.4	--	--	114.8	--	--
38Z T_0	15.3	16.9	15.9	64.2	70.8	66.7
38Z S_1	19.4[§]	25.5	24.1	81.2[§]	106.5	100.8
38E T_0	12.5	14.4	12.9	52.4	60.2	54.1
38E S_1	16.3[§]	21.8	20.2	68.2[§]	91.1	84.6
38 S_1 → 32 TS	37.5	51.2	36.2	156.8	214.4	151.6
38Z T_0 → 38E T_0 TS	22.9	--	--	95.9	--	--
38Z S_1 → 38E S_1 TS	22.9[§]	--	--	95.7[§]	--	--
38 → 39 TS	43.4	59.5	42.2	181.8	249.1	176.7
39	-14.8	-1.2	-13.6	-62.0	-5.2	-56.8
39 → 28 TS	34.0	--	--	142.3	--	--
40	-1.1	-17.1	-7.1	-4.8	-71.5	-29.7
40 → 41 TS	28.6	40.2	27.4	119.7	168.4	114.8
41	-21.6	--	--	-90.5	--	--
41 → 28 TS	13.4	--	--	56.1	--	--
42	60.8	--	--	254.5	--	--
42 → 43 TS	60.6	--	--	253.5	--	--
43	39.9	--	--	166.8	--	--

Table S2. Cartesian Coordinates and Calculated Energies (B3LYP/6-31G*)

Open-shell singlet species were computed at the UB3LYP/6-31G* level. In cases where $<S^2>=1$ (e.g. open-shell singlet nitrenes), the energy was corrected using the sum method of Cramer and Ziegler[1]: "The energy is computed as $E(S_1) = 2\,E(50{:}50) - E(T_0)$ where $E(50{:}50)$ is the energy of the broken symmetry unrestricted DFT wave function having an expectation value of 1 for the $<S^2>$ operator applied to a Slater determinant formed from the DFT orbitals (i.e., the exact wave function for the non-interacting Kohn–Sham reference system), and $E(T_0)$ is the energy of the triplet".

Natural spin densities[2] were computed at the UB3LYP/EPR-III level.

The UV-Vis spectra were calculated at the TD-B3LYP/6-311+G** level using Gaussian03, and convoluted using the SWizard program[3,4], revision 4.6, using the Lorentzian model. The half-bandwidths, $\Delta_{1/2,I}$, were taken to be equal to 3000 cm^{-1}.

(1). Johnson, W. T. G.; Sullivan, M. B.; Cramer, C. J. *Int. J. Quant. Chem.* **2001,** *85*, 492.

(2). NBO Version 3.1, Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. Gaussian 03, Revision E.01.

(3). S. I. Gorelsky, *SWizard program*, http://www.sg-chem.net/, University of Ottawa, Ottawa, Canada, 2009.

(4). S. I. Gorelsky, A. B. P. Lever, *J. Organomet. Chem.* **2001**, *635*, 187-196.

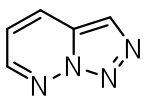
Nitrogen (N_2)

Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.00000000	0.00000000	0.55275074
N	0.00000000	0.00000000	-0.55275074

State=1-Σ^+_g
RB3LYP/6-31G(d), HF= -109.5241291
Zero-point correction= 0.005599 (Hartree/Particle)
Sum of electronic and zero-point Energies= -109.518530

8

[1,2,3]Triazolo[1,5-*b*]pyridazine

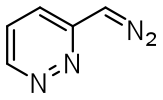


Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.28778315	0.76781820	0.00000000
C	-0.96348815	1.42636700	0.00000000
C	-2.09173133	0.64980057	0.00000000
C	-1.95396545	-0.77177028	0.00000000
C	1.64726027	1.05655870	0.00000000
H	-1.00558980	2.51077729	0.00000000
H	-3.08330072	1.08874273	0.00000000
H	-2.83225797	-1.41073809	0.00000000
H	2.14358511	2.01615028	0.00000000
N	-0.81330840	-1.41949565	0.00000000
N	0.27128778	-0.62557724	0.00000000
N	1.51972036	-1.13366599	0.00000000
N	2.33978987	-0.10358523	0.00000000

State=1-A'
RB3LYP/6-31G(d), HF= -411.8661617
Zero-point correction= 0.093829 (Hartree/Particle)
Sum of electronic and zero-point Energies= -411.772332

9Z

(*s-Z*)-3-(diazomethyl)pyridazine



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.412577	0.000000
C	-1.236521	1.091201	0.000000
C	-2.378089	0.317422	0.000000
C	-2.216335	-1.074288	0.000000
H	-1.276313	2.177020	0.000000
H	-3.368542	0.763199	0.000000
H	-3.069684	-1.746875	0.000000
C	1.247125	1.150179	0.000000
N	0.085131	-0.935011	0.000000
N	-1.021569	-1.670242	0.000000
N	2.391830	0.520071	0.000000
H	1.302345	2.230632	0.000000
N	3.389623	-0.030036	0.000000

State=1-A'
RB3LYP/6-31G(d), HF= -411.8443318
Zero-point correction= 0.090362 (Hartree/Particle)
Sum of electronic and zero-point Energies= -411.753970

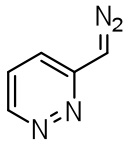
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	84.8	1.9	0

2	A'	121.7	0.0	0
3	A"	201.8	6.6	1
4	A'	319.0	4.9	1
5	A"	370.6	0.0	0
6	A'	446.3	1.1	0
7	A"	458.2	22.7	3
8	A"	517.3	2.7	0
9	A"	548.6	18.8	3
10	A'	624.4	0.0	0
11	A'	665.3	7.8	1
12	A"	737.8	7.4	1
13	A"	792.3	42.4	6
14	A'	836.4	8.1	1
15	A"	903.0	0.3	0
16	A"	970.2	0.1	0
17	A'	997.6	7.4	1
18	A'	1027.9	1.6	0
19	A'	1096.7	13.7	2
20	A'	1135.1	7.7	1
21	A'	1140.2	0.5	0
22	A'	1176.4	4.1	1
23	A'	1201.7	28.1	4
24	A'	1357.3	53.0	8
25	A'	1379.5	5.3	1
26	A'	1428.7	199.4	28
27	A'	1527.7	10.9	2
28	A'	1564.3	123.3	18
29	A'	2141.6	702.6	100
30	A'	3064.6	1.5	0
31	A'	3072.9	14.0	2
32	A'	3087.9	13.4	2
33	A'	3123.2	2.8	0

9E

(*s-E*)-3-(diazomethyl)pyridazine



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.350046	0.000000
C	0.028845	-1.060065	0.000000
C	-1.185998	-1.712981	0.000000
C	-2.344429	-0.925650	0.000000
H	0.969022	-1.604462	0.000000
H	-1.248839	-2.797218	0.000000
H	-3.335771	-1.370416	0.000000
C	1.186609	1.185729	0.000000
H	1.105295	2.264805	0.000000
N	-1.155659	1.050543	0.000000
N	-2.319151	0.409182	0.000000

N	2.385334	0.679007	0.000000
N	3.432350	0.216243	0.000000

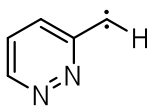
State=1-A'
RB3LYP/6-31G(d), HF= -411.8439885
Zero-point correction= 0.090395 (Hartree/Particle)
Sum of electronic and zero-point Energies= -411.753593

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	79.3	2.2	0
2	A'	124.8	4.5	1
3	A"	203.1	9.0	1
4	A'	337.9	5.9	1
5	A"	371.1	0.0	0
6	A"	451.8	10.8	1
7	A'	453.7	0.1	0
8	A"	518.3	2.6	0
9	A"	588.4	33.2	5
10	A'	622.5	0.1	0
11	A'	665.0	7.9	1
12	A"	736.6	5.1	1
13	A"	791.3	40.8	6
14	A'	823.3	2.3	0
15	A"	903.7	0.0	0
16	A"	971.6	0.0	0
17	A'	993.8	7.5	1
18	A'	1025.6	2.6	0
19	A'	1086.3	20.5	3
20	A'	1128.3	17.3	2
21	A'	1146.7	3.7	1
22	A'	1162.0	1.7	0
23	A'	1228.9	18.5	3
24	A'	1338.8	10.5	1
25	A'	1394.1	23.5	3
26	A'	1421.2	183.2	25
27	A'	1525.3	1.1	0
28	A'	1564.3	74.9	10
29	A'	2114.2	733.8	100
30	A'	3066.2	0.6	0
31	A'	3074.0	10.2	1
32	A'	3089.2	11.0	1
33	A'	3122.0	13.6	2

10Z Triplet T_0

(*s-Z*)-3-pyridazinyl-carbene



Atom	Coordinates (Angstroms)

Type	X	Y	Z
N	-1.217837	-1.002591	0.000000
N	-1.206535	0.319167	0.000000
C	0.000000	0.988460	0.000000
C	1.239748	0.290902	0.000000
C	1.197343	-1.084789	0.000000
C	-0.067124	-1.691713	0.000000
H	2.173665	0.844276	0.000000
H	2.101833	-1.685897	0.000000
H	-0.179920	-2.772349	0.000000
C	-0.073490	2.383799	0.000000
H	-0.903832	3.077983	0.000000

State=3-A"
<S2>= 2.036227
UB3LYP/6-31G(d), HF= -302.2673994
Zero-point correction= 0.077627 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.189773

Natural Atomic Spin Densities (UB3LYP/EPR-III)

1	N	-0.07105
2	N	0.25975
3	C	-0.14835
4	C	0.19103
5	C	-0.08745
6	C	0.20491
7	H	-0.00604
8	H	0.00296
9	H	-0.00626
10	C	1.67529
11	H	-0.01480

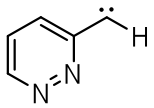
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	179.2	5.1	16
2	A'	333.8	9.2	30
3	A"	348.5	0.0	0
4	A"	445.5	6.7	22
5	A'	555.6	1.0	3
6	A"	555.8	20.8	67
7	A'	615.6	1.3	4
8	A"	716.5	8.8	28
9	A"	778.4	30.7	99
10	A'	804.5	12.2	39
11	A'	852.4	8.4	27
12	A"	900.0	0.1	0
13	A'	937.4	4.9	16
14	A"	969.1	0.0	0
15	A'	1015.5	1.0	3
16	A'	1070.2	11.2	36
17	A'	1095.1	9.3	30
18	A'	1167.7	1.5	5
19	A'	1277.5	2.6	8

20	A'	1297.7	4.5	15
21	A'	1387.8	6.1	20
22	A'	1493.8	10.0	32
23	A'	1530.0	9.0	29
24	A'	3069.0	1.1	3
25	A'	3080.3	10.2	33
26	A'	3092.2	8.3	27
27	A'	3136.6	4.6	15

10Z Singlet S_1

(*s-Z*)-3-pyridazinyl-carbene

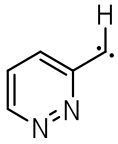


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.240931	-0.989825	0.000000
N	-1.201076	0.328311	0.000000
C	0.000000	0.986568	0.000000
C	1.222486	0.281773	0.000000
C	1.183059	-1.103811	0.000000
C	-0.083136	-1.685346	0.000000
H	2.145841	0.851740	0.000000
H	2.080164	-1.715572	0.000000
H	-0.208804	-2.765301	0.000000
C	0.029871	2.439719	0.000000
H	-1.036835	2.746307	0.000000

State=1-A'
RB3LYP/6-31G(d), HF= -302.2499286
Zero-point correction= 0.077441 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.172487

10E Triplet T_0

(*s-E*)-3-pyridazinyl-carbene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.291063	-0.953506	0.000000
N	-1.227345	0.364896	0.000000
C	0.000000	0.988942	0.000000
C	1.214280	0.240676	0.000000
C	1.117952	-1.132774	0.000000
C	-0.168512	-1.689156	0.000000

H	2.172876	0.751196	0.000000
H	1.999224	-1.767786	0.000000
H	-0.324051	-2.764423	0.000000
C	0.002466	2.386507	0.000000
H	0.783691	3.136109	0.000000

State=3-A"
<S2>= 2.036951
UB3LYP/6-31G(d), HF= -302.2649169
Zero-point correction= 0.077482 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.187434

Natural Atomic Spin Densities (UB3LYP/EPR-III)

1	N	-0.08604
2	N	0.24206
3	C	-0.14936
4	C	0.21299
5	C	-0.08583
6	C	0.20692
7	H	-0.00653
8	H	0.00533
9	H	-0.00686
10	C	1.68407
11	H	-0.01676

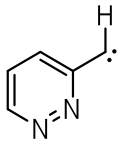
Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	175.5	4.8	15
2	A'	340.0	2.8	9
3	A"	348.5	1.2	4
4	A"	454.9	4.6	14
5	A"	506.7	13.6	43
6	A'	556.3	0.4	1
7	A'	616.6	0.0	0
8	A"	716.1	11.8	37
9	A"	773.5	32.4	101
10	A'	792.9	18.3	57
11	A'	844.1	6.8	21
12	A"	896.8	0.2	1
13	A'	962.9	1.6	5
14	A"	965.0	0.0	0
15	A'	1018.7	0.7	2
16	A'	1080.7	13.0	41
17	A'	1097.8	8.6	27
18	A'	1165.2	3.4	11
19	A'	1272.6	1.4	5
20	A'	1305.6	3.4	11
21	A'	1379.5	8.2	26
22	A'	1489.8	7.2	23
23	A'	1522.6	7.9	25
24	A'	3066.3	0.4	1
25	A'	3077.3	10.5	33
26	A'	3088.4	10.9	34

27	A'	3131.4	0.5	1

10E Singlet S_1

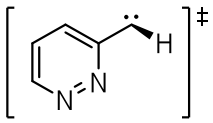
(*s-E*)-3-pyridazinyl-carbene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.008878	-1.244064	0.039633
N	0.307372	-1.234297	0.014285
C	0.988575	-0.043607	0.026696
C	0.299499	1.192486	0.044155
C	-1.083569	1.176227	-0.036383
C	-1.687932	-0.079081	-0.026635
H	0.857078	2.122835	0.107563
H	-1.677556	2.085124	-0.064364
H	-2.768727	-0.188897	-0.064871
C	2.425169	-0.159298	-0.107261
H	2.849294	0.809109	0.240818

State=1-A
RB3LYP/6-31G(d), HF= -302.2433778
Zero-point correction= 0.077170 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.166208

TS 10Z → 10E

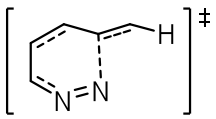


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.008401	-1.230897	0.012305
N	0.316810	-1.238189	-0.010029
C	0.985090	-0.042520	-0.014131
C	0.301474	1.203420	-0.008625
C	-1.074915	1.161068	0.004402
C	-1.698737	-0.092606	0.011797
H	0.842522	2.144398	-0.023491
H	-1.661873	2.074679	0.012385
H	-2.779265	-0.199734	0.018532
C	2.411713	-0.029790	-0.139677
H	2.892011	0.066829	0.854041

State=1-A

RB3LYP/6-31G(d), HF= -302.2368432
Zero-point correction= 0.075123 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.161720
Imaginary frequency: -518.3 cm^{-1}

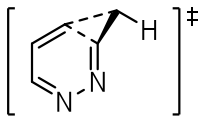
TS 10Z → 11Z



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.92496483	-1.22334613	-0.00481600
N	0.30415818	-1.31688096	0.00651800
C	1.11470698	0.15128816	0.01730500
C	0.21778782	1.25725903	0.02622400
C	-1.14998315	1.10278584	-0.01574300
C	-1.74099398	-0.16251824	-0.00275200
H	0.64769968	2.24973609	0.10000100
H	-1.78337128	1.98483775	-0.02367500
H	-2.80356695	-0.35687839	0.04532200
C	2.41438899	0.04151634	-0.13182000
H	3.14943306	-0.43810056	0.50714600

State=1-A
RB3LYP/6-31G(d), HF= -302.2288074
Zero-point correction= 0.074379 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.154428
Imaginary frequency: -666.7 cm^{-1}

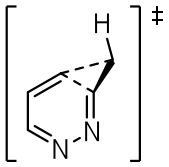
TS 10Z → (16)17



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.95195815	-0.36949061	-0.19872400
C	0.60229558	1.02757425	-0.35190100
C	-0.72156554	1.30560970	0.05111700
C	-1.55754009	0.22973236	0.28638600
H	1.22211328	1.74985750	-0.85974100
H	-1.11377895	2.31947354	0.04694000
H	-2.59109415	0.35210993	0.59276700
N	-1.21322256	-1.05719550	-0.03303300
N	0.02351657	-1.37863599	-0.25075200
C	2.14058801	-0.03098612	0.34985500
H	2.31628914	-0.34526205	1.38612300

State=1-A
RB3LYP/6-31G(d), HF= -302.2321226
Zero-point correction= 0.076643 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.155479
Imaginary frequency: -309.8 cm^{-1}

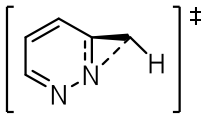
TS 10E → (16)17



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.97225145	-0.38432816	-0.21826200
C	0.57885649	1.02449935	-0.41285814
C	-0.72523129	1.26534711	0.03659788
C	-1.48523813	0.15568006	0.40512621
H	1.15363304	1.71036107	-1.02065388
H	-1.18989619	2.24461142	-0.05568812
H	-2.48711345	0.23893734	0.81097388
N	-1.14457523	-1.09901801	-0.01315068
N	0.05142514	-1.40245698	-0.39794802
C	1.89864869	0.03936898	0.61087293
H	2.73970389	0.71301099	0.61419775

State=1-A
RB3LYP/6-31G(d), HF= -302.226243
Zero-point correction= 0.076085 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.150158
Imaginary frequency: -381.8 cm^{-1}

TS 10Z → 42

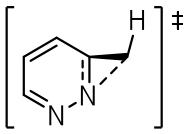


Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.35052720	-1.40884219	0.06547391
N	-0.79890870	-0.78131930	-0.42908714
C	-0.90726396	0.56334129	-0.10757134
C	0.21746769	1.45991399	-0.14119085
C	1.39699886	0.80275548	-0.00191636
C	1.38975178	-0.63507958	0.21848907
H	0.12382750	2.53754604	-0.22814912

H	2.34712356	1.32967727	0.00146988
H	2.31673812	-1.13464740	0.49306546
C	-1.94705334	0.08476161	0.58237849
H	-2.91358869	-0.34032322	0.36962199

State=1-A
RB3LYP/6-31G(d), HF= -302.2274457
Zero-point correction= 0.076580 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.150866
Imaginary frequency: -353.8 cm^{-1}

TS 10E → 42

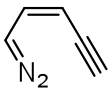


Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.41736932	-1.43058642	0.11735924
N	-0.77153258	-0.84874593	-0.29351418
C	-0.89634543	0.49912738	-0.04032788
C	0.20452302	1.40689446	-0.07031584
C	1.41892777	0.79180123	-0.02284134
C	1.45941138	-0.63844478	0.17155145
H	0.07302576	2.48380056	-0.07702557
H	2.34754421	1.35444743	-0.03870032
H	2.41132705	-1.13084517	0.35816773
C	-2.09797408	0.08749671	0.44561758
H	-2.29357436	0.18412463	1.51826353

State=1-A
RB3LYP/6-31G(d), HF= -302.2261215
Zero-point correction= 0.076718 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.149404
Imaginary frequency: -256.5 cm^{-1}

11Z

(s-Z)-(Z)-5-diazopent-3-en-1-yne



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.723687	-1.445751	0.000000
C	-0.692520	-1.455190	0.000000
C	-1.508915	-0.368718	0.000000
C	-1.206723	1.036979	0.000000

H	-1.166925	-2.434110	0.000000
H	-2.579023	-0.558993	0.000000
H	-1.993341	1.781683	0.000000
C	1.935862	-1.490206	0.000000
H	3.001801	-1.503878	0.000000
N	1.032734	2.033302	0.000000
N	0.000000	1.545643	0.000000

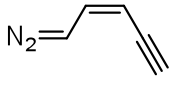
State=1-A'
RB3LYP/6-31G(d), HF= -302.2903369
Zero-point correction= 0.076177 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.214160

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	51.6	1.7	1
2	A'	111.2	0.5	0
3	A'	180.4	0.3	0
4	A"	310.4	3.8	1
5	A'	359.0	8.1	3
6	A"	491.5	47.3	17
7	A"	503.9	6.7	2
8	A'	541.4	12.1	4
9	A"	562.8	45.3	16
10	A"	582.0	24.3	9
11	A'	661.8	35.7	13
12	A"	712.5	18.3	6
13	A'	771.1	9.0	3
14	A'	901.3	1.7	1
15	A"	930.3	0.0	0
16	A'	968.4	7.3	3
17	A'	1163.6	8.4	3
18	A'	1232.2	13.6	5
19	A'	1364.6	38.4	14
20	A'	1406.2	42.6	15
21	A'	1580.6	56.2	20
22	A'	2107.2	218.3	77
23	A'	2124.3	283.8	100
24	A'	3048.8	0.4	0
25	A'	3069.7	12.2	4
26	A'	3106.3	2.1	1
27	A'	3361.4	76.6	27

11E

(s-E)-(Z)-5-diazopent-3-en-1-yne



Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	0.809372	-2.008107	0.000000

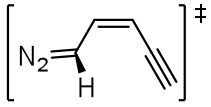
C	-0.537013	-1.566907	0.000000
C	-0.912836	-0.260986	0.000000
H	-1.311555	-2.329650	0.000000
H	-1.974095	-0.025328	0.000000
C	1.959027	-2.395337	0.000000
H	2.967432	-2.741115	0.000000
C	0.000000	0.846629	0.000000
H	1.076584	0.723599	0.000000
N	-0.431619	2.079270	0.000000
N	-0.806905	3.160836	0.000000

State=1-A'
RB3LYP/6-31G(d), HF= -302.2941193
Zero-point correction= 0.076212 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.217908

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A'	98.7	0.5	0
2	A"	101.0	0.7	0
3	A'	201.9	4.0	1
4	A"	273.1	0.9	0
5	A'	350.1	10.9	2
6	A"	479.5	18.7	4
7	A"	502.4	6.6	1
8	A'	537.3	5.5	1
9	A"	577.0	66.1	13
10	A"	629.7	27.7	5
11	A'	662.9	35.6	7
12	A'	684.3	10.1	2
13	A"	711.1	23.9	5
14	A'	909.8	1.5	0
15	A"	928.5	1.1	0
16	A'	1082.6	13.3	3
17	A'	1160.5	8.9	2
18	A'	1213.6	20.4	4
19	A'	1300.4	11.8	2
20	A'	1410.6	43.5	8
21	A'	1573.7	159.8	30
22	A'	2109.2	509.7	97
23	A'	2121.0	526.2	100
24	A'	3055.6	1.2	0
25	A'	3071.8	8.1	2
26	A'	3104.3	5.6	1
27	A'	3361.6	93.6	18

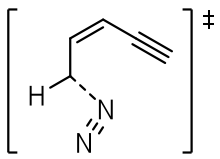
TS 11Z → 11E



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.833222	-0.262523	-0.078734
C	-1.222746	0.991586	-0.357708
C	0.037064	1.335961	-0.030037
H	-1.843727	1.722695	-0.875756
H	0.375288	2.337120	-0.301590
C	-2.401862	-1.310229	0.131901
H	-2.881770	-2.242221	0.327524
C	0.977806	0.456236	0.702725
H	1.057682	0.435446	1.784050
N	1.783825	-0.332925	0.062039
N	2.494789	-1.026964	-0.511054

State=1-A
RB3LYP/6-31G(d), HF= -302.275703
Zero-point correction= 0.075345 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.200358
Imaginary frequency: -172.0 cm^{-1}

TS 11Z → 12E

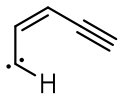


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.48346122	-0.07292679	0.10154913
C	-1.01151363	1.22770815	-0.15029894
C	0.25688358	1.67290583	0.14678890
C	1.24787335	0.88177515	0.79022002
H	-1.69449957	1.89838665	-0.67058393
H	0.46717220	2.71701902	-0.11106486
H	2.26055252	1.23905514	0.54972048
C	-1.92621813	-1.18533166	0.30402540
H	-2.30532486	-2.15685140	0.52776512
N	1.11466550	-1.84395788	-0.63117801
N	1.56686536	-0.84781262	-0.43304254

State=1-A
RB3LYP/6-31G(d), HF= -302.2271093
Zero-point correction= 0.071269 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.155840
Imaginary frequency: -194.4 cm^{-1}

12Z Triplet T_0

(s-Z)-(Z)-2-penten-4-yn-1-ylidene

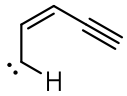


Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.71606748	-0.94354380	0.00000000
C	1.38555825	0.36839475	0.00000000
C	-1.09864544	0.14661636	0.00000000
H	2.19727779	1.09816448	0.00000000
H	1.17923623	-1.88376217	0.00000000
C	0.07437757	0.90782646	0.00000000
H	-0.02994384	1.99086109	0.00000000
C	-2.12998489	-0.50155062	0.00000000
H	-3.03080802	-1.07172231	0.00000000

State=3-A"
<S2>= 2.051086
UB3LYP/6-31G(d), HF= -192.7286523
Zero-point correction= 0.062963 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.665690

12Z Singlet S_1

(s-Z)-(Z)-2-penten-4-yn-1-ylidene

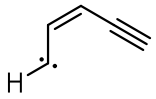


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.77449366	-0.72519171	0.19038333
C	-1.35628298	0.54957701	-0.17538208
C	1.07391006	-0.02845037	0.00356144
H	-2.06659442	1.37507003	-0.23747208
H	-1.06733043	-1.52550270	-0.08622365
C	-0.01234769	0.86949939	0.02109127
H	0.23150520	1.88736923	0.33426049
C	2.06613450	-0.72762370	-0.02873390
H	2.92089827	-1.36380027	-0.07608507

State=1-A
RB3LYP/6-31G(d), HF= -192.704952
Zero-point correction= 0.063419 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.641533

12E Triplet T_0

(s-E)-(Z)-2-penten-4-yn-1-ylidene

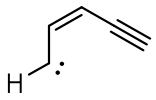


Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.62449916	-1.03676163	0.00000000
C	1.35588879	0.29004137	0.00000000
C	-1.13055560	0.18721957	0.00000000
H	2.20608348	0.98243721	0.00000000
H	2.52380166	-1.63854990	0.00000000
C	0.07748763	0.89124932	0.00000000
H	0.02422273	1.97757942	0.00000000
C	-2.19861659	-0.39811674	0.00000000
H	-3.12632814	-0.92325811	0.00000000

State=3-A"
<S2>= 2.051399
UB3LYP/6-31G(d), HF= -192.7283154
Zero-point correction= 0.062672 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.665643

12E Singlet S_1

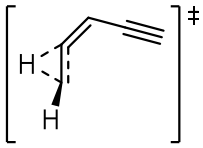
(s-E)-(Z)-2-penten-4-yn-1-ylidene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.66656514	-0.86399617	0.06024863
C	-1.32443553	0.50487549	0.07615811
C	1.10398721	-0.01134693	-0.02109552
H	-2.04942264	1.32806943	0.07919649
H	-2.66279794	-0.98311280	-0.41249681
C	0.00463471	0.87017615	-0.01163839
H	0.24844797	1.92339812	-0.16118478
C	2.12735177	-0.66353263	-0.01859483
H	2.99393455	-1.28541026	-0.01598286

State=1-A
RB3LYP/6-31G(d), HF= -192.7027392
Zero-point correction= 0.063097 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.639643

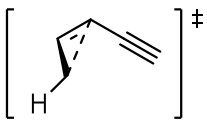
TS 12E → 13



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.17897991	-0.80231967	0.00660310
C	1.19558636	0.08128442	-0.04793177
C	1.87966897	1.23726268	0.12227706
H	0.40191636	-1.86498894	0.00396685
H	2.30131703	-0.28932889	-0.04273162
H	2.29082996	1.65723750	-0.81220262
C	-1.17786185	-0.39495266	0.02123143
C	-2.34683759	-0.07481367	0.03096353
H	-3.37127820	0.21831374	0.05210727

State=1-A
RB3LYP/6-31G(d), HF= -192.6914978
Zero-point correction= 0.060010 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.631488
Imaginary frequency: -356.2 cm^{-1}

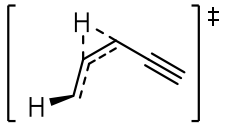
TS 12E → 14



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.11329345	0.77474740	-0.11229385
C	-1.42691798	0.40640090	0.24554767
C	-1.47525521	-0.88003725	-0.17828435
H	0.01573734	1.75683870	-0.58066148
H	-2.20180961	1.14958126	0.45768211
H	-2.35933356	-1.18327783	-0.75776189
C	1.07249075	0.02598870	0.01772496
C	2.18029593	-0.45719049	0.13172799
H	3.12148552	-0.94259766	0.25420670

State=1-A
RB3LYP/6-31G(d), HF= -192.6983526
Zero-point correction= 0.062589 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.635764
Imaginary frequency: -351.2 cm^{-1}

TS 12E → 15

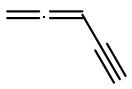


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.22313077	-0.59708822	-0.31562174
C	-1.20924118	0.12041092	-0.01361679
C	1.27770545	0.12410711	0.05408453
H	-1.16238844	0.59564487	1.04863541
H	-3.01893645	-1.02997959	0.27507279
C	0.05079273	0.78634292	-0.07558476
H	0.04043896	1.87433181	-0.06831940
C	2.35185552	-0.43729014	0.15374360
H	3.28795437	-0.94196535	0.22976548

State=1-A
RB3LYP/6-31G(d), HF= -192.672683
Zero-point correction= 0.058806 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.613877
Imaginary frequency: -835.1 cm^{-1}

13

Penta-1,2-dien-4-yne



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.11562417	0.15114251	0.00000000
C	1.30864965	0.07870120	0.00000000
C	2.38947462	-0.46537380	0.00000000
H	3.33434166	-0.95908924	0.00000000
C	-2.27801483	-0.43821209	0.00000000
H	-2.78563919	-0.69850177	-0.92763079
H	-2.78563919	-0.69850177	0.92763079
C	0.05490766	0.75816908	0.00000000
H	0.08057908	1.84953141	0.00000000

State=1-A'
RB3LYP/6-31G(d), HF= -192.800017
Zero-point correction= 0.065308 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.734709

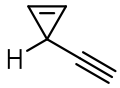
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A'	136.0	1.5	2
2	A"	286.1	12.2	15
3	A"	338.1	0.0	0

4	A'	347.3	2.2	3
5	A'	586.1	10.5	13
6	A"	605.5	29.1	36
7	A"	621.9	18.4	23
8	A'	667.7	41.8	52
9	A'	853.6	51.2	64
10	A"	855.4	19.9	25
11	A'	919.8	9.6	12
12	A"	971.2	0.0	0
13	A'	1102.0	0.8	1
14	A'	1307.8	6.6	8
15	A'	1416.4	4.0	5
16	A'	1974.3	57.8	72
17	A'	2137.0	3.5	4
18	A'	3008.5	1.2	1
19	A'	3012.1	4.5	6
20	A"	3078.5	1.1	1
21	A'	3363.7	79.8	100

14

3-Ethynylcycloprop-1-ene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.31305171	0.00000000	0.58568567
H	0.40655899	0.00000000	1.67557650
C	-1.06318719	0.00000000	0.12692666
C	1.41538891	0.64590770	-0.23358405
C	-2.21561539	0.00000000	-0.23969774
H	-3.22819045	0.00000000	-0.57309360
C	1.41538891	-0.64590770	-0.23358405
H	1.81573487	-1.59090770	-0.56848093
H	1.81573487	1.59090770	-0.56848093

State=1-A'
RB3LYP/6-31G(d), HF=-192.7607009
Zero-point correction= 0.065337 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.695364

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A'	198.3	3.2	4
2	A"	210.4	3.4	4
3	A'	511.8	14.3	18
4	A"	520.9	0.0	0
5	A"	614.7	47.2	59
6	A'	617.0	80.4	100
7	A'	661.9	44.1	55
8	A"	780.6	5.8	7

9	A"	830.8	0.5	1
10	A'	876.8	9.8	12
11	A'	926.2	10.2	13
12	A"	971.4	43.0	54
13	A"	1011.9	3.0	4
14	A'	1117.5	1.6	2
15	A'	1323.5	8.9	11
16	A'	1676.0	32.7	41
17	A'	2135.7	5.6	7
18	A'	2973.3	34.4	43
19	A"	3143.2	1.0	1
20	A'	3190.8	0.3	0
21	A'	3362.3	66.2	83

15

Penta-1,4-diyne

Error! Objects cannot be created from editing field codes.

Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-0.07238103	0.00000000	1.22966233
C	-0.07238103	0.00000000	-1.22966233
C	0.57491253	0.00000000	-2.24715462
H	1.15646847	0.00000000	-3.14091375
C	0.57491253	0.00000000	2.24715462
H	1.15646847	0.00000000	3.14091375
C	-0.87670122	0.00000000	0.00000000
H	-1.54131986	-0.87640746	0.00000000
H	-1.54131986	0.87640746	0.00000000

State=1-A1
RB3LYP/6-31G(d), HF= -192.7828784
Zero-point correction= 0.065320 (Hartree/Particle)
Sum of electronic and zero-point Energies= -192.717559

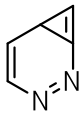
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A1	132.1	1.0	1
2	B1	296.6	16.5	17
3	A2	316.4	0.0	0
4	B2	322.8	3.9	4
5	A1	543.2	8.9	9
6	A2	647.8	0.0	0
7	B1	650.1	89.8	91
8	B2	666.3	26.5	27
9	A1	668.0	53.7	54
10	A1	872.9	8.4	9
11	B1	900.6	0.6	1
12	B2	965.7	4.7	5
13	A2	1202.4	0.0	0
14	B2	1296.5	19.5	20

15	A1	1407.3	6.6	7
16	B2	2158.0	2.6	3
17	A1	2163.4	0.1	0
18	A1	2913.1	8.1	8
19	B1	2935.9	2.5	3
20	B2	3362.4	98.8	100
21	A1	3363.4	30.5	31

(16)

2,3-Diazabicyclo[4.1.0]hepta-1(7),2,4-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.0004568955	0.0003464216	-0.0019091652
N	0.0007806039	-0.0024063969	1.2969470911
C	1.2596367178	-0.0000188180	1.7937953826
C	2.4947844638	-0.8290028756	1.1870178278
C	2.3048404114	-0.7844608764	-0.2361269561
C	1.1531250797	-0.1990471234	-0.7343960178
C	2.4488041910	0.4602095955	1.9911100346
H	3.0254035177	1.3671291402	2.1004668336
H	2.8640500336	-1.7417837577	1.6580747473
H	2.9439753504	-1.3480856852	-0.9154769450
H	0.9913139910	-0.1023952671	-1.8033867118

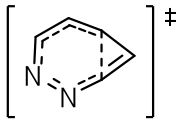
State=1-A
RB3LYP/6-31G(d), HF= -302.2566037
RMSD=4.843e-09|RMSF=1.790e-04, unstable wavefunction.
Zero-point correction= 0.078048 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.178555

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	155.9	15.8	39
2	A	273.5	4.2	10
3	A	338.9	7.5	18
4	A	440.2	11.5	28
5	A	569.5	30.7	75
6	A	580.3	14.5	35
7	A	639.7	9.6	23
8	A	700.6	16.0	39
9	A	786.4	32.1	78
10	A	856.5	4.7	11
11	A	895.0	16.1	39
12	A	924.5	3.8	9
13	A	945.9	17.2	42
14	A	953.2	3.2	8
15	A	995.7	1.8	4

16	A	998.7	19.8	48
17	A	1087.9	9.6	23
18	A	1165.4	7.0	17
19	A	1267.8	32.1	78
20	A	1312.6	26.2	64
21	A	1403.1	2.7	7
22	A	1475.5	4.0	10
23	A	1793.1	41.2	101
24	A	3007.5	27.0	66
25	A	3038.8	12.3	30
26	A	3089.5	10.7	26
27	A	3160.9	4.5	11

TS (16) → 17



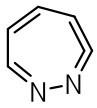
Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.5708803825	-0.2620421970	0.0469559786
C	-0.4573390459	-1.0816968260	-0.1425435083
C	-1.4652832614	-0.6534026869	0.5498231926
C	-1.2808943269	0.4861262129	-0.3724917463
C	-0.2338765274	1.4013652737	-0.0808233804
C	1.0346733565	0.9621676935	0.2873620270
H	-1.9392018530	-0.8135607202	1.4949959710
H	-1.9697338860	0.6745104822	-1.1790107009
H	-0.3506969404	2.4482396373	-0.3053533925
H	1.7778323363	1.6849792582	0.5660259319
N	0.8431366423	-1.2638901831	-0.3361870239

State=1-A
CAS(8,8)/6-31G(d), HF= -300.4724878
Zero-point correction= 0.082085 (Hartree/Particle)
Sum of electronic and zero-point Energies= -300.390402
Imaginary frequency: -758.0 cm^{-1}

Single Point Energy on CAS(8,8)/6-31G* Geometry (above):
RB3LYP/6-31G(d), HF= -302.254594, RMSD=6.200e-09|RMSF=8.729e-03
Zero-point correction= 0.077934 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.176660
Imaginary frequency: -462.0 cm^{-1}

17

1,2-Diazacyclohepta-2,3,5,7-tetraene



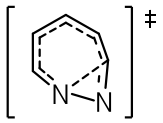
Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.91083661	-0.92374448	-0.07864955
C	0.85142385	1.35094135	-0.09432091
C	-0.50923456	1.32352269	-0.17419152
C	-1.37358076	0.21671002	0.26608828
H	1.38587930	2.28022677	-0.29190980
H	-1.03696774	2.23823833	-0.43315839
H	-2.30787995	0.52852128	0.73829289
N	-1.25235766	-1.07197641	0.23257852
N	-0.08066981	-1.49024527	-0.55731049
C	1.58800076	0.15409506	0.30583043
H	2.48548537	0.15941753	0.91135882

State=1-A
RB3LYP/6-31G(d), HF= -302.2956515
Zero-point correction= 0.079326 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.216326

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	298.7	0.0	0
2	A	311.7	0.1	0
3	A	352.9	11.2	8
4	A	442.1	0.7	1
5	A	546.6	5.7	4
6	A	612.9	1.8	1
7	A	659.3	14.0	10
8	A	697.5	49.6	37
9	A	715.8	25.9	19
10	A	768.1	41.8	31
11	A	848.8	2.3	2
12	A	900.7	2.9	2
13	A	924.9	1.0	1
14	A	944.7	5.9	4
15	A	999.6	0.2	0
16	A	1093.1	6.7	5
17	A	1164.3	2.2	2
18	A	1282.4	12.8	9
19	A	1310.2	1.0	1
20	A	1369.3	12.1	9
21	A	1508.9	14.4	11
22	A	1568.4	9.2	7
23	A	1904.6	134.6	100
24	A	3012.2	4.2	3
25	A	3034.2	14.8	11
26	A	3067.2	10.3	8
27	A	3114.1	0.1	0

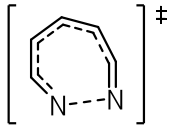
TS 17 → 18



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.34026513	0.32232275	-0.47929559
N	1.43154487	-0.83392917	0.61691284
C	0.42441234	-1.08313834	-0.04727307
C	0.47489779	1.30918432	-0.12725822
C	-0.84636104	1.18784160	0.29595055
C	-1.57000574	-0.01000405	0.07466012
C	-0.94326247	-1.19733814	-0.27024393
H	0.83618328	2.28977604	-0.44227878
H	-1.39575383	2.09483444	0.52529106
H	-2.65683430	0.02984995	0.08420326
H	-1.42435040	-2.07248794	-0.68554902

State=1-A
RB3LYP/6-31G(d), HF= -302.2725673
Zero-point correction= 0.077627 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.194940
Imaginary frequency: -516.9 cm^{-1}

TS 17 → 23ZZ S_1

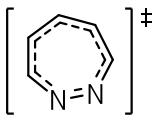


Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.18720850	-1.35351246	-0.46558335
N	1.72734231	0.47872137	0.31392944
C	0.76813008	1.28996970	0.13278961
C	-0.64441552	1.28483751	-0.26190006
C	-1.55834161	0.27950369	-0.02250512
C	-1.19869013	-1.04517100	0.33307561
C	0.08674584	-1.38555092	-0.00710895
H	1.07597035	2.29752972	0.46872095
H	-1.03014448	2.27004249	-0.50486005
H	-2.61753591	0.53147252	-0.06211045
H	-1.87137166	-1.72865388	0.83638451

State=1-A
<S2>= 0.483871, i.e. 75.8% singlet
UB3LYP/6-31G(d), HF= -302.2726391
Zero-point correction= 0.075638 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.197001

Imaginary frequency: -437.6 cm^{-1}

TS 17 → 17’

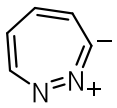


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.28226039	0.78697028	0.12961061
C	-0.05148055	1.42759437	0.02041617
C	1.26905527	0.86540296	-0.11038302
C	1.65790775	-0.44251991	0.06826182
C	0.56618908	-1.35755305	0.25417901
N	-0.56307578	-1.28902985	-0.21128739
N	-1.64930049	-0.49134829	-0.16652571
H	-2.14433180	1.41282152	0.35869581
H	-0.08653900	2.51016005	0.09690770
H	2.07253589	1.59857024	-0.19637485
H	2.68850183	-0.73827275	0.21295552

State=1-A
RB3LYP/6-31G(d), HF= -302.2489988
Zero-point correction= 0.077070 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.171929
Imaginary frequency: -630.8 cm^{-1}

17’

1,2-Diazacyclohepta-1,2,4,6-tetraen-2-ylium-3-ide



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.45739640	0.53920432	0.10386571
C	-0.38430799	1.36181112	0.17634929
C	1.01190880	1.05753371	-0.19390037
C	1.64195427	-0.13790554	-0.09069505
C	0.85365596	-1.25153155	0.51872320
N	-0.25515689	-1.25552566	-0.02710137
N	-1.35331096	-0.78964004	-0.41491153
H	-2.46298265	0.86488930	0.35366405
H	-0.57444496	2.38838249	0.48214112
H	1.61339210	1.91910167	-0.47987368
H	2.68842259	-0.27088591	-0.34789783

State=1-A

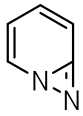
RB3LYP/6-31G(d), HF= -302.2644795
Zero-point correction= 0.079304 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.185176

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	278.6	15.5	5
2	A	320.0	7.5	2
3	A	366.5	23.8	7
4	A	416.2	3.3	1
5	A	524.0	13.9	4
6	A	584.9	6.7	2
7	A	657.3	20.6	6
8	A	724.9	37.9	12
9	A	797.4	14.8	5
10	A	841.9	3.5	1
11	A	870.8	2.5	1
12	A	931.2	14.7	5
13	A	940.3	12.6	4
14	A	951.8	15.9	5
15	A	961.4	4.0	1
16	A	1142.2	9.0	3
17	A	1157.6	6.8	2
18	A	1206.7	7.6	2
19	A	1302.5	28.3	9
20	A	1361.3	0.7	0
21	A	1530.4	3.1	1
22	A	1569.9	1.7	1
23	A	1771.8	322.2	100
24	A	3042.7	3.5	1
25	A	3057.9	3.2	1
26	A	3088.1	17.3	5
27	A	3092.3	6.3	2

18

1,7-diazabicyclo[4.1.0]hepta-2,4,6-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.88984891	-0.77451711	-0.51733400
C	-0.89302507	0.57317989	-0.11727700
C	0.25843683	1.44333603	-0.15071700
C	1.41330491	0.74823417	0.02960700
C	1.39604708	-0.69191883	0.21568000
C	0.25343917	-1.40276497	-0.00917900
H	0.19292670	2.51992102	-0.25026000
H	2.36501185	1.27126628	0.07083600
H	2.32286515	-1.20690272	0.44775000

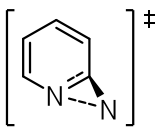
H	0.23512830	-2.48946597	-0.00316800
N	-1.92231502	0.18662777	0.50678500

State=1-A
RB3LYP/6-31G(d), HF= -302.2847793
Zero-point correction= 0.079234 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.205545

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	162.7	3.4	9
2	A	291.9	4.3	11
3	A	400.2	2.2	6
4	A	461.5	7.5	20
5	A	548.3	5.7	15
6	A	587.4	2.6	7
7	A	657.0	4.8	13
8	A	709.3	37.6	99
9	A	790.3	16.8	44
10	A	850.4	4.8	13
11	A	862.3	16.5	43
12	A	924.7	3.4	9
13	A	950.6	1.7	4
14	A	955.5	1.5	4
15	A	1034.8	5.1	13
16	A	1100.4	22.3	59
17	A	1131.5	5.4	14
18	A	1177.7	16.2	43
19	A	1322.0	7.0	18
20	A	1384.3	3.7	10
21	A	1464.8	23.2	61
22	A	1568.9	5.8	15
23	A	1725.6	37.7	99
24	A	3069.8	1.2	3
25	A	3076.3	9.9	26
26	A	3094.0	11.1	29
27	A	3114.9	0.4	1

TS 18 → 19



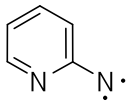
Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.64978844	0.24297472	0.02246635
C	0.80704589	1.39768419	0.03692458
H	2.72960864	0.35515589	0.01440412
H	1.25346488	2.38830782	0.02955024
N	-2.07258091	-0.71800307	-0.47152203

C	1.08360029	-1.01827929	0.09827517
H	1.70381981	-1.91189793	0.13076057
N	-0.23513795	-1.19734512	0.34371944
C	-1.04188967	-0.11763097	0.00776039
C	-0.54802693	1.24481594	-0.02582408
H	-1.23596941	2.07848401	-0.11771130

State=1-A
RB3LYP/6-31G(d), HF= -302.2809623
Zero-point correction= 0.078693 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.202269
Imaginary frequency: -180.0 cm^{-1}

19 Triplet T_0

2-Pyridyl-nitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.03417588	2.36339355	0.00000000
N	-1.22817577	0.41257822	0.00000000
C	0.00000551	1.02679621	0.00000000
C	1.22643033	0.29240292	0.00000000
C	1.17100820	-1.09252788	0.00000000
C	-0.07960282	-1.71668268	0.00000000
C	-1.23528062	-0.91111852	0.00000000
H	2.16716573	0.83272946	0.00000000
H	2.08489222	-1.68005814	0.00000000
H	-0.17051082	-2.79825473	0.00000000
H	-2.21883984	-1.37969839	0.00000000

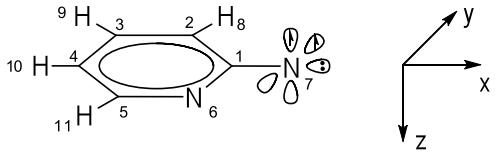
State=3-A"
<S2>= 2.047859
UB3LYP/6-31G(d), HF=-302.3397371
Zero-point correction= 0.079560 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.260177

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	185.2	0.4	1
2	A'	372.2	2.9	6
3	A"	385.3	3.7	7
4	A"	473.2	0.3	1
5	A'	532.6	1.2	2
6	A'	604.9	4.4	9
7	A"	697.4	14.8	30
8	A"	759.5	50.4	101
9	A'	828.1	1.5	3
10	A"	852.6	0.9	2

11	A'	930.6	10.3	21
12	A"	952.0	0.7	1
13	A"	968.3	0.3	1
14	A'	1009.8	4.1	8
15	A'	1068.4	5.8	12
16	A'	1123.1	0.3	1
17	A'	1190.4	11.1	22
18	A'	1211.2	4.0	8
19	A'	1306.9	7.0	14
20	A'	1370.6	11.7	23
21	A'	1397.9	0.4	1
22	A'	1504.2	25.6	51
23	A'	1526.3	0.4	1
24	A'	3039.3	18.2	36
25	A'	3071.9	4.9	10
26	A'	3092.0	8.7	17
27	A'	3098.2	3.7	7

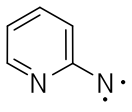
Natural Atomic Spin Densities (UB3LYP/EPR-III)



Net Natural Atomic Valence Orbitals Population						
		2s	2p			Total
			px	py	pz	
C	1	-0.01785	-0.02703	-0.01666	-0.13411	-0.19565
C	2	0.02466	0.01175	0.01813	0.23877	0.29331
C	3	-0.00562	-0.00345	-0.00528	-0.09190	-0.10625
C	4	0.01174	0.00575	0.00600	0.24699	0.27048
C	5	-0.00555	-0.00253	-0.00476	-0.07671	-0.08955
N	6	0.01878	0.01111	0.01532	0.17765	0.22286
N	7	0.02799	0.01121	0.92904	0.63359	1.60183
H	8	-0.00901	(1s)			-0.00901
H	9	0.00535	(1s)			0.00535
H	10	-0.00832	(1s)			-0.00832
H	11	0.00453	(1s)			0.00453

19 Open-Shell Singlet S_1

2-Pyridyl-nitrene



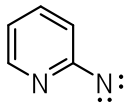
Atom Coordinates (Angstroms)

Type	X	Y	Z
N	0.04000623	2.35006018	0.00000000
N	-1.24020101	0.41110749	0.00000000
C	-0.00271628	1.03817793	0.00000000
C	1.23182707	0.29047304	0.00000000
C	1.17521221	-1.09026941	0.00000000
C	-0.07766303	-1.71544307	0.00000000
C	-1.23829955	-0.90681009	0.00000000
H	2.17141507	0.83208064	0.00000000
H	2.08851239	-1.67877596	0.00000000
H	-0.16929244	-2.79678528	0.00000000
H	-2.21943409	-1.38146348	0.00000000

State=1-A"
<S2>= 1.034647, i.e. 48.3% singlet
UB3LYP/6-31G(d), HF=-302.3265626
Zero-point correction= 0.079299 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.247263
Ziegler-Cramer corrected energy ($2*E(T_0) - E(S_1)$)= -302.234349

19 Closed-Shell Singlet S_2

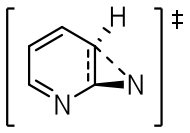
2-Pyridyl-nitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.06611052	2.38067532	0.00000000
N	-1.23703613	0.40511059	0.00000000
C	0.00200707	1.05903985	0.00000000
C	1.20928569	0.28652870	0.00000000
C	1.17964922	-1.10802840	0.00000000
C	-0.07079256	-1.71111248	0.00000000
C	-1.24385502	-0.90978959	0.00000000
H	2.14029463	0.84381116	0.00000000
H	2.09012058	-1.70114810	0.00000000
H	-0.16731936	-2.79402004	0.00000000
H	-2.21719664	-1.40150702	0.00000000

State=1-A'"
RB3LYP/6-31G(d), HF=-302.2805444
Zero-point correction= 0.080176 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.200368

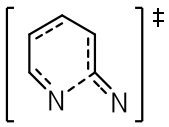
TS 19 S_1 → 20



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.15867212	-1.40100041	-0.27756331
N	2.02513230	-0.01582164	0.54288413
C	1.00367478	-0.31416689	-0.13951010
C	0.58344365	1.07182953	-0.35808724
C	-0.74722417	1.31890411	0.04565238
C	-1.57480969	0.23060243	0.26045491
C	-1.09018206	-1.08958651	-0.05631110
H	1.24986031	1.81639391	-0.76510626
H	-1.14518286	2.33109654	0.05598020
H	-2.62404915	0.36004891	0.50483823
H	-1.81667432	-1.89528105	-0.16615098

State=1-A
<S2>= 0.331612, i.e. 83.4% singlet
UB3LYP/6-31G(d), HF= -302.3027122
Zero-point correction= 0.078359 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.224353
Imaginary frequency: -564.9 cm^{-1}

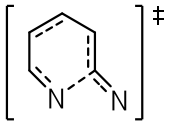
TS 19 T_0 → 23ZZ T_0



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.50002375	-0.14741340	0.00000000
N	0.14864618	-2.44297985	0.00000000
C	-0.16905372	-1.28465128	0.00000000
C	-1.28452528	-0.39478971	0.00000000
C	-1.23613759	0.98919762	0.00000000
C	-0.06051755	1.73468323	0.00000000
C	1.23136099	1.10864743	0.00000000
H	-2.24965159	-0.89361468	0.00000000
H	-2.18459988	1.51991567	0.00000000
H	-0.10399349	2.81878361	0.00000000
H	2.11080141	1.76914597	0.00000000

State=3-A"
<S2>= 2.103161
UB3LYP/6-31G(d), HF= -302.2889592
Zero-point correction= 0.074985 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.213974
Imaginary frequency: -540.0 cm^{-1}

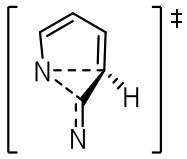
TS 19 S_1 → 23ZZ S_1



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.50167062	-0.04699869	0.00000000
N	-0.46607723	2.40001248	0.00000000
C	-0.00912404	1.29179022	0.00000000
C	1.21896106	0.55725949	0.00000000
C	1.35646873	-0.82266110	0.00000000
C	0.29228363	-1.71346167	0.00000000
C	-1.07652062	-1.25096945	0.00000000
H	2.10750631	1.18181709	0.00000000
H	2.36750345	-1.22155187	0.00000000
H	0.47124527	-2.78331892	0.00000000
H	-1.86443255	-2.01978778	0.00000000

State=1-A"
<S2>= 1.049555, i.e. 47.5% singlet
UB3LYP/6-31G(d), HF= -302.2814719
Zero-point correction= 0.075184 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.206287
Ziegler-Cramer corrected energy ($2*E(T_0) - E(S_1)$)= -302.221661
Imaginary frequency: -561.3 cm^{-1}

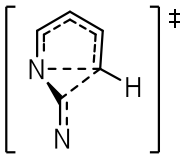
TS 19 → 32



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.29405916	-0.11705824	-0.40648067
N	-0.28885384	-1.25426950	0.48236045
C	0.91130621	-1.25574608	0.00642568
C	1.66290016	-0.09444063	-0.33715388
C	-0.25037990	1.26033697	0.31975927
C	-1.23536260	0.26718600	-0.00819707
H	1.35896602	-2.25113317	-0.12029677
H	2.63968260	-0.18277996	-0.79844029
H	-0.60805378	2.14957435	0.83274168
C	1.07767242	1.13181315	-0.04769118
H	1.69297847	2.02873649	-0.04401998

State=1-A
RB3LYP/6-31G(d), HF= -302.2581948
Zero-point correction= 0.075529 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.182666
Imaginary frequency: -397.1 cm^{-1}

TS 19 → 33

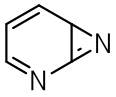


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.31713940	-1.03980709	0.54472620
N	-2.22269765	0.25570457	-0.47819807
C	0.90657820	-1.20682413	-0.04468706
C	1.63930730	-0.12501221	-0.44440763
C	1.03905058	1.11294582	-0.05987819
C	-0.18208585	1.08925412	0.50129061
C	-1.21582186	-0.20023907	-0.02080594
H	1.29785647	-2.21987806	0.00641666
H	2.62895448	-0.20089221	-0.87587712
H	1.57019599	2.06111561	-0.11206990
H	-0.84031783	1.82762510	0.92676264

State=1-A
RB3LYP/6-31G(d), HF= -302.2529578
Zero-point correction= 0.076109 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.176849
Imaginary frequency: -591.1 cm^{-1}

20

2,7-diazabicyclo[4.1.0]hepta-1(7),2,4-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.38639794	0.37523811	0.45870229
C	0.49241799	1.36024502	0.08834737
H	2.37075441	0.64146572	0.83150061
H	0.82448871	2.39568335	0.02802865
N	-1.74447097	0.05603486	0.46463902
C	1.16597714	-0.99812501	0.08219343
H	2.01370352	-1.68190135	0.09343688

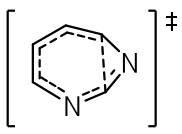
N	0.03167757	-1.48589010	-0.38390160
C	-0.89824805	-0.52083071	-0.26342261
C	-0.79885969	0.97044688	-0.41917546
H	-1.30550478	1.53189319	-1.19799827

State=1-A
RB3LYP/6-31G(d), HF= -302.3194483
Zero-point correction= 0.080211 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.239237

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	254.8	13.4	17
2	A	333.3	3.7	5
3	A	399.3	4.2	5
4	A	485.1	6.9	9
5	A	599.7	2.2	3
6	A	621.6	6.5	8
7	A	645.8	12.3	16
8	A	774.5	65.0	84
9	A	832.6	26.8	35
10	A	890.4	4.8	6
11	A	923.8	10.4	13
12	A	930.6	2.1	3
13	A	946.0	3.3	4
14	A	961.1	2.0	3
15	A	1003.1	16.3	21
16	A	1051.2	1.4	2
17	A	1143.1	5.9	8
18	A	1261.4	11.8	15
19	A	1316.3	25.9	34
20	A	1387.3	4.6	6
21	A	1435.7	61.1	79
22	A	1530.3	14.8	19
23	A	1780.4	76.5	99
24	A	3044.3	4.5	6
25	A	3049.3	9.6	12
26	A	3079.1	13.4	17
27	A	3085.3	8.3	11

TS 20 → 21



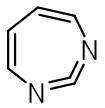
Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	1.16204972	0.89819506	0.29395498
C	-0.09234758	1.42665039	-0.07731743
H	1.98027104	1.57665921	0.51365520

H	-0.13368411	2.46316482	-0.41132643
N	-1.56084233	-0.56405595	0.61950092
C	1.48059087	-0.44305039	0.02901654
H	2.52054580	-0.76081627	0.02198124
N	0.58359121	-1.37954653	-0.36151427
C	-0.60136192	-0.91969274	-0.09220573
C	-1.20714956	0.61425353	-0.30405877
H	-1.97706403	0.86807450	-1.02655406

State=1-A
RB3LYP/6-31G(d), HF= -302.3175151
Zero-point correction= 0.079105 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.238410
Imaginary frequency: -428.2 cm^{-1}

21

1,3-diazacyclohepta-1,2,4,6-tetraene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.14673773	1.07112189	-0.42833708
C	0.00000560	1.22590947	0.00000170
C	-1.56579524	-0.20564742	-0.11261583
C	-0.71152761	-1.24616776	-0.18908760
C	0.71151578	-1.24617362	0.18908973
C	1.56579387	-0.20566232	0.11261394
H	-2.60510873	-0.27088780	-0.41039144
H	-1.12144314	-2.19506021	-0.51901298
H	1.12142058	-2.19506713	0.51902567
H	2.60510434	-0.27090848	0.41039871
N	-1.14672891	1.07113137	0.42833717

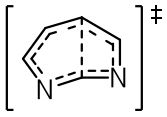
State=1-A
RB3LYP/6-31G(d), HF= -302.336406
Zero-point correction= 0.080348 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.256058

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	288.0	0.5	0
2	A	291.7	17.0	5
3	A	370.4	16.7	5
4	A	482.3	0.2	0
5	A	547.8	29.3	8
6	A	617.6	0.8	0
7	A	678.3	0.7	0
8	A	739.5	58.7	16
9	A	814.1	2.3	1

10	A	822.5	0.5	0
11	A	876.0	5.9	2
12	A	922.6	16.1	4
13	A	927.4	6.7	2
14	A	950.0	6.6	2
15	A	962.3	55.5	15
16	A	1155.7	0.0	0
17	A	1175.3	2.5	1
18	A	1247.9	7.1	2
19	A	1298.7	24.7	7
20	A	1363.6	1.7	0
21	A	1537.5	8.2	2
22	A	1576.8	0.1	0
23	A	1993.1	369.0	100
24	A	3054.9	2.7	1
25	A	3064.5	2.2	1
26	A	3090.8	19.8	5
27	A	3093.0	6.5	2

TS 21 → 24

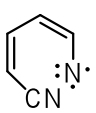


Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.38351970	-0.94632933	-0.27930866
N	-1.03928615	-1.20540842	0.17409713
C	-1.64669786	0.02723691	-0.24204597
C	-0.87887779	1.14781031	-0.20246360
C	0.46326728	1.07538968	0.42824294
C	0.15965456	-0.89107662	0.28645542
C	1.61261452	0.35903126	-0.08832958
H	-2.66149750	-0.04703920	-0.61517849
H	-1.29051818	2.10511328	-0.51599589
H	0.68379450	1.91714527	1.09220344
H	2.59882211	0.77659570	-0.31570366

State=1-A
RB3LYP/6-31G(d), HF= -302.2598589
Zero-point correction= 0.077752 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.182107
Imaginary frequency: -791.9 cm^{-1}

23ZZ T_0

(2Z,3s-Z,4Z)-5-cyanopenta-2,4-dienenitrene



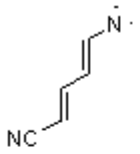
Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.46599583	-1.78048905	0.00000000
N	2.42498206	0.63889777	0.00000000
C	1.29985409	0.95450387	0.00000000
C	0.00000015	1.50768400	0.00000000
C	-1.23299392	0.87417812	0.00000000
C	-1.61137005	-0.47706584	0.00000000
C	-0.80526016	-1.67436992	0.00000000
H	-0.00729575	2.59539400	0.00000000
H	-2.07360185	1.56531020	0.00000000
H	-2.68242906	-0.66107174	0.00000000
H	-1.37490625	-2.61807987	0.00000000

State= 3-A"
<S2>= 2.070425
UB3LYP/6-31G(d), HF= -302.3033377
Zero-point correction= 0.075266 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.228072

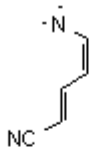
Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	16.6	1.1	2
2	A'	143.3	3.1	6
3	A'	186.7	10.5	20
4	A"	191.1	13.0	24
5	A'	368.9	4.4	8
6	A"	382.5	0.6	1
7	A"	515.9	1.2	2
8	A'	569.6	10.9	21
9	A"	662.1	52.5	99
10	A"	767.7	1.1	2
11	A'	782.5	7.7	15
12	A'	855.0	1.0	2
13	A"	867.5	0.2	0
14	A'	941.3	3.5	7
15	A"	957.4	0.3	1
16	A'	1142.3	2.5	5
17	A'	1214.1	3.6	7
18	A'	1220.8	0.7	1
19	A'	1308.4	0.6	1
20	A'	1412.0	2.6	5
21	A'	1463.7	5.8	11
22	A'	1531.1	8.2	16
23	A'	2185.2	0.8	1
24	A'	2868.7	15.4	29
25	A'	3043.5	2.9	6
26	A'	3060.1	0.7	1
27	A'	3072.0	9.8	18

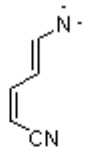
Natural Atomic Spin Density on Nitrene N for Isomers of 23 T_0 (UB3LYP/EPR-III):



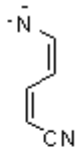
s-E,E,E
ρ= 1.2582



s-E,E,Z
ρ= 1.2679

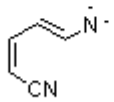


s-E,Z,E
ρ= 1.2636

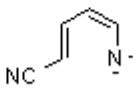


s-E,Z,Z
ρ= 1.2713

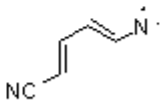
s-Z,Z,Z
ρ= 1.2241



s-Z,Z,E
ρ= 1.2486



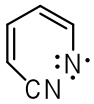
s-Z,E,Z
ρ= 1.2106



s-Z,E,E
ρ= 1.2272

23ZZ S_1

(2Z,3s-Z,4Z)-5-cyanopenta-2,4-dienenitrene

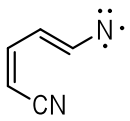


Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.42621335	0.63866327	0.00000000
N	0.46277725	-1.78416777	0.00000000
C	1.30063623	0.95566587	0.00000000
C	0.00357609	1.50732413	0.00000000
C	-1.23942393	0.87095520	0.00000000
C	-1.61551069	-0.46768122	0.00000000
C	-0.79683111	-1.67682615	0.00000000
H	-0.00505673	2.59494180	0.00000000
H	-2.07676621	1.56608751	0.00000000
H	-2.68512733	-0.65911593	0.00000000
H	-1.37066340	-2.62000880	0.00000000

State= 1-A"
<S2>= 1.032388, i.e. 48.3% singlet
UB3LYP/6-31G(d), HF= -302.2970887
Zero-point correction= 0.075129 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.221960
Ziegler-Cramer corrected energy ($2*E(T_0) - E(S_1)$)= -302.234184

23EZ T_0

(2E,3s-Z,4Z)-5-cyanopenta-2,4-dienenitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.91326926	-2.64912592	0.00000000
N	2.50977995	0.54858859	0.00000000
C	1.45166724	1.04383079	0.00000000
C	0.18851023	1.67708430	0.00000000
C	-1.04871155	1.04770717	0.00000000
C	-1.38153230	-0.31477737	0.00000000
C	-0.48557214	-1.44436641	0.00000000
H	0.21568619	2.76319377	0.00000000
H	-1.89767623	1.72784427	0.00000000
H	-2.43906170	-0.56376738	0.00000000
H	0.59930805	-1.28038023	0.00000000

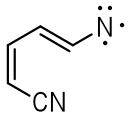
State= 3-A"
<S2>= 2.068785
UB3LYP/6-31G(d), HF= -302.3106982
Zero-point correction= 0.075587 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.235111

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	117.8	4.6	8
2	A'	126.9	4.5	7
3	A"	159.4	5.6	9
4	A'	223.2	6.7	11
5	A"	358.1	0.2	0
6	A'	380.4	13.7	23
7	A'	504.6	2.6	4
8	A"	508.4	2.6	4
9	A"	687.3	60.0	100
10	A'	740.3	0.1	0
11	A"	806.3	6.8	11
12	A"	860.1	2.8	5
13	A'	904.5	0.2	0
14	A"	961.4	0.0	0
15	A'	987.1	4.9	8
16	A'	1132.9	0.1	0
17	A'	1179.8	0.9	1
18	A'	1196.2	6.8	11
19	A'	1347.2	4.0	7
20	A'	1417.3	15.3	26
21	A'	1443.2	0.4	1
22	A'	1493.2	2.8	5
23	A'	2193.6	3.7	6
24	A'	2938.2	6.2	10
25	A'	3052.6	3.1	5
26	A'	3072.9	0.5	1
27	A'	3079.2	3.5	6

23EZ S_1

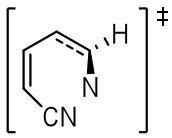
(2E,3s-Z,4Z)-5-cyanopenta-2,4-dienenitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.90539095	-2.64437602	0.00000000
N	2.51265205	0.54937738	0.00000000
C	1.45265401	1.04301763	0.00000000
C	0.19193950	1.67366890	0.00000000
C	-1.05672874	1.04238600	0.00000000
C	-1.39041471	-0.30640682	0.00000000
C	-0.48438431	-1.44965712	0.00000000
H	0.21756003	2.75977234	0.00000000
H	-1.90131906	1.72801056	0.00000000
H	-2.44631418	-0.56045360	0.00000000
H	0.60085096	-1.28039037	0.00000000

State= 1-A"
<S2>= 1.031455, i.e. 48.4% singlet
UB3LYP/6-31G(d), HF= -302.3044962
Zero-point correction= 0.075522 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.228974
Ziegler-Cramer corrected energy ($2*E(T_0) - E(S_1)$)= -302.241248

TS 23ZZ T_0 → 23EZ T_0

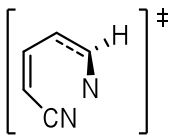


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.62094057	-1.43828377	-0.62141633
N	1.97622306	-1.37002808	0.27062202
C	1.58595376	-0.29026819	0.04950223
C	1.17993852	1.03654553	-0.19471941
C	-0.13067718	1.53139367	-0.09329802
C	-1.29779565	0.84555602	0.16556347
C	-1.43755851	-0.63397777	0.32246363
H	1.97747795	1.73210050	-0.44013240
H	-0.22609908	2.60684612	-0.22841475
H	-2.21946254	1.41373228	0.27208658
H	-1.41805943	-1.02999149	1.35494939

State= 3-A
<S2>= 2.047719
UB3LYP/6-31G(d), HF= -302.2946969
Zero-point correction= 0.074117 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.220580

Imaginary frequency: -169.1 cm^{-1}

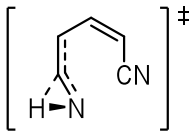
TS 23ZZ S_1 → 23EZ S_1



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.48781320	-1.32141835	-0.63505003
N	1.98229973	-1.41074805	0.16865732
C	1.57357826	-0.33243903	-0.02244297
C	1.15902266	0.99714901	-0.23580251
C	-0.13745906	1.50779048	-0.06671557
C	-1.30209812	0.85425392	0.28338260
C	-1.50199391	-0.61700312	0.40496275
H	1.94724758	1.68782363	-0.52236176
H	-0.22117894	2.58404782	-0.20330863
H	-2.19969359	1.45419835	0.42313671
H	-1.73407973	-1.05941251	1.38697688

State= 1-A
<S2>= 1.001264, i.e. 49.9% singlet
UB3LYP/6-31G(d), HF= -302.2943865
Zero-point correction= 0.074214 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.220173
Ziegler-Cramer corrected energy ($2*E(T_0) - E(S_1)$)= -302.220987
Imaginary frequency: -113.4 cm^{-1}

TS 23ZZ → 26Z

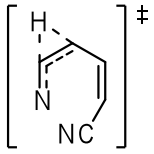


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.86334355	-1.68494301	0.35379818
N	1.50991233	-1.32890288	-0.46413996
C	1.41046420	-0.21250560	-0.11564084
C	1.11993284	1.13012385	0.19368357
C	-0.16711852	1.58941525	0.03927470
C	-1.32034417	0.79757446	-0.21925639
C	-1.31185650	-0.55337881	0.09522111
H	1.92042791	1.78018385	0.52703057
H	-0.33383802	2.65943905	0.15342682
H	-2.27318812	1.25789073	-0.44272841
H	-2.22585033	-1.10796734	0.57497064

State=1-A
RB3LYP/6-31G(d), HF= -302.253361
Zero-point correction= 0.072522 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.180839
Imaginary frequency: -917.3 cm^{-1}

TS 23ZZ → 27Z

~1,2-H shift

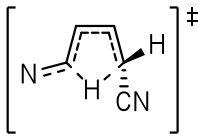


Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.07504164	-1.93598793	-0.35887340
N	1.87656686	0.87400015	0.15564686
C	0.76229643	1.35655544	0.03772563
C	-0.64671995	1.38839385	-0.30939731
C	-1.54400418	0.35930219	0.06134895
C	-1.22334678	-0.95998820	0.28462967
C	0.04487941	-1.50071452	-0.01919870
H	0.59689294	2.21148823	0.78342123
H	-1.04253835	2.37659061	-0.51599138
H	-2.59042882	0.63676432	0.17378938
H	-1.97862529	-1.65036174	0.64747613

State=1-A
RB3LYP/6-31G(d), HF= -302.2551334
Zero-point correction= 0.073062 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.182071
Imaginary frequency: -374.2 cm^{-1}

TS 23EZ → 27Z

~1,4-H shift

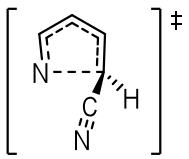


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.11823683	-1.31306177	-0.11798976
N	2.18023054	-1.34576718	-0.34553963
C	1.65230310	-0.37742864	0.04171171
C	1.07070485	0.82228204	0.51495153
C	-0.01674983	1.49254575	-0.11925201

C	-1.23168359	0.91764599	-0.34763545
C	-1.36849559	-0.41992683	0.25620267
H	1.71856039	1.40810778	1.16622148
H	0.09364419	2.55807127	-0.32227373
H	-2.01867553	1.33230725	-0.96584957
H	-0.51053353	-0.53773536	1.01680721

State=1-A
RB3LYP/6-31G(d), HF= -302.2616385
Zero-point correction= 0.073938 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.187701
Imaginary frequency: -288.0 cm^{-1}

TS 23ZZ S_1 → 32

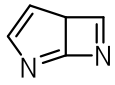


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.44685550	-0.45654217	-0.56735642
N	0.52255474	-1.44495774	0.74856948
C	1.41231570	-1.04443569	-0.04975496
C	1.59355486	0.36372308	-0.44665177
C	0.66962738	1.28733029	-0.10110981
C	-0.60350796	0.97947136	0.51729079
C	-1.58753842	0.16357670	-0.07210428
H	2.10859662	-1.78633563	-0.47050581
H	2.49945898	0.63866961	-0.97895032
H	0.90587841	2.34334641	-0.23413680
H	-0.95053799	1.61682452	1.32908165

State=1-A
<S2>= 0.824212, i.e. 58.8% singlet
UB3LYP/6-31G(d), HF= -302.2882867
Zero-point correction= 0.074503 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.213784
Imaginary frequency: -252.7 cm^{-1}

24

2,7-diazabicyclo[3.2.0]hepta-1,3,6-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.79430989	-1.22145720	-0.05108063

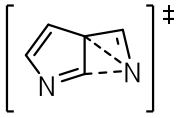
N	-1.62793071	-0.78410219	-0.09520976
C	-0.27231469	-0.66129488	0.41553150
C	-1.55424423	0.49051088	-0.30127009
C	-0.24815723	0.86570536	0.46354509
C	1.10481069	1.09149395	-0.11026860
C	1.67465873	-0.14257254	-0.25494202
H	-2.23302005	1.08713586	-0.90799210
H	-0.47857105	1.40289429	1.38858346
H	1.62179440	2.04089462	-0.18001590
H	2.69662282	-0.35506567	-0.55211806

State=1-A
RB3LYP/6-31G(d), HF= -302.3074558
Zero-point correction= 0.080397 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.227058

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	264.1	1.7	3
2	A	319.3	4.0	6
3	A	490.8	5.6	9
4	A	561.0	25.0	41
5	A	658.4	24.1	40
6	A	714.9	20.5	34
7	A	758.8	13.2	22
8	A	801.3	1.8	3
9	A	831.4	21.5	35
10	A	878.4	10.3	17
11	A	909.0	11.5	19
12	A	930.4	5.5	9
13	A	981.2	28.7	47
14	A	1025.9	29.1	48
15	A	1045.4	2.5	4
16	A	1073.5	18.3	30
17	A	1115.8	16.8	27
18	A	1186.1	6.3	10
19	A	1226.7	6.9	11
20	A	1306.0	18.6	30
21	A	1452.5	4.0	6
22	A	1514.4	25.0	41
23	A	1551.3	60.9	100
24	A	2988.3	3.7	6
25	A	3064.9	1.3	2
26	A	3096.4	6.8	11
27	A	3120.2	10.8	18

TS 24 → 25

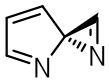


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.78354117	0.57040360	0.43299170
N	0.56282081	-1.26223226	0.03525266
C	1.61670243	-0.47814546	0.40407423
C	1.40453076	0.90111080	0.24722388
C	0.15734012	1.00795533	-0.37057548
C	-0.30838546	-0.40362804	-0.50368344
C	-1.75633348	-0.45477363	-0.29517721
H	2.53228652	-0.94898627	0.75232856
H	2.11117487	1.69450901	0.44930173
H	-0.26256182	1.86778020	-0.87244152
H	-2.51898337	-1.20561628	-0.49807110

State=1-A
RB3LYP/6-31G(d), HF= -302.2928914
Zero-point correction= 0.078480 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.214412
Imaginary frequency: -284.1 cm^{-1}

25

1,4-diazaspiro[2.4]hepta-1,4,6-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.84520348	-0.02518089	-0.71171468
N	-0.33028274	-1.18310979	-0.00261763
C	-1.55695747	-0.75147755	0.01349780
C	-1.67429880	0.70892589	0.01687689
C	-0.40709331	1.18511179	0.00553219
C	0.46327472	-0.00193851	0.02495639
C	1.83402307	-0.05221027	0.53619983
H	-2.39382583	-1.44600417	0.01767432
H	-2.59927438	1.27302136	0.01620695
H	-0.06428493	2.21195685	-0.00714444
H	2.49925065	-0.11140742	1.39121076

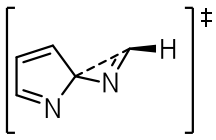
State=1-A
RB3LYP/6-31G(d), HF= -302.3290112
Zero-point correction= 0.079378 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.249633

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	177.1	7.3	12
2	A	318.4	10.4	17
3	A	357.0	3.5	6
4	A	513.0	0.3	0
5	A	573.0	8.7	14

6	A	619.3	4.0	7
7	A	715.4	12.4	20
8	A	772.6	16.4	27
9	A	784.1	35.5	58
10	A	839.3	5.0	8
11	A	859.9	25.6	42
12	A	895.5	5.2	9
13	A	925.2	1.6	3
14	A	962.0	8.6	14
15	A	1005.6	15.8	26
16	A	1057.7	33.3	55
17	A	1138.1	23.4	38
18	A	1187.8	61.0	100
19	A	1292.2	33.4	55
20	A	1333.3	1.5	2
21	A	1443.6	15.0	25
22	A	1562.2	12.4	20
23	A	1721.9	43.0	71
24	A	3068.6	18.6	31
25	A	3108.0	1.0	2
26	A	3110.8	4.2	7
27	A	3132.9	4.0	7

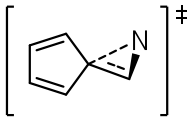
TS 25 → 36



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.71065824	-0.54311055	-0.24260676
N	-0.57016863	-1.24039539	-0.07280313
C	0.33874441	-0.26643860	-0.28327072
C	2.14671859	0.47134943	0.34336124
C	-0.23515455	1.08450895	-0.18639977
C	-1.55673787	0.86397130	0.12600016
C	-1.70457571	-0.56156489	0.16402556
H	2.81954207	0.44533128	1.20791778
H	0.25442363	1.99778901	-0.49407278
H	-2.35325264	1.59131533	0.21397719
H	-2.63810965	-1.10085111	0.29774825

State=1-A
RB3LYP/6-31G(d), HF= -302.266671
Zero-point correction= 0.076185 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.190486
Imaginary frequency: -344.4 cm^{-1}

TS 25 → 38 S_1

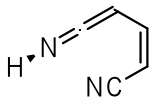


Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.23162400	0.38003758	-0.68239633
N	-0.36393856	-1.22908030	0.18931151
C	-1.61750757	-0.83292085	-0.02188797
C	-1.74941371	0.61373085	-0.17112181
C	-0.48845535	1.10720039	-0.02654097
C	0.34112970	-0.06103135	0.24934694
C	1.81072288	-0.05041583	0.41312408
H	-2.42904291	-1.55481552	-0.04371900
H	-2.66719245	1.15680692	-0.35544916
H	-0.14039609	2.13008766	-0.06405125
H	2.38397773	-0.44815918	1.25729151

State=1-A
<S2>= 0.626254, i.e. 68.7% singlet
UB3LYP/6-31G(d), HF= -302.3023396
Zero-point correction= 0.076589 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.225750
Imaginary frequency: -267.4 cm^{-1}

26Z

(Z)-5-iminopenta-2,4-dienenitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.41302835	-1.83227414	0.15115930
N	2.04003015	-1.08259302	-0.26468533
C	1.50187319	-0.03339369	0.03550207
C	0.98222524	1.18231408	0.20099961
C	-0.40118899	1.54254103	-0.03045007
C	-1.48530625	0.73651405	-0.15428158
C	-1.44256246	-0.67656639	-0.00132519
H	2.05606589	-1.84685398	0.41423839
H	1.66694944	1.95889232	0.53145304
H	-0.58233032	2.61272962	-0.09994910
H	-2.45994198	1.17084777	-0.35372918

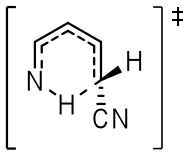
State=1-A
RB3LYP/6-31G(d), HF= -302.3577818
Zero-point correction= 0.077536 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.280245

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	70.6	10.9	2
2	A	104.9	3.0	1
3	A	174.9	4.3	1
4	A	322.8	6.2	1
5	A	383.2	2.0	0
6	A	433.4	71.9	14
7	A	509.8	20.3	4
8	A	569.1	2.6	0
9	A	622.5	17.5	3
10	A	724.5	41.2	8
11	A	769.6	8.0	2
12	A	812.9	60.7	12
13	A	892.4	125.4	24
14	A	905.6	234.7	45
15	A	949.4	9.6	2
16	A	968.6	16.8	3
17	A	1125.1	2.5	0
18	A	1205.6	4.7	1
19	A	1369.7	9.2	2
20	A	1406.3	28.8	6
21	A	1581.1	91.5	18
22	A	2051.1	520.6	100
23	A	2237.1	32.0	6
24	A	3056.9	10.6	2
25	A	3068.4	0.2	0
26	A	3084.3	1.8	0
27	A	3379.1	52.5	10

TS 26Z → 27Z

~1,5-H shift

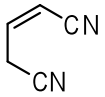


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.42873582	0.43020185	-0.52520434
N	0.60847436	1.56817448	0.35457026
C	1.36198279	0.90325963	-0.30409507
C	1.65255384	-0.43695883	-0.55074873
C	0.68466224	-1.24627446	0.03064128
C	-0.50045884	-0.80489012	0.70084825
C	-1.55330515	-0.11809076	0.01367666
H	0.16295017	0.80476076	1.12236628
H	2.60725528	-0.80247737	-0.90178885
H	0.97341258	-2.28765537	0.16702361
H	-0.87439709	-1.48553506	1.46490318

State=1-A
RB3LYP/6-31G(d), HF= -302.2845308
Zero-point correction= 0.073250 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.211280
Imaginary frequency: -964.0 cm^{-1}

27Z

(Z)-pent-2-enedinitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.74527464	-1.07674195	-0.27867193
N	3.09175841	-0.40174026	-0.59661532
C	0.03670779	0.99957791	0.29175378
C	-1.25016199	1.03381954	-0.08556635
C	0.79368848	-0.25106013	0.67069402
C	2.07744872	-0.34643465	-0.03619038
C	-2.07162441	-0.13167817	-0.19248354
H	0.58758609	1.93496629	0.34503976
H	-1.72781566	1.98027519	-0.32388584
H	0.19775929	-1.14742124	0.46574511
H	1.00073231	-0.24379175	1.75086655

State=1-A
RB3LYP/6-31G(d), HF= -302.3847331
Zero-point correction= 0.078749 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.305984

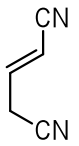
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	44.1	8.7	25
2	A	127.0	11.5	33
3	A	165.8	4.1	12
4	A	290.7	2.2	6
5	A	362.8	0.5	1
6	A	370.3	0.3	1
7	A	479.0	2.8	8
8	A	562.8	2.9	8
9	A	653.3	0.6	2
10	A	737.6	34.6	99
11	A	877.2	7.0	20
12	A	903.8	10.3	29
13	A	935.2	2.2	6
14	A	976.9	0.5	1
15	A	1031.9	2.8	8
16	A	1187.3	1.4	4
17	A	1224.4	0.4	1
18	A	1284.5	5.1	15

19	A	1371.6	0.1	0
20	A	1410.4	12.3	35
21	A	1635.1	7.5	21
22	A	2259.7	6.8	20
23	A	2288.0	5.9	17
24	A	2922.4	0.5	2
25	A	2980.7	0.4	1
26	A	3067.1	1.8	5
27	A	3083.1	0.9	3

27E

(E)-pent-2-enedinitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.33215173	-3.11805475	0.00000000
N	-0.40038494	2.91635511	0.00000000
C	-0.46345150	-0.67577437	0.00000000
C	-0.93282167	-2.02526612	0.00000000
C	1.41573184	1.02068589	0.00000000
C	0.41017577	2.08641214	0.00000000
C	0.84256445	-0.37599810	0.00000000
H	-1.22234995	0.10374060	0.00000000
H	2.06724895	1.15033665	0.87590000
H	2.06724895	1.15033665	-0.87590000
H	1.58226540	-1.17291768	0.00000000

State=1-A'
RB3LYP/6-31G(d), HF= -302.3853781
Zero-point correction= 0.078536 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.306842

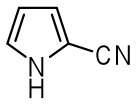
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A'	103.7	8.3	21
2	A"	116.2	7.4	19
3	A"	176.8	1.2	3
4	A'	191.7	3.5	9
5	A"	361.3	0.0	0
6	A'	363.0	2.9	8
7	A"	474.3	5.3	13
8	A'	515.8	0.0	0
9	A'	648.0	1.2	3
10	A"	776.6	0.0	0
11	A'	843.0	0.8	2
12	A"	934.4	9.2	23
13	A"	970.0	38.5	99

14	A'	998.2	1.9	5
15	A'	1010.4	7.3	19
16	A"	1198.4	0.3	1
17	A'	1244.3	3.0	8
18	A'	1292.5	0.3	1
19	A'	1320.7	1.7	4
20	A'	1406.6	19.4	50
21	A'	1647.5	13.5	35
22	A'	2264.5	11.1	29
23	A'	2290.2	2.9	7
24	A'	2924.4	1.4	4
25	A"	2946.8	0.3	1
26	A'	3058.5	2.0	5
27	A'	3069.4	1.8	5

28

2-Cyanopyrrole

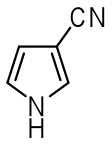


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.02609191	-0.49493102	0.00000000
C	0.06785582	0.35341817	0.00000000
C	1.20931687	-0.43954256	0.00000000
C	0.78592887	-1.78878129	0.00000000
C	-0.59801988	-1.79090484	0.00000000
H	-1.98731309	-0.18764981	0.00000000
H	-1.30318831	-2.60938827	0.00000000
H	1.41942530	-2.66464347	0.00000000
H	2.22404632	-0.06768790	0.00000000
C	-0.08049633	1.76011718	0.00000000
N	-0.21111985	2.91829239	0.00000000

State=1-A'
RB3LYP/6-31G(d), HF= -302.4135317
Zero-point correction= 0.081680 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.331852

29

3-Cyanopyrrole

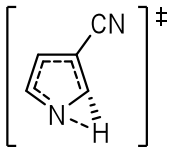


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.85499481	0.06904919	0.00000000

C	-0.77645541	0.90388316	0.00000000
C	0.36235497	0.11001783	0.00000000
C	-0.06889936	-1.25748234	0.00000000
C	-1.44125697	-1.24660467	0.00000000
H	-2.81674161	0.37369913	0.00000000
H	-2.15599003	-2.05606436	0.00000000
H	0.57157102	-2.12737764	0.00000000
H	-0.88021261	1.97831758	0.00000000
C	1.70116122	0.58513505	0.00000000
N	2.80070146	0.96834096	0.00000000

State=1-A'
RB3LYP/6-31G(d), HF= -302.4146745
Zero-point correction= 0.081744 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.332930

TS 29 → 35

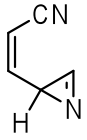


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.12791126	-1.96185430	-0.07086109
N	-0.84001980	2.83167067	0.14668503
C	-0.92017612	-0.76716974	0.09095484
C	-0.07903656	0.36516011	0.00110725
C	1.22795674	-0.12340053	-0.17863898
C	1.15236198	-1.51484166	-0.17253546
C	-0.49458638	1.72223779	0.08002347
H	-0.63669731	-1.60808522	1.04315482
H	2.12259946	0.47896670	-0.27151326
H	1.96675241	-2.22703635	-0.20928493
H	-1.99625503	-0.82447542	-0.01859095

State=1-A
RB3LYP/6-31G(d), HF= -302.3343058
Zero-point correction= 0.076518 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.257787
Imaginary frequency: -1537.9 cm^{-1}

30

3-(2*H*-aziren-2-yl)acrylonitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.68057209	-0.72100078	0.74355700
N	-2.15883785	-1.14688528	-0.06492500
C	-1.61735098	-0.12102221	0.04233000
C	-0.98324715	1.15420087	0.14208100
C	0.32994682	1.36343104	-0.07923800
C	1.36375695	0.35114518	-0.36454100
C	1.12683814	-1.08811085	-0.31846800
H	-1.63569926	1.98634279	0.39170500
H	0.68253169	2.39187809	-0.02950300
H	2.25109090	0.72770130	-0.87050300
H	0.73026626	-1.98858290	-0.77510400

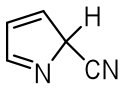
State=1-A
RB3LYP/6-31G(d), HF= -302.3221079
Zero-point correction= 0.077760 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.244347

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	64.0	12.0	22
2	A	123.1	6.5	12
3	A	223.3	13.7	25
4	A	276.4	1.8	3
5	A	368.9	5.1	10
6	A	481.2	0.4	1
7	A	566.0	1.3	2
8	A	667.8	1.9	3
9	A	743.7	4.5	8
10	A	759.1	53.9	100
11	A	783.8	11.6	22
12	A	883.4	7.8	14
13	A	928.9	7.4	14
14	A	965.6	4.2	8
15	A	972.9	25.6	47
16	A	1032.2	7.7	14
17	A	1176.4	4.9	9
18	A	1237.4	18.8	35
19	A	1344.8	6.0	11
20	A	1377.4	1.5	3
21	A	1612.2	14.2	26
22	A	1700.0	17.2	32
23	A	2247.0	14.4	27
24	A	3032.4	17.5	32
25	A	3054.1	9.1	17
26	A	3076.4	2.7	5
27	A	3107.7	2.0	4

32

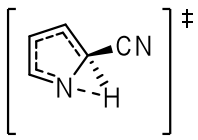
2*H*-Pyrrole-2-carbonitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.69505120	-0.04775579	-0.51726051
N	-0.49152203	-1.20707972	0.21088345
C	1.64305047	-0.05706339	-0.02846525
C	0.31207098	-0.02921024	0.59385603
C	-1.59161649	-0.72854824	-0.26167696
C	-1.66350216	0.74130753	-0.29029630
C	-0.50263791	1.19162631	0.21285573
H	0.44836190	-0.06981562	1.68612542
H	-2.38348794	-1.39437526	-0.59976625
H	-2.50206543	1.32599877	-0.64974369
H	-0.17170209	2.21336891	0.35038433

State=1-A
RB3LYP/6-31G(d), HF= -302.3771838
Zero-point correction= 0.080448 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.296736

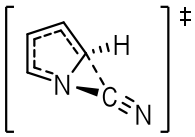
TS 32 → 28



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.49202235	-1.17360858	-0.03205273
N	-2.90891451	-0.06284612	-0.11984643
C	-1.75324931	-0.04007186	0.00463349
C	-0.33524822	0.02642950	0.18059121
C	0.48631979	1.17893068	0.09791841
C	1.78229492	0.72664521	-0.11106392
C	1.74189885	-0.67733707	-0.14222020
H	-0.00474029	-0.80947931	1.10457915
H	0.14206873	2.20107571	0.18128631
H	2.67099069	1.33984780	-0.19748119
H	2.57782991	-1.36384004	-0.20424404

State=1-A
RB3LYP/6-31G(d), HF= -302.3272717
Zero-point correction= 0.076248 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.251024
Imaginary frequency: -1526.0 cm^{-1}

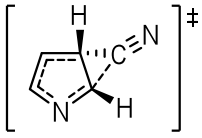
TS 32 → 33



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.17644098	-0.61003501	0.79658100
N	-2.35541800	-0.04211509	-0.64986100
C	-1.33330800	0.02522595	-0.06948800
C	0.83822905	-1.15717597	0.06469200
C	1.65890201	-0.17251494	-0.49401500
C	1.10559296	1.07201304	-0.19978300
C	-0.05513403	0.83394200	0.58021600
H	0.87722709	-2.22993097	-0.07420200
H	2.55035801	-0.35646590	-1.08149000
H	1.48098092	2.04393406	-0.49139600
H	-0.47124306	1.49856898	1.33031400

State=1-A
RB3LYP/6-31G(d), HF= -302.3102016
Zero-point correction= 0.078532 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.231670
Imaginary frequency: -649.0 cm^{-1}

TS 32 → 34

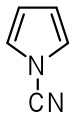


Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.31814050	0.01231762	-0.71917506
N	-0.97159190	-1.17662007	-0.09979354
C	1.30192704	-0.00217530	-0.13473610
C	-0.99835176	1.12884269	-0.06961317
C	-1.57830338	-0.05313838	-0.53472391
C	0.04750736	-0.76370915	0.70351829
C	0.08190652	0.73139356	0.76433456
H	-1.25710452	2.14393044	-0.33834196
H	-2.41949250	-0.12860560	-1.21650807
H	0.53457982	-1.43932627	1.39870559
H	0.58806232	1.32683805	1.51624673

State=1-A
RB3LYP/6-31G(d), HF= -302.3190747
Zero-point correction= 0.078598 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.240477
Imaginary frequency: -698.7 cm^{-1}

33

1-Cyanopyrrole

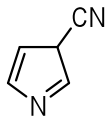


Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.000000	0.000000	0.336268
N	0.000000	0.000000	2.844348
C	0.000000	0.000000	1.679578
C	0.000000	1.140237	-0.475790
C	0.000000	0.717407	-1.774380
C	0.000000	-0.717407	-1.774380
C	0.000000	-1.140237	-0.475790
H	0.000000	2.121431	-0.026187
H	0.000000	1.360337	-2.643681
H	0.000000	-1.360337	-2.643681
H	0.000000	-2.121431	-0.026187

State=1-A1
RB3LYP/6-31G(d), HF= -302.3900591
Zero-point correction= 0.080896 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.309163

34

3*H*-Pyrrole-3-carbonitrile

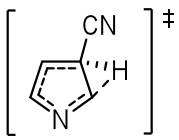


Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.67920095	-0.78302147	-0.31033166
N	-2.72940984	0.00542038	-0.47445771
C	0.54582835	-1.15086625	0.16538979
C	-1.66976502	0.01507330	-0.00062091
C	-0.33305759	0.02164604	0.59678691
C	0.55376714	1.17888648	0.18876918
C	1.68424941	0.64584123	-0.30119873
H	0.25749495	-2.19281580	0.27164314
H	-0.44576707	-0.01110413	1.69356211
H	0.29130112	2.22169945	0.30373932
H	2.56229950	1.16194330	-0.67017644

State=1-A
RB3LYP/6-31G(d), HF= -302.3739672

Zero-point correction= 0.080129 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.293838

TS 34 → 35

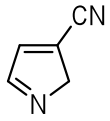


Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.83516404	-0.70937245	-0.10904989
N	-2.93574334	-0.01290344	-0.08065802
C	1.79660901	0.64613130	-0.08060331
C	0.51610794	1.17049281	0.04749893
C	-0.35225251	0.04515297	0.10093133
C	0.56494524	-1.12832238	-0.02132726
C	-1.77653048	0.01624208	0.00492363
H	2.72227426	1.21048651	-0.11142350
H	0.21694878	2.20502972	0.13813080
H	0.25199302	-2.16063857	-0.12553209
H	0.01956390	-0.69712706	1.11824023

State=1-A
RB3LYP/6-31G(d), HF= -302.3369597
Zero-point correction= 0.076729 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.260231
Imaginary frequency: -1220.3 cm^{-1}

35

2*H*-Pyrrole-3-carbonitrile

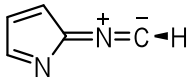


Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.17701849	-1.99325939	0.00000000
N	0.71409813	2.86110929	0.00000000
C	-1.05621093	-1.61044380	0.00000000
C	-1.23419223	-0.15600056	0.00000000
C	0.01254280	0.37565277	0.00000000
C	0.98631429	-0.78330934	0.00000000
C	0.37835459	1.74579502	0.00000000
H	-1.87065273	-2.33167087	0.00000000
H	-2.17589732	0.37915518	0.00000000
H	1.64394130	-0.77629910	0.87999287
H	1.64394130	-0.77629910	-0.87999287

State=1-A'
RB3LYP/6-31G(d), HF= -302.3912314
Zero-point correction= 0.080583 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.310649

36

N-(2*H*-pyrrol-2-ylidene)methanideiminium



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.09531086	1.59134878	-0.01455154
N	-1.15061855	-0.51139729	-0.00037571
C	-0.66802945	-1.73717172	-0.00402836
C	0.78006304	-1.79070271	-0.00610488
C	1.20741957	-0.49069662	-0.00388355
C	-0.00961881	0.28727703	0.00050678
C	-0.19198956	2.77590786	0.13724725
H	-1.33775957	-2.59209838	-0.00364462
H	1.39122154	-2.68468261	-0.00730208
H	2.21635240	-0.10049111	-0.00221337
H	-0.25537728	3.54992864	-0.62477259

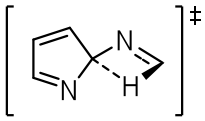
State=1-A
RB3LYP/6-31G(d), HF= -302.3325122
Zero-point correction= 0.078900 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.253612

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	160.9	7.7	1
2	A	173.0	3.3	0
3	A	452.1	52.4	5
4	A	522.3	8.2	1
5	A	556.1	9.3	1
6	A	586.6	161.0	17
7	A	628.3	33.1	3
8	A	651.6	971.5	100
9	A	724.2	65.6	7
10	A	761.2	24.6	3
11	A	846.5	3.8	0
12	A	855.5	3.2	0
13	A	889.0	2.3	0
14	A	902.2	22.7	2
15	A	993.5	6.7	1
16	A	1043.6	14.3	1
17	A	1178.9	25.0	3
18	A	1250.2	3.4	0
19	A	1317.9	7.9	1

20	A	1375.9	118.3	12
21	A	1404.8	0.0	0
22	A	1508.6	14.3	1
23	A	1996.7	642.4	66
24	A	3084.2	13.4	1
25	A	3090.4	19.3	2
26	A	3116.5	5.5	1
27	A	3137.1	5.3	1

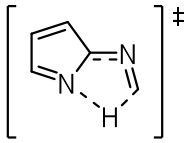
TS 36 → 40



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.32186877	-1.18439918	0.00306896
N	-1.76721710	-0.01675998	-0.66270606
C	1.55346822	-0.75200554	0.00196139
C	1.67114475	0.70500367	0.01419497
C	0.40333981	1.18796047	0.03133150
C	-0.45212767	-0.00515446	-0.00249989
C	-2.12245087	-0.06652497	0.54102183
H	2.38563048	-1.45071938	0.00205757
H	2.59538308	1.26949945	0.01161675
H	0.05164053	2.21087733	0.02803210
H	-1.12393101	-0.04344741	1.27547188

State=1-A
RB3LYP/6-31G(d), HF= -302.2623327
Zero-point correction= 0.074796 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.187537
Imaginary frequency: -910.4 cm^{-1}

TS 36 → 41



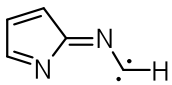
Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.00515648	-0.98192386	-0.29173711
N	1.75207671	0.65656823	-0.19154071
C	-1.28335993	-1.03977456	0.04010231
C	-1.80392432	0.27190616	0.21173880
C	-0.75253992	1.18714099	0.04645546
C	0.34671239	0.40004234	-0.27228514

C	2.11656088	-0.35068656	0.42705752
H	-1.84026504	-1.96789184	-0.00634115
H	-2.85765400	0.51589730	0.28897362
H	-0.77660151	2.26313273	0.14150289
H	1.43319361	-1.34541896	0.24039563

State=1-A
RB3LYP/6-31G(d), HF= -302.2537488
Zero-point correction= 0.073945 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.179804
Imaginary frequency: -1093.2 cm^{-1}

37Z T_0

(s-E,Z)-2*H*-pyrrol-2-imine-*N*-carbene

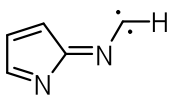


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.88802874	-0.70923908	0.00000000
N	-0.34103712	1.65855542	0.00000000
C	-0.12330593	-1.78369971	0.00000000
C	1.31387312	-1.47405655	0.00000000
C	1.38925089	-0.11451271	0.00000000
C	0.01177473	0.34182353	0.00000000
C	-1.50781241	2.13003199	0.00000000
H	-0.55765973	-2.77961735	0.00000000
H	2.12265780	-2.19375862	0.00000000
H	2.26058767	0.52574631	0.00000000
H	-1.72480705	3.20489595	0.00000000

State= 3-A"
<S2>= 2.026165
UB3LYP/6-31G(d), HF= -302.2935162
Zero-point correction= 0.076977 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.216539

37E T_0

(s-E,E)-2*H*-pyrrol-2-imine-*N*-carbene



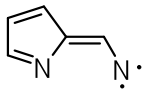
Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.34698561	0.17744600	0.00000000
N	-0.53235191	1.61349232	0.00000000
C	1.50745102	-1.14086993	0.00000000
C	0.23884892	-1.87541940	0.00000000

C	-0.73062605	-0.92376286	0.00000000
C	-0.00692608	0.35086865	0.00000000
C	-1.74565647	1.93245818	0.00000000
H	2.49978337	-1.58178604	0.00000000
H	0.12376404	-2.95212135	0.00000000
H	-1.80648438	-1.03301510	0.00000000
H	-2.09804698	2.97070635	0.00000000

State= 3-A"
<S2>= 2.026724
UB3LYP/6-31G(d), HF= -302.2933804
Zero-point correction= 0.076932 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.216448

38Z T_0

Z-(2*H*-pyrrol-2-ylidene)methylnitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.15998644	-1.78276962	0.00000000
C	1.28673976	-1.50475093	0.00000000
C	1.39321790	-0.14811119	0.00000000
C	0.02504962	0.34308291	0.00000000
N	-0.89533390	-0.69146022	0.00000000
H	-0.61718198	-2.76827775	0.00000000
H	2.08008409	-2.24162504	0.00000000
H	2.28899275	0.45937818	0.00000000
C	-0.36723059	1.72718856	0.00000000
N	-1.57074781	2.15878855	0.00000000
H	0.44393562	2.47138793	0.00000000

State= 3-A"
<S2>= 2.048598
UB3LYP/6-31G(d), HF= -302.3128187
Zero-point correction= 0.077091 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.235728

Natural Atomic Spin Densities (UB3LYP/EPR-III)

1	C	0.31571
2	C	0.19189
3	C	-0.02393
4	C	0.50528
5	N	-0.09861
6	H	-0.00969
7	H	-0.00507
8	H	-0.00011
9	C	-0.23877
10	N	1.27086

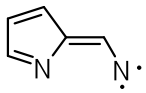
```
    11  H    0.09245
```

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	127.5	0.2	0
2	A'	206.0	2.9	6
3	A"	247.0	15.0	29
4	A'	449.4	6.3	12
5	A"	521.4	3.2	6
6	A"	636.6	2.4	5
7	A'	696.5	29.2	56
8	A"	724.1	51.6	99
9	A'	760.2	3.3	6
10	A"	835.3	2.6	5
11	A"	845.6	13.4	26
12	A"	892.5	1.7	3
13	A'	893.7	15.4	30
14	A'	945.1	7.4	14
15	A'	1028.9	0.9	2
16	A'	1072.4	21.5	41
17	A'	1162.4	1.6	3
18	A'	1216.4	7.5	14
19	A'	1289.6	18.8	36
20	A'	1335.8	48.8	94
21	A'	1405.5	12.5	24
22	A'	1444.8	7.3	14
23	A'	1510.7	8.9	17
24	A'	2896.4	8.9	17
25	A'	3085.0	10.7	21
26	A'	3118.2	3.2	6
27	A'	3137.1	2.4	5

38Z S_1

Z-(2*H*-pyrrol-2-ylidene)methylnitrene

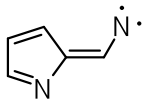


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.15632289	-1.78815881	0.00000000
C	1.28830339	-1.50872714	0.00000000
C	1.39126294	-0.15062485	0.00000000
C	0.02146216	0.33419344	0.00000000
N	-0.89411587	-0.68957648	0.00000000
H	-0.61612506	-2.77209126	0.00000000
H	2.08280182	-2.24407108	0.00000000
H	2.28514512	0.45951693	0.00000000
C	-0.37503644	1.73662465	0.00000000
N	-1.56484365	2.16687331	0.00000000
H	0.44287987	2.47572396	0.00000000

State= 1-A"
<S2>= 1.01651, i.e. 49.2% singlet
UB3LYP/6-31G(d), HF= -302.305986
Zero-point correction= 0.076739 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.229247

38E T_0

E-(2*H*-pyrrol-2-ylidene)methylnitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.45133179	-1.21375482	0.00000000
C	0.14780544	-1.88749221	0.00000000
C	-0.77633350	-0.89143248	0.00000000
C	-0.00068648	0.34686476	0.00000000
N	1.35085743	0.10917785	0.00000000
H	2.42231089	-1.70053083	0.00000000
H	-0.01836479	-2.95724054	0.00000000
H	-1.85563850	-0.96082555	0.00000000
C	-0.50244943	1.69759376	0.00000000
N	-1.74011188	2.00747048	0.00000000
H	0.25846666	2.49138452	0.00000000

State= 3-A"
<S2>= 2.047422
UB3LYP/6-31G(d), HF= -302.3173317
Zero-point correction= 0.077125 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.240207

Natural Atomic Spin Densities (UB3LYP/EPR-III)

1	C	0.38886
2	C	0.09931
3	C	0.04415
4	C	0.49874
5	N	-0.12106
6	H	-0.01122
7	H	-0.00319
8	H	-0.00238
9	C	-0.22830
10	N	1.24288
11	H	0.09221

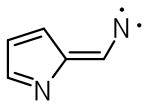
Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	142.0	2.1	4

2	A'	205.4	13.2	26
3	A"	246.9	19.6	39
4	A'	475.0	4.8	10
5	A"	523.4	9.7	19
6	A"	621.5	2.0	4
7	A'	628.3	19.2	38
8	A"	737.6	50.1	100
9	A'	790.3	11.6	23
10	A"	837.1	0.1	0
11	A"	855.8	14.1	28
12	A'	891.0	5.9	12
13	A"	899.6	0.7	1
14	A'	948.5	1.8	4
15	A'	1041.6	14.6	29
16	A'	1059.1	17.7	35
17	A'	1155.6	11.9	24
18	A'	1193.5	11.3	23
19	A'	1285.3	10.9	22
20	A'	1327.7	29.9	60
21	A'	1373.4	31.4	63
22	A'	1485.8	9.9	20
23	A'	1515.3	1.2	2
24	A'	2912.5	4.5	9
25	A'	3088.8	10.4	21
26	A'	3124.2	3.0	6
27	A'	3146.2	1.0	2

38E S_1

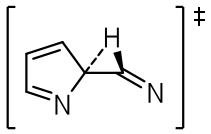
E-(2*H*-pyrrol-2-ylidene)methylnitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.44790667	-1.22208462	0.00000000
C	0.15066992	-1.89398807	0.00000000
C	-0.77369748	-0.89604846	0.00000000
C	0.00573476	0.34290915	0.00000000
N	1.34210545	0.11424817	0.00000000
H	2.42169614	-1.70246568	0.00000000
H	-0.01459532	-2.96357261	0.00000000
H	-1.85324352	-0.96223985	0.00000000
C	-0.50812318	1.70829478	0.00000000
N	-1.73424066	2.01330852	0.00000000
H	0.25614511	2.50088463	0.00000000

State= 1-A"
<S2>= 1.016145, 49.2% singlet
UB3LYP/6-31G(d), HF= -302.3109781
Zero-point correction= 0.076798 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.234181

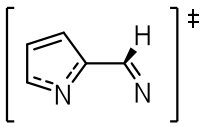
TS 38 S_1 → 32



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.77942039	0.83567452	0.02001566
C	-1.77464716	-0.61701564	-0.07364089
C	0.26476213	-0.02943648	-0.03062196
H	-2.65180934	1.47668377	0.00773290
H	-2.64791476	-1.25640364	-0.15725204
C	1.70814678	-0.17345536	0.06112471
H	1.37413175	-0.26042399	1.19753606
C	-0.46826980	1.21306009	0.10700400
H	-0.04176029	2.20474014	0.16975070
N	2.88364134	-0.22447399	-0.19220327
N	-0.56022374	-1.13803445	-0.05366198

State= 1-A
<S2>= 0.316581, i.e. 84.2% singlet
UB3LYP/6-31G(d), HF= 0.073282
Zero-point correction= 0.073282 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.200473
Imaginary frequency: -1320.7 cm^{-1}

TS 38Z T_0 → 38E T_0

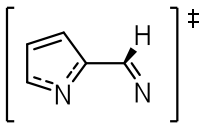


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.69371632	-0.74605925	-0.10218537
C	-1.81924309	0.70869750	-0.11030357
C	-0.55260486	1.18009792	0.05890139
C	0.28593821	-0.01505211	0.15194927
N	-0.42483129	-1.15839907	0.06029652
H	-2.49966488	-1.46476999	-0.21382222
H	-2.73486310	1.27240674	-0.23423145
H	-0.20709814	2.20447361	0.10143651
C	1.76314371	-0.02414353	0.37023770
N	2.63145490	-0.07997284	-0.53019051
H	2.09415495	0.03524983	1.42427862

State= 3-A
<S2>= 2.027119
UB3LYP/6-31G(d), HF= -302.2994816

Zero-point correction= 0.075828 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.223654
Imaginary frequency: -175.2 cm^{-1}

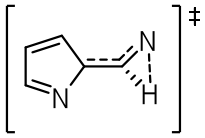
TS 38Z S_1 → 38E S_1



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.65667539	-0.72878889	-0.14736648
C	-1.79089878	0.72800983	-0.11788510
C	-0.53122651	1.20163850	0.09062229
C	0.30471203	0.00977204	0.21035558
N	-0.39601976	-1.13793363	0.03112994
H	-2.45926445	-1.44672268	-0.28584896
H	-2.70774339	1.28999799	-0.24215287
H	-0.19484307	2.22655904	0.17362161
C	1.77827087	0.00260091	0.43366215
N	2.47043105	-0.23058965	-0.58521526
H	2.21587849	0.23043441	1.41664678

State= 1-A
<S2>= 0.921561, i.e. 53.9% singlet
UB3LYP/6-31G(d), HF= -302.2994774
Zero-point correction= 0.075911 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.223567
Ziegler-Cramer corrected energy ($2*E(T_0) - E(S_1)$)= -302.223741
Imaginary frequency: -127.8 cm^{-1}

TS 38 → 39



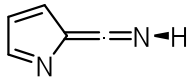
Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.75536932	-0.67987438	-0.02934589
C	-1.80856390	0.75936192	-0.16676749
C	-0.50609554	1.20053370	-0.12972480
C	0.25979756	0.01093608	0.09687121
H	-2.60528088	-1.35505450	-0.01554514
H	-2.70259228	1.36646211	-0.24090550
H	-0.12769185	2.21181499	-0.19130903
C	1.66076008	-0.13198119	0.05836677
H	1.90244191	-0.95275779	-0.71322480

N	2.87282482	-0.03313294	0.21601229
N	-0.52568914	-1.14177015	0.09607138

State=1-A
RB3LYP/6-31G(d), HF= -302.2648026
Zero-point correction= 0.073856 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.190947
Imaginary frequency: -823.9 cm^{-1}

39

(2*H*-pyrrol-2-ylidene)methanimine



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.74169923	-0.75380311	0.01624970
C	-1.86197441	0.69052864	0.02211405
C	-0.58724481	1.17906919	0.00803566
C	0.26238220	0.00108234	-0.00996885
N	-0.50100291	-1.18303817	0.00015046
H	-2.56612760	-1.46135136	0.02494342
H	-2.78313822	1.26016545	0.03232674
H	-0.25397332	2.20846876	0.00258591
C	1.60170795	-0.02392539	-0.00519238
N	2.80772237	-0.03269253	-0.13346237
H	3.41717271	-0.05487794	0.68589828

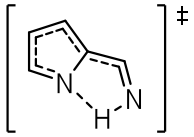
State=1-A
RB3LYP/6-31G(d), HF= -302.3635295
Zero-point correction= 0.079731 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.283799

Vibrational Frequencies (B3LYP/6-311G**, scaled by 0.967):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	141.0	6.9	1
2	A	160.0	1.2	0
3	A	449.0	37.6	4
4	A	549.5	20.3	2
5	A	566.4	2.9	0
6	A	589.7	0.5	0
7	A	621.9	15.5	2
8	A	705.6	68.4	8
9	A	738.8	57.5	6
10	A	847.9	568.2	64
11	A	859.4	26.6	3
12	A	861.8	64.4	7
13	A	891.6	10.9	1
14	A	898.9	2.7	0
15	A	990.2	2.1	0
16	A	1049.0	14.5	2

17	A	1145.4	14.1	2
18	A	1239.7	0.6	0
19	A	1316.0	5.6	1
20	A	1386.5	1.7	0
21	A	1389.8	77.1	9
22	A	1518.4	9.2	1
23	A	2064.3	893.3	100
24	A	3078.9	15.4	2
25	A	3114.3	4.4	0
26	A	3135.4	5.5	1
27	A	3386.2	62.5	7

TS 39 → 28

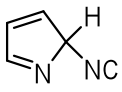


Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.32241324	-1.02228045	0.00012625
C	1.94820458	0.24558700	0.00003350
C	0.94264316	1.21777016	-0.00004455
C	-0.25632735	0.50344413	0.00003123
N	-0.00900058	-0.91038317	0.00013803
H	1.79273164	-1.99885885	0.00019232
H	3.01506661	0.42660021	0.00002858
H	1.05552032	2.29299427	-0.00012716
H	-1.64523372	-1.09834547	-0.00005627
C	-1.63587634	0.47740816	-0.00011502
N	-2.58306065	-0.25446885	-0.00017030

State=1-A
RB3LYP/6-31G(d), HF= -302.2795645
Zero-point correction= 0.073589 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.205975
Imaginary frequency: -1387.4 cm^{-1}

40

2-Isocyano-2*H*-pyrrole

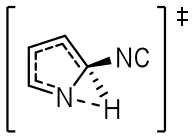


Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.34284406	-0.02942510	0.55250234
C	-1.57190214	-0.73147760	-0.26767965
C	-1.65169286	0.74351408	-0.28446587

C	-0.47605445	1.19242880	0.17828425
H	0.44386467	-0.07811824	1.64796697
H	-2.37264676	-1.39687884	-0.58556474
H	-2.50366679	1.32545661	-0.61587489
H	-0.13805341	2.21229338	0.31225044
N	-0.45355579	-1.20623666	0.15826479
N	1.64500858	-0.04851989	-0.01219485
C	2.72852752	-0.05494969	-0.47551896

State=1-A
RB3LYP/6-31G(d), HF= -302.3419225
Zero-point correction= 0.079934 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.261989

TS 40 → 41

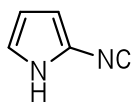


Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.42190617	-1.18087337	-0.01426701
C	-0.36803045	0.03851942	0.16658957
C	0.47202736	1.17188798	0.07229933
C	1.76187198	0.68311395	-0.10405263
C	1.68996276	-0.71842414	-0.11491659
H	-0.04965309	-0.77773291	1.12003571
H	0.14467239	2.20106907	0.12759095
H	2.66667571	1.27385455	-0.17973260
H	2.50941838	-1.42622549	-0.13867471
C	-2.90553825	-0.00802813	-0.14878100
N	-1.73231671	-0.00103801	-0.00802604

State=1-A
RB3LYP/6-31G(d), HF= -302.2902398
Zero-point correction= 0.075657 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.214583
Imaginary frequency: -1548.7 cm^{-1}

41

2-Isocyano-1*H*-pyrrole

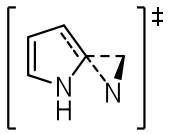


Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.72669355	-0.67929086	0.00000000

C	1.78465459	0.70011620	0.00000000
C	0.45268980	1.19021748	0.00000000
C	-0.37949291	0.08513508	0.00000000
N	0.40588948	-1.04838679	0.00000000
H	0.04629257	-1.99105088	0.00000000
H	2.51056670	-1.42218752	0.00000000
H	2.68778135	1.29421314	0.00000000
H	0.12438624	2.21936438	0.00000000
N	-1.74073921	-0.00815349	0.00000000
C	-2.92205816	-0.08027076	0.00000000

State=1-A'
RB3LYP/6-31G(d), HF= -302.3755225
Zero-point correction= 0.080890 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.294632

TS 41 → 28

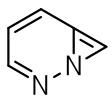


Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.64618078	-0.67675002	0.08014007
C	1.67973193	0.70479956	0.06271978
C	0.34857632	1.16426256	-0.09754177
C	-0.45676087	0.04035296	-0.21030802
N	0.33962196	-1.07270103	-0.05952629
H	2.44122281	-1.40436991	0.15484543
H	2.56560389	1.31649725	0.16181616
H	-0.00191176	2.18553471	-0.12651656
C	-1.97319556	-0.11849968	-0.52530138
N	-2.12302247	0.10694990	0.64549514
H	0.01169302	-2.02239644	-0.15017906

State=1-A
RB3LYP/6-31G(d), HF= -302.3174114
Zero-point correction= 0.078592 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.238820
Imaginary frequency: -433.5 cm^{-1}

42

1,2-Diazabicyclo[4.1.0]hepta-2,4,6-triene



Atom Coordinates (Angstroms)

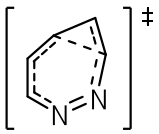
Type	X	Y	Z
N	-0.19095993	-1.43233188	-0.06840100
C	-0.63781238	0.95695541	-0.03692800
C	-1.69143275	0.38219510	0.42630200
C	0.72938989	1.36507253	-0.09074300
C	1.56265720	0.30416499	0.04111500
C	1.00833932	-1.04254065	0.22723200
H	-2.50427383	0.26013763	1.12497700
H	1.05182155	2.39364232	-0.21766100
H	2.64177428	0.42402828	0.03794300
H	1.67756582	-1.82233809	0.59035000
N	-1.05100328	-0.43203232	-0.63695400

State=1-A
RB3LYP/6-31G(d), HF= -302.2406907
Zero-point correction= 0.077462 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.163229

Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	148.3	4.5	8
2	A	304.3	16.5	28
3	A	356.6	8.9	15
4	A	419.7	1.1	2
5	A	549.0	11.0	19
6	A	564.2	1.4	2
7	A	603.8	9.1	15
8	A	654.5	9.1	15
9	A	713.2	59.4	101
10	A	767.0	6.1	10
11	A	850.3	1.8	3
12	A	905.7	4.2	7
13	A	926.3	3.9	7
14	A	947.6	7.4	12
15	A	950.8	2.7	5
16	A	982.2	1.3	2
17	A	1010.2	8.6	15
18	A	1119.6	3.7	6
19	A	1307.5	3.3	6
20	A	1346.4	8.1	14
21	A	1480.2	5.7	10
22	A	1573.9	4.1	7
23	A	1829.8	10.5	18
24	A	3033.4	19.7	33
25	A	3077.7	1.4	2
26	A	3094.8	7.9	13
27	A	3183.9	6.6	11

TS 42 → 43

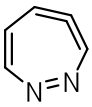


Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.22610231	-1.42444011	-0.09663400
C	-0.61299349	1.00300270	-0.02250800
C	-1.65491420	0.41040319	0.43791800
C	0.76398334	1.35032537	-0.11169000
C	1.56220487	0.26624976	0.05995500
C	0.97415552	-1.06185952	0.23939600
H	-2.45541114	0.29523780	1.15319800
H	1.12211885	2.35722055	-0.30142600
H	2.64454383	0.35123929	0.04224700
H	1.62113091	-1.86597621	0.58807000
N	-1.07775479	-0.42505353	-0.63201100

State=1-A
RB3LYP/6-31G(d), HF= -302.2406546
Zero-point correction= 0.077046 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.163609
Imaginary frequency: -182.5 cm^{-1}

43

1,2-Diazacyclohepta-1,3,4,6-tetraene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.41396631	0.02941632	-0.27724003
C	1.18229604	-0.74247263	0.08016611
N	-1.04167157	-1.15459167	-0.43845544
C	-0.79412338	1.11766828	0.31664271
C	0.53303844	1.48498559	0.19491349
H	0.79977355	2.53118672	0.34892864
H	-1.52497691	1.84973297	0.64886425
C	0.17024199	-1.53294958	0.32540476
H	0.08409034	-2.40668799	0.95997794
C	1.48898870	0.52348152	-0.26327629
H	2.34792737	0.79771663	-0.87100720

State=1-A
RB3LYP/6-31G(d), HF= -302.2755361
Zero-point correction= 0.078875 (Hartree/Particle)
Sum of electronic and zero-point Energies= -302.196661

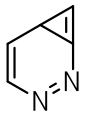
Vibrational Frequencies (B3LYP/6-311G, scaled by 0.967):**

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	263.4	21.8	26
2	A	328.0	2.9	3
3	A	350.1	9.1	11
4	A	435.3	5.5	6
5	A	515.9	15.9	19
6	A	602.8	22.5	27
7	A	663.1	9.6	11
8	A	701.6	48.0	57
9	A	753.7	31.3	37
10	A	807.8	27.5	32
11	A	822.1	8.4	10
12	A	848.6	50.4	59
13	A	915.4	2.7	3
14	A	937.2	3.7	4
15	A	1019.2	7.5	9
16	A	1083.4	2.3	3
17	A	1173.5	19.3	23
18	A	1202.9	8.2	10
19	A	1314.1	8.3	10
20	A	1399.5	9.1	11
21	A	1453.5	12.0	14
22	A	1511.8	84.9	100
23	A	1816.8	3.4	4
24	A	3027.0	20.1	24
25	A	3061.4	9.3	11
26	A	3078.0	8.2	10
27	A	3117.2	1.9	2

Table S3. Cartesian coordinates and CASPT2 energies of species optimized at CASSCF(8,8)/6-31G* level using MOLCAS.

16

2,3-Diazabicyclo[4.1.0]hepta-1(7),2,4-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.4774752	-0.5956947	0.0575605
N	-0.5503553	-1.4172458	-0.1744105
C	0.7140623	-0.8320816	-0.1931738
C	1.6703515	-0.3216284	0.5270965
C	1.0806772	0.6185427	-0.4857561
C	-0.0725271	1.4388329	-0.0579099
C	-1.2196294	0.7855045	0.2521470
H	2.1351355	-0.3206816	1.4890472
H	1.6310305	0.8994088	-1.3688660
H	-0.0436028	2.5141940	-0.0328571
H	-2.0972033	1.3101600	0.5756541

QCISD(T)/6-31G* on CAS(8,8)/6-31G* geometry: -301.4023458

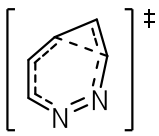
CASSCF Reference energy: -300.4833719120
CASPT2 Total energy: -301.3185401325
Residual norm: 0.0000009957
Reference weight: 0.78371

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of C3-C4 bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.921242	0.848686

TS 16 → 17



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.5707959	-0.2620997	0.0469429
N	0.8428989	-1.2639291	-0.3361654

C	-0.4578175	-1.0816196	-0.1427027
C	-1.4655664	-0.6533612	0.5499319
C	-1.2806560	0.4858345	-0.3726214
C	-0.2337963	1.4014256	-0.0804897
C	1.0347391	0.9623780	0.2871384
H	-1.9393050	-0.8132502	1.4952505
H	-1.9688222	0.6737495	-1.1798046
H	-0.3510678	2.4484764	-0.3039616
H	1.7780942	1.6851917	0.5652350

QCISD(T)/6-31G* on CAS(8,8)/6-31G* geometry: -301.4003518
Barrier is about 1.3 kcal/mol cf. **16**.

CASSCF Reference energy: -300.4724881615
CASPT2 Total energy: -301.3190247140
Residual norm: 0.0000003753
Reference weight: 0.77972

CAS(8,8) active space: 3 π/π^* pairs and σ/σ^* of breaking C3-C4 bond.

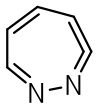
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.914106	0.835590

Imaginary frequency: -756.8 cm^{-1}

17

1,2-Diazacyclohepta-2,3,5,7-tetraene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.6188383	0.0364796	0.2121174
N	1.0478870	-1.0297447	-0.5068398
C	-0.0637449	-1.3717369	-0.0326381
C	-1.2607627	-0.9229212	0.3455433
C	-1.5288088	0.4421654	-0.1318956
C	-0.5054320	1.3273020	-0.2177470
C	0.8819195	1.0915178	0.2526488
H	-1.9311988	-1.4650136	0.9822202
H	-2.5286283	0.7458257	-0.3895322
H	-0.7091336	2.3347691	-0.5358253
H	1.3628571	1.9393120	0.7107251

CASSCF Reference energy: -300.5335373130
CASPT2 Total energy: -301.3587833819
Residual norm: 0.0000003930
Reference weight: 0.78585

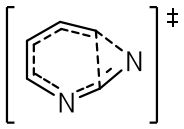
CAS(8,8) active space: 4 π/π* pairs

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.905147	0.819292

TS 17 → 19

NB: the diazirine structure **18** is a TS at the CAS(8,8)/6-31G* level, but an intermediate at the B3LYP/6-31G* level.



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.3335107	0.3471569	-0.4375815
N	1.3001472	-0.6950332	0.6022249
C	0.3838722	-1.1190318	-0.1181254
C	0.4400056	1.3380621	-0.1377111
C	-0.8719521	1.1908390	0.2769910
C	-1.6151648	-0.0117026	0.0939952
C	-1.0041814	-1.1949430	-0.2628298
H	0.7896907	2.3128707	-0.4284905
H	-1.4214230	2.0892659	0.4898067
H	-2.6886436	0.0485591	0.1074659
H	-1.5035724	-2.0370420	-0.6960463

CASSCF Reference energy: -300.4901589243
CASPT2 Total energy: -301.3356436933
Residual norm: 0.0000004153
Reference weight: 0.77877

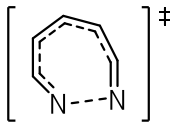
CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.910367	0.828768

Imaginary frequency: -745.0 cm^{-1}

TS 17 → 23ZZ S_1



Atom Type	Coordinates (Angstroms) X	Y	Z

N	1.1201475	-1.2340061	-0.5986258
N	1.7140631	0.4255292	0.2830841
C	0.7583148	1.2679604	0.2017204
C	-0.6642102	1.2618903	-0.2331447
C	-1.5686139	0.2951191	-0.0723658
C	-1.1728067	-1.0375190	0.3778306
C	0.0609987	-1.4005549	-0.0465723
H	1.0513019	2.2332118	0.5981788
H	-1.0051258	2.2311399	-0.5509465
H	-2.6094161	0.5044832	-0.2501523
H	-1.7597554	-1.6280653	1.0518256

CASSCF Reference energy: -300.5266957437
CASPT2 Total energy: -301.3372687687
Residual norm: 0.0000006643
Reference weight: 0.78136

CAS(8,8) active space: 3 π/π^* pairs and σ/σ^* of N1-N2 bond.

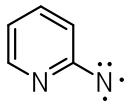
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.868007	0.753436

Imaginary frequency: -446.9 cm^{-1}

19 T_0

2-Pyridyl-nitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.3911211	-1.2133697	0.0000000
N	-2.3631868	-0.0195974	0.0000000
C	1.0782569	1.1857283	0.0000000
C	-0.3109027	1.2183804	0.0000000
C	-1.0146108	-0.0096933	0.0000000
C	0.9273629	-1.2203849	0.0000000
C	1.7169063	-0.0549133	0.0000000
H	1.6464144	2.0976726	0.0000000
H	-0.8584402	2.1417152	0.0000000
H	1.3953693	-2.1885509	0.0000000
H	2.7877755	-0.1326867	0.0000000

CASSCF Reference energy: -300.5894702442
CASPT2 Total energy: -301.3993493799
Residual norm: 0.0000002835
Reference weight: 0.79153

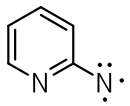
CAS(8,8) active space: 3 π/π^* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222u000	0.912759	0.833129

19 S_1

2-Pyridyl-nitrene



Atom Type	X	Y	Z
N	0.0159740	2.3293780	0.0000000
N	-1.2503770	0.4033240	0.0000000
C	0.0000000	1.0541670	0.0000000
C	1.2537260	0.2826480	0.0000000
C	1.1946790	-1.0863770	0.0000000
C	-0.0710020	-1.7154340	0.0000000
C	-1.2520740	-0.8893970	0.0000000
H	2.1811400	0.8213670	0.0000000
H	2.0936010	-1.6747220	0.0000000
H	-0.1683650	-2.7834420	0.0000000
H	-2.2175250	-1.3657620	0.0000000

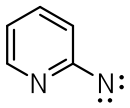
CASSCF Reference energy: -300.5598854554
CASPT2 Total energy: -301.3679226446
Residual norm: 0.0000005313
Reference weight: 0.79137

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222d000	0.916812	0.840544

19 S_2



Atom Type	X	Y	Z
N	-1.1986333	0.4059067	0.0000000
N	0.0337078	2.3828314	0.0000000
C	0.0053437	1.0073353	0.0000000
C	1.2113761	0.2940834	0.0000000
C	1.1670565	-1.1008939	0.0000000
C	-0.0775243	-1.7181387	0.0000000
C	-1.2289406	-0.9165973	0.0000000

H	2.1402237	0.8316956	0.0000000
H	2.0727412	-1.6790783	0.0000000
H	-0.1698087	-2.7883372	0.0000000
H	-2.2042740	-1.3692470	0.0000000

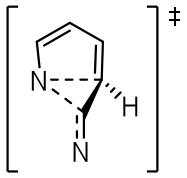
CASSCF Reference energy: -300.5204367231
CASPT2 Total energy: -301.3394930540
Residual norm: 0.0000005443
Reference weight: 0.78868

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	2,2220000	-0.764339	0.584215

TS 19 → 33



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.2980473	-0.8987863	0.6911575
N	-2.2469765	-0.0356512	-0.5978746
C	0.9107505	-1.1657473	0.0251580
C	1.6619958	-0.1141638	-0.3947572
C	1.0573725	1.1389593	-0.0716124
C	-0.2454032	1.0606559	0.4016722
C	-1.1488825	-0.0636510	-0.0484851
H	1.1279586	-2.2065639	-0.1193616
H	2.6031764	-0.2193324	-0.8970963
H	1.5823803	2.0745693	-0.0950136
H	-0.7004442	1.7837038	1.0494853

CASSCF Reference energy: -300.4815749901
CASPT2 Total energy: -301.3240028692
Residual norm: 0.0000001958
Reference weight: 0.77633

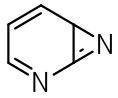
CAS(8,8) active space: 3 π/π* pairs and σ/σ* of new N1-C3 bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.816899	0.667324
18	22202000	-0.397123	0.157707

Imaginary frequency: -694.1 cm^{-1}

20



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.6317404	-0.4328864	0.6902082
N	0.4532494	-1.4431738	-0.1931727
C	1.2462433	0.8520171	0.1927153
C	0.0662103	1.4752390	-0.0629313
C	1.4162130	-0.6032416	-0.0099117
C	-0.7431970	-0.7477093	-0.1346967
C	-1.0571379	0.6077189	-0.4616054
H	2.4176613	-0.9972894	-0.0236403
H	2.1216862	1.4117466	0.4667107
H	-0.0159476	2.5470708	-0.0346315
H	-1.7697314	0.8915892	-1.2103377

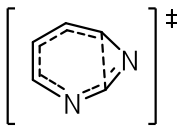
CASSCF Reference energy: -300.5606827649
CASPT2 Total energy: -301.3832684644
Residual norm: 0.0000009972
Reference weight: 0.78799

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of azirene C3-N bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.922280	0.850600

TS 20 → 21



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.4663864	-0.5049669	0.6193171
N	0.6081082	-1.3933502	-0.3641567
C	1.1427358	0.8879992	0.2841518
C	-0.0966195	1.4293716	-0.0983394
C	-0.5988059	-0.9600375	-0.1456898
C	-1.2207758	0.6242695	-0.3173877
C	1.4753570	-0.4565878	0.0455306
H	1.9514619	1.5583657	0.5097608
H	-0.1295885	2.4603233	-0.4066188
H	2.5074176	-0.7541538	0.0629645
H	-2.0183053	0.8886026	-0.9844003

CASSCF Reference energy: -300.5300561875

CASPT2 Total energy: -301.3804825475
Residual norm: 0.0000005280
Reference weight: 0.77952

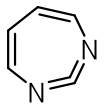
CAS(8,8) active space: 3 π/π* pairs and σ/σ* of breaking C-C bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.925826	0.857153

Imaginary frequency: -891.0 cm^{-1}

21



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.1337848	-1.0410897	0.4442020
N	-1.1336342	-1.0408875	-0.4441576
C	0.0000489	-1.2797882	-0.0000237
C	1.5642903	0.2045207	-0.1186450
C	0.7132113	1.2506975	-0.1986706
C	-0.7132966	1.2508039	0.1986944
C	-1.5643419	0.2046095	0.1186602
H	2.5962859	0.2686199	-0.4027736
H	1.1122206	2.1906219	-0.5360996
H	-1.1121945	2.1907840	0.5360910
H	-2.5963565	0.2685198	0.4027445

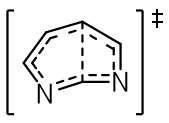
CASSCF Reference energy: -300.5680080915
CASPT2 Total energy: -301.3986077829
Residual norm: 0.0000008171
Reference weight: 0.78576

CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.923982	0.853743

TS 21 → 24



Atom Coordinates (Angstroms)

Type	X	Y	Z
N	1.3562079	-0.9099496	-0.3345003
N	-1.0437026	-1.2100536	0.1941827
C	-1.6556620	0.0307613	-0.2073834
C	-0.8814688	1.1423984	-0.2278035
C	0.4792400	1.0870605	0.3878995
C	0.1634543	-0.8830860	0.2554813
C	1.6276237	0.3727598	-0.0975306
H	-2.6635492	-0.0411703	-0.5642994
H	-1.2880686	2.0825642	-0.5559419
H	0.6654700	1.8845151	1.0952827
H	2.6252504	0.7626690	-0.2234139

CASSCF Reference energy: -300.4772578996
CASPT2 Total energy: -301.3249304819
Residual norm: 0.0000004420
Reference weight: 0.77906

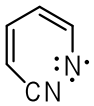
CAS(8,8) active space: 3 π/π* pairs and σ/σ* of new C-C bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.914876	0.836998

Imaginary frequency: -1102.2 cm^{-1}

23ZZ T_0



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.0003763	-1.5340114	0.0000000
N	1.1910971	-1.4539090	0.0000000
C	-1.5900501	-0.4618090	0.0000000
C	-1.2195257	0.9181275	0.0000000
C	0.0297335	1.4988204	0.0000000
C	1.3527061	0.9863635	0.0000000
C	1.8618694	-0.3572208	0.0000000
H	-2.0656285	1.5798105	0.0000000
H	-0.0057935	2.5740994	0.0000000
H	2.1179670	1.7406552	0.0000000
H	2.9383669	-0.4578584	0.0000000

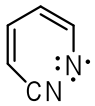
CASSCF Reference energy: -300.5543213940
CASPT2 Total energy: -301.3617603798
Residual norm: 0.0000002000
Reference weight: 0.78517

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222u000	-0.906936	0.822534

23ZZ S_1



Atom Type	X	Y	Z
N	2.4297152	0.6700746	0.0000000
N	0.4445166	-1.8321483	0.0000000
C	1.3253704	0.9925077	0.0000000
C	0.0110854	1.5260187	0.0000000
C	-1.2392001	0.8629464	0.0000000
C	-1.6122772	-0.4629403	0.0000000
C	-0.8146170	-1.7100983	0.0000000
H	-0.0135176	2.5992993	0.0000000
H	-2.0674169	1.5496332	0.0000000
H	-2.6719916	-0.6408996	0.0000000
H	-1.3878436	-2.6285554	0.0000000

CASSCF Reference energy: -300.5426420944
CASPT2 Total energy: -301.3502394249
Residual norm: 0.0000003369
Reference weight: 0.78481

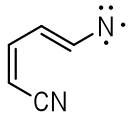
CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222d000	0.921199	0.848607

23EZ T_0

(2E,3s-Z,4Z)-5-cyanopenta-2,4-dienenitrene



Atom Type	X	Y	Z
N	-2.0311679	-1.5858878	0.0000000
N	2.6620615	-0.9381053	0.0000000
C	1.4347188	-0.5452268	0.0000000
C	1.1179194	0.8547504	0.0000000
C	-0.1580975	1.4678449	0.0000000
C	-1.4233226	0.9189266	0.0000000
C	-1.7434417	-0.4739822	0.0000000

H	0.6679662	-1.3011312	0.0000000
H	1.9631236	1.5181211	0.0000000
H	-0.1410006	2.5429806	0.0000000
H	-2.2730027	1.5741031	0.0000000

CASSCF Reference energy: -300.5635446353
CASPT2 Total energy: -301.3704686023
Residual norm: 0.0000001644
Reference weight: 0.78572

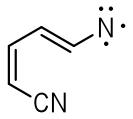
CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222u000	0.906771	0.822233

23EZ S_1

(2E,3s-Z,4Z)-5-cyanopenta-2,4-dienenitrene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.0474478	-1.5748253	0.0000000
N	2.6394639	-0.9659370	0.0000000
C	1.4354424	-0.5669430	0.0000000
C	1.1185441	0.8758745	0.0000000
C	-0.1184613	1.4771950	0.0000000
C	-1.4204355	0.9171994	0.0000000
C	-1.7491324	-0.4633415	0.0000000
H	0.6562148	-1.3112687	0.0000000
H	1.9766633	1.5218116	0.0000000
H	-0.1110225	2.5524078	0.0000000
H	-2.2617127	1.5824794	0.0000000

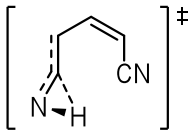
CASSCF Reference energy: -300.5519125942
CASPT2 Total energy: -301.3589529872
Residual norm: 0.0000002915
Reference weight: 0.78539

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222d000	0.922211	0.850472

TS 23EZ → 26Z

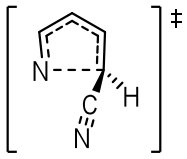


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.526704	-0.181267	0.033780
C	-1.071115	1.122366	0.105947
C	0.302864	1.546349	-0.031876
C	1.441299	0.818970	-0.128777
C	1.498302	-0.612774	-0.003758
N	1.549223	-1.752134	0.122845
N	-2.042176	-1.262538	-0.258732
H	-1.430992	-0.833769	0.991271
H	-1.793630	1.845968	0.432299
H	0.423475	2.614607	-0.067189
H	2.383949	1.314036	-0.257062

CASSCF Reference energy: -300.5024792039
CASPT2 Total energy: -301.3318089537
Residual norm: 0.0000009430
Reference weight: 0.77641

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of breaking C-H bond.

TS 23ZZ → 32



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.3963287	-0.5470579	-0.4871501
N	0.6654827	-1.5552010	0.7789819
C	1.3974378	-1.0749930	-0.1361468
C	1.5585379	0.3741556	-0.3985922
C	0.6538019	1.3258248	-0.0791418
C	-0.6900093	1.1249088	0.4493236
C	-1.6135959	0.1816822	-0.0604113
H	1.9568327	-1.7679546	-0.7495956
H	2.4925455	0.6729588	-0.8388394
H	0.9445795	2.3548614	-0.2022840
H	-1.1013937	1.8716337	1.1012245

CASSCF Reference energy: -300.5425141214
CASPT2 Total energy: -301.3509238749
Residual norm: 0.0000003821
Reference weight: 0.78440

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of new N1-C3 bond.

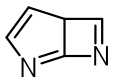
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.722921	0.522615
18	22202000	-0.580152	0.336577

Imaginary frequency: -195.0 cm^{-1}

24

2,7-diazabicyclo[3.2.0]hepta-1,3,6-triene



Atom Type	X	Y	Z
N	-1.6426273	-0.7608699	-0.1230026
N	0.8065958	-1.2198895	-0.0346273
C	-0.2571680	-0.6631235	0.4141463
C	-1.5619806	0.5135369	-0.3168329
C	-0.2618112	0.8414124	0.4309665
C	1.1045808	1.0828678	-0.1360534
C	1.7007143	-0.1348507	-0.2290637
H	-2.2776144	1.1168959	-0.8447048
H	-0.4511322	1.3527583	1.3668202
H	1.6007476	2.0297425	-0.2179627
H	2.7176539	-0.3443378	-0.4949226

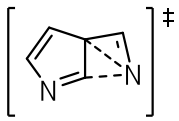
CASSCF Reference energy: -300.5496100247
CASPT2 Total energy: -301.3790610879
Residual norm: 0.0000002666
Reference weight: 0.78529

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of C1-N7 bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.923540	0.852927

TS 24 → 25



Atom Type	X	Y	Z
N	-1.8686721	0.6562185	0.3790679
N	0.5837618	-1.2681430	-0.0286577

C	1.6555112	-0.4637151	0.3773532
C	1.3871002	0.8809789	0.3015801
C	0.1051104	0.9792871	-0.3271864
C	-0.2901917	-0.4370165	-0.5068148
C	-1.7323700	-0.4319351	-0.2682639
H	2.5665895	-0.9290483	0.6975009
H	2.0627326	1.6812735	0.5244902
H	-0.2212564	1.7936492	-0.9391058
H	-2.4932652	-1.1731723	-0.4287397

CASSCF Reference energy: -300.5342278096
CASPT2 Total energy: -301.3629647078
Residual norm: 0.0000007053
Reference weight: 0.78366

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of breaking C1-N7 bond.

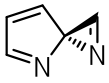
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.883835	0.781164

Imaginary frequency: -334.1 cm^{-1}

25

1,4-diazaspiro[2.4]hepta-1,4,6-triene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.7876386	-0.0326960	-0.6980371
N	-0.3287413	-1.1812136	0.0144410
C	-1.5607773	-0.7563679	0.0102738
C	-1.6708891	0.7162495	0.0093480
C	-0.4101857	1.1859059	0.0146566
C	0.4846195	0.0001991	0.0437464
C	1.8307237	-0.0517817	0.5491341
H	-2.3871624	-1.4426732	0.0006775
H	-2.5863966	1.2734417	-0.0066241
H	-0.0728262	2.2031739	0.0049076
H	2.5297313	-0.1065505	1.3581546

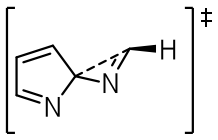
CASSCF Reference energy: -300.5751012351
CASPT2 Total energy: -301.3979184163
Residual norm: 0.0000004157
Reference weight: 0.78681

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of azirene C-N bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.934688	0.873641

TS 25 → 36



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.7329828	-0.2771058	-0.3796518
N	-0.4838502	-1.1072127	0.1016688
C	0.3246746	-0.0901963	-0.1783008
C	2.2190421	0.1287332	0.6979649
C	-0.3851399	1.1853543	-0.2565322
C	-1.6867841	0.8725104	-0.0327525
C	-1.7046778	-0.5682898	0.1866702
H	3.2373444	0.1177232	1.0519435
H	0.0593586	2.1345242	-0.4745170
H	-2.5360671	1.5248826	-0.0194601
H	-2.5647956	-1.1790186	0.3768440

CASSCF Reference energy: -300.5073971641
CASPT2 Total energy: -301.3324021477
Residual norm: 0.0000007407
Reference weight: 0.78667

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of new C-C bond.

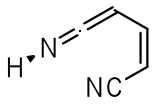
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.766089	0.586893
18	22202000	-0.523796	0.274362

Imaginary frequency: -513.4 cm^{-1}

26Z

(s-Z,Z)-5-Iminopenta-2,4-dienenitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-1.4341479	-1.7740077	0.3497841
N	2.0733510	-0.9948844	-0.4184475
C	1.5200149	0.0171684	0.0037830
C	0.9758636	1.1946989	0.2674259
C	-0.3980873	1.5629704	-0.1001113
C	-1.4587315	0.7704805	-0.1996797

C	-1.4368207	-0.6414179	0.0987330
H	1.9859208	-1.7930066	0.1904218
H	1.5774211	1.9233621	0.7788094
H	-0.5497607	2.6090814	-0.3016018
H	-2.4083465	1.1679530	-0.5029171

CASSCF Reference energy: -300.6183914724
CASPT2 Total energy: -301.4154924170
Residual norm: 0.0000006404
Reference weight: 0.79055

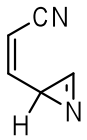
CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.938094	0.880021

30

(Z)-3-(2*H*-azirin-2-yl)acrylonitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.8502010	-0.7490662	-0.7378573
N	-2.2729115	-0.9310095	0.2748188
C	1.1108572	-1.1446390	0.1885307
C	1.3460426	0.2597479	0.3957461
C	0.4090173	1.3353271	-0.0139031
C	-0.9015977	1.2374857	-0.1760680
C	-1.6532992	0.0274148	0.0684535
H	0.6300876	-2.0440412	0.5154779
H	2.1300024	0.5721925	1.0636446
H	0.8591725	2.2965107	-0.1946916
H	-1.4802511	2.0827472	-0.4977987

CASSCF Reference energy: -300.6014492548
CASPT2 Total energy: -301.3906441724
Residual norm: 0.0000008426
Reference weight: 0.79308

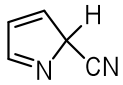
CAS(8,8) active space: 3 π/π* pairs and σ/σ* of azirene C-N bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.938649	0.881062

32

2*H*-Pyrrole-2-carbonitrile



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.4704004	-1.1915459	0.2289863
N	-2.6902971	-0.0037407	-0.4993287
C	-1.6378858	-0.0300169	-0.0174490
C	-0.3011022	-0.0097836	0.6116563
C	0.5358596	1.1828863	0.2010087
C	1.6767400	0.7045707	-0.3195484
C	1.5714004	-0.7685673	-0.2727381
H	-0.4408210	-0.0385998	1.6873075
H	0.2356471	2.2029059	0.3339779
H	2.5120070	1.2588312	-0.6991078
H	2.3240207	-1.4547923	-0.6156037

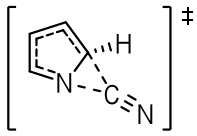
CASSCF Reference energy: -300.6578065280
CASPT2 Total energy: -301.4509614480
Residual norm: 0.0000008676
Reference weight: 0.79758

CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.925462	0.856480

TS 32 → 33



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.1263340	-0.5613110	0.8182420
N	-2.2827450	-0.0438950	-0.6618010
C	0.8630660	-1.1453530	0.0854470
C	1.6726850	-0.1868650	-0.5212930
C	1.1501620	1.0692160	-0.2195060
C	0.0125270	0.8461710	0.5920850
C	-1.2666140	0.0436040	-0.0861640
H	0.8775220	-2.2082390	-0.0356870
H	2.5263240	-0.3907940	-1.1363080
H	1.5123040	2.0243790	-0.5388960
H	-0.3989150	1.5207340	1.3164890

CASSCF Reference energy: -300.5417046639
CASPT2 Total energy: -301.3829899982

Residual norm: 0.0000007328
Reference weight: 0.78180

CAS(8,8) active space: 4 π/π* pairs.

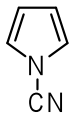
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.925803	0.857112

Imaginary frequency: -1383.6 cm^{-1}

33

1-Cyanopyrrole



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.0000000	0.0000000	0.3377412
N	0.0000000	0.0000000	2.8199254
C	0.0000000	0.0000000	1.6706890
C	0.0000000	1.1345100	-0.4742498
C	0.0000000	-1.1345100	-0.4742498
C	0.0000000	0.7223813	-1.7670273
C	0.0000000	-0.7223813	-1.7670273
H	0.0000000	2.1089129	-0.0364309
H	0.0000000	-2.1089129	-0.0364309
H	0.0000000	1.3600696	-2.6264107
H	0.0000000	-1.3600696	-2.6264107

CASSCF Reference energy: -300.6033328921
CASPT2 Total energy: -301.4601940408
Residual norm: 0.0000006654
Reference weight: 0.77949

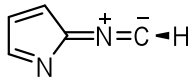
CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a1,b1,a2,b2)	Coef	Weight
111	0,220,20,20	0.947709	0.898152

36

N-(2*H*-pyrrol-2-ylidene)methanideiminium



Atom Coordinates (Angstroms)

Type	X	Y	Z
N	-0.0970659	1.5836753	-0.0364837
N	-1.1280200	-0.5115640	-0.0091340
C	-0.6697923	-1.7319395	-0.0018562
C	0.7831958	-1.7903226	0.0003482
C	1.2099799	-0.4964432	-0.0071537
C	0.0005728	0.2866522	-0.0126789
C	-0.1999168	2.7595836	0.1162585
H	-1.3368900	-2.5731341	0.0027434
H	1.3821243	-2.6791282	0.0077225
H	2.2121366	-0.1176536	-0.0062960
H	-0.2699720	3.5674959	-0.5825927

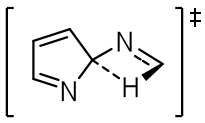
CASSCF Reference energy: -300.5562130329
CASPT2 Total energy: -301.3962691997
Residual norm: 0.0000001924
Reference weight: 0.78208

CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.921150	0.848517

TS 36 → 40



Atom Coordinates (Angstroms)

Type	X	Y	Z
N	-1.7300063	-0.0213260	-0.6455964
N	0.3336795	-1.1711186	0.0015249
C	1.5541576	-0.7568887	0.0010529
C	1.6730655	0.7134060	0.0125568
C	0.4127386	1.1926554	0.0268711
C	-0.4608535	0.0015395	0.0106625
C	-2.1483955	-0.0727550	0.5432782
H	2.3756669	-1.4482747	-0.0034895
H	2.5905063	1.2667318	0.0043430
H	0.0671136	2.2059384	0.0233313
H	-1.1509238	-0.0555781	1.2690162

CASSCF Reference energy: -300.4900926661
CASPT2 Total energy: -301.3322257553
Residual norm: 0.0000002142
Reference weight: 0.78093

CAS(8,8) active space: 3 π/π* pairs and σ/σ* of new C-H bond.

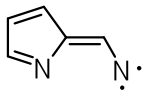
Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight

1	22220000	-0.920689	0.847668

Imaginary frequency: -1267.3 cm^{-1}

38Z T_0



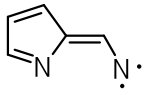
Atom Type	X	Y	Z
N	-0.8730771	-0.6866377	0.0000000
N	-1.5807601	2.1291292	0.0000000
C	-0.3554555	1.7269614	0.0000000
C	-0.1644359	-1.7769488	0.0000000
C	1.2875273	-1.5057268	0.0000000
C	1.4013491	-0.1533815	0.0000000
C	0.0407883	0.3535025	0.0000000
H	-0.6255903	-2.7460342	0.0000000
H	2.0669086	-2.2407938	0.0000000
H	2.2935119	0.4399859	0.0000000
H	0.4167728	2.4827752	0.0000000

CASSCF Reference energy: -300.5624916983
CASPT2 Total energy: -301.3739483677
Residual norm: 0.0000008618
Reference weight: 0.79031

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Conf	Occupation(a',a")	Coef	Weight
1	u,222u000	0.910394	0.828817

38Z S_1



Atom Type	X	Y	Z
N	-0.8658911	-0.6566409	0.0000000
N	-1.5756030	2.1698789	0.0000000
C	-0.1328540	-1.7980163	0.0000000
C	1.2908265	-1.5243237	0.0000000
C	1.3978133	-0.1707876	0.0000000
C	0.0109352	0.3289368	0.0000000
C	-0.3792361	1.7555188	0.0000000
H	-0.6111411	-2.7564878	0.0000000
H	2.0746678	-2.2537393	0.0000000

H	2.2843807	0.4311006	0.0000000
H	0.4115131	2.4942431	0.0000000

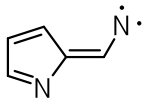
CASSCF Reference energy: -300.5488967669
CASPT2 Total energy: -301.3609718224
Residual norm: 0.0000002668
Reference weight: 0.79004

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222d000	0.925205	0.856005

38E T_0



Atom Type	Coordinates (Angstroms) X	Y	Z
N	1.3461130	0.0897509	0.0000000
N	-1.7375361	1.9929451	0.0000000
C	1.4556728	-1.2139317	0.0000000
C	0.1433269	-1.8845378	0.0000000
C	-0.7746362	-0.8883070	0.0000000
C	-0.0014451	0.3495468	0.0000000
C	-0.4853142	1.6978672	0.0000000
H	2.4145653	-1.6953505	0.0000000
H	-0.0225468	-2.9429566	0.0000000
H	-1.8427945	-0.9590618	0.0000000
H	0.2417826	2.4952504	0.0000000

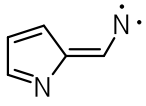
CASSCF Reference energy: -300.5665358313
CASPT2 Total energy: -301.3787410910
Residual norm: 0.0000001574
Reference weight: 0.79022

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222u000	0.911870	0.831506

38E S_1



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.8540757	-0.6207003	0.0000000
N	0.4261477	2.7207865	0.0000000
C	-0.1219586	-1.7916987	0.0000000
C	1.2851312	-1.5335441	0.0000000
C	1.4118843	-0.1733118	0.0000000
C	0.0264903	0.3423053	0.0000000
C	-0.3932084	1.7557637	0.0000000
H	-0.6183665	-2.7403332	0.0000000
H	2.0636292	-2.2686918	0.0000000
H	2.3024595	0.4208628	0.0000000
H	-1.4549316	1.9541350	0.0000000

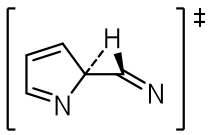
CASSCF Reference energy: -300.5547834683
CASPT2 Total energy: -301.3671333853
Residual norm: 0.0000003884
Reference weight: 0.78994

CAS(8,8) active space: 3 π/π* pairs and p_y/p_z AO on nitrene N.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation(a',a")	Coef	Weight
1	u,222d000	0.924558	0.854808

TS 38 → 32



Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.8913275	-0.2333962	-0.1326847
N	-0.5589864	-1.1184869	-0.0798668
C	-1.7711219	0.8387271	0.0331552
C	-1.7618093	-0.6215230	-0.0683099
C	0.2821046	-0.0156316	-0.0610241
C	1.7039942	-0.1767400	0.0579881
C	-0.4681745	1.2182087	0.0917743
H	-2.6398135	1.4654089	0.0421474
H	-2.6239254	-1.2574583	-0.1265044
H	1.3045958	-0.2707295	1.1487267
H	-0.0515546	2.2025358	0.1503821

CASSCF Reference energy: -300.5078063937
CASPT2 Total energy: -301.3416083966
Residual norm: 0.0000001768
Reference weight: 0.78212

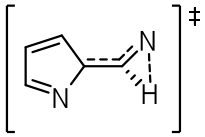
CAS(8,8) active space:
3 π/π* pairs and σ(overlapping with p_z AO on nitrene N)/σ* of new C-H bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.891288	0.794395

Imaginary frequency: -1610.3 cm^{-1}

TS 38 → 39



Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.8343613	-0.2680772	0.2959342
N	-0.5863904	-1.1568670	0.1927304
C	-1.7894203	-0.6867157	0.0357583
C	-1.8100796	0.7566822	-0.1826279
C	-0.5112180	1.1573346	-0.1536918
C	0.2473275	-0.0448144	0.1268458
C	1.6213511	-0.1943658	0.1018731
H	-2.6455914	-1.3332807	0.0710143
H	-2.6825414	1.3629137	-0.3220803
H	-0.1116063	2.1451312	-0.2624753
H	2.0983490	-0.4834029	-0.9227817

CASSCF Reference energy: -300.4945838728
CASPT2 Total energy: -301.3320467591
Residual norm: 0.0000003598
Reference weight: 0.78175

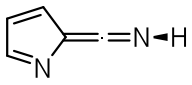
CAS(8,8) active space:
3 π/π^* pairs and σ(overlapping with p_z AO on nitrene N)/σ^* of new N-H bond.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.903347	0.816036

Imaginary frequency: -2001.1 cm^{-1}

39



Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.8251723	-0.0330628	-0.1542614
N	-0.5033942	-1.1699741	-0.0060273

C	-1.7301546	-0.7620390	0.0197886
C	-1.8531212	0.7009074	0.0280391
C	-0.5893077	1.1828784	0.0067869
C	0.2772954	0.0032578	-0.0231783
C	1.6048959	-0.0348224	-0.0160573
H	-2.5465911	-1.4596036	0.0335185
H	-2.7699846	1.2554421	0.0437721
H	-0.2597115	2.2018640	-0.0011295
H	3.3387261	-0.0552219	0.7124292

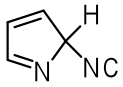
CASSCF Reference energy: -300.5914321861
CASPT2 Total energy: -301.4209687421
Residual norm: 0.0000002886
Reference weight: 0.78672

CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.923802	0.853409

40



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.4611233	-1.1843430	0.1901369
N	1.6173492	-0.0610017	-0.0230447
C	0.3313092	-0.0256756	0.5872963
C	-1.5678671	-0.7335672	-0.2701712
C	-1.6440968	0.7459484	-0.2940566
C	-0.4776591	1.1909550	0.1955907
C	2.6815775	-0.0524309	-0.5137417
H	0.4746175	-0.0747003	1.6595644
H	-2.3422922	-1.3982982	-0.6063904
H	-2.4750043	1.3215208	-0.6502520
H	-0.1441379	2.1996794	0.3330382

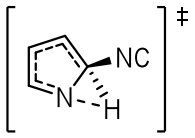
CASSCF Reference energy: -300.6166982998
CASPT2 Total energy: -301.4106696458
Residual norm: 0.0000004551
Reference weight: 0.79724

CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	0.931719	0.868100

TS 40 → 41



Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.4105757	-1.1530272	-0.0128023
N	-1.7266872	-0.0109442	-0.0097631
C	-0.3549767	0.0350572	0.1590189
C	0.4673205	1.1695312	0.0655852
C	1.7601341	0.6795188	-0.0978008
C	1.6833051	-0.7145390	-0.1163269
C	-2.8930775	-0.0054554	-0.1358506
H	-0.0181863	-0.7692510	1.1011558
H	0.1381138	2.1863281	0.1180923
H	2.6581956	1.2611366	-0.1594098
H	2.4862791	-1.4222321	-0.1338337

CASSCF Reference energy: -300.5253397988
CASPT2 Total energy: -301.3556110333
Residual norm: 0.0000004431
Reference weight: 0.78632

CAS(8,8) active space: 4 π/π* pairs.

Occupation of active orbitals, (u,d: Spin up or down):

Conf	Occupation	Coef	Weight
1	22220000	-0.941610	0.886630

Imaginary frequency: -2439.5 cm^{-1}