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SUPPORTING INFORMATION

Interconversion of Nitrenes, Carbenes and Nitrile Ylides by Ring Expansion, Ring Opening, Ring Contraction, and Ring Closure: 3-Quinolylnitrene, 2-Quinoxalylcarbene and 3-Quinolylcarbene

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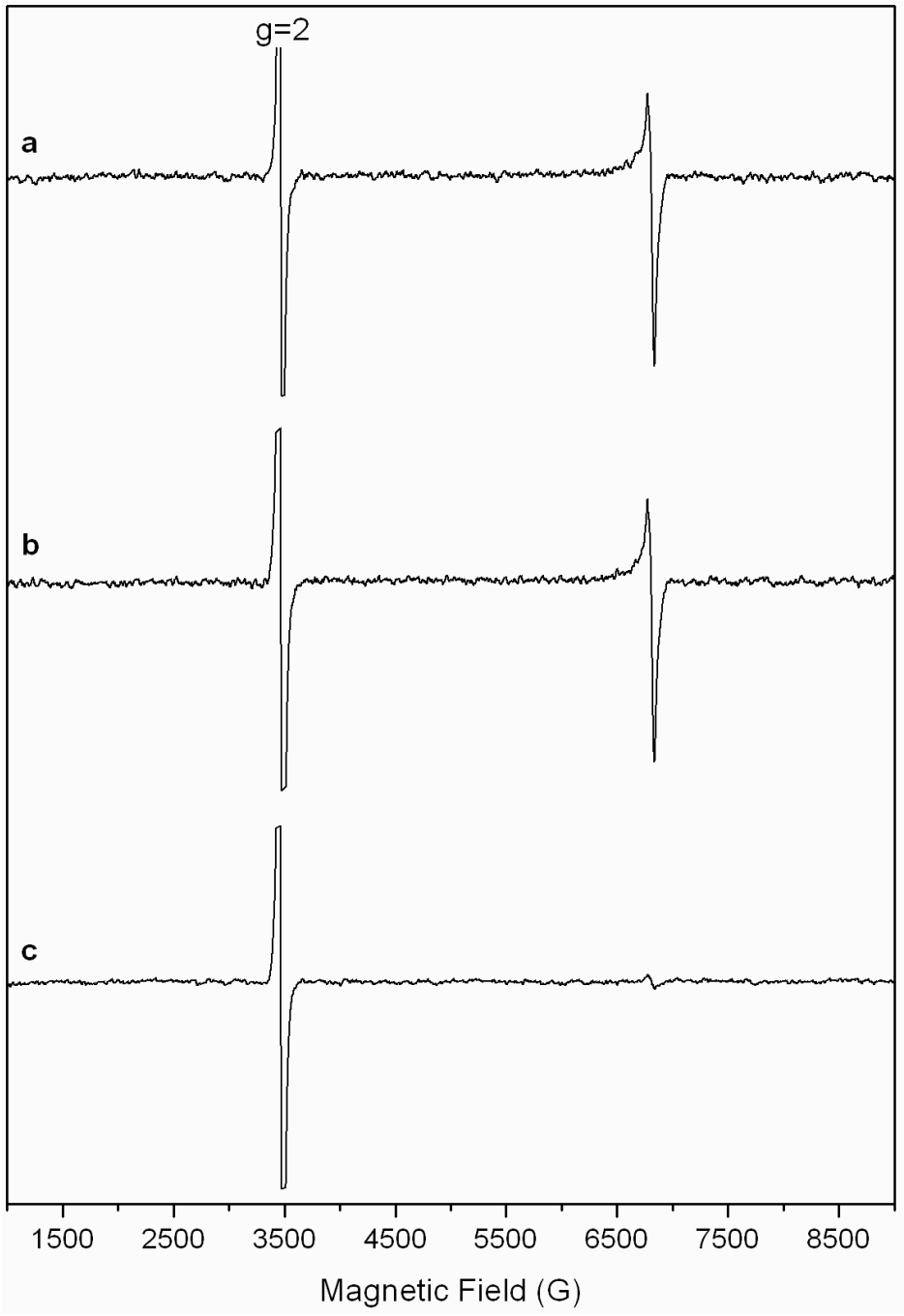


Fig. S1. 3-Quinolylnitrene **7T**, obtained by photolysis of 3-azidoquinoline **6** in Ar matrix at ~15 K at (a) 308nm for 12min, (b) further photolysis > 610 nm for 5 min (no effect), (c) further photolysis > 395 nm for 5 min (nitrene vanishes). For field and zero field splitting parameters, see Fig. 1.

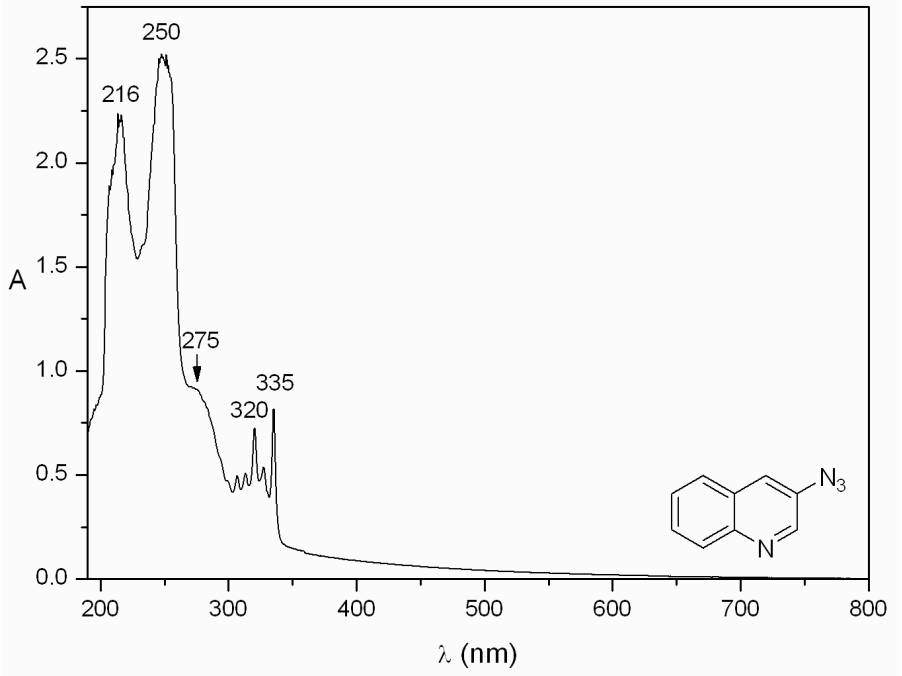


Fig. S2. UV spectrum of 3-azidoquinoline **6** in Ar matrix at ~7 K.

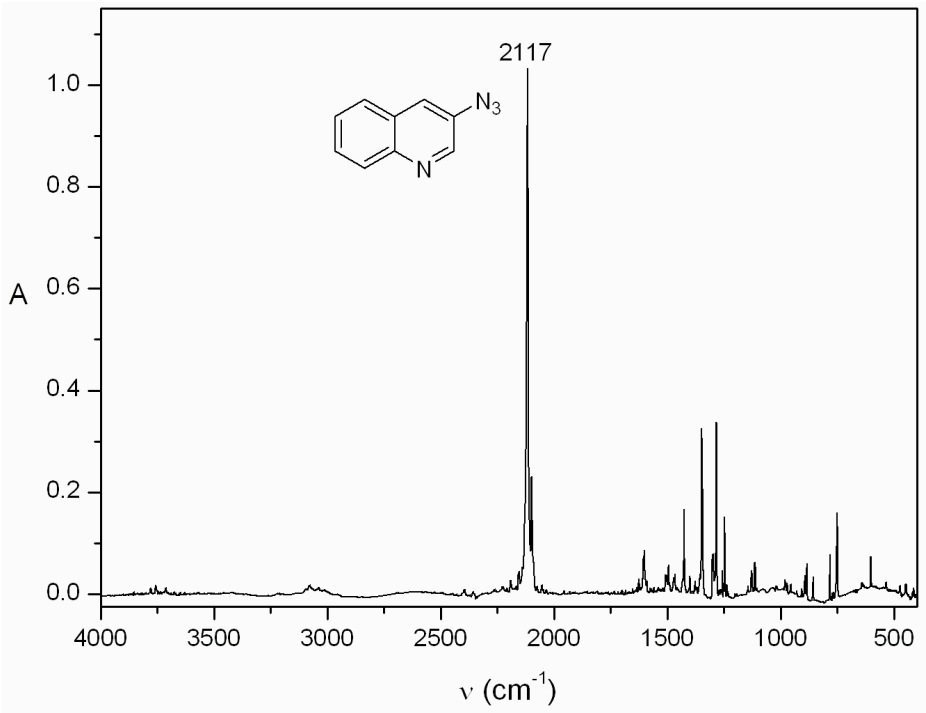


Fig. S3. IR spectrum of 3-azidoquinoline **6** in Ar matrix at ~7 K. See Table 1 for a peak listing and for the calculated wavenumbers.

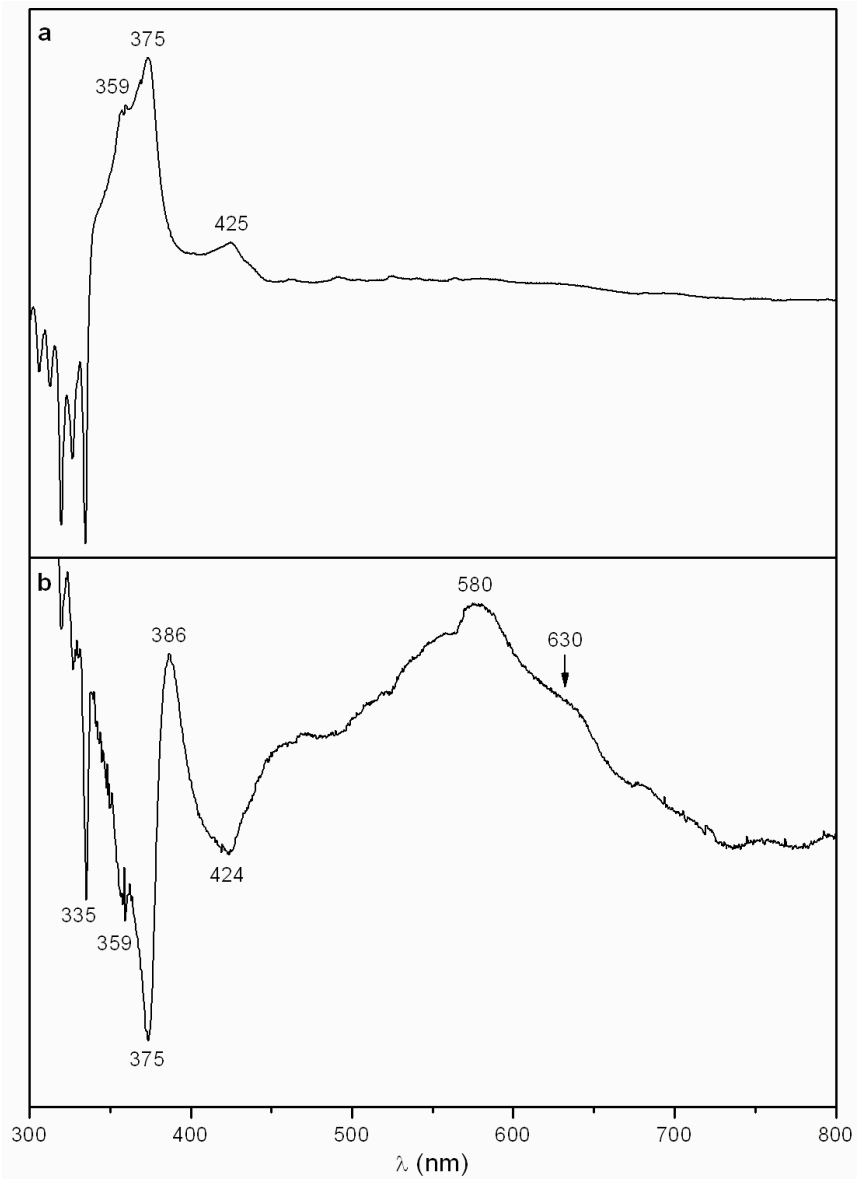


Fig. S4. UV-Vis spectra from the photolysis of 3-azidoquinoline **6** in Ar matrix at ~7 K. (a) Difference spectrum after 30 s of photolysis of 3-azidoquinoline at 308 nm. Positive peaks: nitrene **7** is seen as the major product of photolysis of the azide (cf. Fig. S5). A little nitrile ylide **19** has also formed (λ_{max} ~ 580 nm). Negative peaks: azide **6**. (b) Difference spectrum after further photolysis of the same matrix for another 40 s at 308 nm. This

generates more nitrile ylide **19** (λ_{max} ~ 580 nm) from the nitrene because the nitrene absorbs somewhat at 308 nm, while the ylide does not.

The nitrene is formed first as the azide is depleted, while the nitrile ylide starts appearing at the expense of the nitrene and azide on further photolysis.

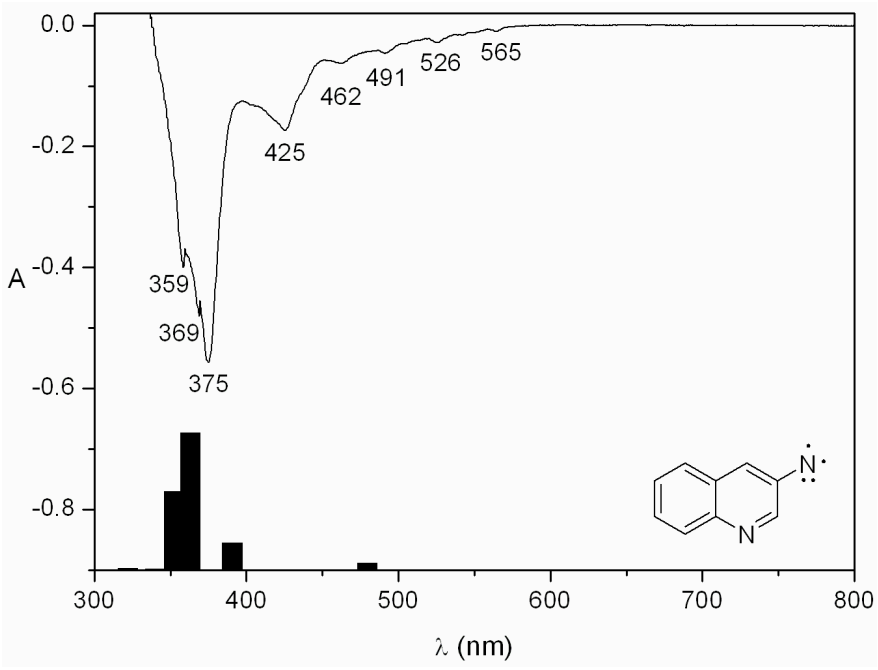


Fig. S5. UV-Vis spectrum of 3-quinolylnitrene **7T** (negative spectrum) and calculated transitions (heavy bars) at the TD-B3LYP/6-31G* level (calculated λ_{max}/nm (oscillator strength) 479 (0.0025), 397(0.0002), 390(0.0097), 363(0.0492), 352(0.0282), 340(0.0003), 322(0.0007), 290(0.0018), 281(0.0034), 273(0.0248), 270(0.0012), 266(0.0105), 252(0.0109).

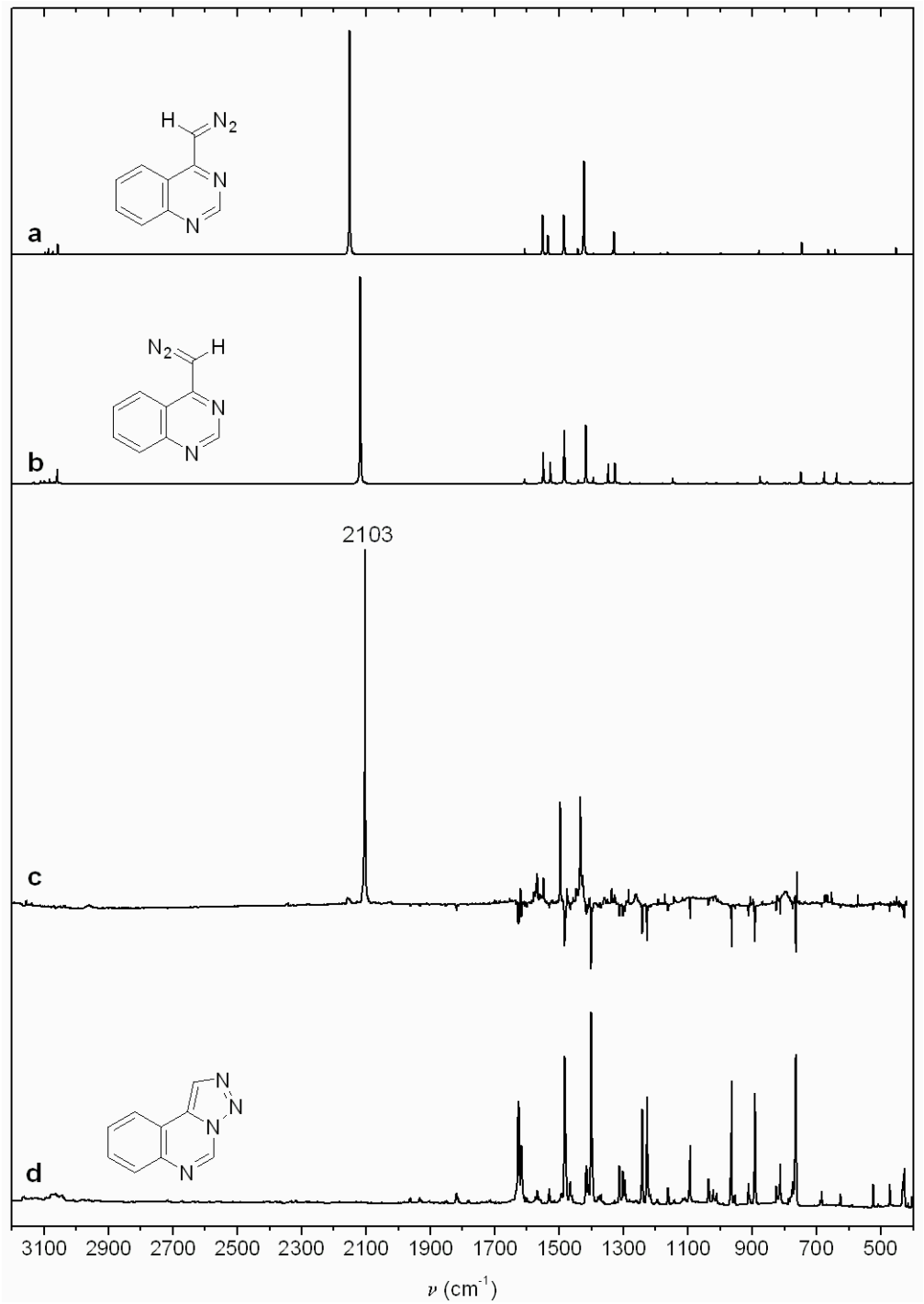


Figure S6. (a) Calculated IR spectrum of the *s*-*Z* conformer of 4-diazomethylquinazoline, *s*-*Z*-**27** (2151, 1551, 1485, 1423, 1330, 746 cm^{-1}; maximum absorbance 819.2 km/mol at 2151 cm^{-1}). (b) Calculated IR spectrum of the *s*-*E* conformer of 4-diazomethylquinazoline, *s*-*E*-**27** (maximum absorbance 669.5 km/mol at 2118 cm^{-1}). (c) IR difference spectrum; photolysis of triazoloquinazoline **26** at 254 nm (low-pressure Hg lamp) in Ar matix at 10 K for 33 min, forming 4-diazomethylquinazoline **27** (positive spectrum; 2103, 1568, 1548, 1496, 1434, 760 cm^{-1}). The negative spectrum is due to **26**. (d) IR spectrum of triazoloquinazoline **26** in Ar matrix at 10K (1625, 1482, 1400, 1241, 1226, 964, 891, 763, 427 cm^{-1}). All calculations at the B3LYP/6-31G* level; wavenumbers scaled by a factor 0.9613.

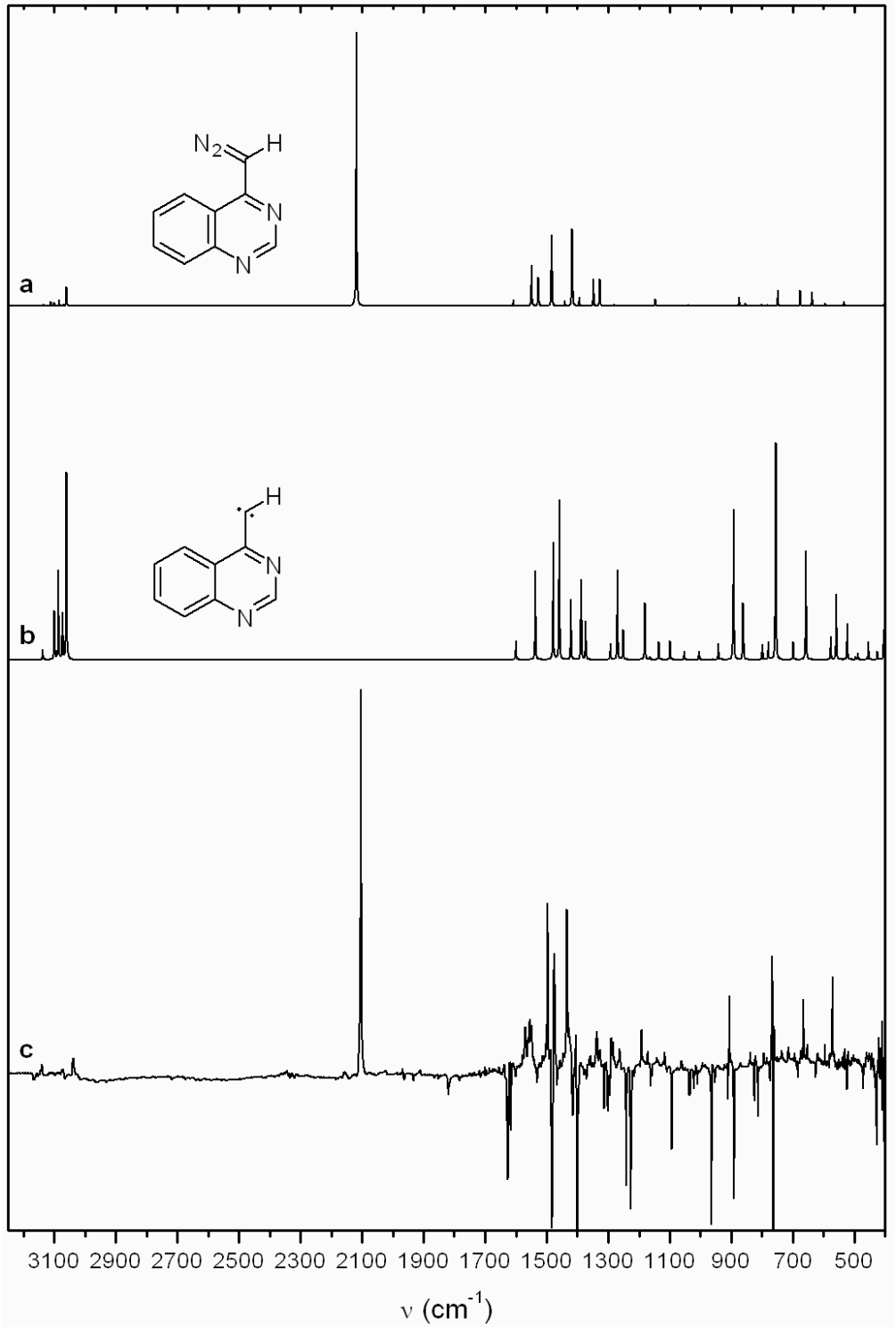


Figure S7. (a) Calculated IR spectrum of the *s*-*E* conformer of 4-diazomethylquinazoline, *s*-*E*-**27** (maximum absorbance 669.5 km/mol at 2118 cm^{-1}). (b) Calculated IR spectrum of the *s*-*Z* conformer of 4-quinazolylcarbene, *s*-*Z*-**28** (1600, 1537, 1478, 1459, 1387, 1269, 1181, 893, 756, 658, 559 cm^{-1}; maximum absorbance 46.1 km/mol at 756 cm^{-1}). (c) IR difference spectrum; photolysis of triazoloquinazoline **26** in Ar matrix at 10 K using the broadband emission of a high-pressure Hg/Xe lamp for 5 min. Positive peaks due to a mixture of diazo compound **27** (see Fig. S6) and carbene **28** (1475, 1405, 1290, 906, 766, 666, 571 cm^{-1}. Negative peaks due to triazole **26** (see Fig S6). All calculations at the B3LYP/6-31G* level; wavenumbers scaled by a factor 0.9613.

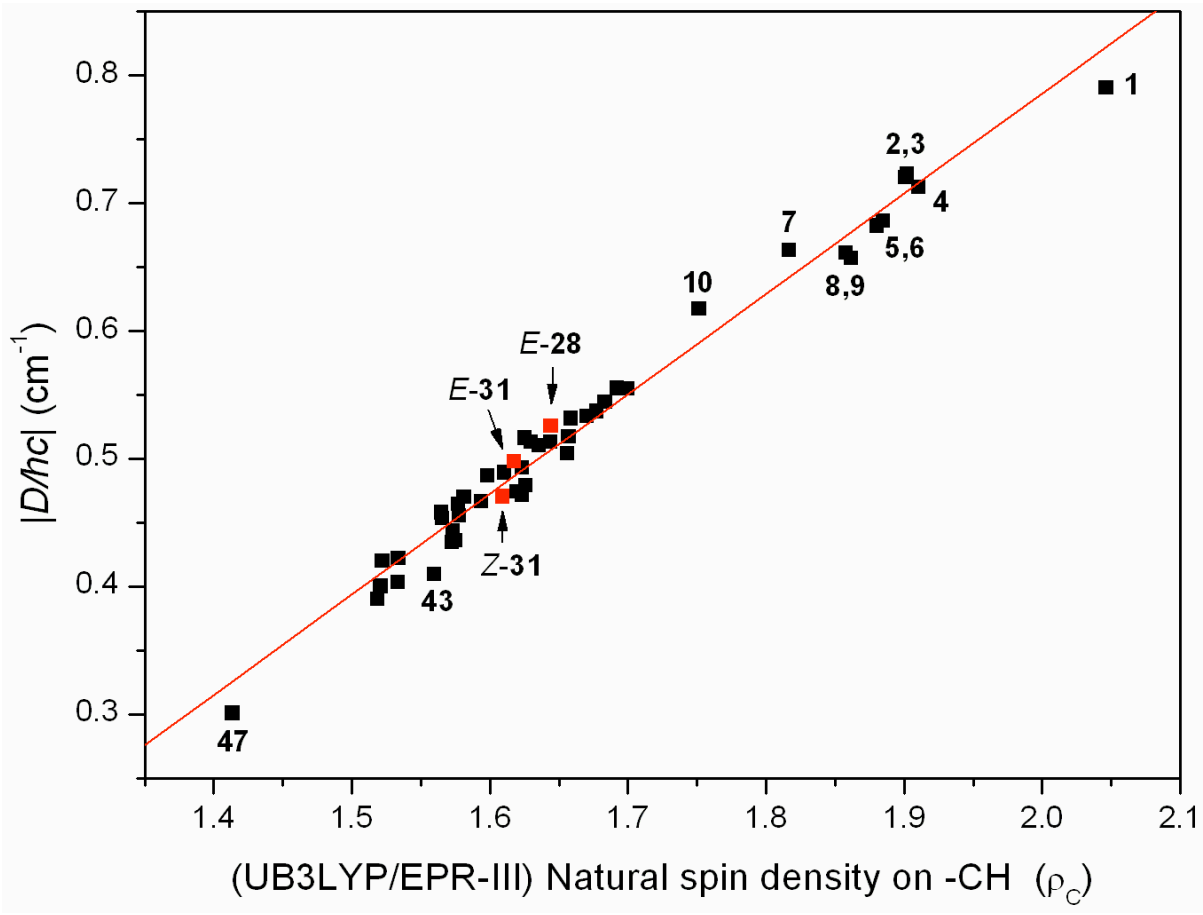


Figure S8. Correlation of the |*D*/*hc*| zfs values of 47 carbenes of the type R-CH with calculated natural spin densities at the UB3LYP/EPR-III level. The data points for *s*-*E*-4-quinazolylcarbene *s*-*E*-**28** and the *s*-*E*- and *s*-*Z*-2-quinolylcarbenes *s*-*E*-**31** and *s*-*Z*-**31** are indicated.

Table S1. Comparison of experimental IR absorptions of matrix-isolated 3-azidoquinoline **6** with theoretical predictions according to B3LYP/6-31G* calculations.

experiment	theoretical data			
	***s-Z* 6**		***s-E* 6**	
ν [cm^{-1}]	ν [cm^{-1}]*	intensity†	ν [cm^{-1}]*	intensity†
	409	0	410	1
	434	0	435	1
	471	0	470	0
	503	1	512	0
	515	0	513	0
	520	0	520	1
604 (w)	591	1	590	2
	625	1	620	0
	627	0	629	0
	736	1	730	2
751 (m)	741	3	741	4
	752	0	755	0
783 (w)	767	1	767	2
	847	0	846	1
856 (w)	867	0	879	3
895 (vw), 885 (w)	885	3	883	1
909 (vw)	905	0	915	0
929 (vw)	931	0	931	1
956 (vw)	951	2	959	1
982 (vw), 979 (vw), 972 (vw)	960	0	961	0
	1005	0	1006	0
	1091	1	1098	3
1115 (w)	1116	1	1116	3
1130 (w)	1138	0	1139	0
	1187	0	1189	1
	1219	0	1218	0
1258 (w), 1248 (m), 1238 (vw)	1243	0	1240	1
1298 (w), 1284 (m)	1308	9	1294	13
1349 (m), 1345 (m)	1349	11	1345	6
	1356	6	1356	1
1378 (vw)	1359	1	1363	7
1426 (m), 1401 (vw)	1417	2	1415	9

1471 (vw), 1466 (vw)	1455	3	1452	1
1509 (vw), 1502 (vw), 1494 (w)	1487	1	1489	3
	1551	1	1555	0
1601 (w)	1594	5	1588	3
	1610	0	1608	0
2117 (vs), 2099 (m)	2175	100	2177	100
3038 (vw), 3015 (vw)	3036	2	3054	2
	3060	0	3059	0
	3071	1	3063	1
	3084	1	3072	1
3079 (vw)	3085	2	3084	3
3097 (vw)	3097	1	3097	2

* scaled by 0.9613. – † normalised to most prominent peak (=100).

Table S2. IR spectroscopic data for the products of photolysis of 3-azidoquinoline **6** in Ar-matrix at 8 K at $\lambda \geq 305$ nm (<u>most prominent bands undelined</u>) compared with the calculated IR spectra for the *s-Z* and *s-E* conformers of 2-(2-imino-vinyl)-isocyanobenzene **20** at the B3LYP/6-31G* level of theory.

experiment	theoretical data			
	***s-Z* 20**		***s-E* 20**	
ν [cm^{-1}]	ν [cm^{-1}]*	intensity†	ν [cm^{-1}]*	Intensity†
	392	2	400	0
<u>417</u> (w)	406	7	406	5
452 (vw)	445	1	441	2
	499	0	493	0
	516	0	528	1
527 (vw)	531	1	539	0
<u>599</u> (w)	591	4	601	3
653 (w)	640	1	625	2
	715	0	737	0
728 (w)	730	0	745	9
762 (m), <u>758</u> (m)	746	10	760	1
829 (m), 813 (w)	827	11	813	0
	836	0	850	3
	854	1	855	5
909 (vw), 904 (vw)	914	1	915	0

936 (m), 927 (m)	946	0	947	0
955 (m), 944 (m), 940 (m), 927m-w	965	68	975	62
1040 (w), 1017 (vw)	1027	2	1031	1
1087 (vw)	1087	2	1064	4
1113 (w), 1103 (w)	1103	2	1110	3
	1150	0	1148	0
	1176	1	1167	0
1203 (w)	1187	1	1198	1
1262 (w)	1249	0	1274	1
1303 (w)	1298	0	1285	1
	1383	0	1380	0
1464 (w)	1447	2	1438	2
1495 (m)	1474	9	1480	3
	1559	0	1559	1
1593 (w)	1590	3	1592	2
2047 (m), 2032 (m, sh), 2025 (s)	2046	100	2043	100
2129 (m), 2125 (m-w)	2114	21	2112	20
3046 (vw)	3054	0	3066	0
	3066	1	3079	0
	3078	2	3082	2
3085 (vw)	3088	3	3088	2
3125 (vw)	3100	2	3101	1
3314 (vw), 3304 (w), 3294 (w)	3318	3	3297	1

* scaled by 0.9613. – † normalised to most prominent peak (=100).

Table S3. IR spectroscopic data for matrix-isolated 3-cyanoindole **22** at 8 K obtained from FVT of **6** at 600 °C. Comparison with IR spectrum of an authentic sample of **22** and the calculated spectrum at the B3LYP/6-31G* level of theory.

22 from FVP of **6**	authentic sample of **22**	theoretical data for **22**	
ν [cm^{-1}]	ν [cm^{-1}]	ν [cm^{-1}]*	intensity†
420 (m)	420 (m)	410	54
458 (w), 453 (w)	457 (vw/sh), 452 (w)	426	34
472 (vw)	470 (vw)	475	2
504 (m)	504 (m)	503	34
522 (w)	515 (vw)	517	0
581 (w), 576 (w)	575 (w)	566	13

600 (vw)	604 (vw)	590	1
612 (vw)	611 (vw)	619	0
	682 (vw), 663 (vw), 656 (vw)	665	0
742 (vs)	742 (vs)	730	75
		749	3
768 (m)	768 (m)	754	6
820 (w)	819 (vw)	789	6
		832	0
876 (vw)	876 (vw)	855	1
918 (vw)	918 (vw)	899	1
957 (vw)	957 (vw)	941	0
1014 (w)	1013 (w)	1002	4
1060 (w)	1059 (w)	1035	8
1105 (m)	1105 (m)	1084	31
1133 (w)	1135 (w)	1117	6
1152 (vw)	1152 (vw)	1142	1
1232 (vw), 1177 (vw)	1232 (w), 1176 (vw)	1212	6
1247 (s)	1246 (s)	1226	36
1305 (vw)	1304 (vw)	1288	6
1332 (w/sh)	1331 (w)	1313	5
1354 (w), 1340 (w), 1335 (m)	1354 (w), 1340 (w), 1335 (m)	1335	19
1418 (s)	1417 (s)	1403	54
1459 (s)	1459 (m)	1444	22
1497 (w)	1497 (w)	1483	4
1537 (m)	1537 (m)	1521	42
		1572	2
1636 (w)	1635 (w)	1613	3
2236 (vs)	2236 (vs)	2252	95
		3065	0
3057 (vw)	3057 (vw)	3073	11
3078 (w)	3078 (w)	3083	24
3096 (vw)	3096 (vw)	3092	19
3141 (vw)	3142 (vw)	3159	1
3506 (vs), 3501 (vs)	3508 (vs)	3521	100

* scaled by 0.9613. – † normalised to most prominent peak (=100).

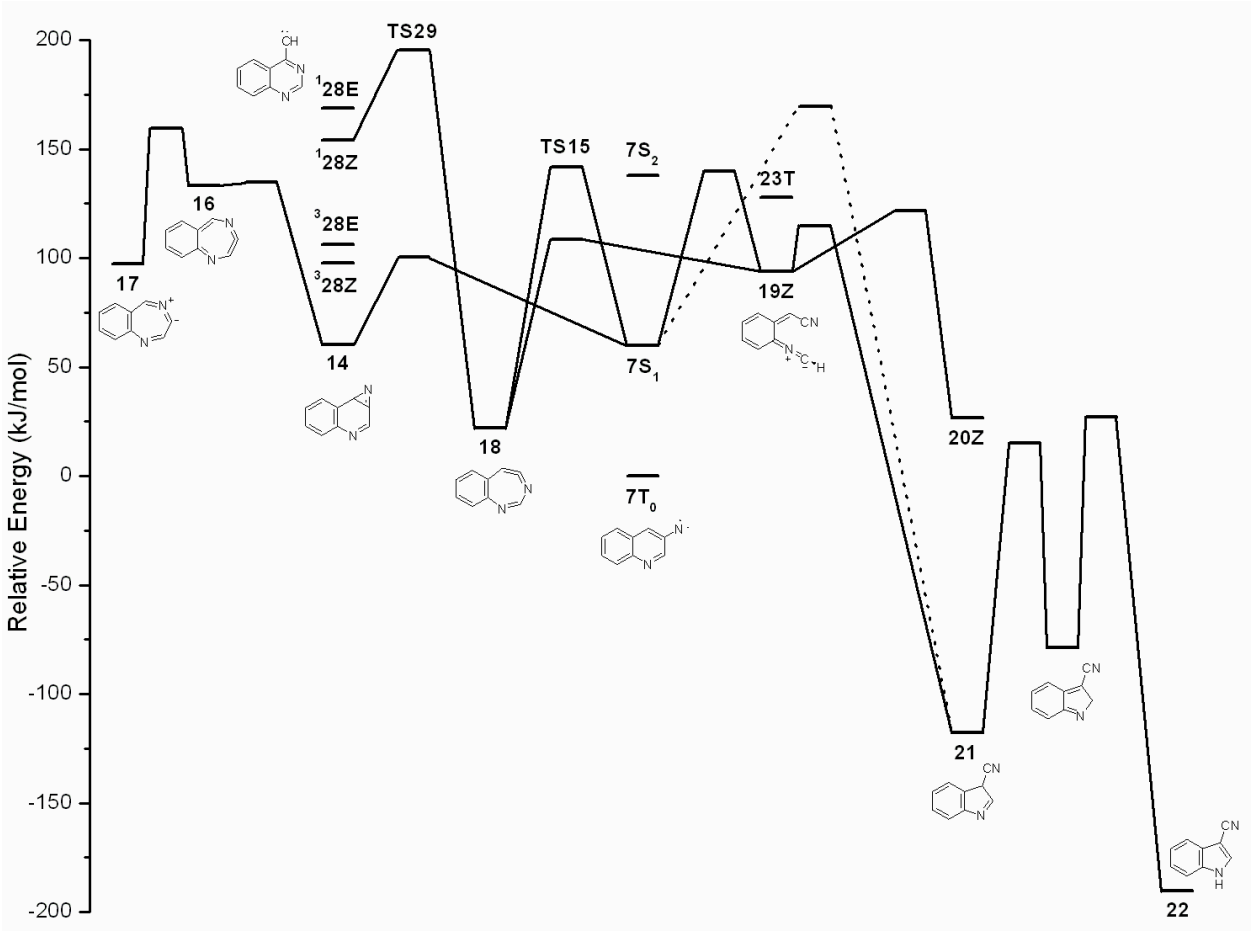
Table S4. Summary of the relative energies pertaining to Schemes 6-7 (B3LYP/6-31G*).

Energies are relative to triplet nitrene 7 (T_0, ^{3}A"). The absolute energy of triplet nitrene 7 at the B3LYP/6-31G* level is -455.863700 Hartree. All energies are corrected for zero-point vibrational energies (ZPVE).

Structure	Energy (kcal/mol) B3LYP/6-31G*	Energy (kJ/mol) B3LYP/6-31G*
6Z - N_2	1.6	6.7
6E - N_2	1.4	5.9
7(T_0, ^{3}A")	0	0
7(S_1, OSS, ^{1}A")	#14.3	#59.9
7(S_2, CSS, ^{1}A')	33.0	137.9
14	14.3	60.0
16	31.8	133.0
17	23.3	97.4
18	5.3	22.1
19Z	22.5	94.1
19E	22.0	92.0
20Z	6.3	26.5
20E	5.2	21.9
(2-isocyanophenyl)acetonitrile (*gauche*)	-18.75	-78.45
(2-isocyanophenyl)acetonitrile (*anti*)	-19.34	-80.92
21	-28.1	-117.6
22	-45.4	-190.1
3-cyano-2*H*-indole	-18.8	-78.8
2-cyano-2*H*-indole	-8.2	-34.3
2-cyanoindole	-43.2	-181.0
23T (T_0, ^{3}A")	30.5	127.7
23S (S_1, OSS, ^{1}A")	#31.4	#131.5
26-N_2	-13.7	-57.2
27Z-N_2	-5.3	-22.1

27E-N_2	-2.2	-9.2
28Z, (T_0, ^{3}A")	23.3	97.7
28Z, (S_1, ^{1}A)	36.8	154.0
28E, (T_0, ^{3}A")	25.4	106.4
28E, (S_1, ^{1}A)	40.3	168.8
15, **TS** (**7→18**)	33.8	141.6
TS (**26→27Z**)-N_2	3.9	16.3
TS (**28Z→28E**) (^{1}A)	40.1	167.9
29, **TS** (**28Z→18**) (^{1}A)	46.7	195.3
TS (**28E→18**) (^{1}A)	49.0	204.8
TS (**7S$_1$→14**) (^{1}A, OSS)	24.0	100.4
TS (**7S$_1$→19Z**) (^{1}A, OSS)	33.4	139.7
TS (**7S$_1$→21**) (^{1}A, OSS)	[§]40.5	[§]169.6
TS (**7T$_0$→23T**) (^{3}A)	34.8	145.4
TS (**7→**2-cyano-2*H*-indole) (^{1}A, CSS)	45.4	190.0
TS (2-cyano-2*H*-indole→2-cyanoindole)	12.8	53.8
TS (**14→16**)	32.2	134.6
TS (**16→17**)	38.1	159.5
TS (**18→19Z**)	25.9	108.5
TS (**19Z→21**)	27.4	114.7
TS (**21→**3-cyano-2*H*-indole)	3.6	15.0
TS (3-cyano-2*H*-indole→**22**)	6.5	27.1
TS (2-cyano-2H-indole→**21**)	16.3	68.3
TS (**19Z→20Z**)	29.1	121.7
TS (**20Z→20E**)	10.6	44.5

[#]: Ziegler-Cramer corrected energy (see Table S6, p. S18). [§]: Single point calculation



Schematic diagram of relative energies pertaining to Schemes 6 and 7 at the B3LYP/6-31G* level

Table S5. Summary of the relative energies pertaining to Scheme 9 (B3LYP/6-31G*).

Energies are relative to triplet carbene 31Z (T_0, ^{3}A"). The absolute energy of triplet carbene 31Z at UB3LYP/6-31G* is -439.775834 Hartree. All energies are corrected for zero-point vibrational energies (ZPVE).

Structure	Energy (kcal/mol) B3LYP/6-31G*	Energy (kJ/mol) B3LYP/6-31G*
30Z-N_2	-24.4	-102.3
30E-N_2	-24.9	-104.0
31Z, (T_0, ^{3}A")	0	0
31Z, (S_1, ^{1}A')	7.7	32.2
31E, (T_0, ^{3}A")	0.3	1.4
31E, (S_1, ^{1}A')	8.4	35.3
3-ethynyl-3*H*-indole	-14.9	-62.2
32	1.3	5.4
33Z	37.9	158.5
33E	35.8	149.6
35Z	-7.0	-29.4
35E	-9.4	-39.1
36	-10.7	-44.8
37	7.9	32.9
39Z, (T_0, ^{3}A")	0.9	3.6
39Z, (S_1, ^{1}A)	12.0	50.1
39E, (T_0, ^{3}A")	2.0	8.2
39E, (S_1, ^{1}A)	15.0	62.7
40	20.7	86.6
41	-17.2	-72.1
43(T_0, ^{3}A")	-26.4	-110.6
43(S_1, OSS, ^{1}A")	$^{\#}$-14.0	$^{\#}$-58.8
43(S_2, CSS, ^{1}A')	4.9	20.3
1-cyano-1*H*-indene	-51.0	-213.5

1-cyano-2*H*-indene	-40.5	-169.4
2-cyano-2*H*-indene	-28.8	-120.5
44	-58.0	-242.5
45	-59.6	-249.3
TS (**31Z**→3-ethynyl-3*H*-indole) (^{1}A)	43.3	181.1
TS (**31Z**→**31E**) (^{1}A)	19.3	80.8
TS (**31Z**→**32**) (^{1}A)	18.2	76.2
TS (**31E**→**32**) (^{1}A)	23.7	99.0
TS (**31Z**→**33Z**) (^{1}A)	46.6	194.9
TS (**31Z**→**36**) (^{1}A)	35.2	147.2
TS (**32**→**37**)	11.9	49.6
TS (**33Z**→3-ethynyl-3*H*-indole)	42.5	177.6
TS (**33Z**→**35**)	39.7	166.0
TS (**33Z**→**36**)	38.2	159.8
TS (**37**→**40**)	22.6	94.7
TS (**40**→**39Z**) (^{1}A)	23.0	96.0
TS (**39Z**→**39E**) (^{1}A)	18.7	78.2
38, **TS** (**39Z**→**41**) (^{1}A)	24.3	101.8
TS (**39E**→**41**) (^{1}A)	27.3	114.3
42, **TS** (**41**→**43**), (^{1}A, CSS)	10.7	44.9
TS (**43**→1-cyano-1*H*-indene), (^{1}A, CSS)	24.8	103.9
TS (**43S$_1$**→1-cyano-1*H*-indene), (^{1}A, OSS)	23.7	99.0
TS (1-cyano-1*H*-indene→1-cyano-2*H*-indene)	-17.7	-74.1
TS (1-cyano-2*H*-indene→**44**)	-22.0	-92.1
TS (1-cyano-1*H*-indene→2-cyano-2*H*-indene)	-5.0	-20.7
TS (2-cyano-2*H*-indene→**45**)	-14.3	-59.7

[#]: Ziegler-Cramer corrected energy (see Table S6, p. S18).

Table S6. Cartesian coordinates and energies at the B3LYP/6-31G* level

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

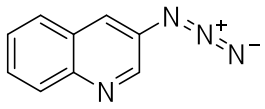
Natural spin densities were computed at the UB3LYP/EPR-III level.
NBO Version 3.1, Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. Gaussian 03, Revision B.05.

Dinitrogen, N_2

Atom Type	Coordinates (Angstroms) X	Y	Z
N	0.000000	0.000000	0.552751
N	0.000000	0.000000	-0.552751

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

(*s*-*Z*)-3-Azidoquinoline 6Z



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.261121	-1.535000	0.000000
C	-1.046102	-0.965067	0.000000
C	-1.168244	0.408289	0.000000
C	0.000000	1.205223	0.000000
C	1.265995	0.535078	0.000000
N	1.366341	-0.827443	0.000000
C	2.457778	1.303897	0.000000
C	2.398204	2.679779	0.000000
C	1.146152	3.344433	0.000000
C	-0.027936	2.625473	0.000000
N	-2.233927	-1.733131	0.000000
N	-2.149346	-2.969248	0.000000
N	-2.238291	-4.106957	0.000000
H	3.402723	0.769742	0.000000
H	3.313918	3.264396	0.000000
H	1.116450	4.430545	0.000000
H	-0.989257	3.133541	0.000000
H	-2.153307	0.866076	0.000000

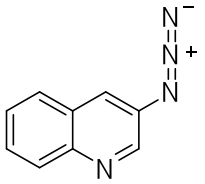
H	0.374235	-2.619476	0.000000

State=1-A'
RB3LYP/6-31G(d), HF= -565.5184875
Zero-point correction= 0.138808 (Hartree/Particle)
Sum of electronic and zero-point Energies= -565.379679

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	48.5	0.1	0
2	A'	117.7	0.3	0
3	A"	125.1	0.0	0
4	A"	182.1	0.1	0
5	A'	268.6	1.8	0
6	A"	297.3	3.2	0
7	A'	392.2	0.8	0
8	A"	409.4	4.4	0
9	A'	434.6	2.3	0
10	A"	470.6	2.0	0
11	A"	503.3	6.4	1
12	A'	515.3	0.7	0
13	A"	520.2	2.5	0
14	A'	592.7	12.4	1
15	A'	624.5	11.3	1
16	A"	627.4	0.3	0
17	A'	736.3	11.2	1
18	A"	741.2	30.0	3
19	A'	752.2	3.8	0
20	A"	767.4	12.4	1
21	A"	846.5	3.9	0
22	A'	867.3	2.5	0
23	A"	885.3	26.0	3
24	A"	905.5	0.0	0
25	A"	930.9	4.5	0
26	A'	951.2	15.0	2
27	A"	960.4	0.0	0
28	A'	1005.8	2.1	0
29	A'	1090.9	8.8	1
30	A'	1116.3	9.2	1
31	A'	1138.6	2.9	0
32	A'	1187.6	0.4	0
33	A'	1219.1	0.6	0
34	A'	1243.9	0.1	0
35	A'	1308.3	87.5	9
36	A'	1348.6	110.8	11
37	A'	1356.4	59.6	6
38	A'	1359.1	8.0	1
39	A'	1417.0	23.6	2
40	A'	1454.5	27.4	3
41	A'	1486.8	11.6	1
42	A'	1551.2	4.9	1
43	A'	1594.1	51.6	5
44	A'	1610.1	2.7	0
45	A'	2175.4	978.2	100
46	A'	3036.4	15.5	2
47	A'	3060.3	1.8	0
48	A'	3071.6	10.5	1
49	A'	3083.9	13.6	1
50	A'	3084.9	16.2	2
51	A'	3097.1	13.8	1

(*s-E*)-3-Azidoquinoline 6E



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.010653	-1.659097	0.000000
C	0.402065	-1.472909	0.000000
C	0.904705	-0.188744	0.000000
C	0.000000	0.900856	0.000000
C	-1.401743	0.606803	0.000000
N	-1.877362	-0.675286	0.000000
C	-2.333053	1.675968	0.000000
C	-1.895322	2.982028	0.000000
C	-0.508669	3.273872	0.000000
C	0.420225	2.257262	0.000000
N	1.168429	-2.664187	0.000000
N	2.402623	-2.563043	0.000000
N	3.542351	-2.610122	0.000000
H	-3.388855	1.423978	0.000000
H	-2.613551	3.797143	0.000000
H	-0.178786	4.309107	0.000000
H	1.484732	2.479397	0.000000
H	1.975989	-0.000121	0.000000
H	-1.397144	-2.677276	0.000000

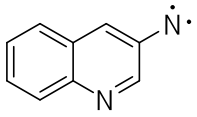
State=1-A'
RB3LYP/6-31G(d), HF= -565.5188434
Zero-point correction= 0.138857 (Hartree/Particle)
Sum of electronic and zero-point Energies= -565.379987

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	56.6	0.1	0
2	A'	104.8	0.4	0
3	A"	125.7	0.2	0
4	A"	184.3	0.0	0
5	A'	279.4	2.1	0
6	A"	297.6	2.5	0
7	A'	396.2	0.5	0
8	A"	410.3	4.6	1
9	A'	435.0	5.7	1
10	A"	469.5	1.9	0
11	A"	512.6	2.4	0
12	A'	513.6	0.1	0
13	A"	520.2	7.2	1
14	A'	590.8	13.5	2
15	A'	620.6	0.5	0
16	A"	629.5	0.2	0
17	A'	730.0	18.6	2
18	A"	740.9	28.9	4
19	A'	755.4	4.0	0

20	A"	767.3	12.7	2
21	A"	845.6	6.5	1
22	A"	878.7	22.9	3
23	A'	882.7	5.3	1
24	A"	915.0	1.2	0
25	A"	930.8	4.8	1
26	A'	958.9	9.7	1
27	A"	960.6	0.1	0
28	A'	1006.6	1.8	0
29	A'	1097.7	25.4	3
30	A'	1116.2	21.0	3
31	A'	1139.8	0.7	0
32	A'	1189.0	4.3	1
33	A'	1218.2	2.3	0
34	A'	1239.8	6.5	1
35	A'	1293.5	107.4	13
36	A'	1344.6	52.7	6
37	A'	1356.4	8.5	1
38	A'	1363.4	56.3	7
39	A'	1415.1	73.3	9
40	A'	1451.7	11.3	1
41	A'	1488.5	20.9	3
42	A'	1555.3	1.3	0
43	A'	1588.4	27.5	3
44	A'	1609.0	0.5	0
45	A'	2177.1	814.3	100
46	A'	3054.8	16.1	2
47	A'	3058.5	1.2	0
48	A'	3063.3	6.9	1
49	A'	3071.6	10.7	1
50	A'	3084.1	22.0	3
51	A'	3096.9	14.7	2

3-Quinolylnitrene 7 (T_0, Triplet, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.227746	1.668282	0.000000
C	-2.796321	0.373604	0.000000
C	-1.986650	-0.749215	0.000000
C	-0.584267	-0.616840	0.000000
C	0.000000	0.693679	0.000000
C	-0.858473	1.827954	0.000000
N	0.182129	-1.763982	0.000000
C	1.476266	-1.654114	0.000000
C	2.196436	-0.377449	0.000000
C	1.403226	0.798778	0.000000
H	-2.876036	2.539909	0.000000
H	-3.876889	0.262477	0.000000
H	-2.401214	-1.752246	0.000000
H	-0.415703	2.820829	0.000000
H	2.067759	-2.567784	0.000000
H	1.890886	1.769116	0.000000
N	3.514494	-0.358929	0.000000

State= 3-A"
<S2>= 2.05789
UB3LYP/6-31G(d), HF= -455.9902408
Zero-point correction= 0.126541 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.863700

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	107.0	0.4	1
2	A"	177.1	0.1	0
3	A"	271.4	7.6	23
4	A'	278.1	1.8	6
5	A"	397.0	5.1	15
6	A'	421.7	11.8	36
7	A'	442.6	2.7	8
8	A"	455.8	1.9	6
9	A"	499.5	0.9	3
10	A'	506.3	0.3	1
11	A'	591.8	6.3	19
12	A"	620.4	0.1	0
13	A'	702.1	2.5	8
14	A"	735.3	21.7	66
15	A'	744.3	0.0	0
16	A"	757.8	15.1	46
17	A"	830.3	22.5	68
18	A"	858.4	8.4	25
19	A'	876.6	0.4	1
20	A"	897.2	5.1	15
21	A'	907.7	15.4	47
22	A"	928.9	3.9	12
23	A"	957.7	0.2	1
24	A'	1006.6	1.1	3
25	A'	1102.6	5.7	17
26	A'	1128.8	0.4	1
27	A'	1167.3	7.4	22
28	A'	1188.5	8.7	26
29	A'	1217.4	1.6	5
30	A'	1259.3	8.2	25
31	A'	1273.7	13.1	40
32	A'	1335.4	4.6	14
33	A'	1358.5	1.8	5
34	A'	1377.5	6.6	20
35	A'	1425.8	2.9	9
36	A'	1465.3	17.0	51
37	A'	1519.2	0.9	3
38	A'	1544.3	33.3	101
39	A'	1588.3	8.1	24
40	A'	3060.4	11.4	35
41	A'	3064.1	1.4	4
42	A'	3075.2	8.6	26
43	A'	3085.7	4.2	13
44	A'	3087.5	20.2	61
45	A'	3099.3	10.9	33

Excitation energies and oscillator strengths:

Excited State	1:	Triplet-A'	2.5858 eV	479.49 nm	f=0.0025
Excited State	2:	Triplet-A"	3.1193 eV	397.47 nm	f=0.0002
Excited State	3:	Triplet-A'	3.1757 eV	390.42 nm	f=0.0097
Excited State	4:	Triplet-A'	3.4168 eV	362.87 nm	f=0.0492

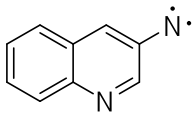
Excited State	5:	Triplet-A'	3.5184 eV	352.39 nm	f=0.0282
Excited State	6:	Triplet-A"	3.6238 eV	342.14 nm	f=0.0000
Excited State	7:	Triplet-A"	3.6471 eV	339.95 nm	f=0.0003
Excited State	8:	Triplet-A'	3.8518 eV	321.88 nm	f=0.0007
Excited State	9:	Triplet-A"	4.1341 eV	299.91 nm	f=0.0000
Excited State	10:	Triplet-A'	4.2809 eV	289.63 nm	f=0.0018
Excited State	11:	Triplet-A"	4.4059 eV	281.40 nm	f=0.0034
Excited State	12:	Triplet-A'	4.5411 eV	273.02 nm	f=0.0248
Excited State	13:	Triplet-A"	4.5918 eV	270.01 nm	f=0.0012
Excited State	14:	Triplet-A'	4.6696 eV	265.51 nm	f=0.0105
Excited State	15:	Triplet-A'	4.9270 eV	251.64 nm	f=0.0109

Natural Atomic Spin Densities of structure optimized at UB3LYP/EPR-III level:

State= 3-A"
<S2>= 2.054665
UB3LYP/EPR-III, HF= -456.1737161

1	C	-0.07118
2	C	0.14814
3	C	-0.07861
4	C	0.13721
5	C	-0.08673
6	C	0.12894
7	C	-0.06475
8	C	0.18267
9	H	-0.20142
10	H	0.41515
11	H	0.00221
12	H	-0.00453
13	H	0.00222
14	C	-0.00402
15	H	-0.00429
16	N	-0.01220
17	N	1.51117

3-Quinolylnitrene 7 (S_1, Open-Shell Singlet, ^{1}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.234176	1.663483	0.000000
C	-2.797554	0.368098	0.000000
C	-1.980527	-0.753484	0.000000
C	-0.582955	-0.615857	0.000000
C	0.000000	0.696831	0.000000
C	-0.864744	1.828111	0.000000
N	0.189727	-1.765069	0.000000
C	1.479096	-1.657663	0.000000
C	2.208202	-0.371872	0.000000
C	1.398770	0.810039	0.000000
H	-2.885052	2.533160	0.000000
H	-3.877433	0.251499	0.000000
H	-2.391979	-1.757839	0.000000

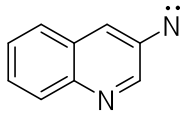
H	-0.425749	2.822595	0.000000
H	2.073171	-2.569442	0.000000
H	1.884347	1.780839	0.000000
N	3.505420	-0.358778	0.000000

State= 1-A"
<S2>= 1.037979
UB3LYP/6-31G(d), HF= -455.9786386
Zero-point correction= 0.126350 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.852289
Ziegler-Cramer corrected energy= -455.840878 (see Table S6, p. S18)

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	101.0	0.7	2
2	A"	176.3	0.1	0
3	A"	257.0	7.6	23
4	A'	280.2	2.0	6
5	A"	392.1	5.3	16
6	A'	422.9	12.1	37
7	A'	440.8	4.2	13
8	A"	449.3	1.7	5
9	A"	497.1	0.7	2
10	A'	503.6	0.1	0
11	A'	588.7	6.5	20
12	A"	618.9	0.2	1
13	A'	698.1	2.5	8
14	A"	731.5	16.1	49
15	A'	741.6	0.2	1
16	A"	753.2	18.1	55
17	A"	810.0	29.0	88
18	A"	852.4	3.2	10
19	A'	870.2	1.8	5
20	A"	890.5	7.4	22
21	A'	893.2	13.9	42
22	A"	927.0	3.9	12
23	A"	954.4	0.3	1
24	A'	1006.6	1.0	3
25	A'	1099.5	4.4	13
26	A'	1129.2	0.8	2
27	A'	1164.7	2.5	8
28	A'	1190.8	4.4	13
29	A'	1222.7	1.7	5
30	A'	1243.2	2.0	6
31	A'	1293.0	17.6	53
32	A'	1344.8	3.0	9
33	A'	1356.0	0.1	0
34	A'	1397.0	9.8	30
35	A'	1421.6	2.0	6
36	A'	1463.8	15.9	48
37	A'	1518.1	0.2	1
38	A'	1551.2	32.5	99
39	A'	1580.7	7.2	22
40	A'	3062.8	10.6	32
41	A'	3064.8	1.4	4
42	A'	3076.2	8.2	25
43	A'	3087.7	19.0	58
44	A'	3091.2	4.4	13
45	A'	3099.3	11.2	34

3-Quinolylnitrene 7 (S_2, Closed-Shell Singlet, $^1A'$)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.211350	1.698798	0.000000
C	-2.782676	0.401479	0.000000
C	-1.993239	-0.732896	0.000000
C	-0.585655	-0.623421	0.000000
C	0.000000	0.693829	0.000000
C	-0.844307	1.842472	0.000000
N	0.153776	-1.786204	0.000000
C	1.455105	-1.667204	0.000000
C	2.204422	-0.405178	0.000000
C	1.398512	0.773749	0.000000
H	-2.857357	2.571325	0.000000
H	-3.864703	0.299970	0.000000
H	-2.424612	-1.728370	0.000000
H	-0.384722	2.827466	0.000000
H	2.053245	-2.579066	0.000000
H	1.914225	1.731912	0.000000
N	3.520374	-0.358512	0.000000

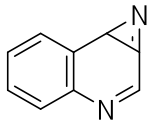
State= 1-A'
RB3LYP/6-31G(d), HF= -455.9386479
Zero-point correction= 0.127477 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.811171

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	95.9	4.3	2
2	A"	171.3	0.0	0
3	A"	232.5	18.1	10
4	A'	293.8	1.9	1
5	A"	398.4	2.7	2
6	A'	436.4	12.2	7
7	A'	448.5	2.1	1
8	A"	471.2	3.5	2
9	A"	484.1	0.2	0
10	A'	509.9	6.5	4
11	A'	592.9	7.8	4
12	A"	629.7	0.5	0
13	A'	695.3	8.9	5
14	A"	746.5	29.8	16
15	A'	747.6	0.0	0
16	A"	771.4	14.5	8
17	A"	863.0	4.9	3
18	A'	877.1	5.1	3
19	A"	932.7	1.5	1
20	A'	941.5	10.6	6
21	A"	958.1	9.0	5
22	A"	963.2	5.7	3
23	A"	976.7	0.6	0
24	A'	1003.8	1.3	1
25	A'	1109.7	9.6	5
26	A'	1139.0	10.7	6

27	A'	1166.6	25.1	14
28	A'	1193.6	1.6	1
29	A'	1231.3	9.4	5
30	A'	1266.4	2.1	1
31	A'	1300.8	140.0	77
32	A'	1345.5	22.4	12
33	A'	1358.4	1.8	1
34	A'	1388.4	98.5	54
35	A'	1429.4	65.9	36
36	A'	1465.9	40.1	22
37	A'	1522.4	34.0	19
38	A'	1555.5	180.8	100
39	A'	1604.2	119.6	66
40	A'	3049.3	14.0	8
41	A'	3070.3	0.4	0
42	A'	3076.3	1.7	1
43	A'	3077.7	8.4	5
44	A'	3093.8	15.4	9
45	A'	3104.4	5.9	3

Azirene 14



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.240958	-0.243115	-0.016848
C	-1.215211	-1.240745	-0.345372
C	0.128192	-0.669931	-0.167797
C	0.201866	0.750058	-0.017576
N	-0.891402	1.623177	-0.178814
C	-2.105372	1.190036	-0.223190
C	1.454881	1.356259	0.183542
C	2.613931	0.592520	0.201229
C	2.546505	-0.791629	-0.013092
C	1.316187	-1.411275	-0.207829
H	1.262368	-2.485989	-0.363005
H	3.457091	-1.384533	-0.017972
H	3.576023	1.071014	0.360872
H	1.485491	2.434734	0.303682
H	-1.401761	-2.050947	-1.045122
H	-2.926626	1.869009	-0.439332
N	-2.201844	-1.144086	0.870597

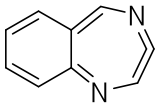
RB3LYP/6-31G(d), HF= -455.9684324
Zero-point correction= 0.127598 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.840834

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	131.5	3.2	8
2	A	146.3	2.5	6
3	A	294.2	4.9	11
4	A	327.4	0.7	2
5	A	364.8	3.2	7

6	A	429.7	3.9	9
7	A	473.1	0.8	2
8	A	496.4	1.0	2
9	A	526.9	1.7	4
10	A	581.4	7.0	16
11	A	592.9	2.3	5
12	A	645.9	10.9	25
13	A	725.3	2.7	6
14	A	729.0	0.5	1
15	A	753.3	32.2	75
16	A	769.0	15.4	36
17	A	819.9	6.5	15
18	A	841.6	2.6	6
19	A	864.8	3.8	9
20	A	895.5	7.1	17
21	A	927.1	3.0	7
22	A	956.1	1.4	3
23	A	966.9	33.4	78
24	A	1018.4	1.8	4
25	A	1081.4	1.0	2
26	A	1105.8	19.0	44
27	A	1143.8	2.6	6
28	A	1164.9	4.1	9
29	A	1194.9	1.8	4
30	A	1230.9	1.1	3
31	A	1283.7	3.5	8
32	A	1310.4	1.6	4
33	A	1324.9	4.0	9
34	A	1437.2	2.4	5
35	A	1446.2	4.9	11
36	A	1524.7	11.6	27
37	A	1551.5	6.6	15
38	A	1598.4	2.6	6
39	A	1721.1	43.3	101
40	A	3058.6	12.9	30
41	A	3062.1	4.3	10
42	A	3071.5	14.6	34
43	A	3072.6	11.0	26
44	A	3084.0	22.0	51
45	A	3095.6	12.1	28

Cyclic Ketenimine 16



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.558083	-0.686476	-0.203289
C	-1.392078	-1.369655	-0.358875
C	-0.105794	-0.764384	-0.076406
C	-0.105502	0.719973	0.128112
C	-1.384862	1.359314	0.358807
C	-2.558965	0.694449	0.194427
N	0.892154	-1.616888	0.072900
C	2.109975	-1.099275	0.546012
C	2.481055	0.037162	-0.033614
N	2.170433	1.098713	-0.652330

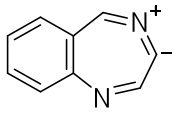
C	0.973292	1.555674	-0.086878
H	-1.380795	2.417705	0.607842
H	-3.504616	1.208481	0.339424
H	-3.507169	-1.191381	-0.361905
H	-1.375726	-2.425068	-0.609251
H	2.707687	-1.695921	1.223773
H	0.868282	2.632708	0.046349

RB3LYP/6-31G(d), HF= -455.939357
Zero-point correction= 0.126332 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.813025

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	145.4	1.2	1
2	A	152.7	1.0	1
3	A	246.0	6.6	7
4	A	319.5	6.7	7
5	A	361.4	15.4	15
6	A	384.0	5.9	6
7	A	395.9	6.4	6
8	A	414.1	5.0	5
9	A	508.1	7.5	7
10	A	537.6	2.7	3
11	A	559.7	16.4	16
12	A	616.4	1.9	2
13	A	651.2	22.5	23
14	A	685.0	20.8	21
15	A	733.9	14.5	14
16	A	736.6	45.8	46
17	A	746.2	0.6	1
18	A	827.2	5.2	5
19	A	868.9	1.7	2
20	A	902.5	14.2	14
21	A	934.6	4.2	4
22	A	962.7	1.0	1
23	A	983.4	3.5	4
24	A	1035.5	26.6	27
25	A	1050.4	25.5	26
26	A	1107.9	13.1	13
27	A	1122.1	3.7	4
28	A	1147.3	5.7	6
29	A	1190.6	1.7	2
30	A	1209.0	6.4	6
31	A	1274.2	28.1	28
32	A	1332.6	12.5	12
33	A	1368.5	0.1	0
34	A	1421.9	8.3	8
35	A	1448.6	33.1	33
36	A	1492.5	25.0	25
37	A	1516.4	4.3	4
38	A	1621.5	7.5	8
39	A	1818.4	100.2	100
40	A	3039.8	15.7	16
41	A	3060.7	2.6	3
42	A	3071.5	14.8	15
43	A	3087.6	21.0	21
44	A	3102.5	7.6	8
45	A	3114.7	9.7	10

Cyclic Nitrile Ylide 17



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.953186	1.577278	-0.294193
N	-2.037586	1.101169	0.223221
C	-2.512650	0.071730	0.774382
C	-2.261436	-1.092503	-0.125452
N	-1.051897	-1.386396	-0.428968
C	0.121008	-0.655929	-0.130472
C	0.253248	0.764338	-0.166226
C	1.531516	1.341771	-0.077815
C	1.276497	-1.431955	0.068851
C	2.658803	0.552826	0.111379
C	2.525199	-0.838881	0.208243
H	1.622600	2.423192	-0.147780
H	3.639880	1.013863	0.181420
H	3.403029	-1.460300	0.361122
H	1.163910	-2.511769	0.081308
H	-3.068595	-1.744801	-0.459655
H	-0.968431	2.544343	-0.788360

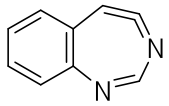
RB3LYP/6-31G(d), HF= -455.9533895
Zero-point correction= 0.126789 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.826600

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	137.3	3.3	2
2	A	143.9	0.8	0
3	A	310.1	4.0	2
4	A	316.7	2.1	1
5	A	332.9	18.7	11
6	A	396.8	5.5	3
7	A	439.5	16.2	10
8	A	449.1	2.2	1
9	A	523.2	13.6	8
10	A	556.7	18.2	11
11	A	577.3	4.4	3
12	A	615.4	16.7	10
13	A	645.6	9.1	6
14	A	710.4	2.8	2
15	A	739.6	1.6	1
16	A	746.8	43.2	26
17	A	793.5	12.0	7
18	A	832.3	5.7	3
19	A	859.1	2.0	1
20	A	878.4	74.6	45
21	A	906.5	15.8	10
22	A	922.3	3.8	2
23	A	951.3	0.0	0
24	A	1022.4	2.8	2
25	A	1084.1	3.7	2
26	A	1134.5	12.8	8
27	A	1149.8	3.1	2

28	A	1191.7	23.6	14
29	A	1196.1	30.4	19
30	A	1237.5	3.1	2
31	A	1289.6	9.4	6
32	A	1314.2	18.9	12
33	A	1375.3	32.2	20
34	A	1445.2	7.7	5
35	A	1451.7	21.4	13
36	A	1542.9	19.1	12
37	A	1546.8	4.6	3
38	A	1595.3	1.1	1
39	A	1705.8	164.0	100
40	A	3042.8	36.5	22
41	A	3059.8	3.1	2
42	A	3071.8	6.9	4
43	A	3079.8	13.3	8
44	A	3084.6	19.5	12
45	A	3094.1	14.4	9

Cyclic Ketenimine 18



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.673081	0.517953	0.163742
C	2.517196	-0.874597	0.194185
C	1.261301	-1.436075	0.014078
C	0.118956	-0.632059	-0.168328
C	0.277948	0.788517	-0.172104
C	1.563451	1.334088	-0.012522
N	-1.070016	-1.346284	-0.429354
C	-2.256444	-1.025165	-0.093119
C	-1.955543	1.086047	0.235244
C	-0.916970	1.632699	-0.374967
H	3.659819	0.959929	0.271038
H	3.381440	-1.517362	0.335769
H	1.126099	-2.513047	-0.001552
H	1.675590	2.415013	-0.035983
H	-3.094220	-1.663324	-0.368970
N	-2.574341	0.123333	0.723822
H	-0.936085	2.531005	-0.978831

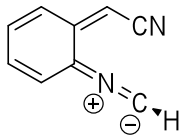
RB3LYP/6-31G(d), HF= -455.9825811
Zero-point correction= 0.127289 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.855293

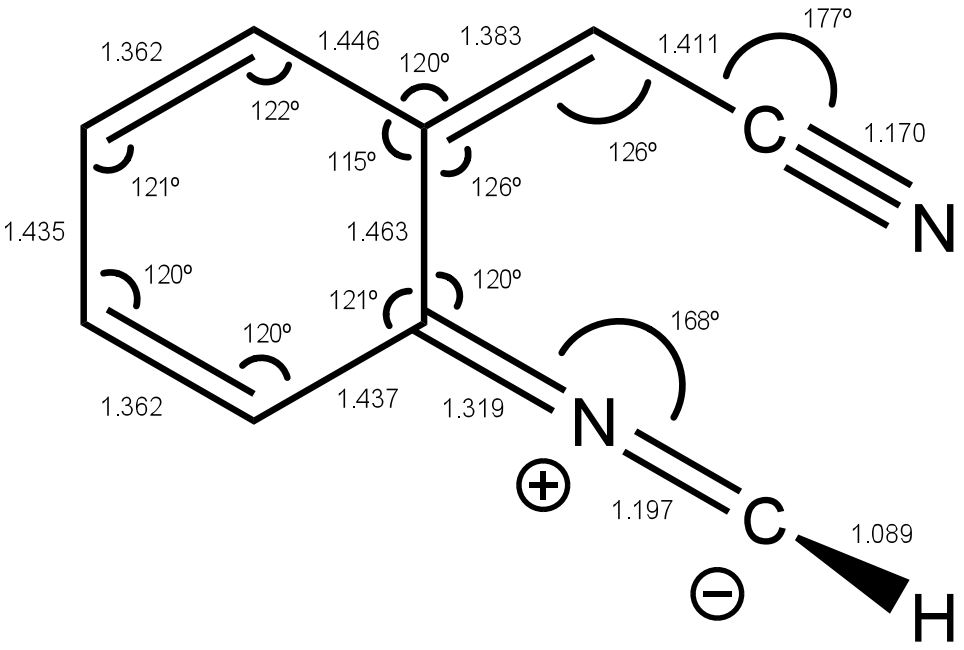
Vibrational frequencies (scaled by 0.9613):

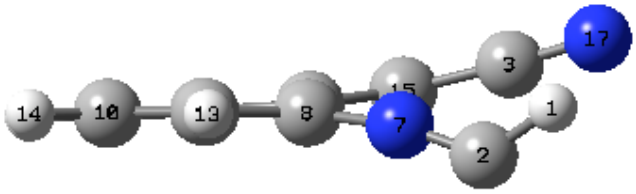
ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	134.7	1.3	0
2	A	145.9	1.7	1
3	A	304.3	2.1	1
4	A	329.5	9.5	4
5	A	346.2	4.6	2
6	A	417.1	7.9	3
7	A	459.2	7.0	3

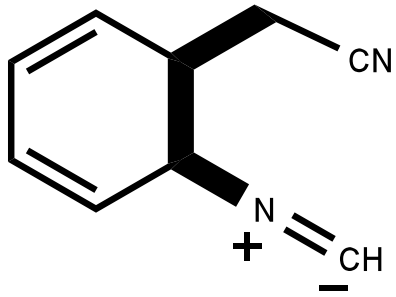
8	A	465.6	2.0	1
9	A	523.7	17.0	7
10	A	567.7	5.3	2
11	A	576.2	4.9	2
12	A	612.6	6.6	3
13	A	654.3	3.4	1
14	A	709.1	0.7	0
15	A	737.8	20.1	8
16	A	747.0	21.8	8
17	A	764.6	35.4	14
18	A	828.2	1.3	0
19	A	857.3	3.9	1
20	A	894.2	64.4	25
21	A	919.5	26.0	10
22	A	927.6	11.6	4
23	A	951.4	0.1	0
24	A	1023.4	2.0	1
25	A	1079.6	8.0	3
26	A	1101.8	30.3	12
27	A	1140.7	4.2	2
28	A	1153.3	1.6	1
29	A	1178.7	11.0	4
30	A	1224.8	3.3	1
31	A	1278.3	0.9	0
32	A	1310.5	4.8	2
33	A	1334.0	11.2	4
34	A	1434.9	3.8	1
35	A	1446.5	15.4	6
36	A	1541.1	1.9	1
37	A	1569.5	13.0	5
38	A	1606.1	15.2	6
39	A	1917.2	261.1	100
40	A	3062.4	1.1	0
41	A	3065.8	31.3	12
42	A	3072.8	10.5	4
43	A	3084.1	22.0	8
44	A	3095.0	13.4	5
45	A	3116.6	2.1	1

(*Z*)-Ylide 19Z









ϕ= -12°

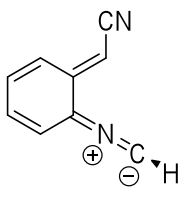
Atom Type	Coordinates (Angstroms) X	Y	Z
H	2.625204	2.392135	-0.084309
C	1.758248	2.056351	0.482231
C	2.287839	-1.005972	-0.132294
C	-0.179685	-0.765071	0.114911
C	-1.449435	-1.452761	0.192820
C	-2.638351	-0.809777	0.022531
N	0.800708	1.435565	0.119926
C	-0.278137	0.688744	-0.017309
C	-1.544448	1.331721	-0.236717
C	-2.695308	0.603983	-0.219519
H	-1.425033	-2.527133	0.353321
H	-3.564662	-1.376451	0.060264
H	-1.550314	2.408132	-0.377346
H	-3.654846	1.089018	-0.367071
C	0.994939	-1.494767	0.151561
H	0.926805	-2.563665	0.332692
N	3.357702	-0.626528	-0.415190

RB3LYP/6-31G(d), HF= -455.9512066
Zero-point correction= 0.123335 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.827872

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	45.3	6.2	1
2	A	124.6	2.0	0
3	A	143.2	0.1	0
4	A	150.3	2.7	0
5	A	214.9	6.0	1
6	A	320.0	7.1	1
7	A	365.0	6.0	1
8	A	393.6	6.3	1
9	A	455.3	6.1	1
10	A	487.0	9.3	2
11	A	511.2	8.1	1
12	A	519.9	12.2	2
13	A	533.0	6.7	1
14	A	618.8	39.7	7
15	A	659.2	41.5	7
16	A	681.5	179.9	30
17	A	695.5	37.6	6
18	A	706.1	595.9	100
19	A	716.1	2.6	0
20	A	760.1	84.4	14
21	A	819.0	13.4	2
22	A	853.1	0.4	0
23	A	916.1	0.7	0
24	A	949.3	0.6	0
25	A	980.7	4.6	1
26	A	1024.2	2.2	0
27	A	1108.7	4.5	1
28	A	1147.2	1.2	0
29	A	1188.3	12.3	2
30	A	1225.0	2.6	0
31	A	1262.6	3.1	1
32	A	1360.2	8.0	1
33	A	1384.7	2.6	0
34	A	1442.7	2.0	0
35	A	1501.7	103.1	17
36	A	1519.9	26.7	4
37	A	1615.5	34.9	6
38	A	1973.2	398.3	67
39	A	2198.7	99.3	17
40	A	3065.4	1.5	0
41	A	3071.1	0.2	0
42	A	3072.6	9.9	2
43	A	3078.9	7.9	1
44	A	3084.9	16.7	3
45	A	3098.5	15.6	3

(*E*)-Ylide 19E



Atom Type	Coordinates (Angstroms) X	Y	Z
H	1.410184	3.723937	0.622700
C	1.316298	2.962822	-0.157013
C	-2.766840	0.262484	-0.005181
C	-0.335272	-0.061225	0.014922
C	-0.431547	-1.505366	0.013328
C	0.671907	-2.301027	0.003264
N	1.218585	1.775528	0.031823
C	1.030404	0.477200	0.011125
C	2.173542	-0.398318	-0.005016
C	1.999541	-1.746778	-0.009695
H	-1.426576	-1.939081	0.019728
H	0.553503	-3.380936	0.002666
H	3.160529	0.053130	-0.015859
H	2.858804	-2.409783	-0.023373
C	-1.443881	0.757937	0.012759
H	-1.334535	1.837542	0.015138
N	-3.862416	-0.142841	-0.016390

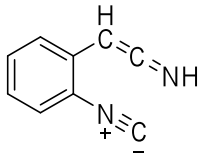
RB3LYP/6-31G(d), HF= -455.9521573
Zero-point correction= 0.123499 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.828659

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	91.1	0.4	0
2	A	100.7	1.8	0
3	A	106.8	3.6	0
4	A	144.8	3.4	0
5	A	211.9	5.2	0
6	A	323.8	0.8	0
7	A	348.4	5.2	0
8	A	390.2	11.3	1
9	A	448.5	9.3	1
10	A	482.4	6.2	1
11	A	484.4	4.2	0
12	A	514.5	2.1	0
13	A	559.9	16.4	2
14	A	597.9	21.9	2
15	A	675.5	44.2	4
16	A	686.0	7.9	1
17	A	747.3	18.6	2
18	A	753.9	7.6	1
19	A	763.3	41.1	4
20	A	775.1	1055.9	100
21	A	820.0	16.5	2
22	A	821.7	4.6	0
23	A	921.6	0.3	0
24	A	959.7	0.2	0
25	A	983.5	5.6	1
26	A	1007.8	3.2	0
27	A	1098.6	9.0	1
28	A	1144.1	0.5	0
29	A	1190.6	4.8	0
30	A	1249.5	7.5	1
31	A	1284.3	1.9	0
32	A	1321.5	9.8	1
33	A	1409.1	0.4	0
34	A	1437.9	2.0	0

35	A	1514.1	51.6	5
36	A	1516.5	62.5	6
37	A	1620.7	21.6	2
38	A	1950.4	549.3	52
39	A	2215.0	90.8	9
40	A	3004.1	17.0	2
41	A	3072.7	7.9	1
42	A	3083.0	1.7	0
43	A	3085.9	3.9	0
44	A	3093.2	5.8	1
45	A	3099.6	15.3	1

(*s*-*Z*)-3-(2-Isocyanophenyl)ketenimine 20Z



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.200583	-0.698153	-0.100052
C	0.371446	0.704958	-0.024338
C	1.642464	1.278615	0.107137
C	2.774639	0.472549	0.149161
C	2.632722	-0.914319	0.052679
C	1.369097	-1.481867	-0.070497
N	-0.724405	1.547429	-0.110804
C	-1.649147	2.274877	-0.217263
C	-1.091803	-1.371286	-0.231085
C	-2.294881	-0.886372	0.044835
N	-3.406128	-0.546299	0.424208
H	1.719393	2.359508	0.163693
H	3.757321	0.922952	0.249182
H	3.508858	-1.556083	0.076692
H	1.268127	-2.561903	-0.135753
H	-1.072191	-2.404716	-0.570354
H	-3.998495	-0.041675	-0.240755

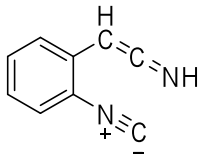
RB3LYP/6-31G(d), HF= -455.9779373
Zero-point correction= 0.124344 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.853593

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	45.7	3.2	1
2	A	121.0	1.5	0
3	A	137.4	2.4	0
4	A	153.4	3.0	1
5	A	208.7	4.9	1
6	A	303.9	3.0	1
7	A	341.5	2.8	1
8	A	391.5	12.2	2
9	A	406.0	39.0	7
10	A	445.3	6.8	1
11	A	499.3	0.8	0
12	A	516.5	2.3	0

13	A	530.7	4.8	1
14	A	591.6	22.1	4
15	A	639.5	5.1	1
16	A	715.4	0.8	0
17	A	730.0	2.6	0
18	A	746.0	58.8	10
19	A	827.4	62.9	11
20	A	836.9	1.0	0
21	A	853.9	4.0	1
22	A	914.2	3.4	1
23	A	946.5	0.6	0
24	A	965.4	384.3	68
25	A	1027.5	12.1	2
26	A	1087.7	10.0	2
27	A	1103.9	13.9	2
28	A	1150.2	1.0	0
29	A	1176.1	3.7	1
30	A	1187.8	7.5	1
31	A	1249.8	0.4	0
32	A	1298.2	5.4	1
33	A	1383.2	1.2	0
34	A	1447.5	10.6	2
35	A	1474.7	49.4	9
36	A	1559.0	1.3	0
37	A	1590.1	19.3	3
38	A	2046.0	561.1	100
39	A	2114.9	118.7	21
40	A	3054.8	2.2	0
41	A	3065.7	4.9	1
42	A	3077.9	9.0	2
43	A	3088.3	16.5	3
44	A	3100.0	9.6	2
45	A	3318.1	14.6	3

(*s-E*)-3-(2-Isocyanophenyl)ketenimine 20E



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.033808	0.575075	0.002003
C	2.240733	-0.135812	0.024980
C	2.229929	-1.525509	0.022161
C	1.006939	-2.204145	-0.006447
C	-0.189503	-1.497429	-0.031807
C	-0.214319	-0.090821	-0.026866
H	3.172075	0.420486	0.045830
H	3.166102	-2.074857	0.040379
H	0.986949	-3.290266	-0.012645
H	-1.132190	-2.036979	-0.063123
C	-1.458898	0.677488	-0.056086
C	-2.668502	0.143976	0.006450
H	-1.400242	1.760440	-0.111407
N	1.074194	1.959972	0.008090
C	1.097130	3.141402	0.015298

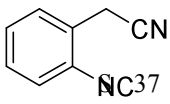
N	-3.785129	-0.355118	-0.066993
H	-4.280046	-0.518145	0.815174

RB3LYP/6-31G(d), HF= -455.979836
Zero-point correction= 0.124483 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.855353

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	58.3	2.2	0
2	A	102.5	2.7	0
3	A	128.1	3.5	1
4	A	143.4	1.0	0
5	A	213.0	4.7	1
6	A	305.9	0.3	0
7	A	341.7	2.0	0
8	A	400.1	2.1	0
9	A	406.0	30.4	5
10	A	441.4	11.6	2
11	A	493.9	0.4	0
12	A	528.1	3.5	1
13	A	539.6	2.0	0
14	A	601.8	20.3	3
15	A	625.1	13.5	2
16	A	736.9	2.2	0
17	A	744.8	59.3	9
18	A	759.9	9.4	1
19	A	813.0	1.0	0
20	A	850.5	20.6	3
21	A	855.1	33.3	5
22	A	915.2	2.2	0
23	A	947.7	0.1	0
24	A	975.9	418.2	62
25	A	1031.2	4.3	1
26	A	1064.6	28.2	4
27	A	1110.0	19.2	3
28	A	1148.4	0.5	0
29	A	1167.2	1.9	0
30	A	1197.9	4.0	1
31	A	1274.5	4.1	1
32	A	1285.3	6.8	1
33	A	1380.2	0.2	0
34	A	1437.6	11.3	2
35	A	1480.3	43.8	7
36	A	1559.8	4.3	1
37	A	1592.0	15.8	2
38	A	2043.4	670.2	100
39	A	2112.8	132.4	20
40	A	3066.8	2.1	0
41	A	3079.0	2.9	0
42	A	3081.7	13.7	2
43	A	3088.8	16.0	2
44	A	3100.9	9.4	1
45	A	3297.3	7.3	1

(**2-Isocyanophenyl)acetonitrile** *gauche* conformation



centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.717389405	0.392857383	0.543075314
2	C	–0.67937405	0.401179066	1.943749627
3	C	0.541877985	0.296539156	2.601774299
4	C	1.723548622	0.187728011	1.86593778
5	C	1.677956354	0.183517283	0.472432466
6	C	0.46471874	0.285537957	–0.212891738
7	H	–1.61034715	0.489058666	2.493528985
8	H	0.569500081	0.301924507	3.687203222
9	H	2.679316938	0.107062242	2.374890401
10	H	2.598962905	0.096250781	–0.098057998
11	N	–1.941259111	0.502213519	–0.096859849
12	C	–2.987063279	0.601208934	–0.639044461
13	C	0.431110863	0.2695161	–1.733317886
14	C	0.43491091	–1.095419599	–2.279562447
15	N	0.451660161	–2.176113247	–2.701986116
16	H	–0.457326754	0.788477487	–2.107916024
17	H	1.305306188	0.798538678	–2.130644547

HF = –456.1597983 Hartree

Zero-point correction = 0.125715 Hartree

Sum of electronic and zero-point energies = –456.0340833 Hartree

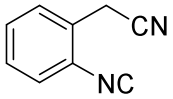
Vibrational frequencies

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	9.8076	3.1546	1	9
2	89.8513	3.1909	1	86
3	137.7563	1.5927	0	132
4	148.4703	5.8642	3	142
5	239.069	1.4797	0	229
6	318.4492	3.7957	2	306
7	350.73	0.7711	0	337
8	370.9659	0.2309	0	356
9	406.3207	2.9153	1	390
10	459.1545	2.7781	1	441
11	519.1778	0.1631	0	499

12	536.2468	1.2653	0	515
13	558.3615	0.1211	0	536
14	629.7273	2.807	1	605
15	731.1001	3.5442	2	702
16	773.8292	7.8453	4	743
17	780.9404	43.3014	25	750
18	845.2782	1.9233	1	812
19	893.3158	0.5985	0	858
20	938.7064	1.1572	0	902
21	946.3088	3.0992	1	909
22	963.0714	0.3986	0	925
23	995.8479	0.0033	0	957
24	1071.672	1.4369	0	1030
25	1123.588	6.6254	3	1080
26	1197.47	0.0583	0	1151
27	1206.372	2.2372	1	1159
28	1232.717	0.7461	0	1185
29	1247.501	3.8062	2	1199
30	1321.593	0.8961	0	1270
31	1353.226	0.5957	0	1300
32	1363.989	1.6797	0	1311
33	1491.905	13.2416	7	1434
34	1498.292	7.3001	4	1440
35	1536.097	18.4337	10	1476
36	1635.973	0.9138	0	1572
37	1658.433	0.5121	0	1594
38	2199.764	170.7312	100	2114
39	2371.396	6.3103	3	2279
40	3069.483	4.045	2	2950
41	3114.99	0.3636	0	2994
42	3193.223	2.721	1	3069
43	3204.963	5.5574	3	3080
44	3217.89	12.7735	7	3093
45	3229.527	4.8734	2	3104

[*] scaling factor = 0.9613, [#] rounded

(2-Isocyanophenyl)acetonitrile *anti* conformation



centre No.	atom type	coordinates [Å]		
		x	y	z
1	C	–0.047028297	–0.002162446	–0.245364474
2	C	–0.067798533	0.010925357	1.163142732
3	C	1.116950847	0.017068554	1.907320589
4	C	2.342611528	0.010167027	1.246934155
5	C	2.379815365	–0.002781335	–0.147510654
6	C	1.193522924	–0.008862495	–0.884068996
7	N	–1.286681547	0.017838259	1.822802055
8	C	–2.338025413	0.023550285	2.363393785
9	C	–1.371233942	–0.008270067	–0.995682915
10	C	–1.231559443	–0.022296203	–2.45329131
11	N	–1.114608846	–0.033386789	–3.607620267
12	H	1.058026826	0.027150224	2.990508946
13	H	3.263704539	0.014906058	1.821778137
14	H	3.332786072	–0.008212381	–0.66808484
15	H	1.230111239	–0.018962612	–1.969123094
16	H	–1.970241621	–0.878875101	–0.696963596
17	H	–1.968884522	0.86880146	–0.713625546

HF = –456.1618161 Hartree

Zero-point correction = 0.125582 Hartree

Sum of electronic and zero-point energies = –456.0362341 Hartree

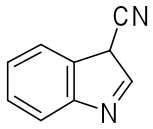
Vibrational frequencies

mode No.	unscaled frequency	absolute intensity	relative intensity[#]	scaled frequency[*#]
1	41.2697	8.2564	5	39
2	112.7296	8.7853	5	108
3	133.6491	4.4076	2	128
4	149.495	1.3556	0	143
5	204.8252	1.6978	1	196
6	298.579	0.8485	0	287
7	348.9041	0.583	0	335
8	372.5131	0.4832	0	358
9	409.9811	2.632	1	394
10	456.6966	4.1556	2	439
11	503.679	0.0034	0	484
12	552.8282	0.8989	0	531

13	555.7205	0.0601	0	534
14	624.0638	0.8228	0	599
15	722.0244	2.6134	1	694
16	776.9716	1.9668	1	746
17	781.2456	47.956	30	751
18	823.4207	3.2966	2	791
19	885.0662	0.8063	0	850
20	949.8906	0.0371	0	913
21	968.3732	2.843	1	930
22	976.1425	3.4835	2	938
23	999.2471	0.3103	0	960
24	1073.476	3.0721	1	1031
25	1116.745	6.1826	3	1073
26	1195.842	0.4175	0	1149
27	1205.986	1.1796	0	1159
28	1243.729	2.8992	1	1195
29	1252.685	0.1152	0	1204
30	1314.441	1.7448	1	1263
31	1331.374	0.4738	0	1279
32	1377.799	6.1453	3	1324
33	1479.118	5.2508	3	1421
34	1500.376	15.3593	9	1442
35	1533.755	20.4559	12	1474
36	1635.047	1.6599	1	1571
37	1659.251	1.093	0	1595
38	2197.708	158.7499	100	2112
39	2375.869	5.9963	3	2283
40	3047.937	1.0148	0	2929
41	3077.097	0.3848	0	2958
42	3200.105	0.8779	0	3076
43	3210.653	5.152	3	3086
44	3219.522	8.6775	5	3094
45	3228.372	5.582	3	3103

- scaling factor = 0.9613, # rounded

3-Cyano-3*H*-indole 21



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.035756	-0.286987	0.313475
C	0.668029	0.911108	-0.059834
C	2.025572	0.947786	-0.358376
C	2.741093	-0.252110	-0.283440
C	2.110919	-1.446852	0.080889
C	0.742735	-1.476821	0.386118
C	-1.414590	0.065581	0.592325
C	-1.387974	1.562520	0.243530
H	2.501184	1.880758	-0.643127
H	3.802671	-0.257103	-0.514176
H	2.688128	-2.365864	0.126492
H	0.258006	-2.409022	0.662741
H	-2.270254	2.194929	0.293771
N	-0.233969	2.010720	-0.088729
H	-1.652888	-0.044293	1.662234
C	-2.407107	-0.693951	-0.171343
N	-3.196523	-1.293727	-0.775272

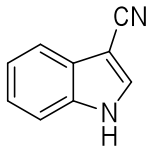
RB3LYP/6-31G(d), HF= -456.0363223
Zero-point correction= 0.127821 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.908501

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	81.6	2.7	14
2	A	104.2	5.2	26
3	A	218.9	1.5	7
4	A	235.7	5.8	29
5	A	364.4	4.3	22
6	A	392.8	0.7	3
7	A	410.3	3.5	17
8	A	486.8	0.6	3
9	A	498.4	1.0	5
10	A	544.1	0.9	4
11	A	581.4	1.3	7
12	A	620.8	0.8	4
13	A	716.0	7.3	36
14	A	728.9	16.3	81
15	A	748.5	14.8	74
16	A	776.9	18.6	93
17	A	832.2	4.6	23
18	A	844.9	0.7	3
19	A	886.6	6.9	34
20	A	915.2	1.3	6
21	A	947.7	13.1	66
22	A	952.7	0.0	0
23	A	986.4	1.4	7
24	A	1004.8	2.1	11
25	A	1072.2	0.2	1
26	A	1128.9	1.0	5
27	A	1140.5	10.2	51
28	A	1144.5	3.2	16
29	A	1176.8	1.5	8

30	A	1243.4	0.9	4
31	A	1266.5	1.0	5
32	A	1287.6	2.7	14
33	A	1330.6	0.9	4
34	A	1441.4	15.1	75
35	A	1454.5	5.0	25
36	A	1569.9	19.7	99
37	A	1586.4	13.6	68
38	A	1604.8	3.0	15
39	A	2275.1	15.0	75
40	A	2906.8	0.8	4
41	A	3068.6	0.3	1
42	A	3077.6	9.0	45
43	A	3088.9	18.3	91
44	A	3091.1	4.2	21
45	A	3099.3	9.0	45

3-Cyanoindole 22



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.274596	0.000000
C	-0.722085	-0.944711	0.000000
C	-2.119791	-0.984250	0.000000
C	-2.790384	0.232954	0.000000
C	-2.088527	1.456315	0.000000
C	-0.700319	1.490370	0.000000
H	-2.660555	-1.926719	0.000000
H	-3.876601	0.241562	0.000000
H	-2.647227	2.387848	0.000000
H	-0.162199	2.433811	0.000000
C	1.403573	-0.078324	0.000000
N	0.206679	-1.974424	0.000000
C	1.474506	-1.457709	0.000000
H	-0.013876	-2.958668	0.000000
H	2.344461	-2.098433	0.000000
C	2.506267	0.812566	0.000000
N	3.398544	1.561531	0.000000

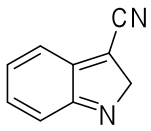
RB3LYP/6-31G(d), HF= -456.0650926
Zero-point correction= 0.128989 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.936104

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	112.4	0.9	1
2	A'	116.1	4.3	5
3	A"	214.0	9.6	11
4	A"	258.0	1.8	2
5	A'	365.8	3.5	4
6	A"	409.6	45.5	54
7	A"	426.2	28.7	34
8	A'	475.0	1.4	2

9	A"	502.7	29.0	34
10	A'	517.0	0.2	0
11	A"	565.6	10.5	13
12	A'	590.4	0.5	1
13	A"	618.7	0.0	0
14	A'	665.0	0.1	0
15	A"	730.9	62.8	75
16	A"	749.1	2.2	3
17	A'	754.1	5.0	6
18	A"	788.6	5.4	6
19	A"	832.0	0.3	0
20	A'	855.9	0.5	1
21	A"	899.2	1.1	1
22	A"	941.6	0.0	0
23	A'	1002.5	3.7	4
24	A'	1035.8	7.0	8
25	A'	1084.1	26.1	31
26	A'	1117.7	5.2	6
27	A'	1141.9	0.7	1
28	A'	1211.6	5.2	6
29	A'	1225.9	30.1	36
30	A'	1288.3	5.4	6
31	A'	1312.7	4.3	5
32	A'	1335.0	15.9	19
33	A'	1403.4	45.1	54
34	A'	1444.1	18.6	22
35	A'	1483.1	3.3	4
36	A'	1521.5	35.6	42
37	A'	1572.4	1.4	2
38	A'	1613.3	2.7	3
39	A'	2252.5	79.7	95
40	A'	3065.3	0.3	0
41	A'	3073.4	9.2	11
42	A'	3083.5	19.9	24
43	A'	3091.8	16.1	19
44	A'	3159.3	0.5	1
45	A'	3521.2	83.9	100

3-Cyano-2*H*-indole



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.045800	-0.278988	0.000769
C	0.786850	0.942395	-0.000435
C	2.225240	0.808626	-0.000938
C	2.756500	-0.442943	-0.000778
C	1.929143	-1.635515	0.000303
C	0.568076	-1.574252	0.001212
C	-1.345769	0.157958	0.000946
C	-1.294445	1.668113	0.000704
H	2.838808	1.703507	-0.001676
H	3.835282	-0.573076	-0.001489
H	2.425896	-2.601711	0.000293
H	-0.043911	-2.471221	0.002009

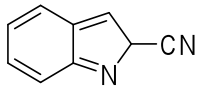
H	-1.798828	2.098792	-0.876984
N	0.103853	2.053809	-0.000201
H	-1.798054	2.098602	0.879039
C	-2.522954	-0.621891	0.001596
N	-3.503886	-1.253224	-0.002866

RB3LYP/6-31G(d), HF= -456.0209629
Zero-point correction= 0.127268 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.893695

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	106.8	3.1	6
2	A	115.6	5.0	10
3	A	184.4	2.8	6
4	A	236.0	8.1	16
5	A	324.8	8.9	18
6	A	366.7	8.7	17
7	A	448.5	5.6	11
8	A	469.4	0.8	2
9	A	494.6	0.3	1
10	A	510.2	4.6	9
11	A	539.2	0.1	0
12	A	572.8	0.9	2
13	A	619.7	6.7	13
14	A	717.4	8.8	18
15	A	745.2	36.6	73
16	A	752.7	22.6	45
17	A	839.3	0.3	1
18	A	852.2	9.0	18
19	A	868.8	0.1	0
20	A	945.2	0.1	0
21	A	950.6	1.2	2
22	A	972.1	0.0	0
23	A	992.0	6.1	12
24	A	1009.7	17.0	34
25	A	1096.9	1.5	3
26	A	1105.8	0.3	1
27	A	1133.5	11.9	24
28	A	1157.8	4.4	9
29	A	1176.8	4.1	8
30	A	1262.3	1.4	3
31	A	1331.0	8.1	16
32	A	1365.6	21.6	43
33	A	1372.7	1.8	4
34	A	1409.7	2.5	5
35	A	1490.6	8.3	17
36	A	1523.9	17.3	35
37	A	1564.3	3.5	7
38	A	1630.6	1.2	2
39	A	2230.4	50.2	100
40	A	2923.2	0.0	0
41	A	2949.0	0.7	1
42	A	3069.9	6.3	13
43	A	3080.0	6.1	12
44	A	3092.6	12.4	25
45	A	3102.0	10.2	20

2-Cyano-2*H*-indole



Atom Type	Coordinates (Angstroms) X	Y	Z
N	3.807921	-0.052953	-0.924875
C	2.868608	-0.049145	-0.243913
C	1.682491	-0.007640	0.624089
C	-0.361248	-0.700338	0.189879
C	-0.427799	0.782484	0.157776
C	0.829123	1.223955	0.405092
H	2.032919	-0.028760	1.670185
H	1.197038	2.241060	0.458649
N	0.823973	-1.184553	0.431019
C	-1.569049	-1.461692	-0.037657
H	-1.522710	-2.545399	-0.014741
C	-2.721660	-0.784247	-0.278994
H	-3.642186	-1.333531	-0.457776
C	-2.783293	0.668601	-0.310680
H	-3.744290	1.134334	-0.509604
C	-1.684627	1.439785	-0.099792
H	-1.739305	2.524241	-0.124527

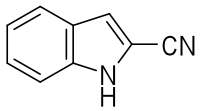
RB3LYP/6-31G(d), HF= -456.0038907
Zero-point correction= 0.127128 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.876763

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	67.7	1.6	5
2	A	122.4	2.3	7
3	A	207.0	1.2	4
4	A	236.4	2.4	8
5	A	356.0	8.9	28
6	A	376.1	9.2	29
7	A	439.8	3.0	9
8	A	461.4	3.3	10
9	A	484.0	1.0	3
10	A	544.7	1.9	6
11	A	565.2	2.9	9
12	A	579.5	0.7	2
13	A	693.1	6.5	20
14	A	732.5	7.3	23
15	A	750.3	15.6	49
16	A	781.8	32.3	101
17	A	812.9	20.4	64
18	A	838.7	0.2	1
19	A	859.9	14.7	46
20	A	877.9	2.9	9
21	A	942.7	0.2	1
22	A	945.5	0.8	3
23	A	972.1	0.0	0
24	A	995.0	4.6	14
25	A	1009.7	12.8	40
26	A	1103.1	8.5	27
27	A	1141.8	1.7	5
28	A	1143.9	0.2	1
29	A	1160.8	1.8	5

30	A	1202.9	3.8	12
31	A	1244.7	7.9	25
32	A	1327.7	5.9	18
33	A	1364.9	0.6	2
34	A	1404.5	4.2	13
35	A	1505.7	24.6	77
36	A	1527.1	18.5	58
37	A	1578.0	3.5	11
38	A	1643.6	16.5	52
39	A	2281.0	10.7	34
40	A	2891.7	2.6	8
41	A	3068.3	3.5	11
42	A	3077.1	8.0	25
43	A	3090.5	20.7	65
44	A	3102.7	8.2	26
45	A	3130.6	0.4	1

2-Cyanoindole



Atom Type	Coordinates (Angstroms) X	Y	Z
N	3.512103	-2.364622	0.000000
C	2.510140	-1.770470	0.000000
C	1.297547	-1.036683	0.000000
C	0.000000	0.804080	0.000000
C	-0.850483	-0.339536	0.000000
C	-0.005936	-1.491110	0.000000
H	2.129702	0.926327	0.000000
H	-0.304306	-2.529849	0.000000
N	1.299038	0.354204	0.000000
C	-0.505715	2.110944	0.000000
H	0.155129	2.973267	0.000000
C	-1.884835	2.259421	0.000000
H	-2.311248	3.258582	0.000000
C	-2.748349	1.139870	0.000000
H	-3.822599	1.300516	0.000000
C	-2.247164	-0.151238	0.000000
H	-2.915892	-1.007583	0.000000

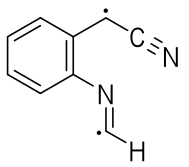
State= 1-A'
RB3LYP/6-31G(d), HF= -456.0611764
Zero-point correction= 0.128554 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.932622

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	89.8	0.8	1
2	A'	130.9	5.6	5
3	A"	230.9	5.2	5
4	A"	246.8	5.0	5
5	A"	366.9	87.9	82
6	A'	369.7	5.4	5
7	A"	414.6	1.3	1
8	A'	433.2	0.4	0

9	A"	483.7	0.7	1
10	A"	555.1	0.8	1
11	A'	562.2	0.8	1
12	A'	592.9	3.8	4
13	A'	612.4	3.9	4
14	A"	633.5	19.1	18
15	A"	725.7	27.7	26
16	A"	738.8	16.2	15
17	A'	794.0	0.1	0
18	A"	795.6	34.5	32
19	A"	831.4	3.5	3
20	A'	871.8	0.7	1
21	A"	899.6	1.5	1
22	A"	939.9	0.0	0
23	A'	960.5	2.2	2
24	A'	1001.7	1.2	1
25	A'	1106.2	1.5	1
26	A'	1120.0	27.7	26
27	A'	1143.4	3.6	3
28	A'	1198.0	9.0	8
29	A'	1215.6	11.0	10
30	A'	1281.8	14.5	14
31	A'	1320.2	2.9	3
32	A'	1341.2	36.1	34
33	A'	1393.8	13.2	12
34	A'	1427.3	5.3	5
35	A'	1487.8	1.1	1
36	A'	1515.1	12.2	11
37	A'	1570.0	0.6	1
38	A'	1611.5	6.4	6
39	A'	2251.1	107.2	100
40	A'	3064.8	0.3	0
41	A'	3071.6	2.0	2
42	A'	3080.8	27.7	26
43	A'	3090.3	23.3	22
44	A'	3150.3	0.5	1
45	A'	3522.7	78.7	74

Diradical 23T (Triplet, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.990858	-1.954799	0.000000
C	-1.827159	-1.813021	0.000000
C	-0.425283	-1.797367	0.000000
C	0.000000	0.688347	0.000000
C	-2.012154	1.987643	0.000000
H	0.039586	-2.780356	0.000000
H	-3.108087	2.038821	0.000000
C	0.443157	-0.670735	0.000000
N	-1.380286	0.919051	0.000000
C	0.933133	1.731959	0.000000
H	0.560327	2.751536	0.000000

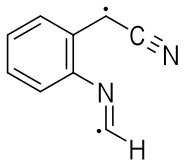
C	2.298626	1.466502	0.000000
H	3.009029	2.288132	0.000000
C	2.755362	0.137484	0.000000
H	3.821005	-0.072060	0.000000
C	1.847173	-0.904649	0.000000
H	2.199009	-1.932814	0.000000

State= 3-A"
<S2>= 2.043259
UB3LYP/6-31G(d), HF= -455.9370907
Zero-point correction= 0.122018 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.815073

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	52.8	0.1	0
2	A"	62.6	2.9	5
3	A'	120.6	4.2	7
4	A"	179.3	0.7	1
5	A'	211.4	1.1	2
6	A"	245.6	7.7	12
7	A'	304.8	10.8	17
8	A'	400.2	8.3	13
9	A"	417.9	5.9	9
10	A"	455.2	5.9	9
11	A'	484.7	12.7	20
12	A"	496.1	1.1	2
13	A'	535.0	16.2	25
14	A'	622.4	3.1	5
15	A"	627.7	2.9	4
16	A"	681.1	4.7	7
17	A'	723.4	4.7	7
18	A"	744.6	12.0	19
19	A"	753.2	64.4	101
20	A'	842.0	0.1	0
21	A"	851.7	0.0	0
22	A"	924.3	2.7	4
23	A"	948.6	0.2	0
24	A'	1006.7	2.5	4
25	A'	1041.3	3.1	5
26	A'	1060.5	20.1	31
27	A'	1095.1	17.7	28
28	A'	1142.7	2.2	3
29	A'	1165.5	3.7	6
30	A'	1206.1	6.2	10
31	A'	1246.6	2.1	3
32	A'	1308.4	6.5	10
33	A'	1370.3	2.6	4
34	A'	1428.8	0.7	1
35	A'	1449.1	25.7	40
36	A'	1526.0	9.7	15
37	A'	1561.2	9.4	15
38	A'	1726.6	35.1	55
39	A'	2127.8	1.6	3
40	A'	2947.6	22.1	35
41	A'	3062.8	0.3	1
42	A'	3068.1	2.1	3
43	A'	3076.7	8.1	13
44	A'	3088.2	13.3	21
45	A'	3095.8	13.0	20

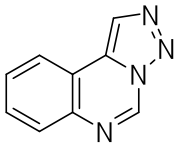
Diradical 23S (Open-Shell Singlet, ^{1}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-2.986052	-1.965997	0.000000
C	-1.822823	-1.820701	0.000000
C	-0.421431	-1.798675	0.000000
C	0.000000	0.689173	0.000000
C	-2.019661	1.982718	0.000000
H	0.047166	-2.779882	0.000000
H	-3.116547	2.025213	0.000000
C	0.445260	-0.667787	0.000000
N	-1.382663	0.918644	0.000000
C	0.928980	1.734022	0.000000
H	0.553209	2.752545	0.000000
C	2.296747	1.472079	0.000000
H	3.004738	2.295774	0.000000
C	2.755842	0.145705	0.000000
H	3.821812	-0.062100	0.000000
C	1.848457	-0.898832	0.000000
H	2.202402	-1.926286	0.000000

State= 1-A"
<S2>= 1.030571
UB3LYP/6-31G(d), HF= -455.9359598
Zero-point correction= 0.121610 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.814350
Ziegler-Cramer corrected energy= -455.813627
Negative frequency= -188.3cm^{-1} (out-of-plane N=C-H vibration)

[1,2,3]Triazolo[1,5-*c*]quinazoline 26



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.872088	2.945621	0.000000
C	-2.185289	2.442917	0.000000
C	-2.411059	1.075530	0.000000
C	-1.328518	0.176893	0.000000
C	0.000000	0.689112	0.000000
C	0.210523	2.079609	0.000000
N	-1.610001	-1.188779	0.000000
C	-0.629544	-2.021583	0.000000
N	0.690046	-1.610381	0.000000
C	1.059665	-0.282626	0.000000
C	2.443783	-0.345439	0.000000

N	2.825212	-1.652579	0.000000
N	1.781093	-2.433238	0.000000
H	-0.703725	4.018645	0.000000
H	-3.026065	3.130568	0.000000
H	-3.414618	0.662584	0.000000
H	1.225094	2.467681	0.000000
H	-0.781692	-3.096707	0.000000
H	3.171711	0.451870	0.000000

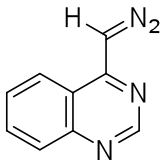
RB3LYP/6-31G(d), HF= -565.5451254
Zero-point correction= 0.141096 (Hartree/Particle)
Sum of electronic and zero-point Energies= -565.404030

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	107.3	0.9	2
2	A"	136.0	0.0	0
3	A"	231.6	0.1	0
4	A'	243.5	0.5	1
5	A"	294.3	6.7	11
6	A'	420.1	2.7	5
7	A"	422.7	8.2	14
8	A'	458.9	3.8	6
9	A"	500.1	0.3	1
10	A'	513.4	2.9	5
11	A"	581.0	1.0	2
12	A'	613.6	2.1	4
13	A'	667.0	2.6	4
14	A"	669.9	0.0	0
15	A"	670.6	0.3	1
16	A"	750.0	33.4	57
17	A"	757.2	18.1	31
18	A'	769.1	1.3	2
19	A"	780.7	21.5	36
20	A"	854.9	0.0	0
21	A'	864.9	23.5	40
22	A"	890.0	6.6	11
23	A"	926.4	2.6	4
24	A'	939.4	23.5	40
25	A"	959.5	0.1	0
26	A'	992.7	3.1	5
27	A'	1019.7	4.6	8
28	A'	1072.2	7.3	12
29	A'	1102.2	0.8	1
30	A'	1124.2	0.8	1
31	A'	1145.9	0.8	1
32	A'	1179.9	0.7	1
33	A'	1209.3	12.2	21
34	A'	1246.6	42.2	71
35	A'	1281.6	15.4	26
36	A'	1299.0	2.1	4
37	A'	1318.5	1.3	2
38	A'	1354.7	6.2	10
39	A'	1373.2	59.0	100
40	A'	1449.6	4.1	7
41	A'	1464.6	37.4	63
42	A'	1508.0	4.3	7
43	A'	1548.3	4.7	8
44	A'	1603.8	12.2	21
45	A'	1609.8	41.1	70

46	A'	3070.1	0.1	0
47	A'	3079.2	8.0	14
48	A'	3090.4	17.1	29
49	A'	3100.8	9.9	17
50	A'	3104.2	0.9	2
51	A'	3166.3	0.9	1

(*s*-*Z*)-4-(Diazomethyl)quinazoline 27Z



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.130933	2.994289	0.000000
C	-1.281763	3.072629	0.000000
C	-2.045596	1.926622	0.000000
C	-1.425244	0.651145	0.000000
C	0.000000	0.571672	0.000000
C	0.759970	1.767405	0.000000
N	-2.215211	-0.464780	0.000000
C	-1.579006	-1.616524	0.000000
N	-0.244451	-1.833673	0.000000
C	0.544023	-0.760110	0.000000
C	1.972159	-0.986364	0.000000
N	2.421991	-2.216515	0.000000
N	2.800132	-3.289026	0.000000
H	0.721362	3.906132	0.000000
H	-1.763217	4.046816	0.000000
H	-3.130495	1.957349	0.000000
H	1.845086	1.726383	0.000000
H	-2.193204	-2.515737	0.000000
H	2.730382	-0.217571	0.000000

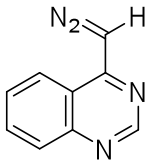
RB3LYP/6-31G(d), HF= -565.5290107
Zero-point correction= 0.138360 (Hartree/Particle)
Sum of electronic and zero-point Energies= -565.390651

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	65.6	0.0	0
2	A"	103.8	1.2	0
3	A'	114.3	0.4	0
4	A"	173.8	0.0	0
5	A'	239.5	1.5	0
6	A"	250.8	1.5	0
7	A'	397.8	0.4	0
8	A"	419.9	5.1	1
9	A'	438.7	1.5	0
10	A"	453.9	27.7	3
11	A"	462.4	5.8	1
12	A'	495.8	0.8	0
13	A"	525.5	1.9	0
14	A'	531.1	1.9	0
15	A"	583.4	3.5	0

16	A'	642.9	20.3	2
17	A"	663.6	20.7	3
18	A"	746.6	46.8	6
19	A'	773.3	4.3	1
20	A"	786.3	2.8	0
21	A'	804.4	7.3	1
22	A"	851.7	4.8	1
23	A'	879.5	18.1	2
24	A"	916.9	0.5	0
25	A"	948.4	2.3	0
26	A"	963.3	0.5	0
27	A'	998.0	8.5	1
28	A'	1014.7	1.5	0
29	A'	1105.8	5.2	1
30	A'	1139.4	1.7	0
31	A'	1162.3	10.2	1
32	A'	1186.5	9.4	1
33	A'	1225.7	3.0	0
34	A'	1259.4	6.1	1
35	A'	1268.0	12.4	2
36	A'	1330.4	83.9	10
37	A'	1336.6	7.4	1
38	A'	1393.3	7.7	1
39	A'	1423.0	342.2	42
40	A'	1442.3	23.0	3
41	A'	1485.4	146.7	18
42	A'	1535.1	72.2	9
43	A'	1551.2	146.5	18
44	A'	1608.0	24.9	3
45	A'	2151.2	819.2	100
46	A'	3058.6	38.9	5
47	A'	3065.5	0.1	0
48	A'	3074.9	14.9	2
49	A'	3087.2	23.2	3
50	A'	3098.4	11.2	1
51	A'	3148.8	2.4	0

(*s*-*E*)-4-(Diazomethyl)quinazoline 27E



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.453157	2.155542	0.000000
C	0.326200	3.009200	0.000000
C	-0.943855	2.479468	0.000000
C	-1.137948	1.074275	0.000000
C	0.000000	0.206254	0.000000
C	1.295102	0.785684	0.000000
N	-2.419587	0.602314	0.000000
C	-2.545759	-0.706726	0.000000
N	-1.565626	-1.635133	0.000000
C	-0.302708	-1.202949	0.000000
C	0.642533	-2.303309	0.000000
N	1.944481	-2.232310	0.000000

N	3.087624	-2.235989	0.000000
H	2.452386	2.581389	0.000000
H	0.468220	4.086455	0.000000
H	-1.830278	3.105476	0.000000
H	2.179744	0.163105	0.000000
H	-3.559672	-1.103646	0.000000
H	0.241029	-3.309586	0.000000

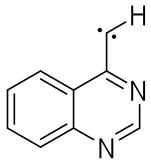
RB3LYP/6-31G(d), HF= -565.5241755
Zero-point correction= 0.138454 (Hartree/Particle)
Sum of electronic and zero-point Energies= -565.385722

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	13.8	1.1	0
2	A	124.2	1.0	0
3	A	136.0	2.0	0
4	A	175.5	0.1	0
5	A	244.4	0.9	0
6	A	268.9	2.4	0
7	A	404.6	5.6	1
8	A	409.9	0.7	0
9	A	438.7	0.1	0
10	A	459.8	3.3	0
11	A	496.8	1.7	0
12	A	508.8	3.2	0
13	A	534.5	11.1	2
14	A	539.1	2.7	0
15	A	595.1	7.1	1
16	A	638.2	35.3	5
17	A	677.1	38.7	6
18	A	702.3	1.7	0
19	A	749.4	38.8	6
20	A	784.2	3.6	1
21	A	801.5	5.2	1
22	A	855.0	6.4	1
23	A	875.6	22.8	3
24	A	922.6	0.1	0
25	A	947.3	3.0	0
26	A	965.9	0.5	0
27	A	1013.2	2.8	0
28	A	1042.7	3.9	1
29	A	1101.5	0.6	0
30	A	1147.6	18.1	3
31	A	1151.1	1.4	0
32	A	1180.1	0.8	0
33	A	1212.5	0.2	0
34	A	1252.8	0.9	0
35	A	1281.7	5.6	1
36	A	1327.6	65.8	10
37	A	1348.8	65.4	10
38	A	1394.9	21.5	3
39	A	1417.3	188.3	28
40	A	1441.9	12.3	2
41	A	1484.1	173.5	26
42	A	1527.7	70.2	10
43	A	1549.5	101.0	15
44	A	1608.5	15.8	2
45	A	2118.5	669.3	100
46	A	3060.3	46.2	7

47	A	3069.7	5.3	1
48	A	3083.8	14.9	2
49	A	3099.8	10.3	2
50	A	3111.1	10.5	2
51	A	3134.4	5.4	1

(*s*-*Z*)-4-Quinazolylcarbene 28Z (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.358380	1.033255	0.000000
C	2.671790	-0.346738	0.000000
C	1.670534	-1.294448	0.000000
C	0.311206	-0.890847	0.000000
C	0.000000	0.499315	0.000000
C	1.041847	1.450663	0.000000
N	-0.667694	-1.845362	0.000000
C	-1.917247	-1.406195	0.000000
N	-2.354541	-0.133369	0.000000
C	-1.406413	0.834808	0.000000
C	-1.868544	2.151612	0.000000
H	3.160336	1.766009	0.000000
H	3.712942	-0.657684	0.000000
H	1.884146	-2.358484	0.000000
H	0.794008	2.508877	0.000000
H	-2.697448	-2.165752	0.000000
H	-2.867650	2.569591	0.000000

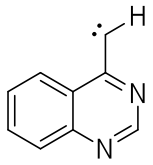
State= 3-A"
<S2>= 2.041779
UB3LYP/6-31G(d), HF= -455.9523295
Zero-point correction= 0.125838 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.826491

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	112.5	0.0	0
2	A"	167.7	0.5	1
3	A"	238.3	0.9	2
4	A'	260.3	3.6	8
5	A"	405.4	6.4	14
6	A'	426.8	1.8	4
7	A"	455.8	3.9	8
8	A'	489.3	1.4	3
9	A'	496.7	0.6	1
10	A"	523.8	7.6	17
11	A'	559.7	13.9	30
12	A"	577.3	4.9	11
13	A"	658.4	23.0	50
14	A'	699.6	3.8	8
15	A"	756.3	46.1	100
16	A"	780.6	3.8	8

17	A'	799.8	3.2	7
18	A"	860.5	1.3	3
19	A'	862.5	11.8	26
20	A'	893.5	31.9	69
21	A"	930.3	0.1	0
22	A"	942.0	3.4	7
23	A"	964.2	0.1	0
24	A'	1005.1	1.7	4
25	A'	1053.4	1.8	4
26	A'	1099.6	4.0	9
27	A'	1136.7	3.8	8
28	A'	1164.8	0.7	1
29	A'	1181.3	12.1	26
30	A'	1251.9	6.4	14
31	A'	1270.8	19.0	41
32	A'	1293.4	3.4	7
33	A'	1373.4	8.2	18
34	A'	1388.8	17.0	37
35	A'	1421.2	12.9	28
36	A'	1459.2	33.9	74
37	A'	1479.1	24.8	54
38	A'	1537.1	18.8	41
39	A'	1600.6	4.0	9
40	A'	3060.2	39.6	86
41	A'	3064.9	0.0	0
42	A'	3073.1	9.7	21
43	A'	3086.7	18.9	41
44	A'	3099.0	10.2	22
45	A'	3137.4	2.2	5

(*s*-*Z*)-4-Quinazolylcarbene 28Z (S_1, ^{1}A)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.341014	1.063336	-0.025452
C	-2.672421	-0.314327	0.031184
C	-1.687673	-1.277605	0.045283
C	-0.323670	-0.888504	0.014559
C	0.004956	0.500240	0.003919
C	-1.022374	1.468120	-0.037836
N	0.647957	-1.844357	-0.040730
C	1.899857	-1.422155	-0.073380
N	2.342143	-0.152787	0.070064
C	1.405797	0.816437	0.064694
C	1.916701	2.144236	-0.105774
H	-3.136218	1.802233	-0.066366
H	-3.718138	-0.608976	0.045788
H	-1.916864	-2.338067	0.068371
H	-0.749719	2.518346	-0.087913
H	2.671798	-2.184295	-0.161459
H	2.837493	2.252099	0.493047

State= 1-A

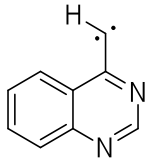
RB3LYP/6-31G(d), HF= -455.9303735
Zero-point correction= 0.125340 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.805033

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	101.6	7.9	8
2	A	164.1	6.2	6
3	A	182.1	8.5	8
4	A	267.6	1.1	1
5	A	351.5	102.6	100
6	A	400.0	12.0	12
7	A	455.5	6.6	6
8	A	466.5	72.2	70
9	A	494.7	1.5	1
10	A	508.4	37.4	36
11	A	541.1	1.0	1
12	A	570.5	33.2	32
13	A	644.3	47.2	46
14	A	707.1	8.8	9
15	A	756.3	48.9	47
16	A	784.0	11.8	11
17	A	802.2	1.8	2
18	A	865.0	3.0	3
19	A	876.8	13.1	13
20	A	930.3	22.1	21
21	A	945.0	2.8	3
22	A	970.6	7.2	7
23	A	977.9	67.5	65
24	A	1000.8	1.5	1
25	A	1053.6	31.0	30
26	A	1097.0	2.0	2
27	A	1143.4	4.3	4
28	A	1162.0	22.8	22
29	A	1200.9	19.8	19
30	A	1259.4	0.9	1
31	A	1272.6	7.0	7
32	A	1305.1	19.3	19
33	A	1378.2	10.8	10
34	A	1391.5	2.9	3
35	A	1426.4	13.8	13
36	A	1467.2	43.3	42
37	A	1495.4	32.9	32
38	A	1540.1	21.1	20
39	A	1602.5	2.8	3
40	A	2922.2	50.9	49
41	A	3067.4	34.2	33
42	A	3069.7	4.0	4
43	A	3079.6	5.8	6
44	A	3090.4	11.5	11
45	A	3100.4	10.0	10

State= 1-A'
RB3LYP/6-31G(d), HF= -455.9286104
Zero-point correction= 0.125159 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.803452
Negative frequency= -305.3 cm^{-1} (out-of-plane C-H vibration)

(*s*-*E*)-4-Quinazolylcarbene 28E (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.387294	0.916812	0.000000
C	2.638075	-0.474867	0.000000
C	1.591527	-1.370927	0.000000
C	0.251748	-0.904345	0.000000
C	0.000000	0.499901	0.000000
C	1.091601	1.395828	0.000000
N	-0.761440	-1.820358	0.000000
C	-1.993210	-1.329961	0.000000
N	-2.380546	-0.044788	0.000000
C	-1.401745	0.894065	0.000000
C	-1.804269	2.227009	0.000000
H	3.220865	1.613451	0.000000
H	3.663296	-0.834516	0.000000
H	1.750473	-2.444505	0.000000
H	0.913055	2.466925	0.000000
H	-2.801745	-2.059347	0.000000
H	-1.318167	3.192921	0.000000

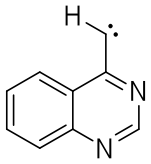
State= 3-A"
<S2>= 2.044258
UB3LYP/6-31G(d), HF= -455.9487298
Zero-point correction= 0.125562 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.823168

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	95.8	0.2	0
2	A"	165.6	0.0	0
3	A"	238.0	0.8	2
4	A'	282.8	1.1	2
5	A"	411.5	3.5	7
6	A'	429.5	6.7	14
7	A"	443.0	15.1	32
8	A'	483.9	2.0	4
9	A"	492.1	5.9	13
10	A'	498.5	2.2	5
11	A"	563.2	4.5	10
12	A'	566.9	5.8	12
13	A"	648.8	12.1	26
14	A'	708.3	4.0	8
15	A"	750.3	47.4	101
16	A"	775.9	4.1	9
17	A'	800.1	3.3	7
18	A'	815.3	13.7	29
19	A"	853.3	2.0	4
20	A'	884.8	15.1	32
21	A"	923.1	0.4	1
22	A"	944.7	2.7	6
23	A"	963.0	0.2	0

24	A'	1008.6	1.7	4
25	A'	1056.1	4.8	10
26	A'	1100.1	2.4	5
27	A'	1140.2	5.6	12
28	A'	1171.9	6.5	14
29	A'	1192.4	6.8	15
30	A'	1245.7	16.6	35
31	A'	1253.0	7.4	16
32	A'	1296.1	6.0	13
33	A'	1359.3	14.3	30
34	A'	1389.0	17.0	36
35	A'	1423.4	11.7	25
36	A'	1459.4	43.2	92
37	A'	1472.7	12.5	27
38	A'	1534.8	13.7	29
39	A'	1599.5	2.6	5
40	A'	3060.1	40.9	87
41	A'	3067.5	0.6	1
42	A'	3077.2	9.8	21
43	A'	3088.4	20.4	43
44	A'	3099.6	9.8	21
45	A'	3148.8	0.6	1

(*s*-*E*)-4-Quinazolylcarbene 28E (S_1, ^{1}A)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.352469	1.019679	0.010473
C	-2.656858	-0.363137	-0.013171
C	-1.651452	-1.305408	-0.020479
C	-0.294030	-0.894596	-0.005741
C	0.008799	0.498067	-0.004872
C	-1.040092	1.445571	0.008043
N	0.690597	-1.841053	0.041796
C	1.932373	-1.398544	0.052950
N	2.358807	-0.119909	-0.070641
C	1.411531	0.829154	-0.045647
C	1.956255	2.154321	-0.090951
H	-3.159238	1.746676	0.027813
H	-3.696275	-0.679351	-0.020156
H	-1.859215	-2.370526	-0.036006
H	-0.811759	2.508908	0.005126
H	2.719795	-2.146607	0.123086
H	1.576518	2.757001	0.758407

State= 1-A
RB3LYP/6-31G(d), HF= -455.9238802
Zero-point correction= 0.124473 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.799407

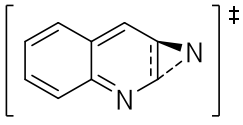
Vibrational frequencies (scaled by 0.9613):

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

1	A	75.0	5.7	4
2	A	153.3	13.0	9
3	A	171.3	1.6	1
4	A	256.3	35.1	24
5	A	288.5	148.9	100
6	A	395.7	39.6	27
7	A	439.0	44.5	30
8	A	455.0	8.0	5
9	A	490.5	4.7	3
10	A	505.0	20.8	14
11	A	537.9	36.8	25
12	A	569.5	4.9	3
13	A	632.7	16.7	11
14	A	706.0	1.0	1
15	A	747.5	47.7	32
16	A	771.3	22.1	15
17	A	797.3	7.8	5
18	A	854.3	6.8	5
19	A	860.3	45.9	31
20	A	923.1	8.8	6
21	A	939.2	68.2	46
22	A	945.0	24.4	16
23	A	966.6	0.3	0
24	A	1005.3	1.7	1
25	A	1030.5	14.7	10
26	A	1098.7	1.6	1
27	A	1143.6	6.9	5
28	A	1167.0	26.4	18
29	A	1217.1	36.1	24
30	A	1251.9	5.8	4
31	A	1276.8	9.5	6
32	A	1299.2	5.3	4
33	A	1356.4	25.8	17
34	A	1390.7	6.6	4
35	A	1433.8	5.5	4
36	A	1475.1	44.1	30
37	A	1495.1	67.8	46
38	A	1543.8	21.2	14
39	A	1603.3	9.0	6
40	A	2869.5	59.5	40
41	A	3057.3	3.0	2
42	A	3067.4	33.8	23
43	A	3073.2	7.8	5
44	A	3087.8	15.9	11
45	A	3099.6	9.3	6

State= 1-A'
RB3LYP/6-31G(d), HF= -455.9195893
Zero-point correction= 0.124787 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.794802
Negative frequency= -456.2 cm^{-1} (out-of-plane C-H vibration)

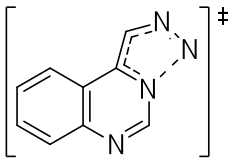
15, TS connecting 7 and 18



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.657347	0.756204	0.061784
C	-2.681081	-0.660639	0.192384
C	-1.513152	-1.384458	0.139234
C	-0.261316	-0.731910	0.003342
C	-0.224930	0.716406	-0.100173
C	-1.471827	1.422480	-0.107514
N	0.850266	-1.481263	-0.228261
C	2.004745	-0.911215	-0.406371
C	2.161263	0.579388	0.016829
C	0.999083	1.372165	-0.216798
H	-3.591008	1.310977	0.087354
H	-3.632352	-1.170823	0.312192
H	-1.511051	-2.468219	0.194858
H	-1.452778	2.505331	-0.197372
H	2.883061	-1.453707	-0.718673
H	1.078285	2.405125	-0.541627
N	3.163052	0.327089	0.709258

RB3LYP/6-31G(d), HF= -455.934249
Zero-point correction= 0.124478 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.809771
Negative frequency= -163.4 cm^{-1}

TS connecting 26 and 27Z

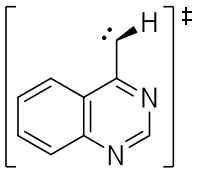


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.438875	2.996720	0.000000
C	-1.827135	2.739398	0.000000
C	-2.301893	1.443329	0.000000
C	-1.401722	0.351601	0.000000
C	0.000000	0.615236	0.000000
C	0.462035	1.949571	0.000000
N	-1.911361	-0.924931	0.000000
C	-1.036595	-1.899576	0.000000
N	0.309418	-1.764520	0.000000
C	0.855844	-0.544306	0.000000
C	2.282955	-0.528470	0.000000
N	2.738321	-1.786598	0.000000
N	2.195286	-2.823362	0.000000
H	-0.079429	4.021658	0.000000
H	-2.525729	3.571652	0.000000
H	-3.364297	1.222348	0.000000
H	1.528777	2.152973	0.000000
H	-1.407466	-2.922071	0.000000
H	2.958812	0.308304	0.000000

State= 1-A'
RB3LYP/6-31G(d), HF= -565.514289
Zero-point correction= 0.138276 (Hartree/Particle)
Sum of electronic and zero-point Energies= -565.376013

Negative frequency= -180.5 cm^{-1}

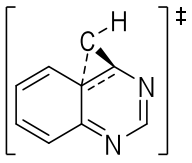
TS connecting 28Z and 28E, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.356503	1.037004	-0.000934
C	-2.664459	-0.344541	0.000870
C	-1.663095	-1.293051	0.000545
C	-0.304598	-0.889947	0.000371
C	-0.000999	0.500134	-0.018439
C	-1.041434	1.455458	-0.016671
N	0.680875	-1.840668	0.047146
C	1.921042	-1.403799	0.039230
N	2.346715	-0.121215	-0.092369
C	1.399081	0.820584	-0.058859
C	2.016380	2.113498	-0.054441
H	-3.160464	1.767199	0.004939
H	-3.705046	-0.657215	0.004318
H	-1.878122	-2.356891	0.001247
H	-0.802697	2.516768	-0.041795
H	2.710642	-2.150195	0.099976
H	1.810057	2.641466	0.897836

State= 1-A
RB3LYP/6-31G(d), HF= -455.9238455
Zero-point correction= 0.124092 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.799754
Negative frequency= -121.3 cm^{-1}

29, TS connecting 28Z and 18, (singlet)

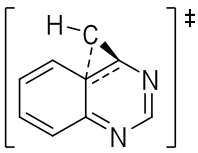


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.430491	0.683002	-0.321325
C	-2.512973	-0.671974	0.083867
C	-1.381081	-1.425949	0.314869
C	-0.094126	-0.843530	0.195434
C	-0.021458	0.586181	-0.060124
C	-1.202757	1.301015	-0.413531
N	1.001493	-1.644164	0.134165
C	2.135831	-1.079800	-0.280932
N	2.428850	0.223086	-0.374156
C	1.419108	1.018461	-0.037623
C	0.972925	2.038579	0.689123

H	-3.335582	1.235697	-0.552413
H	-3.490421	-1.140347	0.166354
H	-1.434447	-2.488739	0.527882
H	-1.107480	2.341095	-0.701305
H	2.942369	-1.760836	-0.545753
H	1.103294	2.124768	1.766611

State= 1-A
RB3LYP/6-31G(d), HF= -455.9140665
Zero-point correction= 0.124747 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.789320
Negative frequency= -212.3cm^{-1}

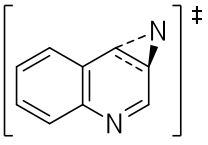
TS connecting 28E and 18, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.428866	0.668665	-0.345306
C	-2.504932	-0.695504	0.014593
C	-1.365723	-1.429929	0.284487
C	-0.088277	-0.821526	0.251729
C	-0.036661	0.598041	0.012039
C	-1.205056	1.306697	-0.362735
N	1.029674	-1.608786	0.238066
C	2.125490	-1.063226	-0.278619
N	2.383522	0.231019	-0.537250
C	1.440896	1.041340	-0.076909
C	1.068695	1.854996	0.883361
H	-3.330368	1.216162	-0.601917
H	-3.474789	-1.185170	0.039251
H	-1.407229	-2.497003	0.478170
H	-1.128340	2.358900	-0.620740
H	2.929755	-1.751228	-0.534553
H	0.485196	2.745389	1.038231

State= 1-A
RB3LYP/6-31G(d), HF= -455.9099904
Zero-point correction= 0.124311 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.785679
Negative frequency= -293.3 cm^{-1}

TS connecting 7S$_1$ and 14, (singlet)

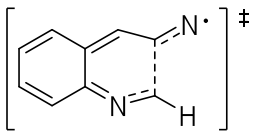


Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.803770	-1.004051	0.772759

C	-2.689339	0.503682	0.221090
C	-1.561668	1.318420	0.166939
C	-0.292903	0.762361	-0.035855
C	-0.160323	-0.658589	-0.163507
C	-1.321888	-1.458722	-0.147846
C	-2.570367	-0.884070	0.047009
C	1.156413	-1.154835	-0.415049
C	2.228089	-0.240820	-0.050073
C	1.993088	1.211931	-0.200762
H	-3.668020	0.946627	0.381921
H	-1.637663	2.396949	0.263071
H	-1.222957	-2.533646	-0.275556
H	-3.456921	-1.511298	0.073215
H	1.371607	-2.156721	-0.755446
H	2.813827	1.914689	-0.341051
N	0.783876	1.653658	-0.183879

State= 1-A
<S2>= 0.216662 (11% triplet contamination, i.e. 89% singlet)
UB3LYP/6-31G(d), HF= -455.9510699
Zero-point correction= 0.125621 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.825448
Negative frequency= -545.7 cm^{-1}

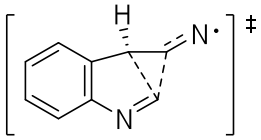
TS connecting $7S_1$ and 19Z, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-3.265960	-0.390532	0.735721
C	-2.237539	-0.620439	0.151871
C	-1.069692	-1.256710	-0.325592
C	0.340102	0.749214	-0.003644
C	-1.909970	1.052919	-0.472782
H	-1.180520	-2.203999	-0.845026
H	-2.863508	1.527500	-0.646812
C	0.205827	-0.672103	-0.129975
N	-0.781099	1.518610	-0.230118
C	1.597918	1.347514	0.171481
H	1.651017	2.428814	0.246940
C	2.735271	0.559998	0.227831
H	3.708535	1.019149	0.371729
C	2.630112	-0.837547	0.072927
H	3.526425	-1.450755	0.104696
C	1.400939	-1.439214	-0.118226
H	1.329655	-2.519042	-0.214082

State= 1-A
<S2>= 0.096554 (5% triplet contamination, i.e. 95% singlet)
UB3LYP/6-31G(d), HF= -455.933115
Zero-point correction= 0.122630 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.810485
Negative frequency= -680.0 cm^{-1}

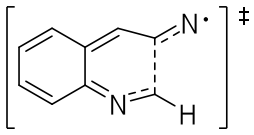
TS connecting $7S_1$ to 21, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-3.360706	-0.517055	0.770688
C	-2.253553	-0.499146	0.239526
C	-1.154222	-1.066871	-0.422457
C	0.419019	0.779878	-0.042865
C	-1.815681	0.995178	-0.409727
H	-1.321166	-1.920026	-1.075924
H	-2.763888	1.486444	-0.633176
C	0.208799	-0.590557	-0.208363
N	-0.718754	1.625950	-0.276921
C	1.696099	1.294269	0.206512
H	1.825117	2.363068	0.322718
C	2.761621	0.428489	0.287792
H	3.756861	0.807927	0.479931
C	1.315414	-1.454817	-0.153025
H	1.171187	-2.519038	-0.288277
C	2.567688	-0.947062	0.099962
H	3.416999	-1.616804	0.154218

State= 1-A
<S2>= 0.249637 (12% triplet contamination, i.e. 88% singlet)
Single-point calculation using the structure from a UHF/6-31G* calculation
UB3LYP/6-31G(d), HF= -455.9226561
Zero-point correction= 0.123545 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.799112
Negative frequency= -988.6 cm^{-1}

TS connecting $7T_0$ and diradical 23T, (triplet)

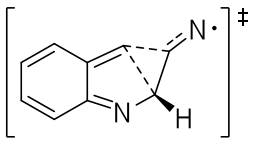


Atom Type	Coordinates (Angstroms) X	Y	Z
N	3.602973	-0.666294	-0.112443
C	2.426430	-0.732920	-0.029055
C	1.118770	-1.245829	0.033953
C	-0.434688	0.789338	-0.017022
C	1.767112	1.617999	0.162535
H	1.105896	-2.334426	0.053318
H	2.536152	2.395045	0.134795
C	-0.158407	-0.619173	0.028403
N	0.549576	1.789141	-0.026523
C	-1.756673	1.241151	-0.061681
H	-1.915658	2.313769	-0.106146
C	-2.830172	0.354800	-0.041470
H	-3.847646	0.732772	-0.071273
C	-2.586085	-1.025183	0.016910

H	-3.413819	-1.728057	0.033545
C	-1.285209	-1.492840	0.047856
H	-1.099240	-2.563093	0.085948

State= 3-A
<S2>= 2.053346
UB3LYP/6-31G(d), HF= -455.9299379
Zero-point correction= 0.121620 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.808318
Negative frequency= -168.9 cm^{-1}

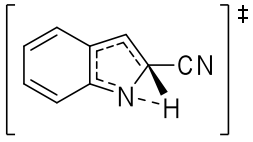
TS connecting 7 and 2-cyano-2*H*-indole, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.895562	-0.868160	1.056197
C	2.304310	-0.159896	0.296910
C	1.882856	1.019665	-0.460263
C	-0.334711	0.821120	-0.056537
C	-0.140952	-0.606227	-0.311156
C	1.148018	-0.974800	-0.634078
H	2.579375	1.360751	-1.224321
H	1.499895	-1.985379	-0.804148
N	0.722280	1.603275	-0.276483
C	-1.621949	1.304518	0.312160
H	-1.739999	2.360490	0.531810
C	-2.678197	0.431915	0.356976
H	-3.664956	0.796716	0.628872
C	-2.516273	-0.957160	0.051388
H	-3.382603	-1.610965	0.092471
C	-1.286314	-1.469005	-0.258884
H	-1.157340	-2.528197	-0.461768

State= 1-A
RB3LYP/6-31G(d), HF= -455.9150255
Zero-point correction= 0.123704 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.791321
Negative frequency= -523.1 cm^{-1}

TS connecting 2-cyano-2*H*-indole and 2-cyanoindole

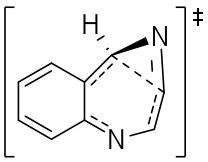


Atom Type	Coordinates (Angstroms) X	Y	Z
N	4.195586	-0.042475	-0.292631
C	3.053736	-0.022664	-0.077339
C	1.649284	0.039824	0.207704
C	-0.440227	-0.678823	0.027450

C	-0.481306	0.761143	0.032436
C	0.839541	1.203607	0.143416
H	1.407829	-0.686792	1.192423
H	1.204532	2.221438	0.179107
N	0.821005	-1.179282	0.069180
C	-1.637084	-1.441131	-0.012483
H	-1.589201	-2.525281	-0.003515
C	-2.828065	-0.761618	-0.093798
H	-3.761110	-1.315085	-0.151356
C	-2.876831	0.667890	-0.103342
H	-3.846419	1.154523	-0.163150
C	-1.736854	1.429867	-0.033556
H	-1.784938	2.514926	-0.032269

RB3LYP/6-31G(d), HF= -455.9665091
Zero-point correction= 0.123283 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.843226
Negative frequency= -1484.3 cm^{-1}

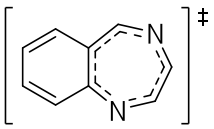
TS connecting 14 and 16



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.430666	0.065074	0.036668
C	1.043484	1.489084	-0.020850
C	-0.101145	0.710070	-0.085741
C	-0.134302	-0.756271	0.099954
N	0.866526	-1.604229	-0.155661
C	2.093842	-1.120143	-0.515168
C	-1.420566	-1.360056	0.338859
C	-2.578277	-0.649928	0.210496
C	-2.545535	0.729382	-0.169848
C	-1.355054	1.373379	-0.340611
H	-1.331781	2.432183	-0.586649
H	-3.478507	1.268267	-0.308993
H	-3.537136	-1.138191	0.360244
H	-1.423472	-2.423503	0.554414
H	1.082583	2.490879	-0.447563
H	2.750725	-1.726222	-1.126660
N	2.181890	1.063235	0.760327

RB3LYP/6-31G(d), HF= -455.9378646
Zero-point correction= 0.125426 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.812439
Negative frequency= -310.3 cm^{-1}

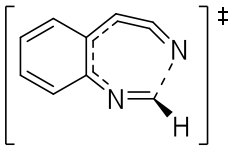
TS connecting 16 and 17



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.575148	-0.734271	-0.179760
C	-1.372089	-1.402037	-0.234240
C	-0.130738	-0.740337	0.000122
C	-0.183218	0.708643	0.157317
C	-1.451450	1.353863	0.221369
C	-2.628047	0.657259	0.073608
N	0.939456	-1.561567	0.131959
C	2.178826	-1.094087	0.392948
C	2.646178	-0.001698	-0.314148
N	2.139758	1.201443	-0.416819
C	0.958249	1.555768	0.059345
H	-1.468443	2.430137	0.377850
H	-3.584536	1.166650	0.135685
H	-3.499970	-1.286726	-0.324730
H	-1.327018	-2.473434	-0.399111
H	2.861595	-1.759088	0.920597
H	0.808491	2.624734	0.224358

RB3LYP/6-31G(d), HF= -455.9286052
Zero-point correction= 0.125646 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.802960
Negative frequency= -455.5 cm^{-1}

TS connecting 18 and 19Z

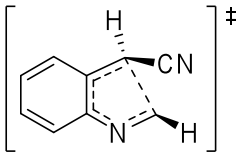


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.672133	-0.665488	0.011063
C	-2.637671	0.737674	0.252979
C	-1.437762	1.398622	0.222143
C	-0.232812	0.676940	-0.010691
C	-0.225708	-0.768960	-0.131405
C	-1.520293	-1.382370	-0.186528
N	0.898211	1.357084	-0.284046
C	2.082800	1.495719	-0.365535
C	2.156517	-1.010868	0.214926
C	0.952677	-1.531517	-0.238714
H	-3.630461	-1.177827	-0.005485
H	-3.559940	1.281494	0.430826
H	-1.378224	2.475577	0.348053
H	-1.563239	-2.456663	-0.345907
H	2.791869	1.870372	-1.090588
N	3.049172	-0.377604	0.665321
H	0.914626	-2.547820	-0.615247

RB3LYP/6-31G(d), HF= -455.945635

Zero-point correction= 0.123256 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.822379
Negative frequency= -197.7 cm^{-1}

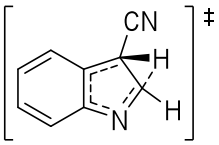
TS connecting 19Z and 21



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-0.719355	1.537054	-0.174277
C	-1.774714	1.413982	-0.758322
C	-2.303247	-0.803921	0.263719
C	-1.126119	-1.195539	-0.405395
C	0.157350	-0.651272	-0.165736
C	0.365796	0.763007	0.034170
H	-2.806038	1.635023	-0.473826
H	-1.181136	-2.150936	-0.921524
N	-3.270665	-0.458272	0.830885
C	1.644874	1.308792	0.293484
H	1.734648	2.377388	0.459426
C	2.741508	0.479533	0.295623
H	3.730912	0.882321	0.488380
C	2.581531	-0.904555	0.023816
C	1.339843	-1.448306	-0.212521
H	1.234936	-2.516006	-0.383038
H	3.455887	-1.549596	0.021301

RB3LYP/6-31G(d), HF= -455.9430951
Zero-point correction= 0.123068 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.820027
Negative frequency= -266.1 cm^{-1}

TS connecting 21 and 3-cyano-2*H*-indole

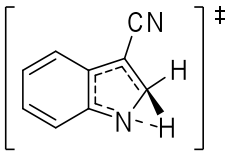


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.005090	-0.279225	0.026038
C	0.779465	0.919763	-0.038114
C	2.193231	0.832444	-0.058327
C	2.767664	-0.419989	-0.038002
C	1.981018	-1.604731	0.020997
C	0.603330	-1.551268	0.067330
C	-1.359359	0.162614	0.057164
C	-1.254156	1.656391	0.024302
H	2.787738	1.739470	-0.096569
H	3.849840	-0.514086	-0.064883
H	2.482004	-2.568423	0.033000

H	0.003338	-2.455116	0.118212
H	-2.093564	2.326431	-0.129487
N	0.029528	2.055428	-0.039530
H	-1.482315	1.046129	1.122931
C	-2.551798	-0.602340	-0.037242
N	-3.525653	-1.234908	-0.121622

RB3LYP/6-31G(d), HF= -455.981822
Zero-point correction= 0.123844 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.857978
Negative frequency= -1259.3cm^{-1}

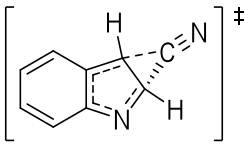
TS connecting 3-cyano-2*H*-indole and 3-cyanoindole 22



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.029589	-0.270122	-0.029295
C	0.792023	0.902444	-0.028611
C	2.202931	0.803869	0.015797
C	2.758126	-0.456027	0.016392
C	1.943405	-1.625554	0.003068
C	0.567485	-1.553577	-0.012199
C	-1.372655	0.186088	-0.015862
C	-1.312931	1.600329	-0.015509
H	2.810335	1.703288	0.026157
H	3.838250	-0.570059	0.028201
H	2.427549	-2.598247	0.008678
H	-0.046002	-2.449467	-0.013227
H	-2.105967	2.294813	-0.270084
N	0.059275	2.055988	-0.078797
H	-0.738843	2.105106	0.989046
C	-2.550552	-0.600387	0.004780
N	-3.512814	-1.257104	0.021634

RB3LYP/6-31G(d), HF= -455.9770703
Zero-point correction= 0.123673 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.853397
Negative frequency= -1510.7 cm^{-1}

TS connecting 2-cyano-2*H*-indole and 3-cyano-3*H*-indole 21

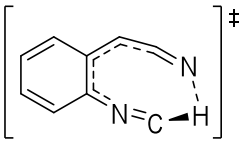


Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.920731	-0.673420	1.358675
C	2.259997	-0.311631	0.458829
C	1.725823	0.691001	-0.710410

C	-0.356816	0.838589	-0.120023
C	-0.185573	-0.558992	-0.431878
C	1.165684	-0.694199	-0.845832
H	2.604167	1.050822	-1.239342
H	1.628927	-1.518955	-1.374158
N	0.766035	1.572452	-0.283684
C	-1.618258	1.306422	0.337290
H	-1.745229	2.355205	0.584708
C	-2.645369	0.398132	0.447768
H	-3.622434	0.732750	0.785963
C	-2.468436	-0.983597	0.139950
H	-3.313561	-1.657295	0.247650
C	-1.250896	-1.473619	-0.280314
H	-1.116172	-2.528388	-0.502031

RB3LYP/6-31G(d), HF= -455.9633002
Zero-point correction= 0.125624 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.837677
Negative frequency= -679.5 cm^{-1}

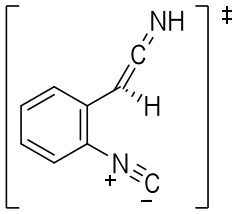
TS connecting 19Z and 20Z



Atom Type	Coordinates (Angstroms) X	Y	Z
H	-2.959659	0.930674	-0.023386
C	-2.031598	1.557573	-0.595983
C	-2.153652	-0.978357	0.239892
C	0.229953	-0.746288	-0.161750
C	1.496113	-1.392243	-0.175885
C	2.664156	-0.691970	0.041357
N	-0.901024	1.365553	-0.283889
C	0.255580	0.685400	-0.041853
C	1.451780	1.388567	0.224333
C	2.646249	0.702851	0.274579
H	1.521696	-2.468396	-0.325184
H	3.612312	-1.222585	0.050428
H	1.408850	2.466242	0.347020
H	3.572642	1.234598	0.467392
C	-0.995160	-1.480899	-0.281755
H	-0.993956	-2.462818	-0.743261
N	-3.033606	-0.329199	0.725230

RB3LYP/6-31G(d), HF= -455.9376329
Zero-point correction= 0.120289 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.817344
Negative frequency= -1108.5 cm^{-1}

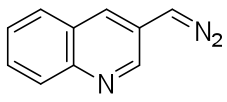
TS connecting 20Z and 20E



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.006762	-0.462404	0.375710
C	-0.567197	0.792022	0.054491
C	-1.910639	0.911547	-0.324966
C	-2.713363	-0.223462	-0.389248
C	-2.177855	-1.474169	-0.076646
C	-0.839234	-1.585286	0.300349
N	0.216119	1.933037	0.108785
C	0.893371	2.899750	0.151011
C	1.415151	-0.590229	0.810213
C	2.412078	-0.731226	-0.039025
N	3.323708	-0.984583	-0.821821
H	-2.303765	1.893591	-0.566070
H	-3.754352	-0.129520	-0.684148
H	-2.799759	-2.363157	-0.128468
H	-0.418172	-2.556690	0.541009
H	1.654623	-0.530908	1.870388
H	3.809344	-0.171754	-1.212795

RB3LYP/6-31G(d), HF= -455.9707658
Zero-point correction= 0.124014 (Hartree/Particle)
Sum of electronic and zero-point Energies= -455.846752
Negative frequency= -76.7 cm^{-1}

3-(Diazomethyl)quinoline 30Z



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.128584	3.379363	0.000000
C	2.386151	2.726326	0.000000
C	2.456025	1.350117	0.000000
C	1.271590	0.571879	0.000000
C	0.000000	1.229113	0.000000
C	-0.039135	2.649234	0.000000
N	1.381371	-0.791211	0.000000
C	0.281103	-1.504345	0.000000
C	-1.044006	-0.960416	0.000000
C	-1.159816	0.420307	0.000000
H	1.088718	4.465301	0.000000
H	3.297098	3.318430	0.000000
H	3.405340	0.823499	0.000000
H	-1.004785	3.149742	0.000000
H	0.412009	-2.586834	0.000000
H	-2.140156	0.892619	0.000000
C	-2.226855	-1.803878	0.000000
H	-3.229570	-1.393941	0.000000

N	-2.160693	-3.104669	0.000000
N	-2.099320	-4.249122	0.000000

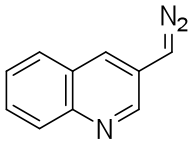
State= 1-A'
RB3LYP/6-31G(d), HF= -549.4832505
Zero-point correction= 0.149932 (Hartree/Particle)
Sum of electronic and zero-point Energies= -549.333319

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	50.1	0.1	0
2	A'	107.5	1.3	0
3	A"	121.6	3.7	0
4	A"	181.8	0.1	0
5	A'	249.9	2.1	0
6	A"	280.8	0.3	0
7	A'	384.6	0.5	0
8	A"	400.8	0.0	0
9	A'	407.6	1.1	0
10	A"	462.9	17.5	2
11	A"	477.1	2.7	0
12	A"	499.9	3.4	0
13	A'	514.4	0.3	0
14	A"	550.2	23.5	2
15	A'	584.6	11.5	1
16	A'	613.6	2.1	0
17	A"	636.6	1.7	0
18	A"	739.2	28.1	3
19	A'	745.0	6.3	1
20	A'	754.7	6.2	1
21	A"	768.6	9.5	1
22	A"	843.1	7.5	1
23	A'	865.8	0.0	0
24	A"	875.9	26.4	3
25	A"	909.4	0.3	0
26	A"	927.4	4.3	0
27	A'	950.9	6.7	1
28	A"	956.7	0.1	0
29	A'	1006.2	3.0	0
30	A'	1107.1	4.8	0
31	A'	1127.6	5.4	1
32	A'	1145.5	4.4	0
33	A'	1177.9	5.1	1
34	A'	1207.4	7.7	1
35	A'	1226.2	2.6	0
36	A'	1254.0	6.4	1
37	A'	1316.5	23.3	2
38	A'	1349.1	9.8	1
39	A'	1364.7	16.1	2
40	A'	1398.0	49.1	5
41	A'	1420.0	4.7	0
42	A'	1461.8	22.6	2
43	A'	1486.2	9.9	1
44	A'	1551.9	7.5	1
45	A'	1589.5	52.4	5
46	A'	1607.8	3.0	0
47	A'	2109.3	1001.6	100
48	A'	3033.2	19.0	2
49	A'	3054.0	4.1	0
50	A'	3056.7	13.9	1

51	A'	3069.2	13.2	1
52	A'	3082.1	27.2	3
53	A'	3095.3	16.9	2
54	A'	3107.8	3.2	0

3-(Diazomethyl)quinoline 30E



Atom Type	Coordinates (Angstroms) X	Y	Z
C	3.115949	-1.172930	0.000000
C	2.556553	-2.475165	0.000000
C	1.189412	-2.645853	0.000000
C	0.326180	-1.521584	0.000000
C	0.888705	-0.204694	0.000000
C	2.302490	-0.061993	0.000000
N	-1.025055	-1.730550	0.000000
C	-1.813639	-0.683915	0.000000
C	-1.368409	0.676929	0.000000
C	0.000000	0.895167	0.000000
H	4.196053	-1.053854	0.000000
H	3.213910	-3.340222	0.000000
H	0.733975	-3.631297	0.000000
H	2.730204	0.937926	0.000000
H	-2.886502	-0.883345	0.000000
H	0.406277	1.904529	0.000000
C	-2.378148	1.722088	0.000000
H	-3.439131	1.504992	0.000000
N	-2.062334	2.984663	0.000000
N	-1.751088	4.087739	0.000000

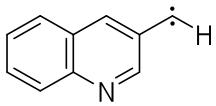
State= 1-A'
RB3LYP/6-31G(d), HF= -549.4839275
Zero-point correction= 0.149945 (Hartree/Particle)
Sum of electronic and zero-point Energies= -549.333982

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	56.2	0.9	0
2	A'	94.8	1.5	0
3	A"	122.5	5.2	1
4	A"	182.9	0.0	0
5	A'	258.8	2.7	0
6	A"	283.4	0.5	0
7	A'	388.3	0.0	0
8	A"	402.5	0.0	0
9	A'	412.8	2.0	0
10	A"	462.5	17.2	2
11	A"	482.9	8.4	1
12	A"	503.8	0.2	0
13	A'	513.6	0.1	0
14	A"	544.5	24.2	3
15	A'	573.6	11.9	1
16	A'	611.9	1.4	0

17	A"	635.2	0.8	0
18	A'	731.7	8.1	1
19	A"	739.4	30.2	3
20	A'	758.3	5.0	1
21	A"	768.7	9.3	1
22	A"	843.6	5.9	1
23	A"	877.9	24.9	3
24	A'	892.3	4.4	0
25	A"	908.3	0.6	0
26	A"	927.9	4.3	0
27	A"	956.8	0.1	0
28	A'	966.0	7.8	1
29	A'	1006.1	3.6	0
30	A'	1106.0	8.1	1
31	A'	1115.5	14.3	2
32	A'	1143.3	2.3	0
33	A'	1181.8	8.4	1
34	A'	1189.7	7.6	1
35	A'	1226.3	1.9	0
36	A'	1248.9	4.4	0
37	A'	1332.3	0.1	0
38	A'	1350.3	15.3	2
39	A'	1356.8	4.7	1
40	A'	1388.5	19.3	2
41	A'	1431.7	73.3	8
42	A'	1455.4	11.4	1
43	A'	1484.8	23.7	3
44	A'	1551.0	3.0	0
45	A'	1589.8	29.0	3
46	A'	1607.7	0.8	0
47	A'	2108.8	878.9	100
48	A'	3022.4	35.8	4
49	A'	3055.9	0.8	0
50	A'	3058.3	10.0	1
51	A'	3069.5	11.0	1
52	A'	3082.3	25.3	3
53	A'	3095.2	17.8	2
54	A'	3111.7	4.7	1

(*s*-*Z*)-3-Quinolylcarbene 31Z (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.203974	1.729282	0.000000
C	-2.806673	0.449472	0.000000
C	-2.024640	-0.690770	0.000000
C	-0.617095	-0.592188	0.000000
C	0.000000	0.701314	0.000000
C	-0.831139	1.854945	0.000000
N	0.123064	-1.753293	0.000000
C	1.422347	-1.665217	0.000000
C	2.175150	-0.416186	0.000000
C	1.408254	0.767208	0.000000
C	3.559550	-0.434143	0.000000
H	-2.829812	2.617547	0.000000

H	-3.889861	0.366013	0.000000
H	-2.462401	-1.684189	0.000000
H	-0.365053	2.837465	0.000000
H	1.979935	-2.601777	0.000000
H	1.907266	1.732429	0.000000
H	4.307800	-1.216748	0.000000

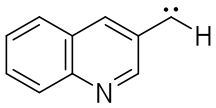
State= 3-A"
<S2>= 2.048562
UB3LYP/6-31G(d), HF= -439.9131727
Zero-point correction= 0.137339 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.775834

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	107.4	0.9	3
2	A"	177.9	0.5	2
3	A'	265.2	1.5	5
4	A"	270.0	0.3	1
5	A"	399.2	1.7	6
6	A'	408.4	4.6	17
7	A'	445.8	0.2	1
8	A"	459.7	5.9	22
9	A"	474.3	20.3	75
10	A"	507.6	6.5	24
11	A'	509.0	0.1	0
12	A'	595.7	9.4	35
13	A"	622.6	0.0	0
14	A'	704.7	4.8	18
15	A"	735.0	27.2	101
16	A'	748.0	0.0	0
17	A"	761.2	12.3	46
18	A"	833.5	14.9	55
19	A'	844.6	24.6	91
20	A"	859.9	12.8	47
21	A'	888.0	6.4	24
22	A"	898.8	2.7	10
23	A"	924.9	4.0	15
24	A'	933.2	11.4	42
25	A"	953.0	0.1	1
26	A'	1006.6	2.7	10
27	A'	1104.7	4.8	18
28	A'	1129.6	2.2	8
29	A'	1172.6	0.6	2
30	A'	1194.0	0.4	1
31	A'	1223.1	1.7	6
32	A'	1267.5	4.7	18
33	A'	1308.6	5.8	21
34	A'	1338.6	7.2	27
35	A'	1365.3	1.0	4
36	A'	1396.8	1.6	6
37	A'	1436.5	0.8	3
38	A'	1468.1	14.0	52
39	A'	1525.7	0.0	0
40	A'	1542.2	19.0	70
41	A'	1592.5	1.8	7
42	A'	3036.9	25.2	93
43	A'	3058.5	2.1	8
44	A'	3070.7	7.6	28
45	A'	3074.6	11.0	41

46	A'	3082.9	25.4	94
47	A'	3095.4	15.5	57
48	A'	3132.4	2.2	8

(*s*-*Z*)-3-Quinolylcarbene 31Z (S_1, ^{1}A')



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.188898	1.740291	0.000000
C	-2.792870	0.458389	0.000000
C	-2.026750	-0.689663	0.000000
C	-0.614674	-0.605270	0.000000
C	0.000000	0.692551	0.000000
C	-0.817765	1.855903	0.000000
N	0.108086	-1.773393	0.000000
C	1.414273	-1.675240	0.000000
C	2.162651	-0.439953	0.000000
C	1.407365	0.739712	0.000000
C	3.595665	-0.321283	0.000000
H	-2.813669	2.628586	0.000000
H	-3.876883	0.382328	0.000000
H	-2.475714	-1.677551	0.000000
H	-0.340109	2.832448	0.000000
H	1.974145	-2.611970	0.000000
H	1.940803	1.687327	0.000000
H	4.000842	-1.360045	0.000000

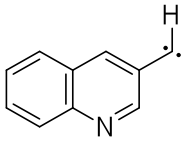
State= 1-A'
RB3LYP/6-31G(d), HF= -439.9013293
Zero-point correction= 0.137764 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.763565

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	99.5	0.4	0
2	A"	169.0	3.2	1
3	A"	234.8	0.7	0
4	A'	278.6	3.0	1
5	A"	326.8	50.1	20
6	A'	423.2	10.5	4
7	A"	430.3	1.6	1
8	A'	450.5	4.3	2
9	A"	480.4	2.0	1
10	A'	512.6	4.4	2
11	A"	518.0	28.4	12
12	A'	600.3	7.2	3
13	A"	629.6	0.5	0
14	A'	701.8	4.4	2
15	A"	745.8	29.6	12
16	A'	750.4	2.4	1
17	A"	774.0	13.5	6
18	A"	860.1	3.8	2
19	A'	875.4	0.4	0
20	A"	923.3	7.1	3

21	A"	939.0	3.9	2
22	A"	953.4	9.1	4
23	A'	967.0	5.6	2
24	A"	970.9	0.2	0
25	A'	1005.4	1.3	1
26	A'	1090.7	14.6	6
27	A'	1111.9	10.4	4
28	A'	1138.8	2.2	1
29	A'	1162.6	87.3	36
30	A'	1205.7	15.8	6
31	A'	1223.2	21.8	9
32	A'	1265.2	79.9	33
33	A'	1332.7	13.7	6
34	A'	1350.0	10.8	4
35	A'	1358.3	22.8	9
36	A'	1393.9	14.9	6
37	A'	1444.5	17.1	7
38	A'	1477.2	38.2	16
39	A'	1543.6	12.7	5
40	A'	1566.6	244.9	100
41	A'	1606.4	80.5	33
42	A'	2796.3	167.3	68
43	A'	3032.1	20.7	8
44	A'	3066.5	0.4	0
45	A'	3074.5	8.4	3
46	A'	3079.6	2.4	1
47	A'	3089.6	19.8	8
48	A'	3101.2	8.9	4

(*s*-*E*)-3-quinolylcarbene 31E (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.20264100	1.71186700	0.00000000
C	-2.80620400	0.43259900	0.00000000
C	-2.02505900	-0.70835600	0.00000000
C	-0.61733900	-0.61223700	0.00000000
C	0.00000000	0.68137100	0.00000000
C	-0.82964000	1.83593200	0.00000000
N	0.12073400	-1.77506900	0.00000000
C	1.42040600	-1.68591100	0.00000000
C	2.17286000	-0.44188900	0.00000000
C	1.40890300	0.74643800	0.00000000
C	3.55736500	-0.46323900	0.00000000
H	-2.82755100	2.60078900	0.00000000
H	-3.88946400	0.34993800	0.00000000
H	-2.46360800	-1.70140600	0.00000000
H	-0.36268000	2.81810500	0.00000000
H	1.98105900	-2.62014800	0.00000000
H	1.90533000	1.71365200	0.00000000
H	4.33986300	0.28509000	0.00000000

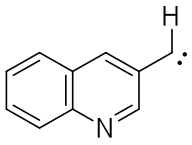
State= 3-A"
<S2>= 2.04875

UB3LYP/6-31G(d), HF= -439.9126477
Zero-point correction= 0.137350 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.775298

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	107.7	1.1	5
2	A"	178.3	0.0	0
3	A'	263.5	2.8	11
4	A"	269.4	0.1	0
5	A"	392.6	0.1	0
6	A'	404.5	2.8	11
7	A'	450.9	0.6	3
8	A"	457.7	8.2	33
9	A"	476.1	11.6	46
10	A'	508.9	0.1	0
11	A"	524.6	12.8	51
12	A'	594.9	5.0	20
13	A"	625.3	0.0	0
14	A'	711.4	2.8	11
15	A"	734.5	24.4	98
16	A'	746.4	0.6	2
17	A"	761.9	12.8	51
18	A'	816.3	19.5	78
19	A"	828.2	24.0	96
20	A"	855.9	8.0	32
21	A'	897.5	6.5	26
22	A"	908.5	1.5	6
23	A"	925.2	4.5	18
24	A'	949.3	8.7	35
25	A"	953.0	0.2	1
26	A'	1007.0	2.1	8
27	A'	1104.5	4.3	17
28	A'	1130.0	1.6	6
29	A'	1173.4	0.3	1
30	A'	1197.3	0.1	0
31	A'	1223.2	1.0	4
32	A'	1267.8	3.0	12
33	A'	1304.0	9.1	36
34	A'	1337.1	6.1	25
35	A'	1360.7	0.2	1
36	A'	1397.4	2.2	9
37	A'	1433.0	0.4	2
38	A'	1467.9	15.4	62
39	A'	1522.6	0.2	1
40	A'	1546.8	16.6	66
41	A'	1592.4	1.7	7
42	A'	3043.5	21.3	85
43	A'	3057.6	1.9	7
44	A'	3066.4	7.9	32
45	A'	3070.7	14.7	59
46	A'	3082.8	25.3	101
47	A'	3095.6	15.2	61
48	A'	3132.4	1.3	5

(*s*-*E*)-3-Quinolylcarbene 31E (S_1, ^{1}A')



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.190947	1.728507	0.000000
C	-2.793284	0.444568	0.000000
C	-2.025967	-0.701534	0.000000
C	-0.612566	-0.616747	0.000000
C	0.000000	0.683811	0.000000
C	-0.821069	1.846218	0.000000
N	0.110066	-1.782059	0.000000
C	1.417816	-1.681866	0.000000
C	2.162892	-0.447551	0.000000
C	1.406404	0.732851	0.000000
C	3.599928	-0.530622	0.000000
H	-2.817510	2.615568	0.000000
H	-3.877215	0.367308	0.000000
H	-2.472993	-1.690195	0.000000
H	-0.345936	2.824171	0.000000
H	1.996719	-2.604374	0.000000
H	1.913782	1.696568	0.000000
H	3.973454	0.519547	0.000000

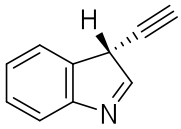
State= 1-A'
RB3LYP/6-31G(d), HF= -439.9000103
Zero-point correction= 0.137605 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.762405

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	86.6	11.7	5
2	A"	157.3	14.4	6
3	A"	204.4	19.4	8
4	A'	279.4	4.3	2
5	A"	325.2	7.7	3
6	A'	424.5	11.3	5
7	A"	426.3	18.8	8
8	A'	450.2	1.4	1
9	A"	479.5	0.8	0
10	A'	512.3	1.8	1
11	A"	514.3	13.4	6
12	A'	599.9	4.4	2
13	A"	628.7	0.9	0
14	A'	709.2	3.8	2
15	A"	742.9	33.8	15
16	A'	749.8	3.8	2
17	A"	774.7	12.0	5
18	A"	858.5	5.8	3
19	A'	875.6	3.8	2
20	A"	915.7	10.3	4
21	A"	942.1	7.9	3
22	A"	955.2	2.3	1
23	A'	965.6	4.7	2
24	A"	971.2	0.3	0
25	A'	1004.5	1.8	1
26	A'	1084.5	20.2	9

27	A'	1112.2	8.8	4
28	A'	1139.8	0.9	0
29	A'	1171.6	81.1	35
30	A'	1207.9	10.7	5
31	A'	1225.8	21.9	9
32	A'	1262.0	100.7	43
33	A'	1337.1	1.8	1
34	A'	1343.3	15.8	7
35	A'	1352.5	36.9	16
36	A'	1398.3	16.3	7
37	A'	1441.3	16.9	7
38	A'	1477.0	43.8	19
39	A'	1541.2	21.2	9
40	A'	1566.0	232.1	100
41	A'	1607.0	77.1	33
42	A'	2796.9	155.0	67
43	A'	3055.0	7.4	3
44	A'	3061.3	8.3	4
45	A'	3064.6	1.9	1
46	A'	3074.0	9.9	4
47	A'	3089.1	20.1	9
48	A'	3102.2	8.3	4

3-Ethynyl-3*H*-indole



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.085914	-1.497235	0.083679
C	2.749534	-0.326161	-0.298300
C	2.068632	0.893127	-0.381971
C	0.712367	0.900919	-0.073342
C	0.045588	-0.272121	0.318848
C	0.719620	-1.480714	0.398333
C	-1.393769	0.122095	0.604504
C	-2.427997	-0.618929	-0.115584
C	-3.290649	-1.225789	-0.702565
N	-0.157129	2.027098	-0.110887
C	-1.319451	1.610244	0.238552
H	2.635728	-2.432920	0.135284
H	3.809063	-0.365283	-0.536150
H	2.570010	1.808281	-0.680947
H	0.206984	-2.394135	0.687938
H	-1.594883	0.053123	1.687441
H	-4.043342	-1.761505	-1.235104
H	-2.182392	2.270135	0.284831

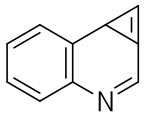
RB3LYP/6-31G(d), HF= -439.9375876
Zero-point correction= 0.138046 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.799542

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	?A	78.9	0.0	0

2	?A	101.0	0.4	1
3	?A	217.0	1.7	2
4	?A	230.2	1.6	2
5	?A	348.8	0.8	1
6	?A	370.5	3.3	5
7	?A	407.6	2.3	3
8	?A	484.2	5.4	8
9	?A	490.2	0.6	1
10	?A	542.5	0.8	1
11	?A	576.1	0.8	1
12	?A	591.9	42.2	59
13	?A	602.1	42.5	60
14	?A	622.0	5.2	7
15	?A	716.0	9.2	13
16	?A	728.9	17.1	24
17	?A	748.0	14.1	20
18	?A	775.1	15.0	21
19	?A	831.9	5.5	8
20	?A	843.6	0.8	1
21	?A	888.7	7.1	10
22	?A	910.8	1.3	2
23	?A	947.2	0.0	0
24	?A	952.7	13.6	19
25	?A	997.4	1.3	2
26	?A	1004.6	2.7	4
27	?A	1073.0	0.3	0
28	?A	1130.1	0.2	0
29	?A	1141.1	0.9	1
30	?A	1148.4	10.7	15
31	?A	1175.2	2.8	4
32	?A	1242.5	4.8	7
33	?A	1265.1	1.2	2
34	?A	1288.2	4.2	6
35	?A	1330.2	0.7	1
36	?A	1441.0	16.2	23
37	?A	1454.0	4.6	7
38	?A	1569.4	22.8	32
39	?A	1585.8	14.1	20
40	?A	1605.0	3.6	5
41	?A	2154.7	4.6	6
42	?A	2878.6	5.6	8
43	?A	3063.8	0.1	0
44	?A	3073.7	11.5	16
45	?A	3082.4	11.4	16
46	?A	3085.0	22.8	32
47	?A	3095.3	13.0	18
48	?A	3359.6	71.2	100

Cyclopropene 32



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.537018	-0.832890	-0.000214
C	2.634189	0.547530	0.219542
C	1.491375	1.335480	0.192528

C	0.224646	0.762445	-0.025437
C	0.121124	-0.650973	-0.192204
C	1.292293	-1.418271	-0.214820
N	-0.845647	1.668895	-0.160495
C	-2.067847	1.250895	-0.182970
C	-2.293999	-0.164775	-0.018322
C	-1.240505	-1.210116	-0.400487
C	-2.229933	-1.226657	0.734933
H	3.432823	-1.448315	-0.000280
H	3.604698	1.004573	0.392194
H	1.543658	2.412010	0.323829
H	1.215619	-2.490486	-0.381162
H	-2.869519	1.971057	-0.340539
H	-1.396914	-1.858121	-1.266447
H	-2.420992	-1.628996	1.720569

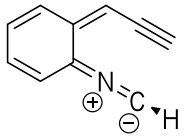
RB3LYP/6-31G(d), HF= -439.912772
Zero-point correction= 0.138995 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.773777

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	?A	128.0	0.4	1
2	?A	141.7	2.0	4
3	?A	268.9	2.3	5
4	?A	318.7	2.7	6
5	?A	363.2	0.6	1
6	?A	418.2	5.1	12
7	?A	474.3	3.1	7
8	?A	487.7	0.3	1
9	?A	518.0	8.1	18
10	?A	578.5	1.5	3
11	?A	587.4	5.4	12
12	?A	657.8	18.9	43
13	?A	703.0	11.2	26
14	?A	720.5	4.6	11
15	?A	742.9	7.0	16
16	?A	757.1	12.6	29
17	?A	775.7	43.7	99
18	?A	838.7	2.8	6
19	?A	856.4	2.4	5
20	?A	871.6	6.7	15
21	?A	921.7	3.9	9
22	?A	934.1	13.9	32
23	?A	952.5	0.1	0
24	?A	973.5	0.8	2
25	?A	1010.2	30.7	70
26	?A	1020.8	5.3	12
27	?A	1074.6	0.3	1
28	?A	1098.2	13.0	30
29	?A	1141.4	0.4	1
30	?A	1163.7	0.6	1
31	?A	1194.9	1.6	4
32	?A	1240.0	0.4	1
33	?A	1281.6	2.4	5
34	?A	1319.5	1.1	3
35	?A	1341.5	4.3	10
36	?A	1436.6	5.7	13
37	?A	1445.1	5.0	11
38	?A	1528.6	8.4	19

39	?A	1555.2	12.7	29
40	?A	1597.8	1.8	4
41	?A	1746.9	30.9	70
42	?A	2978.5	44.2	100
43	?A	3048.2	28.1	64
44	?A	3055.2	3.6	8
45	?A	3067.4	12.7	29
46	?A	3080.0	26.8	61
47	?A	3092.6	15.7	36
48	?A	3142.1	1.0	2

(*Z*)-Ylide 33Z



Atom Type	Coordinates (Angstroms) X	Y	Z
H	2.343948	2.661704	-0.296368
C	1.609194	2.250892	0.403497
C	2.333116	-1.003567	-0.077989
C	-0.167536	-0.760811	0.089433
C	-1.415461	-1.496363	0.149305
C	-2.630013	-0.900279	0.014951
N	0.720484	1.497589	0.079900
C	-0.313437	0.696240	-0.014275
C	-1.617087	1.289478	-0.191810
C	-2.738351	0.521042	-0.176962
H	-1.346340	-2.573579	0.277061
H	-3.534290	-1.501775	0.045152
H	-1.666397	2.368252	-0.303944
H	-3.716821	0.976925	-0.293198
C	1.017629	-1.468144	0.110820
C	3.495167	-0.702948	-0.272034
H	4.509900	-0.421888	-0.437157
H	0.927288	-2.546004	0.239533

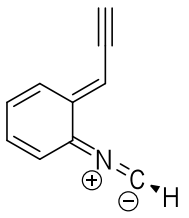
RB3LYP/6-31G(d), HF= -439.8486861
Zero-point correction= 0.133211 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.715475

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	27.0	0.2	0
2	A	129.1	0.3	0
3	A	142.4	1.8	0
4	A	147.0	0.1	0
5	A	209.5	1.4	0
6	A	316.3	1.0	0
7	A	353.7	5.6	1
8	A	374.6	13.8	2
9	A	429.8	30.9	4
10	A	450.5	1.3	0
11	A	469.8	20.5	3
12	A	507.3	5.9	1
13	A	514.3	8.7	1

14	A	523.0	2.2	0
15	A	595.1	33.5	4
16	A	614.2	8.8	1
17	A	668.3	26.4	3
18	A	689.9	0.7	0
19	A	695.8	14.1	2
20	A	731.1	7.3	1
21	A	776.2	31.3	4
22	A	801.2	810.1	100
23	A	819.2	17.2	2
24	A	851.6	9.9	1
25	A	916.8	1.1	0
26	A	943.9	0.4	0
27	A	978.2	6.7	1
28	A	1031.8	0.2	0
29	A	1107.7	10.0	1
30	A	1144.8	0.4	0
31	A	1188.9	2.3	0
32	A	1221.1	0.4	0
33	A	1273.3	2.7	0
34	A	1367.2	9.3	1
35	A	1387.5	3.2	0
36	A	1438.8	0.8	0
37	A	1507.1	27.9	3
38	A	1528.8	5.4	1
39	A	1618.2	15.5	2
40	A	1935.6	390.1	48
41	A	2095.9	13.4	2
42	A	2985.4	29.1	4
43	A	3032.5	5.0	1
44	A	3060.8	0.5	0
45	A	3073.5	9.9	1
46	A	3081.8	21.2	3
47	A	3094.3	21.5	3
48	A	3358.8	84.2	10

(*E*)-Ylide 33E



Atom Type	Coordinates (Angstroms) X	Y	Z
H	1.442697	3.691402	0.652376
C	1.346095	2.965638	-0.165752
C	-2.756847	0.287230	-0.004131
C	-0.314956	-0.064657	0.016521
C	-0.411136	-1.509288	0.015777
C	0.688827	-2.308279	0.003860
N	1.245960	1.772770	0.035699
C	1.051942	0.478996	0.011254
C	2.192383	-0.403328	-0.007286
C	2.016817	-1.751177	-0.012227
H	-1.408665	-1.936711	0.024533

H	0.571354	-3.388460	0.004207
H	3.180712	0.045568	-0.020256
H	2.876787	-2.413872	-0.028432
C	-1.426767	0.750043	0.014876
C	-3.914061	-0.083105	-0.017877
H	-4.928886	-0.408624	-0.031510
H	-1.289508	1.828870	0.019097

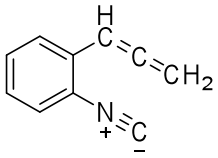
RB3LYP/6-31G(d), HF= -439.852283
Zero-point correction= 0.133443 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.718840

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	88.5	0.4	0
2	A	100.6	0.5	0
3	A	107.2	0.5	0
4	A	145.1	0.2	0
5	A	210.5	1.1	0
6	A	318.8	4.4	0
7	A	340.3	4.3	0
8	A	381.9	6.9	1
9	A	436.0	7.8	1
10	A	456.3	6.2	1
11	A	473.4	9.9	1
12	A	479.1	33.9	3
13	A	505.9	21.9	2
14	A	558.2	8.6	1
15	A	592.4	3.3	0
16	A	607.0	54.7	5
17	A	676.9	37.8	4
18	A	688.6	2.8	0
19	A	745.0	3.1	0
20	A	756.6	28.8	3
21	A	790.4	11.6	1
22	A	815.6	27.8	3
23	A	817.8	36.7	4
24	A	838.9	1013.6	100
25	A	920.5	0.7	0
26	A	953.2	0.1	0
27	A	980.1	5.9	1
28	A	1012.7	11.0	1
29	A	1100.9	8.1	1
30	A	1141.6	0.3	0
31	A	1186.4	1.2	0
32	A	1248.0	1.4	0
33	A	1287.8	0.7	0
34	A	1319.4	13.5	1
35	A	1411.3	1.1	0
36	A	1436.4	1.5	0
37	A	1513.9	22.9	2
38	A	1516.5	7.4	1
39	A	1619.6	15.3	2
40	A	1924.6	541.7	53
41	A	2103.7	10.6	1
42	A	2948.0	67.3	7
43	A	3057.1	5.2	1
44	A	3068.1	10.1	1
45	A	3078.9	4.7	0
46	A	3092.0	11.0	1

47	A	3096.6	18.7	2
48	A	3359.7	108.6	11

(*s*-*Z*)-1-Isocyano-2-(propa-1,2-dienyl)benzene 35Z



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.206749	-0.697053	-0.000059
C	-0.400841	0.704652	-0.000012
C	-1.688859	1.257189	0.000062
C	-2.809955	0.434380	0.000094
C	-2.643740	-0.952063	0.000045
C	-1.364118	-1.497080	-0.000036
N	0.671368	1.578533	-0.000065
C	1.551494	2.366751	-0.000124
C	1.093204	-1.384438	-0.000137
C	2.316232	-0.895229	-0.000066
H	-1.786018	2.337887	0.000091
H	-3.803175	0.873034	0.000154
H	-3.509299	-1.608287	0.000063
H	-1.241372	-2.577068	-0.000078
H	1.012095	-2.473142	-0.000317
C	3.558787	-0.500566	0.000211
H	4.097878	-0.310503	-0.926440
H	4.097586	-0.310909	0.927114

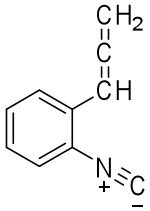
RB3LYP/6-31G(d), HF= -439.9228039
Zero-point correction= 0.135756 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.787048

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	19.9	1.1	1
2	A	125.0	2.2	2
3	A	133.8	1.0	1
4	A	152.7	1.0	1
5	A	195.9	0.1	0
6	A	298.5	0.0	0
7	A	323.9	4.3	3
8	A	340.9	0.1	0
9	A	384.0	0.4	0
10	A	426.4	1.0	1
11	A	490.6	6.1	5
12	A	515.0	1.7	1
13	A	527.1	0.7	1
14	A	588.7	0.4	0
15	A	633.5	9.5	8
16	A	714.2	2.4	2
17	A	732.6	1.1	1
18	A	747.6	47.8	38
19	A	834.7	2.1	2
20	A	844.0	49.4	39

21	A	849.4	3.0	2
22	A	881.2	14.9	12
23	A	918.5	5.3	4
24	A	949.0	0.2	0
25	A	984.4	0.1	0
26	A	1026.9	2.5	2
27	A	1079.4	2.9	2
28	A	1094.1	3.2	3
29	A	1151.0	0.2	0
30	A	1182.1	2.6	2
31	A	1197.8	2.7	2
32	A	1246.4	1.0	1
33	A	1298.1	4.6	4
34	A	1352.5	0.3	0
35	A	1422.5	1.1	1
36	A	1456.6	9.1	7
37	A	1476.1	29.6	23
38	A	1562.0	1.6	1
39	A	1590.2	2.4	2
40	A	1973.7	65.8	52
41	A	2117.6	125.6	100
42	A	3006.3	6.5	5
43	A	3021.4	3.9	3
44	A	3064.3	5.4	4
45	A	3077.3	8.0	6
46	A	3086.8	1.9	2
47	A	3088.6	17.9	14
48	A	3100.3	9.8	8

(*s*-*E*)-1-Isocyano-2-(propa-1,2-dienyl)benzene 35E



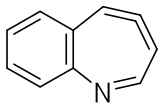
Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.198971	-0.080273	-0.000784
C	-1.063039	0.555858	-0.000071
C	-2.253187	-0.184211	0.000376
C	-2.205923	-1.573174	0.000360
C	-0.966953	-2.223011	-0.000012
C	0.210939	-1.485206	-0.000480
N	-1.143576	1.939637	0.000297
C	-1.216952	3.118963	0.000484
C	1.437633	0.714097	-0.001315
C	2.655606	0.216058	-0.001131
H	-3.198795	0.347741	0.000776
H	-3.128678	-2.145428	0.000831
H	-0.921387	-3.308358	0.000109
H	1.171395	-1.992274	-0.000664
H	1.323403	1.796547	-0.001910
C	3.864189	-0.275878	0.001452
H	4.393956	-0.486273	0.929675
H	4.397436	-0.488758	-0.924169

RB3LYP/6-31G(d), HF= -439.9266779
Zero-point correction= 0.135937 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.790741

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	53.8	0.0	0
2	A	106.2	2.7	2
3	A	125.5	1.9	1
4	A	145.3	1.2	1
5	A	204.0	0.1	0
6	A	300.9	0.3	0
7	A	327.2	4.9	3
8	A	340.9	0.0	0
9	A	389.6	0.9	1
10	A	425.5	1.5	1
11	A	485.2	2.1	1
12	A	525.0	0.5	0
13	A	537.3	1.7	1
14	A	592.0	0.4	0
15	A	616.8	11.7	8
16	A	736.9	0.5	0
17	A	749.1	49.0	32
18	A	756.2	6.3	4
19	A	808.9	0.6	0
20	A	845.8	50.2	33
21	A	857.9	0.4	0
22	A	888.1	16.4	11
23	A	922.5	2.5	2
24	A	953.0	0.1	0
25	A	986.7	0.0	0
26	A	1030.2	2.5	2
27	A	1054.0	6.3	4
28	A	1096.6	2.7	2
29	A	1148.5	0.2	0
30	A	1167.6	2.7	2
31	A	1201.1	1.4	1
32	A	1268.3	3.3	2
33	A	1281.2	3.8	2
34	A	1345.8	1.0	1
35	A	1431.7	4.8	3
36	A	1442.2	4.7	3
37	A	1477.9	28.5	19
38	A	1562.4	0.7	0
39	A	1592.2	2.9	2
40	A	1973.7	75.9	50
41	A	2114.0	151.1	100
42	A	3015.9	6.2	4
43	A	3052.8	4.9	3
44	A	3070.4	1.0	1
45	A	3080.9	2.8	2
46	A	3081.9	4.2	3
47	A	3089.9	16.4	11
48	A	3101.0	9.5	6

Cyclic Allene 36



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.689640	0.521729	0.188380
C	2.529786	-0.872673	0.218140
C	1.278901	-1.432344	0.019274
C	0.126982	-0.631811	-0.163811
C	0.295223	0.790860	-0.165002
C	1.584245	1.334407	-0.010033
N	-1.034788	-1.368183	-0.437527
C	-2.251098	-1.077826	-0.128091
C	-1.977162	1.198010	0.221571
C	-0.890623	1.623045	-0.406130
H	3.675968	0.961872	0.307367
H	3.391955	-1.516229	0.370493
H	1.144626	-2.509360	-0.002505
H	1.697257	2.415325	-0.042420
H	-3.012325	-1.803459	-0.429268
H	-0.868886	2.459507	-1.101843
C	-2.634833	0.129532	0.635696
H	-3.291438	0.072045	1.500894

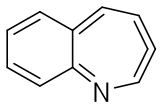
RB3LYP/6-31G(d), HF= -439.9319013
Zero-point correction= 0.139017 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.792885

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	130.9	1.9	3
2	A	138.6	1.9	3
3	A	309.0	0.4	1
4	A	320.0	5.4	9
5	A	343.2	1.4	2
6	A	406.9	7.5	12
7	A	434.8	6.8	11
8	A	448.2	1.6	3
9	A	493.6	16.2	27
10	A	554.5	2.2	4
11	A	574.1	4.8	8
12	A	617.5	16.8	28
13	A	686.5	42.1	69
14	A	707.8	4.2	7
15	A	740.9	4.8	8
16	A	750.3	18.1	30
17	A	770.6	30.2	50
18	A	814.5	19.6	32
19	A	832.6	1.3	2
20	A	859.6	13.0	21
21	A	873.8	21.4	35
22	A	925.9	4.0	7
23	A	954.1	0.1	0
24	A	990.3	8.5	14
25	A	1023.2	3.6	6
26	A	1072.0	4.6	8
27	A	1089.3	1.7	3
28	A	1140.2	2.0	3
29	A	1159.6	0.7	1

30	A	1180.5	2.6	4
31	A	1221.5	8.4	14
32	A	1265.3	13.9	23
33	A	1282.3	3.6	6
34	A	1346.4	13.4	22
35	A	1366.0	8.5	14
36	A	1433.5	6.0	10
37	A	1446.2	10.3	17
38	A	1534.7	1.8	3
39	A	1563.2	13.9	23
40	A	1597.4	1.9	3
41	A	1848.7	16.5	27
42	A	2993.7	60.6	99
43	A	3051.7	10.5	17
44	A	3059.6	2.3	4
45	A	3060.6	19.7	32
46	A	3069.7	13.2	22
47	A	3082.3	25.3	42
48	A	3093.8	14.0	23

Cyclic Allene 37



Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	2.588306	0.698911	0.185916
C	2.586334	-0.672431	-0.224491
C	1.413585	-1.348389	-0.378215
C	0.129911	-0.745719	-0.086387
C	0.128141	0.727090	0.140191
C	1.409192	1.357551	0.364419
N	-0.854547	-1.625410	0.060782
C	-2.072449	-1.162842	0.531092
C	-2.622261	-0.077229	-0.027694
C	-0.958054	1.578265	-0.051209
C	-2.225784	1.108644	-0.521340
H	3.532480	1.216645	0.328074
H	3.532293	-1.179447	-0.394691
H	1.391173	-2.402604	-0.633027
H	1.406679	2.413739	0.622361
H	-2.575779	-1.794329	1.262124
H	-0.767149	2.650618	0.038674
H	-2.799396	1.690142	-1.242682

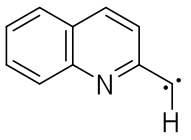
RB3LYP/6-31G(d), HF= -439.9018181
Zero-point correction= 0.138519 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.763300

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	140.1	1.4	3
2	A	144.0	1.0	3
3	A	280.1	0.7	2
4	A	315.1	22.9	59
5	A	325.2	2.4	6

6	A	380.5	8.4	22
7	A	385.5	21.5	55
8	A	406.0	3.5	9
9	A	504.0	14.8	38
10	A	532.2	28.2	72
11	A	557.2	18.4	47
12	A	631.5	5.0	13
13	A	653.7	27.6	71
14	A	706.4	35.0	90
15	A	732.5	21.4	55
16	A	749.1	6.3	16
17	A	791.3	28.6	73
18	A	827.8	9.2	24
19	A	834.9	6.8	17
20	A	880.2	7.0	18
21	A	891.6	20.0	51
22	A	935.1	3.2	8
23	A	962.9	1.3	3
24	A	993.1	0.6	2
25	A	1027.0	2.4	6
26	A	1085.2	9.7	25
27	A	1119.2	9.0	23
28	A	1131.3	12.9	33
29	A	1142.6	2.5	7
30	A	1184.1	6.0	15
31	A	1209.5	6.2	16
32	A	1300.3	19.5	50
33	A	1321.3	31.0	80
34	A	1339.1	11.0	28
35	A	1375.0	2.1	5
36	A	1427.5	2.6	7
37	A	1452.9	23.7	61
38	A	1499.4	19.4	50
39	A	1517.8	6.2	16
40	A	1617.7	8.9	23
41	A	1746.5	3.9	10
42	A	2999.7	25.7	66
43	A	3031.7	39.0	100
44	A	3041.5	36.7	94
45	A	3060.2	2.0	5
46	A	3071.1	15.1	39
47	A	3086.7	22.4	58
48	A	3102.3	8.3	21

(*s*-*Z*)-2-Quinolylcarbene 39Z (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.029612	-0.765490	0.000000
C	-2.809919	0.374352	0.000000
C	-2.203745	1.653789	0.000000
C	-0.832032	1.778417	0.000000
C	0.000000	0.623673	0.000000
C	-0.619653	-0.672184	0.000000

C	2.133120	-0.296613	0.000000
C	1.594780	-1.633932	0.000000
C	0.241428	-1.808936	0.000000
C	3.515931	-0.082592	0.000000
H	-2.491758	-1.750178	0.000000
H	-3.893210	0.291945	0.000000
H	-2.829576	2.542156	0.000000
H	-0.344021	2.747987	0.000000
H	2.279535	-2.476238	0.000000
H	-0.193648	-2.805793	0.000000
H	4.117923	0.817854	0.000000
N	1.344709	0.801338	0.000000

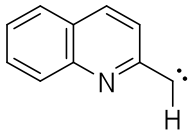
State= 3-A"
<S2>= 2.042906
UB3LYP/6-31G(d), HF= -439.9119507
Zero-point correction= 0.137474 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.774476

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	113.6	0.8	2
2	A"	168.9	2.4	5
3	A'	265.3	2.0	4
4	A"	271.4	2.8	6
5	A"	381.5	0.0	0
6	A'	403.4	7.1	15
7	A'	460.4	1.1	2
8	A"	460.5	6.8	14
9	A"	497.3	6.5	14
10	A'	507.2	0.5	1
11	A"	551.0	13.5	29
12	A'	600.9	4.3	9
13	A"	656.8	4.8	10
14	A'	712.3	0.2	0
15	A"	739.1	21.0	45
16	A'	739.7	3.7	8
17	A"	763.0	7.3	16
18	A"	807.7	47.2	100
19	A'	825.1	17.0	36
20	A"	852.9	1.0	2
21	A'	896.4	0.9	2
22	A"	919.7	1.8	4
23	A"	951.7	1.1	2
24	A"	956.1	0.0	0
25	A'	966.4	3.5	7
26	A'	1006.7	1.5	3
27	A'	1092.7	4.1	9
28	A'	1122.1	1.3	3
29	A'	1134.1	1.6	3
30	A'	1191.5	1.1	2
31	A'	1229.1	3.8	8
32	A'	1271.2	5.4	11
33	A'	1282.6	1.1	2
34	A'	1290.3	7.5	16
35	A'	1345.4	2.0	4
36	A'	1405.1	7.4	16
37	A'	1414.5	0.1	0
38	A'	1486.9	7.1	15
39	A'	1509.9	11.5	24

40	A'	1572.1	9.4	20
41	A'	1596.8	3.4	7
42	A'	3055.9	3.4	7
43	A'	3062.3	9.0	19
44	A'	3068.3	13.8	29
45	A'	3083.4	27.3	58
46	A'	3090.1	13.1	28
47	A'	3096.1	12.6	27
48	A'	3133.4	2.4	5

(*s*-*Z*)-2-Quinolylcarbene 39Z (S_1, ^{1}A)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	1.767594	1.263114	0.002488
C	2.805094	0.357716	-0.013285
C	2.551313	-1.040206	-0.019499
C	1.261626	-1.511096	-0.010402
C	0.160638	-0.603333	0.007256
C	0.422659	0.813717	0.011549
C	-2.137851	-0.266468	0.022073
C	-1.957043	1.153969	-0.007823
C	-0.692817	1.688246	0.018368
C	-3.484191	-0.788887	-0.089537
H	1.965951	2.332036	0.005659
H	3.832089	0.712441	-0.020438
H	3.387214	-1.733774	-0.030978
H	1.033992	-2.572242	-0.012625
H	-2.846416	1.772657	-0.058509
H	-0.530313	2.763525	0.013732
H	-3.408666	-1.863124	0.178117
N	-1.087999	-1.116022	0.056844

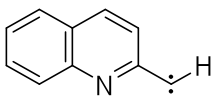
State= 1-A
RB3LYP/6-31G(d), HF= -439.8939875
Zero-point correction= 0.137220 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.756767

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	94.9	25.1	26
2	A	145.0	27.6	29
3	A	203.4	52.2	55
4	A	287.0	50.2	53
5	A	290.2	16.3	17
6	A	412.4	18.3	19
7	A	443.2	62.0	65
8	A	459.2	1.2	1
9	A	477.3	14.0	15
10	A	509.7	1.0	1
11	A	517.6	23.7	25
12	A	606.5	3.1	3
13	A	646.8	4.5	5

14	A	708.3	3.2	3
15	A	742.0	21.6	23
16	A	746.5	14.9	16
17	A	778.5	5.7	6
18	A	829.8	50.2	53
19	A	864.7	6.2	7
20	A	881.3	19.7	21
21	A	932.7	3.4	4
22	A	937.7	2.6	3
23	A	966.5	0.3	0
24	A	969.3	0.1	0
25	A	1001.2	2.0	2
26	A	1076.7	18.0	19
27	A	1098.8	13.2	14
28	A	1123.3	3.2	3
29	A	1139.0	10.8	11
30	A	1190.2	49.1	52
31	A	1227.0	9.6	10
32	A	1259.3	80.2	84
33	A	1294.8	22.2	23
34	A	1310.1	1.6	2
35	A	1360.3	11.8	12
36	A	1412.7	6.7	7
37	A	1423.3	24.8	26
38	A	1487.7	0.6	1
39	A	1517.7	0.5	0
40	A	1565.7	34.8	37
41	A	1606.9	10.4	11
42	A	2858.6	95.5	101
43	A	3062.5	0.2	0
44	A	3066.4	9.8	10
45	A	3074.9	13.3	14
46	A	3086.7	21.1	22
47	A	3100.5	10.5	11
48	A	3106.9	3.6	4

(*s*-*E*)-2-quinolylcarbene 39E (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.037776	-0.734005	0.000000
C	-2.812301	0.409683	0.000000
C	-2.199658	1.686286	0.000000
C	-0.827624	1.804187	0.000000
C	0.000000	0.645415	0.000000
C	-0.627533	-0.646789	0.000000
C	2.131938	-0.276410	0.000000
C	1.583203	-1.616031	0.000000
C	0.229061	-1.785720	0.000000
C	3.518298	-0.099968	0.000000
H	-2.504721	-1.716440	0.000000
H	-3.896005	0.332769	0.000000
H	-2.821287	2.577588	0.000000
H	-0.334371	2.771045	0.000000
H	2.257942	-2.466821	0.000000

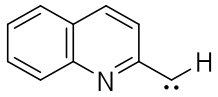
H	-0.208037	-2.781905	0.000000
H	4.358731	-0.783443	0.000000
N	1.343157	0.821045	0.000000

State= 3-A"
<S2>= 2.044151
UB3LYP/6-31G(d), HF= -439.9099998
Zero-point correction= 0.137283 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.772717

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	112.2	0.7	1
2	A"	168.0	4.8	9
3	A'	269.0	4.1	8
4	A"	270.0	1.8	3
5	A"	384.6	1.2	2
6	A'	414.6	0.1	0
7	A'	452.2	0.5	1
8	A"	462.5	0.3	1
9	A"	491.1	16.0	30
10	A'	507.3	0.1	0
11	A"	521.5	5.0	9
12	A'	600.8	5.9	11
13	A"	647.6	1.2	2
14	A'	707.9	0.2	0
15	A"	737.1	17.5	33
16	A'	740.9	0.7	1
17	A"	763.2	9.1	17
18	A"	800.6	53.1	100
19	A'	846.8	16.6	31
20	A"	852.8	0.6	1
21	A'	895.2	8.1	15
22	A"	919.7	1.5	3
23	A'	932.2	2.3	4
24	A"	946.4	1.4	3
25	A"	956.8	0.0	0
26	A'	1006.0	2.3	4
27	A'	1100.0	3.5	7
28	A'	1126.0	0.7	1
29	A'	1134.3	1.8	3
30	A'	1194.1	1.7	3
31	A'	1228.1	6.1	11
32	A'	1257.8	7.0	13
33	A'	1291.7	3.5	7
34	A'	1296.2	3.7	7
35	A'	1347.0	2.1	4
36	A'	1398.2	6.1	12
37	A'	1416.2	0.4	1
38	A'	1480.7	4.7	9
39	A'	1509.4	11.9	22
40	A'	1569.0	7.1	13
41	A'	1596.8	3.2	6
42	A'	3055.5	2.0	4
43	A'	3059.0	9.7	18
44	A'	3068.4	13.2	25
45	A'	3083.4	28.3	53
46	A'	3084.2	15.4	29
47	A'	3096.9	12.1	23
48	A'	3128.3	2.3	4

(*s*-*E*)-2-quinolylcarbene 39E (S_1, ^1A)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.754088	1.279962	-0.018511
C	-2.806358	0.391183	-0.002497
C	-2.574649	-1.010155	0.018528
C	-1.292574	-1.502053	0.023155
C	-0.176556	-0.612284	0.006441
C	-0.417736	0.807708	-0.011975
C	2.128223	-0.324103	0.004460
C	1.967445	1.104104	0.031738
C	0.713813	1.660928	-0.012729
C	3.421590	-0.972022	-0.067031
H	-1.935095	2.351928	-0.033503
H	-3.827591	0.762231	-0.006560
H	-3.421553	-1.690266	0.029282
H	-1.080921	-2.566338	0.034389
H	2.852936	1.730783	0.083370
H	0.572622	2.739517	-0.011487
H	4.162225	-0.226332	0.303491
N	1.060389	-1.148732	-0.032637

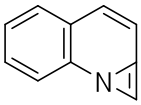
State= 1-A
RB3LYP/6-31G(d), HF= -439.8889404
Zero-point correction= 0.136970 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.751970

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	104.5	3.5	2
2	A	152.2	39.8	23
3	A	236.1	6.7	4
4	A	251.0	126.3	73
5	A	302.4	53.8	31
6	A	413.5	42.4	25
7	A	435.6	10.3	6
8	A	459.4	5.8	3
9	A	476.3	14.6	8
10	A	505.3	8.9	5
11	A	518.1	28.4	16
12	A	605.0	4.3	3
13	A	649.7	2.2	1
14	A	706.2	5.9	3
15	A	740.7	20.9	12
16	A	746.1	6.6	4
17	A	777.1	3.3	2
18	A	814.6	50.8	30
19	A	862.2	3.5	2
20	A	883.3	4.7	3
21	A	933.3	0.5	0
22	A	937.1	1.1	1
23	A	955.5	1.6	1

24	A	968.6	0.0	0
25	A	1001.3	1.3	1
26	A	1072.7	42.5	25
27	A	1108.1	9.1	5
28	A	1131.0	3.9	2
29	A	1139.6	8.4	5
30	A	1183.1	42.3	25
31	A	1220.6	10.0	6
32	A	1242.2	10.1	6
33	A	1301.0	13.1	8
34	A	1316.5	56.7	33
35	A	1361.0	10.6	6
36	A	1405.0	6.7	4
37	A	1428.4	37.8	22
38	A	1482.9	2.1	1
39	A	1518.8	1.0	1
40	A	1564.8	28.3	16
41	A	1606.5	9.2	5
42	A	2807.1	172.0	100
43	A	3059.4	3.7	2
44	A	3062.7	6.1	4
45	A	3074.8	12.6	7
46	A	3085.7	13.9	8
47	A	3086.9	19.7	11
48	A	3102.4	8.4	5

Azireno[1,2-a]quinoline 40



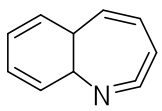
Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-1.523306	1.341329	0.159796
C	-2.647501	0.521231	0.205183
C	-2.505581	-0.857825	0.023115
C	-1.244824	-1.412990	-0.195837
C	-0.106630	-0.604801	-0.201639
C	-0.240687	0.805270	-0.041369
C	2.236720	-0.232750	0.052161
C	2.195928	1.193483	-0.069569
C	0.931651	1.678863	-0.124797
C	2.134645	-1.389498	0.603351
H	-1.629988	2.415985	0.291967
H	-3.629868	0.953664	0.372147
H	-3.380912	-1.501804	0.046225
H	-1.124933	-2.479734	-0.363309
H	3.084324	1.815426	-0.072246
H	0.759033	2.751144	-0.180670
H	2.331412	-2.164150	1.324312
N	1.172635	-1.149201	-0.554399

RB3LYP/6-31G(d), HF= -439.879909
Zero-point correction= 0.137062 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.742847

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	117.3	1.0	2
2	A	145.7	2.2	5
3	A	268.8	6.8	15
4	A	307.0	7.8	17
5	A	341.4	0.9	2
6	A	392.4	10.3	22
7	A	447.9	2.6	6
8	A	460.8	11.8	26
9	A	481.4	3.9	8
10	A	508.4	3.0	6
11	A	550.2	6.0	13
12	A	574.1	7.1	15
13	A	595.1	3.0	6
14	A	677.4	6.5	14
15	A	707.6	7.1	15
16	A	735.1	8.1	18
17	A	758.2	45.5	99
18	A	766.2	8.0	17
19	A	809.4	6.3	14
20	A	854.5	0.2	0
21	A	903.8	1.1	2
22	A	911.8	5.6	12
23	A	925.9	2.6	6
24	A	942.7	1.5	3
25	A	944.2	5.6	12
26	A	998.1	8.5	19
27	A	1023.0	3.0	6
28	A	1094.5	14.0	30
29	A	1123.1	0.7	2
30	A	1142.6	0.2	1
31	A	1167.0	14.1	31
32	A	1186.7	8.1	18
33	A	1251.5	1.1	2
34	A	1292.9	0.2	1
35	A	1359.0	0.1	0
36	A	1427.7	8.0	17
37	A	1450.4	1.4	3
38	A	1535.4	19.1	42
39	A	1576.3	11.4	25
40	A	1591.1	21.4	46
41	A	1831.4	22.2	48
42	A	3052.7	6.0	13
43	A	3063.5	2.1	4
44	A	3065.6	13.6	29
45	A	3078.2	21.1	46
46	A	3086.7	25.1	55
47	A	3100.4	9.4	21
48	A	3209.7	10.9	24

Cyclic Ketenimine 41



Atom	Coordinates (Angstroms)		
Type	X	Y	Z
C	-2.694793	-0.528572	0.188691

C	-2.549599	0.861653	0.219412
C	-1.294283	1.432472	0.038902
C	-0.134723	0.652381	-0.146813
C	-0.318736	-0.761328	-0.185954
C	-1.580604	-1.335154	-0.024851
C	2.403510	0.989959	-0.020339
C	1.810659	-1.204477	0.103877
H	-3.675721	-0.980442	0.306705
H	-3.415892	1.498856	0.372909
H	-1.190845	2.514775	0.060780
H	-1.668715	-2.415147	-0.089986
H	3.230670	1.673703	-0.210383
N	0.809115	-1.588868	-0.518025
C	2.664086	-0.322321	0.594531
H	3.344622	-0.490512	1.420043
C	1.142825	1.373741	-0.345297
H	1.022024	2.370726	-0.766851

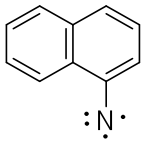
RB3LYP/6-31G(d), HF= -439.9425239
Zero-point correction= 0.139211 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.803313

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	126.4	2.1	1
2	A	149.9	0.6	0
3	A	305.2	2.8	1
4	A	313.9	2.5	1
5	A	367.0	6.9	4
6	A	414.9	2.5	1
7	A	430.5	1.2	1
8	A	461.9	4.9	3
9	A	504.4	5.3	3
10	A	559.7	0.7	0
11	A	563.2	1.7	1
12	A	622.5	4.8	2
13	A	671.3	35.4	18
14	A	692.8	8.1	4
15	A	723.9	9.5	5
16	A	746.7	37.0	19
17	A	749.0	5.7	3
18	A	793.6	42.7	22
19	A	824.6	10.2	5
20	A	860.2	1.4	1
21	A	916.2	3.6	2
22	A	929.7	5.5	3
23	A	947.6	0.2	0
24	A	980.7	0.9	0
25	A	1026.8	2.4	1
26	A	1064.9	13.4	7
27	A	1101.1	4.3	2
28	A	1133.9	6.6	3
29	A	1148.8	2.2	1
30	A	1169.3	16.9	9
31	A	1197.2	0.4	0
32	A	1251.9	4.2	2
33	A	1288.0	1.0	1
34	A	1321.8	2.0	1
35	A	1372.4	7.7	4
36	A	1428.2	10.8	6

37	A	1452.9	10.8	6
38	A	1543.7	4.7	2
39	A	1572.7	11.9	6
40	A	1589.3	10.3	5
41	A	1928.2	191.6	100
42	A	3028.1	7.3	4
43	A	3047.4	32.0	17
44	A	3059.0	7.4	4
45	A	3070.8	10.4	5
46	A	3084.2	22.5	12
47	A	3094.1	13.7	7
48	A	3111.0	4.0	2

1-Naphthylnitrene 43 (T_0, ^{3}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.351123	1.100476	0.000000
C	1.018861	1.479347	0.000000
C	0.000000	0.507990	0.000000
C	0.346253	-0.874957	0.000000
C	1.717907	-1.232833	0.000000
C	2.702404	-0.264206	0.000000
H	3.128940	1.858895	0.000000
H	0.743644	2.529489	0.000000
C	-1.420897	0.885748	0.000000
C	-0.684260	-1.861793	0.000000
H	1.982793	-2.287394	0.000000
H	3.749756	-0.553201	0.000000
C	-2.025140	-1.497773	0.000000
C	-2.404141	-0.157012	0.000000
H	-0.402127	-2.911223	0.000000
H	-2.792507	-2.267091	0.000000
H	-3.450013	0.131302	0.000000
N	-1.796164	2.141327	0.000000

State= 3-A"
<S2>= 2.064188
UB3LYP/6-31G(d), HF= -439.956555
Zero-point correction= 0.138599 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.817956

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	119.3	3.4	7
2	A"	168.7	0.6	1
3	A"	234.9	0.1	0
4	A'	273.1	6.6	14
5	A"	403.9	0.7	1
6	A'	428.2	3.2	7
7	A"	456.7	0.2	0
8	A'	459.2	1.0	2
9	A'	495.7	1.3	3

10	A"	521.1	8.2	17
11	A'	556.0	3.1	7
12	A"	615.5	0.7	2
13	A'	696.9	0.3	1
14	A"	706.5	6.3	13
15	A"	750.4	47.2	100
16	A'	765.2	0.7	2
17	A"	773.4	33.5	71
18	A"	838.2	0.0	0
19	A'	860.4	0.7	1
20	A"	860.7	1.0	2
21	A"	925.7	1.1	2
22	A"	932.4	0.4	1
23	A"	957.6	0.0	0
24	A'	1006.5	4.8	10
25	A'	1032.6	0.3	1
26	A'	1072.1	2.4	5
27	A'	1113.6	0.2	0
28	A'	1127.4	2.5	5
29	A'	1146.7	0.8	2
30	A'	1195.5	4.4	9
31	A'	1211.8	12.8	27
32	A'	1262.8	4.8	10
33	A'	1300.2	4.0	8
34	A'	1334.8	1.1	2
35	A'	1362.2	2.6	6
36	A'	1418.9	2.1	4
37	A'	1422.2	0.6	1
38	A'	1479.3	12.9	28
39	A'	1504.0	0.9	2
40	A'	1545.7	4.6	10
41	A'	1595.0	4.0	8
42	A'	3059.6	1.9	4
43	A'	3065.5	1.7	4
44	A'	3071.6	10.5	22
45	A'	3080.0	19.6	42
46	A'	3083.4	20.5	44
47	A'	3093.4	12.9	28
48	A'	3098.5	7.5	16

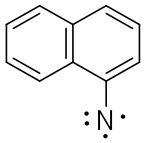
Natural Atomic Spin Densities of structure optimized at UB3LYP/EPR-III level:

State= 3-A"
<S2>= 2.059167
UB3LYP/EPR-III, HF= -440.1336156

1	C	0.08990
2	C	-0.05685
3	C	0.18116
4	C	-0.07577
5	C	0.08024
6	C	-0.05657
7	H	-0.00240
8	H	0.00089
9	C	-0.20581
10	C	0.34384
11	H	-0.00212
12	H	0.00165
13	C	-0.13183

14	C	0.39932
15	H	-0.01044
16	H	0.00654
17	H	-0.01220
18	N	1.45045

1-Naphthylnitrene 43 (S_1, ^{1}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.344494	1.125887	0.000000
C	1.004241	1.489541	0.000000
C	0.000000	0.509923	0.000000
C	0.357963	-0.868357	0.000000
C	1.731666	-1.211933	0.000000
C	2.708633	-0.232204	0.000000
H	3.113073	1.893574	0.000000
H	0.716122	2.536307	0.000000
C	-1.434825	0.880069	0.000000
C	-0.662706	-1.868603	0.000000
H	2.008170	-2.263527	0.000000
H	3.758527	-0.511884	0.000000
C	-2.013926	-1.518081	0.000000
C	-2.411929	-0.191194	0.000000
H	-0.369302	-2.914675	0.000000
H	-2.769633	-2.299136	0.000000
H	-3.460345	0.085824	0.000000
N	-1.819753	2.111889	0.000000

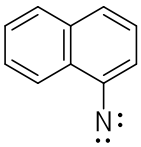
State= 1-A"
<S2>= 1.035141
UB3LYP/6-31G(d), HF= -439.9465575
Zero-point correction= 0.138470 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.808087
Ziegler-Cramer corrected energy= -439.798218

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	109.2	4.0	8
2	A"	167.2	0.4	1
3	A"	222.5	0.0	0
4	A'	275.7	6.9	14
5	A"	400.2	0.5	1
6	A'	427.7	3.4	7
7	A"	453.0	0.6	1
8	A'	455.3	2.5	5
9	A'	492.6	1.8	4
10	A"	510.9	6.9	14
11	A'	553.7	2.9	6
12	A"	616.1	0.3	1
13	A'	693.8	0.3	1
14	A"	697.7	11.9	24
15	A"	746.6	48.9	100

16	A'	763.7	0.9	2
17	A"	770.4	27.5	56
18	A"	822.5	0.1	0
19	A"	858.5	1.1	2
20	A'	858.5	0.9	2
21	A"	926.2	1.4	3
22	A"	930.9	0.2	0
23	A"	956.6	0.1	0
24	A'	1001.6	5.2	11
25	A'	1030.3	0.1	0
26	A'	1067.3	1.9	4
27	A'	1112.4	1.0	2
28	A'	1125.6	0.6	1
29	A'	1146.6	0.4	1
30	A'	1194.1	6.6	13
31	A'	1216.5	6.1	12
32	A'	1255.3	4.3	9
33	A'	1302.8	4.7	10
34	A'	1337.4	0.1	0
35	A'	1404.8	3.7	8
36	A'	1413.8	0.2	0
37	A'	1442.3	2.5	5
38	A'	1481.9	13.2	27
39	A'	1494.8	1.1	2
40	A'	1545.1	3.4	7
41	A'	1589.0	4.4	9
42	A'	3059.7	2.5	5
43	A'	3065.9	2.7	6
44	A'	3072.0	9.7	20
45	A'	3080.7	19.6	40
46	A'	3083.5	19.1	39
47	A'	3093.3	13.2	27
48	A'	3103.3	6.5	13

1-Naphthylnitrene 43 (S_2, ^{1}A')



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.347969	1.083108	0.000000
C	1.020095	1.472316	0.000000
C	0.000000	0.507208	0.000000
C	0.354915	-0.877695	0.000000
C	1.725772	-1.254347	0.000000
C	2.705685	-0.285656	0.000000
H	3.131486	1.836620	0.000000
H	0.711748	2.513588	0.000000
C	-1.425621	0.913763	0.000000
C	-0.682867	-1.842833	0.000000
H	1.987587	-2.309819	0.000000
H	3.754227	-0.569382	0.000000
C	-2.032588	-1.499250	0.000000
C	-2.390355	-0.151777	0.000000
H	-0.403252	-2.895358	0.000000
H	-2.788071	-2.279959	0.000000

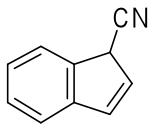
H	-3.431561	0.158502	0.000000
N	-1.814314	2.165255	0.000000

State= 1-A'
RB3LYP/6-31G(d), HF= -439.9078957
Zero-point correction= 0.139811 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.768085

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	120.3	7.7	6
2	A"	169.4	0.6	0
3	A"\par	250.4	0.6	0
4	A'	284.6	12.5	9
5	A"	403.1	0.0	0
6	A'\par	450.6	1.9	1
7	A'	458.2	3.1	2
8	A"	459.7	0.6	0
9	A'\par	518.9	1.0	1
10	A"	521.5	14.7	11
11	A'	562.5	8.6	6
12	A"\par	625.8	0.2	0
13	A'	692.6	2.0	1
14	A"	734.3	0.3	0
15	A"\par	759.3	45.8	33
16	A'	763.2	2.4	2
17	A"	811.1	28.9	21
18	A'\par	859.0	3.5	3
19	A"	886.7	0.1	0
20	A"	936.2	0.5	0
21	A"\par	964.5	0.7	1
22	A"	981.7	0.1	0
23	A"	992.2	1.3	1
24	A'\par	1001.7	2.1	2
25	A'	1029.0	1.2	1
26	A'	1064.0	11.9	9
27	A'\par	1117.8	4.2	3
28	A'	1133.7	13.0	9
29	A'	1151.0	9.1	7
30	A'\par	1196.9	36.0	26
31	A'	1225.6	39.2	29
32	A'	1265.1	29.1	21
33	A'\par	1331.1	19.1	14
34	A'	1344.7	137.1	100
35	A'	1379.6	78.1	57
36	A'\par	1422.3	5.6	4
37	A'	1422.7	9.1	7
38	A'	1489.4	78.4	57
39	A'\par	1528.1	20.1	15
40	A'	1549.3	36.8	27
41	A'	1602.8	34.5	25
42	A'\par	3052.3	3.3	2
43	A'	3060.1	3.2	2
44	A'	3069.5	15.1	11
45	A'\par	3075.9	15.6	11
46	A'	3085.9	18.7	14
47	A'	3093.9	17.1	12
48	A'\par	3096.2	4.2	3

1-Cyano-1*H*-indene



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.042155	-0.252908	0.308299
C	0.695735	0.936090	-0.070286
C	2.061147	0.924663	-0.356731
C	2.753556	-0.287004	-0.267894
C	2.095818	-1.464652	0.100435
C	0.725414	-1.455972	0.394094
C	-1.422568	0.070209	0.589781
C	-1.500411	1.559290	0.267356
H	2.577498	1.835873	-0.646876
H	3.816786	-0.314148	-0.490530
H	2.650679	-2.396783	0.157827
H	0.214674	-2.373942	0.672915
H	-2.424049	2.120337	0.339146
H	-1.648715	-0.091469	1.655865
C	-2.371264	-0.741983	-0.183959
N	-3.124635	-1.385389	-0.789153
C	-0.289004	2.023327	-0.084614
H	-0.057895	3.051503	-0.343166

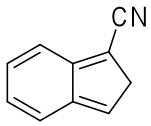
RB3LYP/6-31G(d), HF= -439.9968495
Zero-point correction= 0.139680 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.857170

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	81.8	2.0	5
2	A	105.1	4.3	10
3	A	213.3	2.1	5
4	A	235.6	1.3	3
5	A	356.3	1.2	3
6	A	383.8	2.4	6
7	A	409.5	4.6	11
8	A	477.0	2.2	5
9	A	498.3	1.4	3
10	A	532.7	3.4	8
11	A	575.5	0.5	1
12	A	614.4	1.9	5
13	A	694.1	6.7	16
14	A	718.7	18.1	44
15	A	724.2	7.9	19
16	A	759.1	40.6	99
17	A	820.9	4.8	12
18	A	837.8	1.0	2
19	A	863.7	5.1	12
20	A	909.0	0.5	1
21	A	926.7	2.4	6
22	A	932.2	14.4	35
23	A	949.5	0.3	1
24	A	995.6	1.5	4
25	A	1010.5	1.7	4

26	A	1051.2	0.8	2
27	A	1101.0	0.5	1
28	A	1132.1	0.3	1
29	A	1147.1	0.3	1
30	A	1165.0	4.2	10
31	A	1190.5	0.5	1
32	A	1250.4	2.3	6
33	A	1262.5	1.7	4
34	A	1305.9	1.0	2
35	A	1349.6	1.1	3
36	A	1446.9	5.4	13
37	A	1451.5	7.4	18
38	A	1561.5	1.7	4
39	A	1594.9	0.0	0
40	A	1602.1	0.9	2
41	A	2273.1	14.3	35
42	A	2900.7	1.6	4
43	A	3063.0	1.4	3
44	A	3070.1	2.6	6
45	A	3078.5	24.5	60
46	A	3089.0	21.8	53
47	A	3098.7	7.1	17
48	A	3129.5	4.7	11

1-Cyano-2*H*-indene



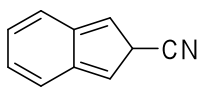
Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.245163	0.000000
C	0.667352	-1.069657	0.000000
C	2.107343	-1.125984	0.000000
C	2.812404	0.037541	0.000000
C	2.150171	1.325891	0.000000
C	0.792316	1.441475	0.000000
H	2.608669	-2.089960	0.000000
H	3.898619	0.016604	0.000000
H	2.767408	2.220244	0.000000
H	0.304693	2.411884	0.000000
C	-1.364556	0.053703	0.000000
C	-1.642095	-1.430120	0.000000
H	-2.233848	-1.734916	0.876967
C	-2.359057	1.054382	0.000000
N	-3.186771	1.877996	0.000000
C	-0.280354	-2.051378	0.000000
H	-0.105434	-3.121005	0.000000
H	-2.233848	-1.734916	-0.876967

State= 1-A'
RB3LYP/6-31G(d), HF= -439.9790203
Zero-point correction= 0.138653 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.840367

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	107.1	2.2	2
2	A'	117.1	4.8	5
3	A"	179.8	5.2	5
4	A"	224.4	1.4	1
5	A"	316.0	3.3	3
6	A'	360.8	7.1	7
7	A"	451.1	11.1	11
8	A'	464.1	1.1	1
9	A"	487.2	0.2	0
10	A'	508.6	3.9	4
11	A"	529.1	0.2	0
12	A'	574.0	1.2	1
13	A'	618.5	5.2	5
14	A"	680.4	0.0	0
15	A'	709.4	4.0	4
16	A"	745.1	7.7	8
17	A"	761.7	54.0	54
18	A"	835.5	0.2	0
19	A'	848.9	1.2	1
20	A"	862.7	6.1	6
21	A"	937.4	0.2	0
22	A'	939.5	13.9	14
23	A'	958.6	2.5	2
24	A"	964.6	0.1	0
25	A'	993.8	11.1	11
26	A"	1071.3	0.6	1
27	A'	1100.2	0.8	1
28	A'	1140.1	6.5	6
29	A'	1156.9	15.0	15
30	A'	1171.9	0.4	0
31	A'	1210.6	0.4	0
32	A'	1276.6	7.3	7
33	A'	1345.6	0.6	1
34	A'	1367.9	16.3	16
35	A'	1370.2	11.0	11
36	A'	1413.0	3.7	4
37	A'	1486.2	20.6	21
38	A'	1525.4	5.6	6
39	A'	1558.7	0.9	1
40	A'	1631.0	8.1	8
41	A'	2222.2	99.9	100
42	A'	2914.7	0.3	0
43	A"	2938.3	1.9	2
44	A'	3065.2	1.6	2
45	A'	3073.1	7.2	7
46	A'	3085.1	20.5	21
47	A'	3091.8	18.2	18
48	A'	3115.0	2.4	2

2-Cyano-2*H*-indene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-3.860346	-0.000918	-0.928523
C	-2.922921	0.000504	-0.243452

C	-1.740212	0.000521	0.627094
C	0.424829	0.742671	0.168633
C	0.424589	-0.742446	0.168866
C	-0.832409	-1.194476	0.414403
H	-2.097368	0.000744	1.672224
H	-1.176407	-2.219321	0.470950
C	1.664222	1.444433	-0.069440
H	1.675967	2.530842	-0.071780
C	2.795872	0.726362	-0.290851
H	3.736540	1.238333	-0.474852
C	2.795637	-0.727041	-0.290618
H	3.736140	-1.239373	-0.474455
C	1.663758	-1.444680	-0.068976
H	1.675157	-2.531092	-0.070972
C	-0.832021	1.195172	0.414046
H	-1.175673	2.220149	0.470319

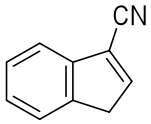
RB3LYP/6-31G(d), HF= -439.9602857
Zero-point correction= 0.138543 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.821742

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A	65.5	1.8	3
2	A	116.9	3.2	5
3	A	203.8	2.5	4
4	A	230.0	0.0	0
5	A	356.4	6.0	10
6	A	364.6	7.2	12
7	A	433.2	2.0	3
8	A	459.7	11.0	18
9	A	479.3	0.2	0
10	A	542.5	1.2	2
11	A	554.5	1.0	2
12	A	569.7	0.8	1
13	A	660.0	0.3	0
14	A	680.9	2.3	4
15	A	726.0	8.7	14
16	A	748.7	0.5	1
17	A	776.6	19.4	32
18	A	815.8	60.1	100
19	A	830.3	0.2	0
20	A	867.6	13.4	22
21	A	870.3	0.5	1
22	A	936.7	0.3	1
23	A	949.8	0.7	1
24	A	961.8	0.0	0
25	A	988.3	2.2	4
26	A	1005.1	11.1	18
27	A	1083.0	3.4	6
28	A	1144.7	0.1	0
29	A	1144.9	0.3	0
30	A	1166.7	3.4	6
31	A	1171.6	0.1	0
32	A	1216.8	2.5	4
33	A	1244.1	1.2	2
34	A	1346.4	0.3	1
35	A	1356.8	1.0	2
36	A	1410.4	1.1	2
37	A	1510.8	0.4	1

38	A	1537.4	3.8	6
39	A	1573.7	0.4	1
40	A	1642.8	2.0	3
41	A	2272.6	24.7	41
42	A	2880.3	2.0	3
43	A	3063.0	0.8	1
44	A	3070.4	1.8	3
45	A	3081.7	28.6	48
46	A	3089.1	24.1	40
47	A	3128.5	1.3	2
48	A	3130.4	0.5	1

3-Cyano-1*H*-indene 44



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.240025	0.000000
C	0.829980	-0.897763	0.000000
C	2.211903	-0.753520	0.000000
C	2.754771	0.537214	0.000000
C	1.924742	1.663822	0.000000
C	0.534328	1.527339	0.000000
H	2.864645	-1.623146	0.000000
H	3.833727	0.665256	0.000000
H	2.366514	2.656431	0.000000
H	-0.113479	2.399590	0.000000
C	-1.399562	-0.227493	0.000000
C	-1.432710	-1.582011	0.000000
H	-2.329581	-2.189811	0.000000
C	-2.532658	0.639121	0.000000
N	-3.436468	1.372092	0.000000
C	-0.033390	-2.139684	0.000000
H	0.144513	-2.777636	0.878390
H	0.144513	-2.777636	-0.878390

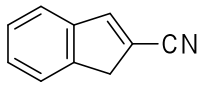
State= 1-A'
RB3LYP/6-31G(d), HF= -440.0077787
Zero-point correction= 0.139586 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.868192

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	108.5	1.7	4
2	A'	115.6	4.4	11
3	A"	195.3	2.6	7
4	A"	218.8	0.6	1
5	A'	356.3	2.1	5
6	A"	369.5	6.8	17
7	A"	414.2	6.2	15
8	A'	462.0	1.3	3
9	A"	498.7	1.7	4
10	A'	505.1	0.0	0
11	A'	590.0	0.1	0

12	A"	615.6	0.6	2
13	A'	638.9	0.5	1
14	A"	710.6	12.0	30
15	A'	729.8	2.4	6
16	A"	756.1	40.1	100
17	A"	776.1	10.4	26
18	A'	815.5	0.3	1
19	A"	849.7	0.1	0
20	A"	904.1	2.5	6
21	A"	927.3	0.0	0
22	A'	944.3	11.5	29
23	A"	950.5	0.0	0
24	A'	1010.1	3.6	9
25	A'	1025.1	2.3	6
26	A'	1091.3	1.6	4
27	A"	1111.2	1.1	3
28	A'	1142.1	0.4	1
29	A'	1151.6	1.5	4
30	A'	1192.5	0.3	1
31	A'	1225.4	1.4	4
32	A'	1280.7	5.1	13
33	A'	1290.2	2.3	6
34	A'	1336.1	4.9	12
35	A'	1404.1	11.7	29
36	A'	1449.5	8.8	22
37	A'	1451.2	6.4	16
38	A'	1564.1	2.0	5
39	A'	1587.0	1.1	3
40	A'	1602.0	0.7	2
41	A'	2258.2	19.8	50
42	A'	2915.9	8.6	21
43	A"	2939.6	6.7	17
44	A'	3060.2	3.2	8
45	A'	3069.2	7.3	18
46	A'	3079.1	20.1	50
47	A'	3088.8	19.7	49
48	A'	3122.6	0.5	1

2-Cyano-1*H*-indene 45



Atom Type	Coordinates (Angstroms) X	Y	Z
C	0.000000	0.865025	0.000000
C	0.846819	-0.266195	0.000000
C	2.226799	-0.111707	0.000000
C	2.758868	1.183781	0.000000
C	1.920421	2.305108	0.000000
C	0.532586	2.157315	0.000000
H	2.887242	-0.975276	0.000000
H	3.836780	1.320163	0.000000
H	2.355714	3.300547	0.000000
H	-0.117650	3.028083	0.000000
C	-1.381658	0.403491	0.000000
C	-1.411133	-0.954369	0.000000
C	0.001056	-1.517335	0.000000
H	0.181347	-2.149509	0.880146

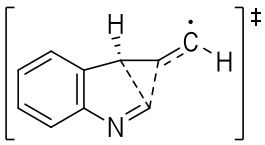
H	0.181347	-2.149509	-0.880146
H	-2.253375	1.048587	0.000000
C	-2.573892	-1.767869	0.000000
N	-3.512942	-2.458080	0.000000

State= 1-A'
RB3LYP/6-31G(d), HF= -440.0105735
Zero-point correction= 0.139783 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.870790

Vibrational frequencies (scaled by 0.9613):

ModeNr.	Symmetry	Wavenumber	Abs.Int.	Rel.Int.
1	A"	86.9	2.4	3
2	A'	130.0	5.3	7
3	A"	201.9	0.5	1
4	A"	233.4	5.7	8
5	A'	361.0	2.8	4
6	A"	374.9	1.8	2
7	A'	411.8	0.2	0
8	A"	414.2	6.2	8
9	A"	526.2	5.5	7
10	A"	536.9	2.8	4
11	A'	555.9	2.9	4
12	A'	581.0	0.7	1
13	A'	606.5	8.5	11
14	A"	706.1	15.9	21
15	A"	745.1	27.0	36
16	A'	768.0	0.4	1
17	A"	844.5	0.0	0
18	A'	852.0	1.0	1
19	A'	865.9	0.8	1
20	A"	876.4	9.9	13
21	A"	911.4	8.0	11
22	A"	929.4	0.3	0
23	A"	951.2	0.1	0
24	A'	1009.6	0.9	1
25	A'	1083.8	0.5	1
26	A'	1109.0	14.8	20
27	A"	1116.7	0.6	1
28	A'	1144.0	0.2	0
29	A'	1152.4	2.1	3
30	A'	1191.5	0.5	1
31	A'	1207.0	6.0	8
32	A'	1277.4	0.0	0
33	A'	1292.3	0.1	0
34	A'	1341.8	5.0	7
35	A'	1410.8	10.3	14
36	A'	1447.2	1.8	2
37	A'	1451.7	4.9	7
38	A'	1552.9	17.4	23
39	A'	1585.0	2.2	3
40	A'	1601.0	1.1	1
41	A'	2241.8	74.8	100
42	A'	2930.0	4.3	6
43	A"	2958.9	5.2	7
44	A'	3061.6	2.6	3
45	A'	3067.9	1.8	2
46	A'	3077.4	26.0	35
47	A'	3088.5	26.3	35
48	A'	3112.0	5.5	7

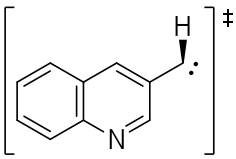
TS connecting 31Z and 3-ethynyl-3*H*-indole, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.199946	-0.605468	0.218478
C	-1.109314	-1.137017	-0.490934
C	0.359280	0.770274	-0.065008
C	-1.843221	0.900679	-0.556793
H	-1.276870	-1.954262	-1.189730
H	-2.774358	1.300355	-0.936480
C	0.220780	-0.639441	-0.224429
N	-0.767656	1.530431	-0.348988
C	1.604420	1.339837	0.220502
H	1.677476	2.417515	0.327305
C	2.722925	0.520497	0.333478
H	3.692713	0.957858	0.552980
C	2.607385	-0.864281	0.140869
H	3.487980	-1.496070	0.217155
C	1.372696	-1.440002	-0.143081
H	1.287886	-2.516439	-0.265198
C	-3.182349	-0.446918	0.998082
H	-4.037183	0.189070	1.149904

State= 1-A
RB3LYP/6-31G(d), HF= -439.8410374
Zero-point correction= 0.134194 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.706843
Negative frequency= -501.7 cm^{-1}

TS connecting 31Z and 31E, (singlet)

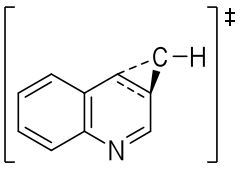


Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.624147	-0.947488	0.006342
C	2.805124	0.457684	0.021150
C	1.712724	1.297216	0.017672
C	0.401304	0.761325	0.000689
C	0.213465	-0.654241	-0.012718
C	1.359586	-1.493581	-0.010894
N	-0.662637	1.617781	-0.008978
C	-1.878570	1.138347	-0.025236
C	-2.189131	-0.281962	-0.012487
C	-1.109020	-1.156743	-0.019605
C	-3.564473	-0.663717	-0.100056
H	3.493824	-1.599159	0.007895

H	3.810372	0.869240	0.034413
H	1.818039	2.377706	0.026871
H	1.223007	-2.572378	-0.022611
H	-2.689224	1.862021	-0.054481
H	-1.269002	-2.231149	-0.034703
H	-3.999492	-0.771790	0.916325

State= 1-A
RB3LYP/6-31G(d), HF= -439.8804839
Zero-point correction= 0.135426 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.745058
Negative frequency= -796.9 cm^{-1}

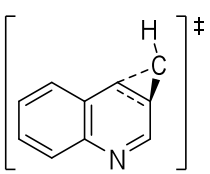
TS connecting 31Z and 32 (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.557493	-0.940680	0.052616
C	2.723280	0.447432	0.198052
C	1.624542	1.293929	0.150566
C	0.330354	0.774001	-0.027817
C	0.157410	-0.638598	-0.138869
C	1.289626	-1.475867	-0.120557
N	-0.720708	1.687921	-0.130903
C	-1.937036	1.241373	-0.188821
C	-2.237460	-0.177950	-0.170410
C	-1.184321	-1.122286	-0.355375
C	-2.924842	-1.073678	0.585345
H	3.423948	-1.595506	0.078621
H	3.718577	0.860322	0.336836
H	1.731524	2.370434	0.239669
H	1.154011	-2.549107	-0.230146
H	-2.744401	1.972288	-0.241894
H	-1.359832	-2.113725	-0.743631
H	-3.273141	-0.726215	1.568474

State= 1-A
RB3LYP/6-31G(d), HF= -439.8839755
Zero-point correction= 0.137157 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.746818
Negative frequency= -347.5 cm^{-1}

TS connecting 31E and 32 (singlet)

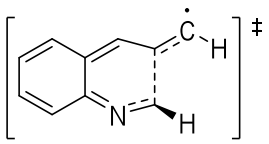


Atom Coordinates (Angstroms)

Type	X	Y	Z
C	2.539601	-0.901401	0.019521
C	2.679375	0.478247	0.236680
C	1.563379	1.304776	0.202929
C	0.284159	0.769562	-0.020233
C	0.133097	-0.642694	-0.184073
C	1.282740	-1.452410	-0.196753
N	-0.772467	1.683737	-0.162169
C	-1.991475	1.261896	-0.210109
C	-2.250828	-0.173154	-0.104775
C	-1.212050	-1.118256	-0.426764
C	-2.614929	-1.012999	0.856632
H	3.417152	-1.542391	0.026115
H	3.663841	0.902584	0.412674
H	1.649986	2.379681	0.328739
H	1.173211	-2.522376	-0.358150
H	-2.792436	1.990106	-0.336959
H	-1.410005	-2.010983	-1.007093
H	-2.772908	-2.064184	1.031518

State= 1-A
RB3LYP/6-31G(d), HF= -439.8745741
Zero-point correction= 0.136449 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.738125
Negative frequency= -530.3 cm^{-1}

TS connecting 31Z and 33Z, (singlet)

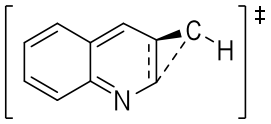


Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.350281	-0.658894	-0.037813
C	1.077059	-1.241631	0.146094
C	-0.427867	0.770507	-0.027353
C	1.794521	1.437062	0.389551
H	1.091601	-2.319092	0.303958
H	2.669616	2.049625	0.164627
C	-0.200550	-0.643652	0.065852
N	0.635926	1.645919	-0.012540
C	-1.730032	1.286745	-0.123928
H	-1.846936	2.363684	-0.195916
C	-2.826470	0.439851	-0.111602
H	-3.830909	0.847062	-0.177954
C	-2.631816	-0.954231	-0.008449
H	-3.490082	-1.620475	-0.003149
C	-1.359172	-1.477636	0.079760
H	-1.215622	-2.553499	0.143821
C	3.553134	-0.619678	-0.332216
H	4.576324	-0.319403	-0.386983

State= 1-A
<S2>= 0.736905 (37% triplet contamination, i.e. 63% singlet)
UB3LYP/6-31G(d), HF= -439.8330541
Zero-point correction= 0.131446 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.701609

Negative frequency= -450.2 cm^{-1}

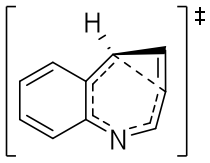
TS connecting 31Z and 36 (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.671894	0.662692	0.095477
C	2.620824	-0.760603	0.220785
C	1.426758	-1.421933	0.131447
C	0.197127	-0.710395	-0.045092
C	0.243293	0.752372	-0.119152
C	1.529731	1.389629	-0.092128
N	-0.911616	-1.409958	-0.345592
C	-2.066527	-0.743216	-0.450723
C	-2.108263	0.701633	-0.001587
C	-0.941682	1.474987	-0.218851
C	-2.922263	0.169730	0.880241
H	3.633471	1.166687	0.143031
H	3.543937	-1.315707	0.361940
H	1.368297	-2.504870	0.178084
H	1.569599	2.472932	-0.175047
H	-2.855009	-1.172787	-1.056981
H	-0.963288	2.535080	-0.454686
H	-3.821033	-0.401006	1.020301

State= 1-A
RB3LYP/6-31G(d), HF= -439.8551187
Zero-point correction= 0.135351 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.719768
Negative frequency= -588.7 cm^{-1}

TS connecting 32 and 37

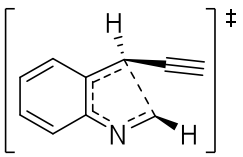


Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.562164	-0.754244	-0.121267
C	2.607545	0.615762	0.245781
C	1.446728	1.341393	0.325662
C	0.167154	0.746662	0.088308
C	0.115670	-0.696922	-0.115822
C	1.355104	-1.375264	-0.329301
N	-0.835325	1.621718	-0.190391
C	-2.070308	1.192345	-0.449154
C	-2.497341	-0.015925	0.054326
C	-1.080488	-1.455645	-0.166292
C	-2.199426	-1.109728	0.703968
H	3.486137	-1.315789	-0.229933

H	3.566339	1.096488	0.419076
H	1.457872	2.409028	0.520677
H	1.323172	-2.433363	-0.578437
H	-2.726112	1.855799	-1.008445
H	-1.122276	-2.329238	-0.822243
H	-2.578674	-1.565556	1.614782

RB3LYP/6-31G(d), HF= -439.894188
Zero-point correction= 0.137241 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.756947
Negative frequency= -358.3 cm^{-1}

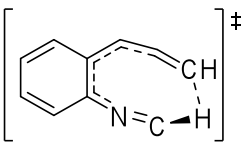
TS connecting 33Z and 3-ethynyl-3*H*-indole



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.292299	-0.825589	0.243981
C	-1.110485	-1.196454	-0.416110
C	0.375638	0.764935	0.037074
C	-1.722276	1.433120	-0.846635
H	-1.144228	-2.143160	-0.954425
H	-2.758631	1.619638	-0.531239
C	0.172405	-0.648570	-0.183263
N	-0.695163	1.543433	-0.198055
C	1.653146	1.299373	0.339410
H	1.743457	2.364663	0.526413
C	2.746835	0.467955	0.346550
H	3.732929	0.865030	0.567905
C	2.593608	-0.910985	0.036847
H	3.468404	-1.555569	0.034405
C	1.356311	-1.445015	-0.235373
H	1.252211	-2.508125	-0.435542
C	-3.318854	-0.462022	0.799493
H	-4.152181	-0.306998	1.447022

RB3LYP/6-31G(d), HF= -439.8409694
Zero-point correction= 0.132786 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.708183
Negative frequency= -262.8 cm^{-1}

TS connecting 33Z and 35

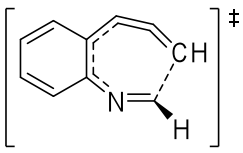


Atom Type	Coordinates (Angstroms) X	Y	Z
H	-2.913826	1.295885	-0.282705
C	-1.925348	1.618668	-0.762302

C	-2.164608	-0.999940	0.258092
C	0.236396	-0.740718	-0.188327
C	1.506289	-1.391881	-0.252674
C	2.669909	-0.716998	0.024407
N	-0.847627	1.374473	-0.299665
C	0.270605	0.693855	-0.012046
C	1.475955	1.368401	0.327034
C	2.655517	0.667622	0.353846
H	1.525599	-2.456999	-0.469528
H	3.617057	-1.249376	0.010662
H	1.443263	2.437988	0.510242
H	3.585021	1.174393	0.594751
C	-0.982105	-1.455404	-0.282941
H	-0.958033	-2.449481	-0.726318
C	-3.158544	-0.399600	0.697740
H	-3.870080	-0.237752	1.483577

RB3LYP/6-31G(d), HF= -439.8444737
Zero-point correction= 0.131873 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.712601
Negative frequency= -371.3 cm^{-1}

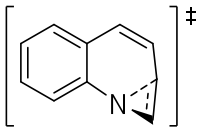
TS connecting 33Z and 36



Atom Type	Coordinates (Angstroms) X	Y	Z
C	2.669976	-0.745309	0.015539
C	2.669798	0.651839	-0.314104
C	1.500324	1.351273	-0.318739
C	0.260453	0.688465	-0.015825
C	0.217405	-0.765787	0.152945
C	1.504261	-1.411058	0.254565
N	-0.807228	1.410092	0.258468
C	-1.925141	1.846760	0.394847
C	-2.209931	-1.054544	-0.186331
C	-0.952194	-1.511035	0.221888
H	3.615731	-1.278572	0.058911
H	3.608156	1.153176	-0.531139
H	1.474675	2.419491	-0.512433
H	1.513561	-2.476522	0.471155
H	-2.322255	2.272796	1.320267
H	-0.871285	-2.547963	0.543802
C	-3.270346	-0.577599	-0.556044
H	-4.155610	-0.251078	-1.052285

State= 1-A
<S2>= 0.
UB3LYP/6-31G(d), HF= -439.8482194
Zero-point correction= 0.133247 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.714973
Negative frequency= -85.0 cm^{-1}

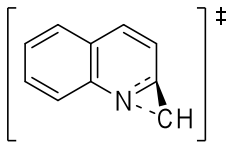
TS connecting 37 and 40



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.451880	1.357210	0.254325
C	-2.617440	0.610334	0.226391
C	-2.549218	-0.760398	-0.066452
C	-1.322821	-1.369867	-0.291247
C	-0.119770	-0.650143	-0.170407
C	-0.183491	0.768754	0.045875
C	2.375216	-0.211236	0.097180
C	2.246071	1.148927	-0.240244
C	0.970053	1.622574	-0.160483
C	2.017895	-1.305794	0.667198
H	-1.499329	2.428548	0.436791
H	-3.577319	1.086722	0.403513
H	-3.460016	-1.351553	-0.116465
H	-1.259192	-2.428093	-0.525919
H	3.089261	1.756510	-0.552196
H	0.778839	2.678397	-0.342116
H	2.199155	-1.982664	1.493634
N	1.077273	-1.350004	-0.424293

RB3LYP/6-31G(d), HF= -439.8764014
Zero-point correction= 0.136628 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.739774
Negative frequency= -330.3 cm^{-1}

TS connecting 40 and 39Z

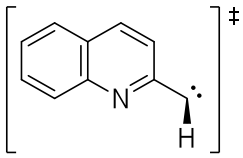


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.620296	1.298076	0.118524
C	-2.698037	0.420846	0.171039
C	-2.478787	-0.958048	0.043112
C	-1.193394	-1.460637	-0.139344
C	-0.097619	-0.589786	-0.167756
C	-0.310659	0.815559	-0.040218
C	2.201821	-0.184450	-0.019648
C	2.116034	1.248102	-0.055150
C	0.837223	1.709556	-0.085849
C	2.400987	-1.328013	0.617826
H	-1.782453	2.369773	0.212553
H	-3.705682	0.802714	0.306232
H	-3.321456	-1.643407	0.084234
H	-1.016450	-2.525395	-0.258395
H	2.983406	1.894656	0.018691
H	0.643890	2.780489	-0.074638

H	2.906810	-2.274440	0.534347
N	1.192615	-1.033090	-0.496892

RB3LYP/6-31G(d), HF= -439.8757318
Zero-point correction= 0.136474 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.739258
Negative frequency= -301.8 cm^{-1}

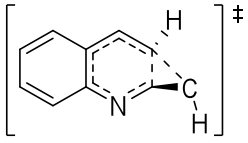
TS connecting 39Z and 39E, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-1.768674	1.246235	0.020634
C	-2.802927	0.335248	0.033307
C	-2.525933	-1.053405	0.017077
C	-1.227548	-1.515001	-0.013234
C	-0.145864	-0.598514	-0.022794
C	-0.421462	0.807180	-0.003499
C	2.131695	-0.197343	-0.039695
C	1.972255	1.216586	-0.015766
C	0.688028	1.699075	-0.010728
C	3.304442	-1.050573	-0.050931
H	-1.971587	2.314924	0.031999
H	-3.833148	0.678789	0.055029
H	-3.349991	-1.761872	0.026214
H	-0.997111	-2.575441	-0.031758
H	2.835180	1.874926	-0.000557
H	0.501748	2.770923	0.001150
H	3.652276	-1.196445	0.993403
N	1.134081	-1.063248	-0.080243

State= 1-A
RB3LYP/6-31G(d), HF= -439.8817918
Zero-point correction= 0.135750 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.746041
Negative frequency= -334.7 cm^{-1}

38, TS connecting 39Z and 41, (singlet)

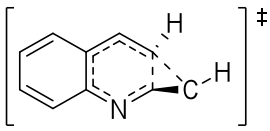


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.639989	-0.808524	-0.001212
C	-2.717694	0.605187	0.178191
C	-1.576682	1.363118	0.189470
C	-0.293834	0.752978	0.043074
C	-0.212962	-0.691144	-0.100305

C	-1.432182	-1.437153	-0.151596
C	2.104149	0.847605	-0.372990
C	2.053754	-0.604467	-0.100445
C	3.263047	-0.437372	0.495778
H	-3.557683	-1.390399	-0.017661
H	-3.689413	1.076302	0.294033
H	-1.628652	2.443483	0.301895
H	-1.355121	-2.512537	-0.275511
H	2.898468	1.349280	-0.904365
H	3.271436	-0.577186	1.584919
C	0.881844	1.496236	-0.148468
H	0.804145	2.571954	-0.299848
N	0.954302	-1.354239	-0.124635

State= 1-A
RB3LYP/6-31G(d), HF= -439.8733085
Zero-point correction= 0.136248 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.737061
Negative frequency= -315.8 cm^{-1}

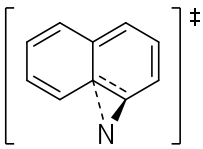
TS connecting 39E and 41, (singlet)



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.689107	-0.749451	-0.005640
C	-2.729287	0.645520	0.146148
C	-1.545535	1.371486	0.152715
C	-0.302641	0.722497	0.045896
C	-0.269195	-0.698009	-0.075954
C	-1.475654	-1.415279	-0.125741
C	2.167680	0.872291	-0.221627
C	2.036707	-0.746520	-0.046889
C	3.181485	-0.405089	0.572548
H	-3.615889	-1.316371	-0.029792
H	-3.682522	1.156309	0.245138
H	-1.568334	2.454944	0.246019
H	-1.429517	-2.494095	-0.234579
H	2.959004	1.420327	-0.717917
H	4.108726	-0.299279	0.010429
C	0.932751	1.443971	-0.157277
H	0.847675	2.476254	-0.494237
N	0.933946	-1.378084	-0.104306

State= 1-A
RB3LYP/6-31G(d), HF= -439.8681243
Zero-point correction= 0.135825 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.732299
Negative frequency= -437.8 cm^{-1}

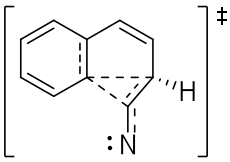
42, TS connecting 41 and 43



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.434234	-0.729949	-0.357737
C	-1.199577	-1.324623	-0.385261
C	-0.041482	-0.563325	-0.071433
C	-0.157564	0.862991	0.190374
C	-1.478696	1.409919	0.308047
C	-2.574515	0.636253	0.039162
H	-3.318351	-1.306440	-0.612451
H	-1.077067	-2.378042	-0.610746
C	1.354275	-1.087514	0.039731
C	0.998222	1.640893	0.108570
H	-1.586691	2.455111	0.587302
H	-3.570420	1.064761	0.113840
C	2.250630	1.088889	-0.283066
C	2.472189	-0.261151	-0.363076
H	0.913184	2.719094	0.213757
H	3.060337	1.772413	-0.526179
H	3.401753	-0.694307	-0.715737
N	1.005967	-1.952412	0.885479

State= 1-A
RB3LYP/6-31G(d), HF= -439.8961313
Zero-point correction= 0.137383 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.758748
Negative frequency= -184.0 cm^{-1}

TS connecting 43 and 1-cyano-1*H*-indene (closed-shell singlet ^{1}A')

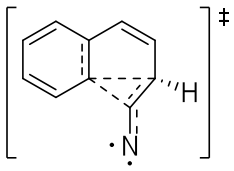


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.345892	-0.899479	-0.336516
C	-1.027774	-1.345722	-0.422610
C	-0.020036	-0.415008	-0.216578
C	-0.254163	0.921750	0.150606
C	-1.602367	1.306335	0.343587
C	-2.628563	0.412730	0.079259
H	-3.154370	-1.578656	-0.592153
H	-0.787873	-2.377524	-0.653306
C	1.556349	-1.105080	0.245021
C	0.879296	1.801231	0.196372
H	-1.818626	2.310997	0.698834
H	-3.661508	0.728206	0.196158
C	2.063257	1.289702	-0.263896
C	2.205663	-0.092152	-0.533806
H	0.761307	2.849201	0.452164
H	2.889584	1.940415	-0.539544

H	2.809044	-0.441971	-1.370265
N	1.429689	-2.096644	0.908497

State= 1-A
RB3LYP/6-31G(d), HF= -439.8717513
Zero-point correction= 0.135482 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.736270
Negative frequency= -500.4 cm^{-1}

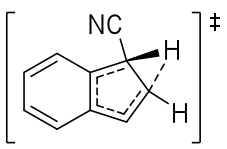
TS connecting 43S_1 and 1-cyano-1*H*-indene (open-shell singlet ^{1}A")



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-2.327670	-0.922886	-0.338635
C	-1.001559	-1.344446	-0.440821
C	-0.003347	-0.409432	-0.199021
C	-0.263251	0.922803	0.166262
C	-1.611710	1.288849	0.354393
C	-2.628267	0.379843	0.086423
H	-3.126982	-1.617118	-0.582199
H	-0.749617	-2.370456	-0.685269
C	1.554860	-1.090314	0.260177
C	0.868021	1.819387	0.201676
H	-1.845555	2.295237	0.693141
H	-3.665193	0.682310	0.202210
C	2.035898	1.310357	-0.281491
C	2.132742	-0.083167	-0.584877
H	0.751819	2.861326	0.481294
H	2.883707	1.943576	-0.530959
H	2.657036	-0.438281	-1.470688
N	1.508640	-2.083223	0.935422

State= 1-A
Note: *<S2>= 0.266904 (13% triplet contamination, i.e. 87% singlet)*
UB3LYP/6-31G(d), HF= -439.8729258
Zero-point correction= 0.134800 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.738125
Negative frequency= -906.9 cm^{-1}

TS connecting 1-cyano-1*H*-indene and 1-cyano-2*H*-indene

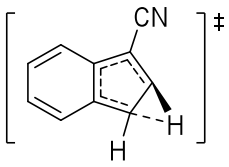


Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.001227	-0.245010	0.030549
C	0.819077	0.931602	-0.043366
C	2.231304	0.790086	-0.062202

C	2.774796	-0.475224	-0.038248
C	1.952248	-1.633909	0.024658
C	0.578011	-1.531921	0.073104
C	-1.367630	0.170878	0.076738
C	-1.348396	1.675175	0.033488
H	2.867425	1.670070	-0.105900
H	3.854128	-0.598353	-0.066057
H	2.420696	-2.614000	0.037818
H	-0.051075	-2.415993	0.126626
H	-2.239029	2.273190	-0.116924
H	-1.510561	1.034666	1.125818
C	-2.527017	-0.637436	-0.042789
N	-3.470999	-1.314268	-0.136831
C	-0.006617	2.079362	-0.047955
H	0.328117	3.108677	-0.067425

RB3LYP/6-31G(d), HF= -439.9394565
Zero-point correction= 0.135408 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.804048
Negative frequency= -1282.0 cm^{-1}

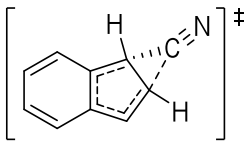
TS connecting 1-cyano-2*H*-indene and 44



Atom Type	Coordinates (Angstroms) X	Y	Z
C	-0.022989	-0.238811	-0.036183
C	0.830746	0.918048	-0.028192
C	2.238641	0.768308	0.004411
C	2.767662	-0.503018	0.010569
C	1.922609	-1.648542	0.010628
C	0.549861	-1.534152	-0.002696
C	-1.379362	0.189535	-0.038247
C	-1.390311	1.613125	-0.022873
H	2.883661	1.643033	0.010592
H	3.845057	-0.641423	0.019506
H	2.377714	-2.635302	0.023665
H	-0.088511	-2.412896	0.003537
H	-2.247755	2.249938	-0.207254
H	-0.853942	2.016807	1.045569
C	-2.526094	-0.638223	-0.002783
N	-3.462734	-1.332928	0.018724
C	0.011412	2.073629	-0.044188
H	0.309869	3.110945	-0.129340

RB3LYP/6-31G(d), HF= -439.9465846
Zero-point correction= 0.135663 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.810922
Negative frequency= -1227.2 cm^{-1}

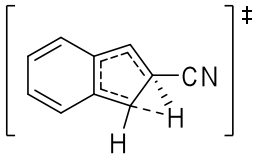
TS connecting 1-cyano-1*H*-indene and 2-cyano-2*H*-indene



Atom Type	Coordinates (Angstroms) X	Y	Z
N	2.934230	-0.709445	1.361641
C	2.278876	-0.338466	0.457121
C	1.811816	0.644799	-0.721601
C	-0.398450	0.864868	-0.112386
C	-0.193005	-0.530663	-0.426467
C	1.159958	-0.707977	-0.821651
H	2.689507	0.922444	-1.297858
H	1.580769	-1.550441	-1.356051
C	-1.679118	1.293131	0.342327
H	-1.846268	2.335277	0.600018
C	-2.691192	0.369374	0.440179
H	-3.676480	0.683459	0.774314
C	-2.481748	-1.005612	0.121083
H	-3.312581	-1.699381	0.213062
C	-1.249508	-1.461212	-0.290554
H	-1.089399	-2.511056	-0.520307
C	0.798586	1.567608	-0.300134
H	0.977562	2.610711	-0.072156

RB3LYP/6-31G(d), HF= -439.9209899
Zero-point correction= 0.137259 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.783731
Negative frequency= -657.8 cm^{-1}

TS connecting 2-cyano-2*H*-indene and 45



Atom Type	Coordinates (Angstroms) X	Y	Z
N	-4.255758	0.021019	-0.250756
C	-3.108377	0.020404	-0.062994
C	-1.694553	0.025071	0.174713
C	0.477166	0.723395	0.017435
C	0.498183	-0.726229	0.012464
C	-0.821114	-1.195189	0.070299
H	-1.439928	-0.594026	1.216392
H	-1.205437	-2.204760	0.019130
C	1.712111	1.436984	-0.013837
H	1.712381	2.523496	0.000292
C	2.886829	0.731379	-0.073100
H	3.833970	1.262954	-0.109648
C	2.901279	-0.698846	-0.084367
H	3.856968	-1.213229	-0.134049
C	1.737205	-1.423636	-0.028974
H	1.753210	-2.510193	-0.032201
C	-0.843682	1.172227	0.096743
H	-1.191124	2.195272	0.145088

RB3LYP/6-31G(d), HF= -439.9338315
Zero-point correction= 0.135270 (Hartree/Particle)
Sum of electronic and zero-point Energies= -439.798562
Negative frequency= -1224.9 cm^{-1}