NMR Spectroscopic and Computational Study of Conformational Isomerism in Substituted 2-Aryl-3*H*-1-benzazepines: Toward Isolable Atropisomeric Benzazepine Enantiomers

Keith Ramig,*[†] Edyta M. Greer,*[†] David J. Szalda,[†] Sasan Karimi,[‡] Allen Ko,[†] Laura Boulos,[†] Jiansan Gu,[†] Nathan Dvorkin,[†] Hema Bhramdat,[§] Gopal Subramaniam*[§]

[†]Department of Natural Sciences, Baruch College of the City University of New York, 17 Lexington Ave., New York, NY 10010, USA [‡] Department of Chemistry, Queensborough Community College of the City University of New York, 222-05 56th Ave., Bayside, NY 11364, USA [§]Department of Chemistry and Biochemistry, Queens College of the City University of New York, 65-30 Kissena Blvd., Flushing, NY 11367, USA

Supporting Information

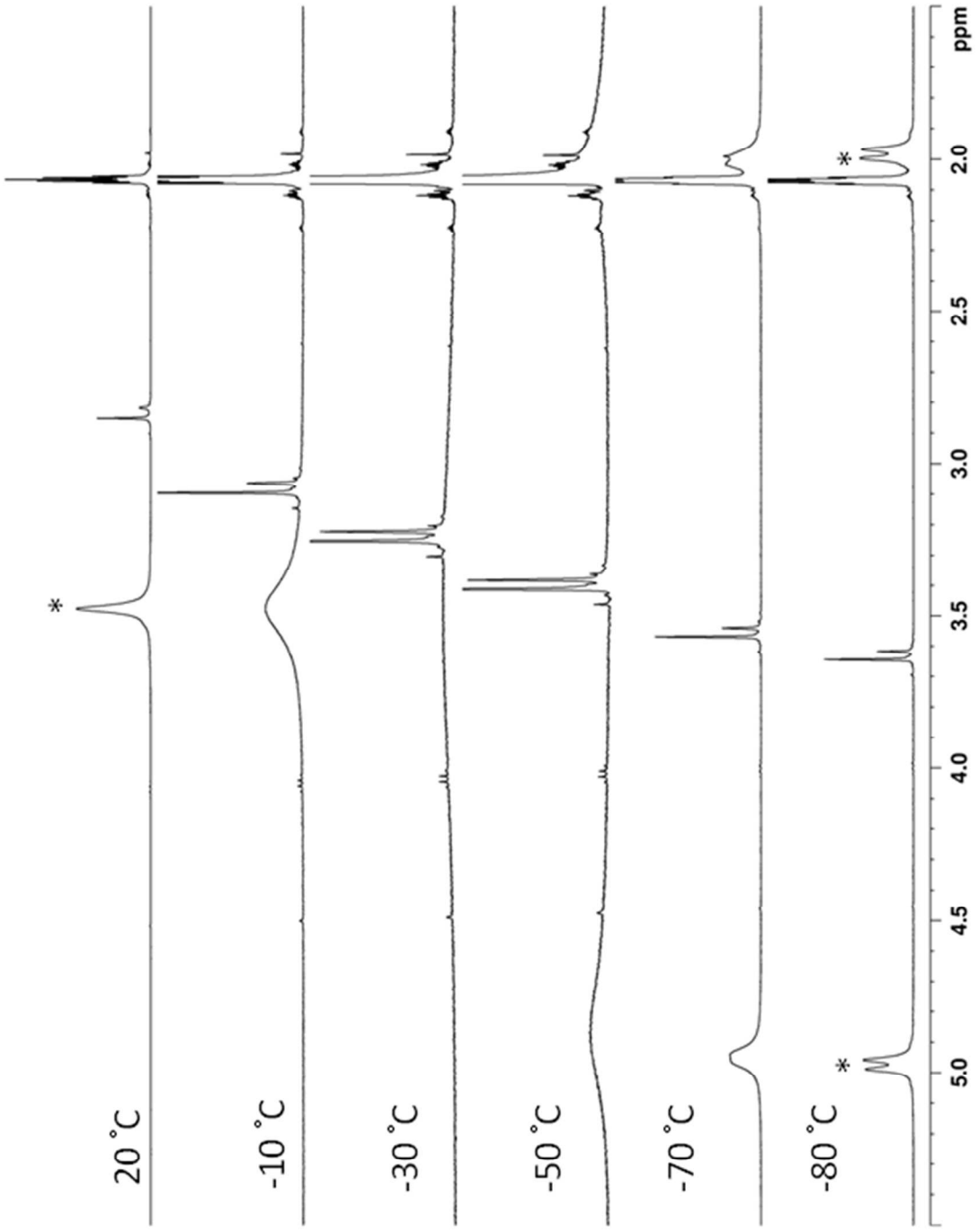
Table of Contents

Page

Full Gaussian reference 44.

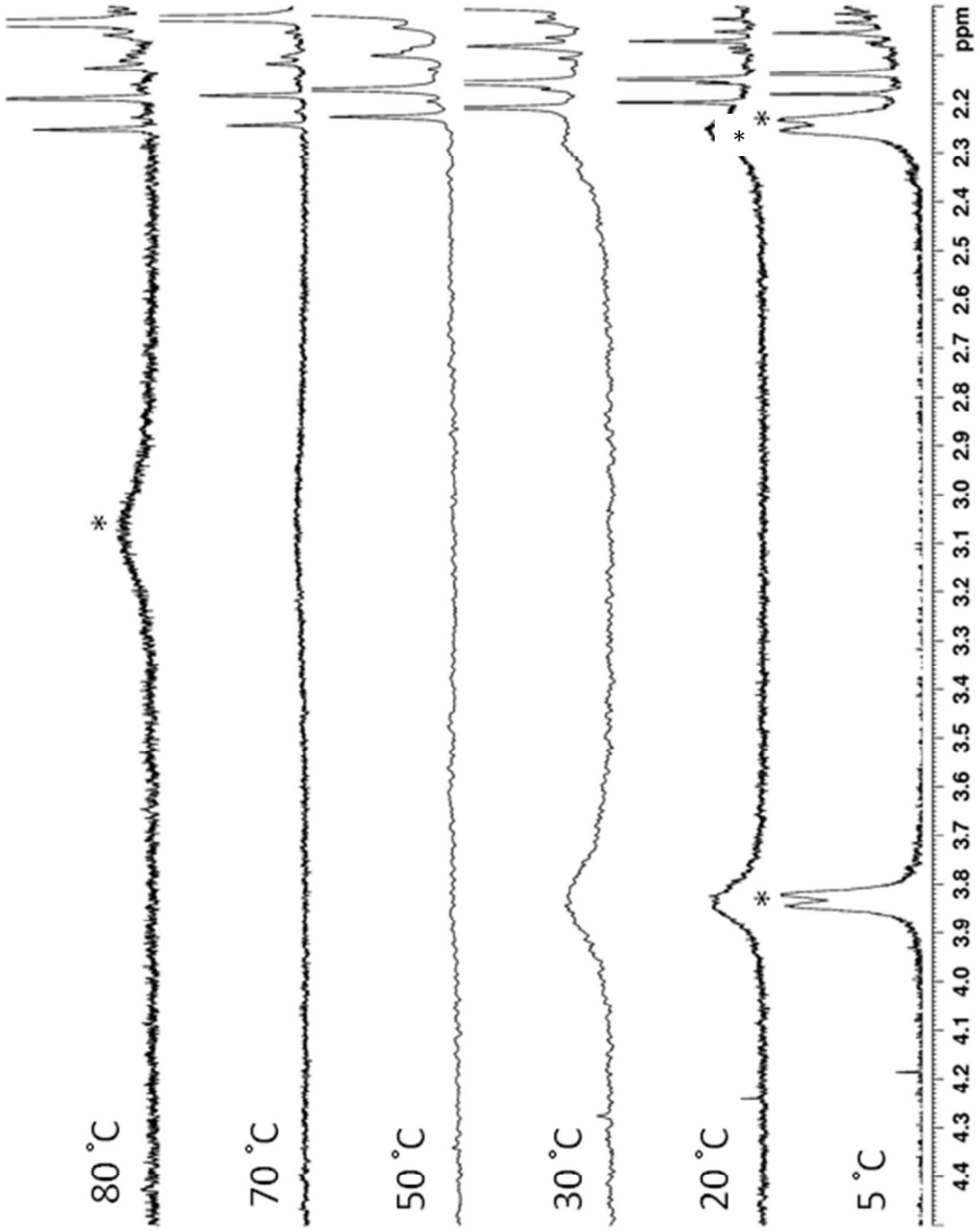
Gaussian 09, Revision **C.01**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Benzazepine 2a variable temperature (VT) data plot



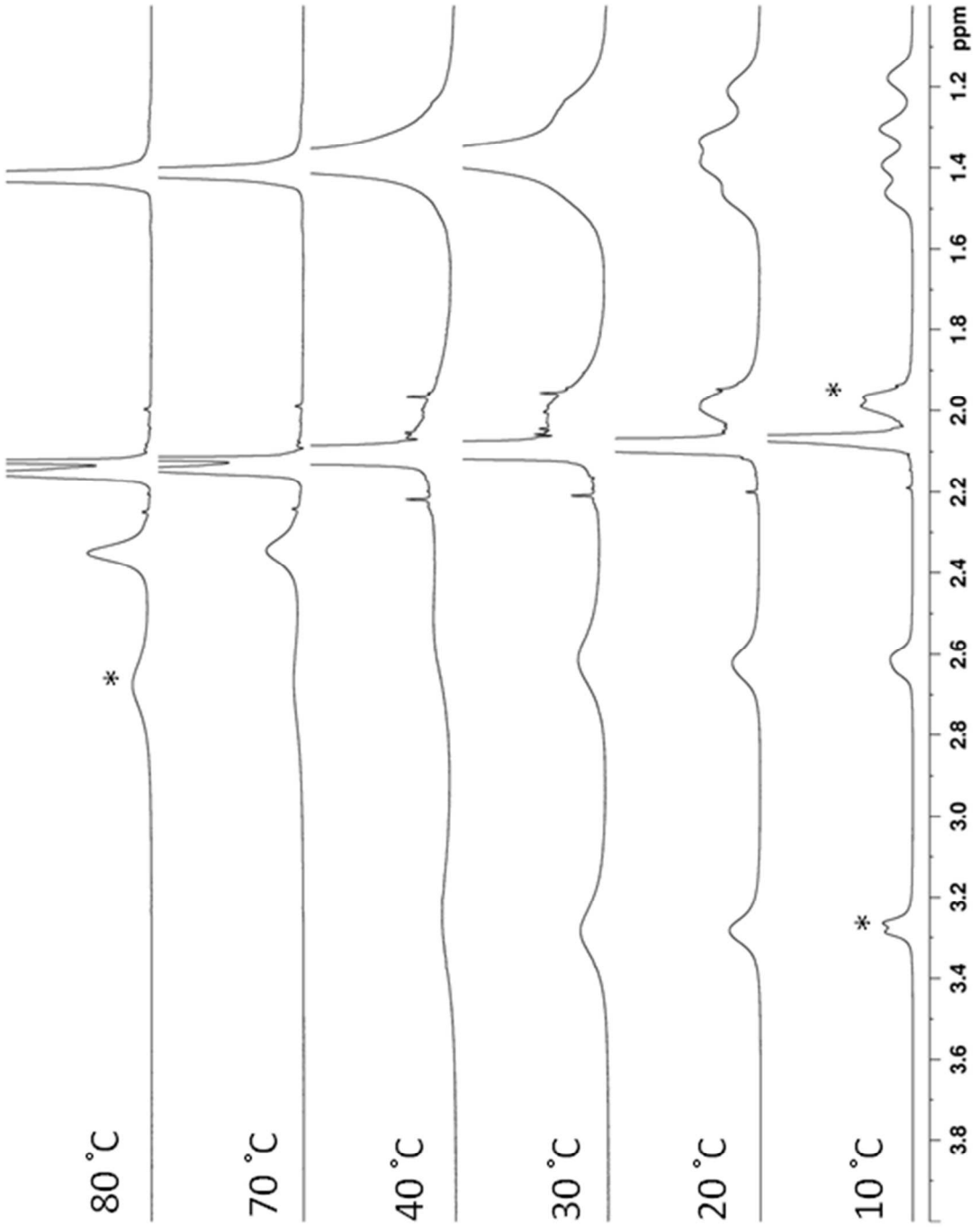
Solvent: acetone-d_6 NMR: 400 MHz
Temperatures are listed from bottom to top and marked on the spectrum. The $3CH_2$ protons are marked with a * at the lowest and highest temperatures.

Benzazepine 2b variable temperature (VT) data plot



Solvent: C_6D_6 NMR: 500 MHz
Temperatures are listed from bottom to top and marked on the spectrum. The $3CH_2$ protons are marked with a * at the lowest and highest temperatures.

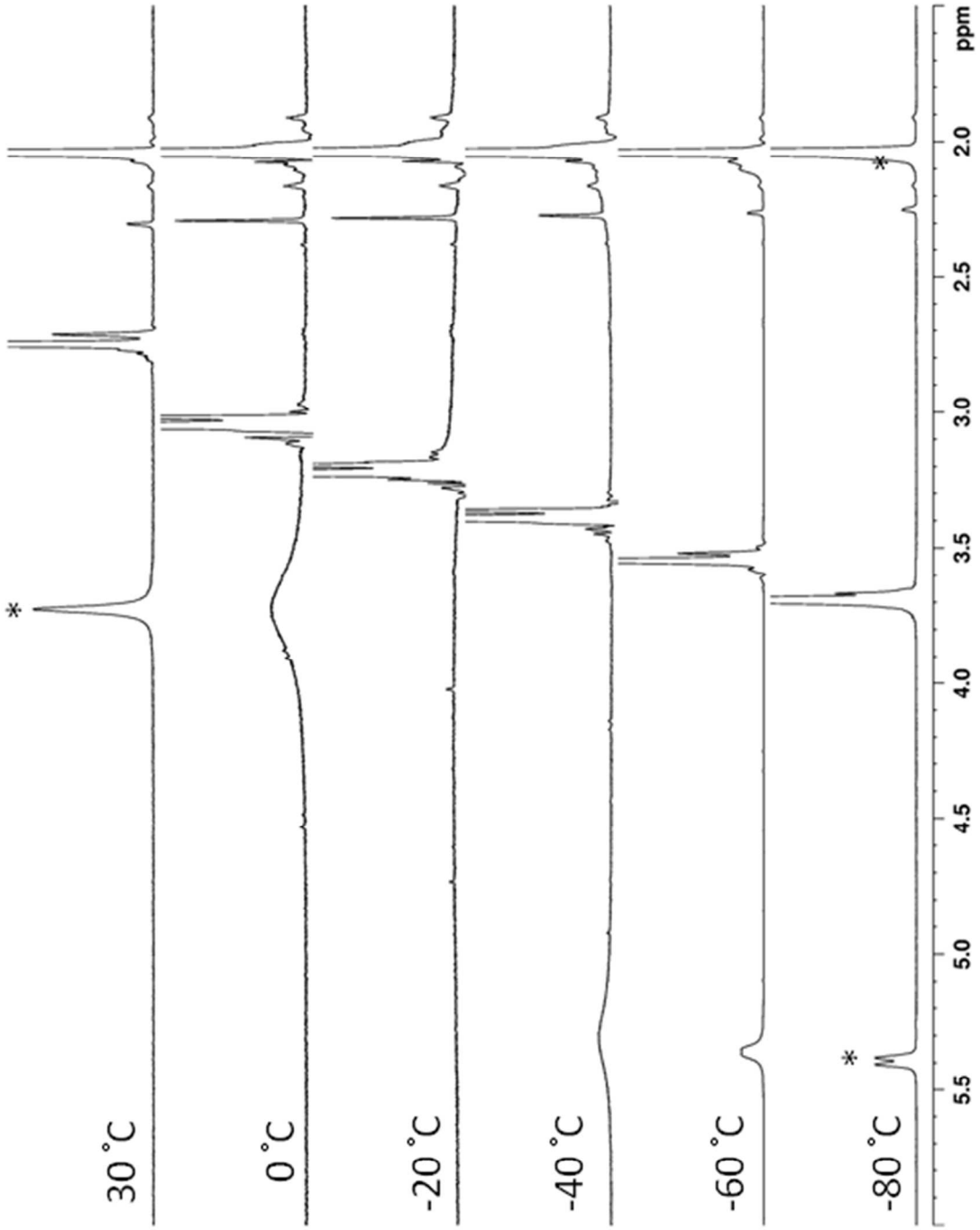
Benzazepine 2c variable temperature (VT) data plot



Solvent: C_6D_6 NMR: 400 MHz

Temperatures are listed from bottom to top and marked on the spectrum. The $3CH_2$ protons are marked with a * at the lowest and highest temperatures.

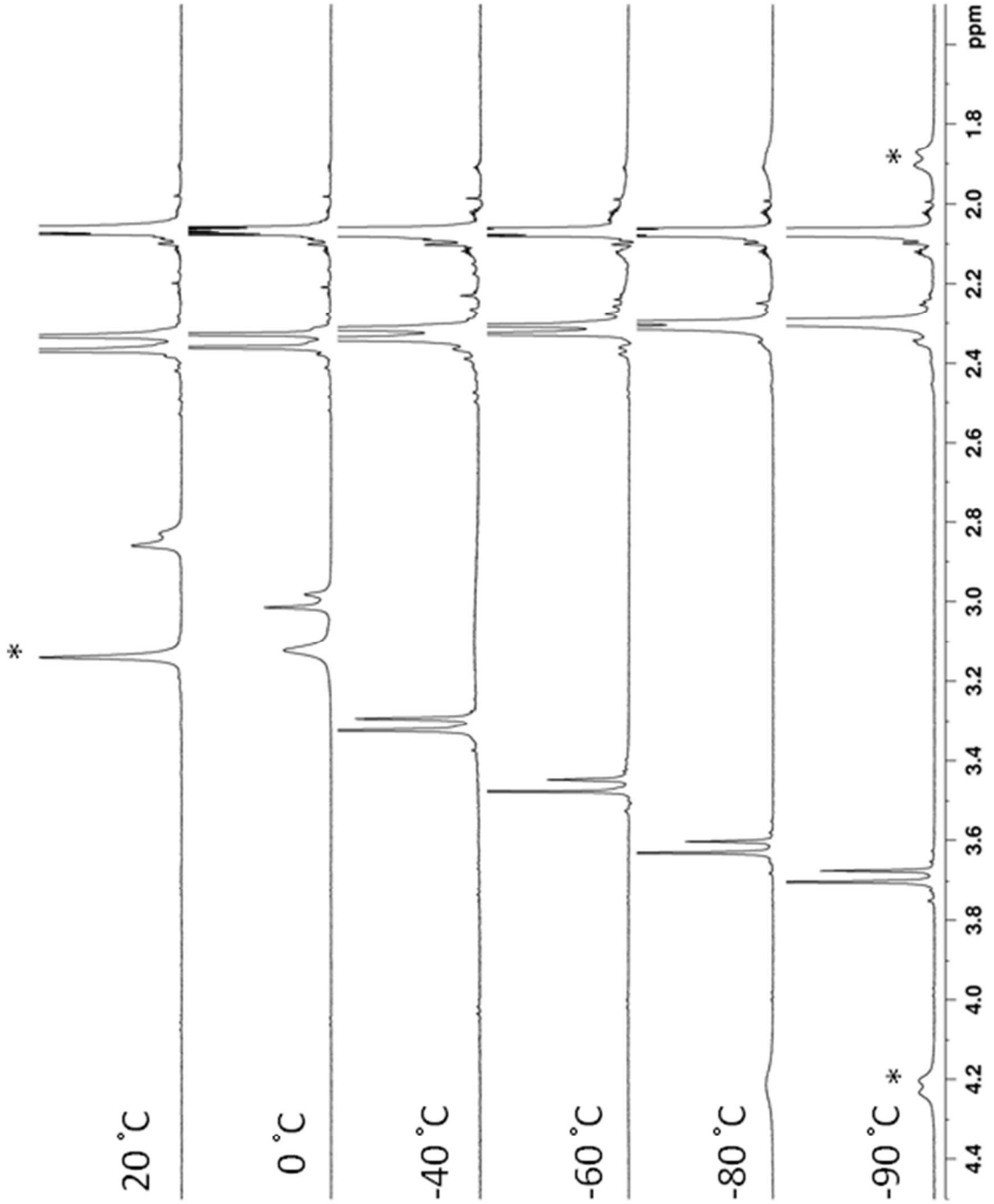
Benzazepine 2d variable temperature (VT) data plot



Solvent: acetone-d_6 NMR: 500 MHz

Temperatures are listed from bottom to top and marked on the spectrum. The $3CH_2$ protons are marked with a * at the lowest and highest temperatures. The second methylene proton is hidden underneath a solvent signal at 2.05 ppm.

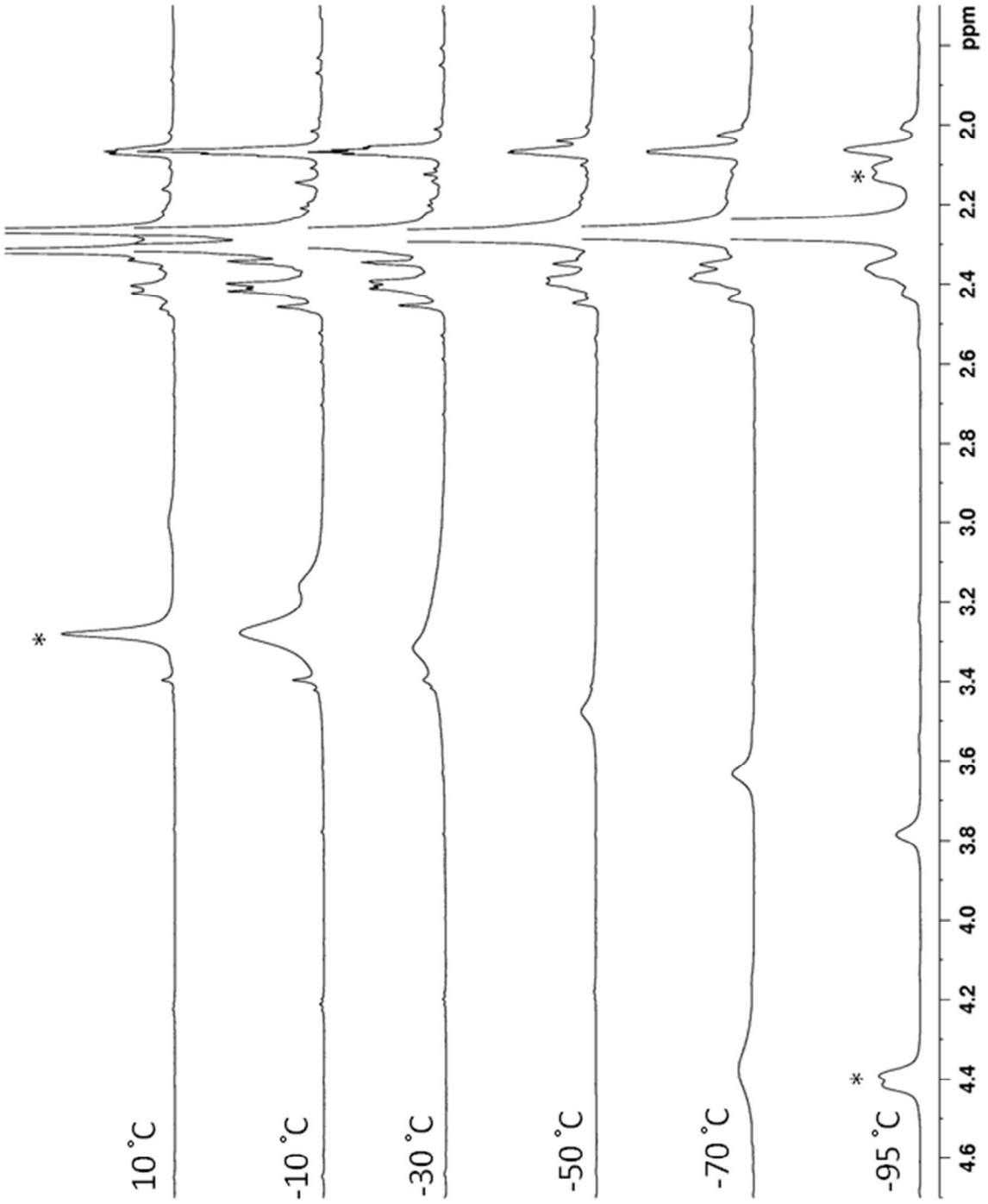
Benzazepine 2e variable temperature (VT) data plot



Solvent: acetone-d_6 NMR: 400 MHz

Temperatures are listed from bottom to top and marked on the spectrum. The $3CH_2$ protons are marked with a * at the lowest and highest temperatures.

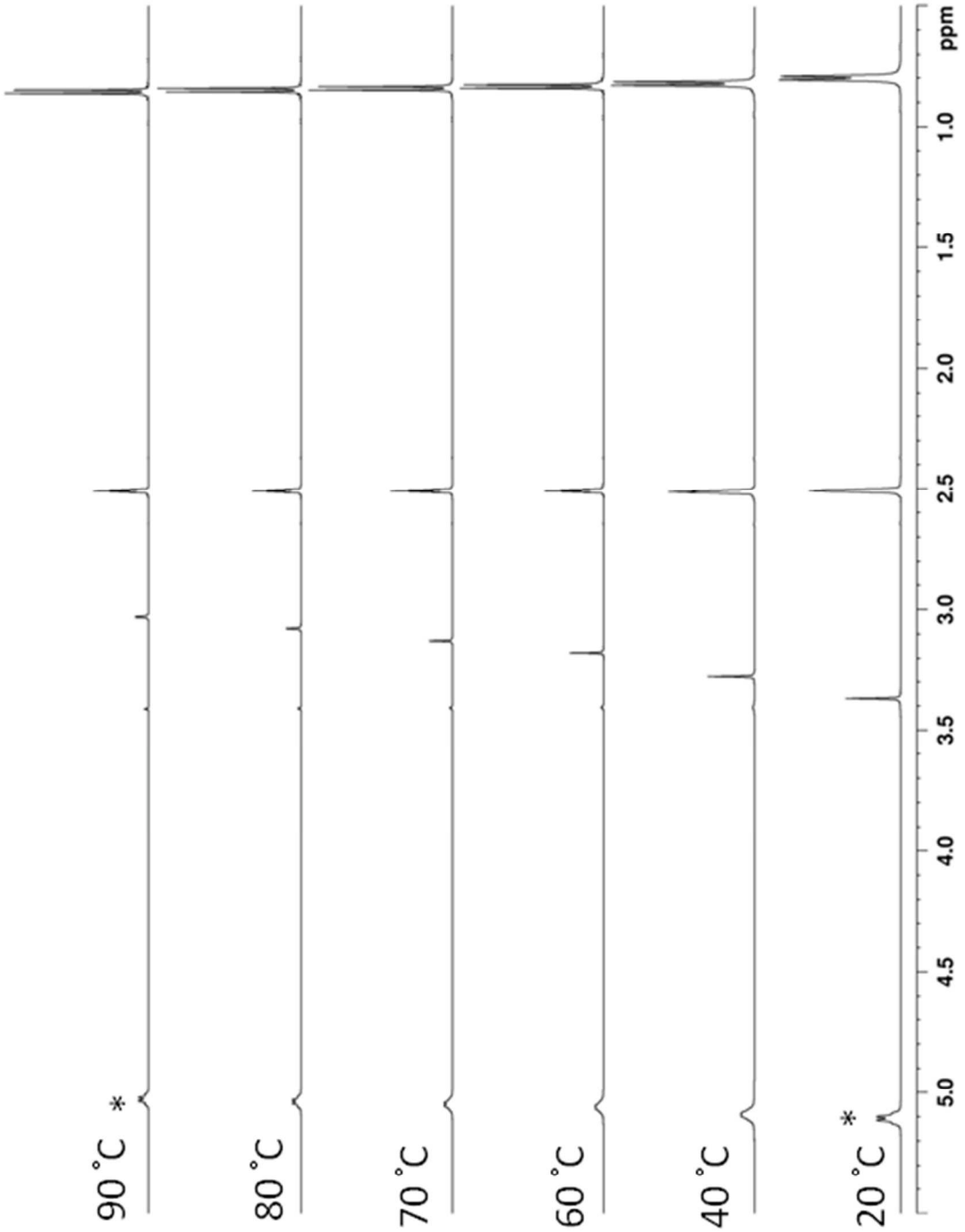
Benzazepine 2f variable temperature (VT) data plot



Solvent: acetone-d_6 NMR: 400 MHz

Temperatures are listed from bottom to top and marked on the spectrum. The $3CH_2$ protons are marked with a * at the lowest and highest temperatures.

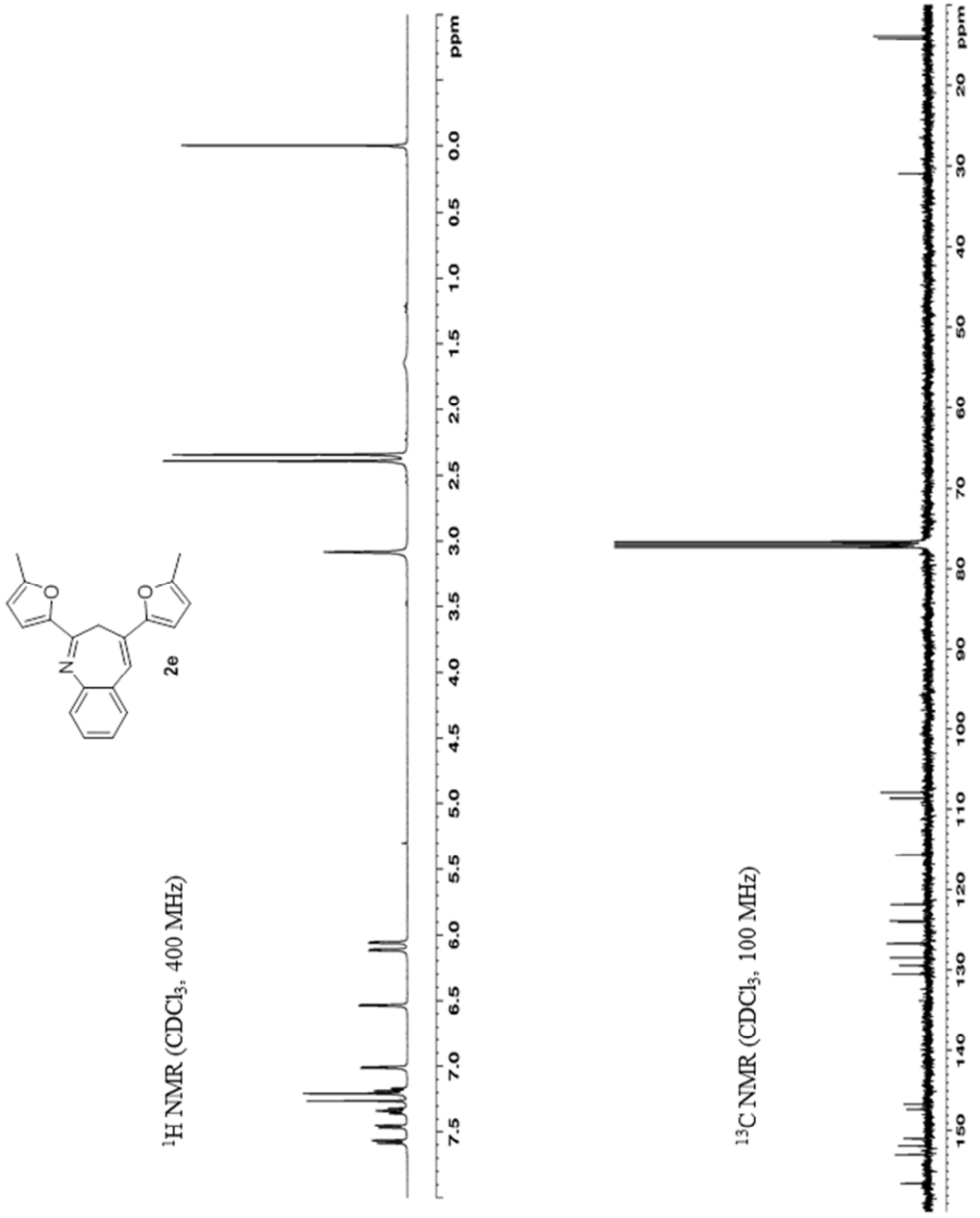
Benzazepine 2g variable temperature (VT) data plot



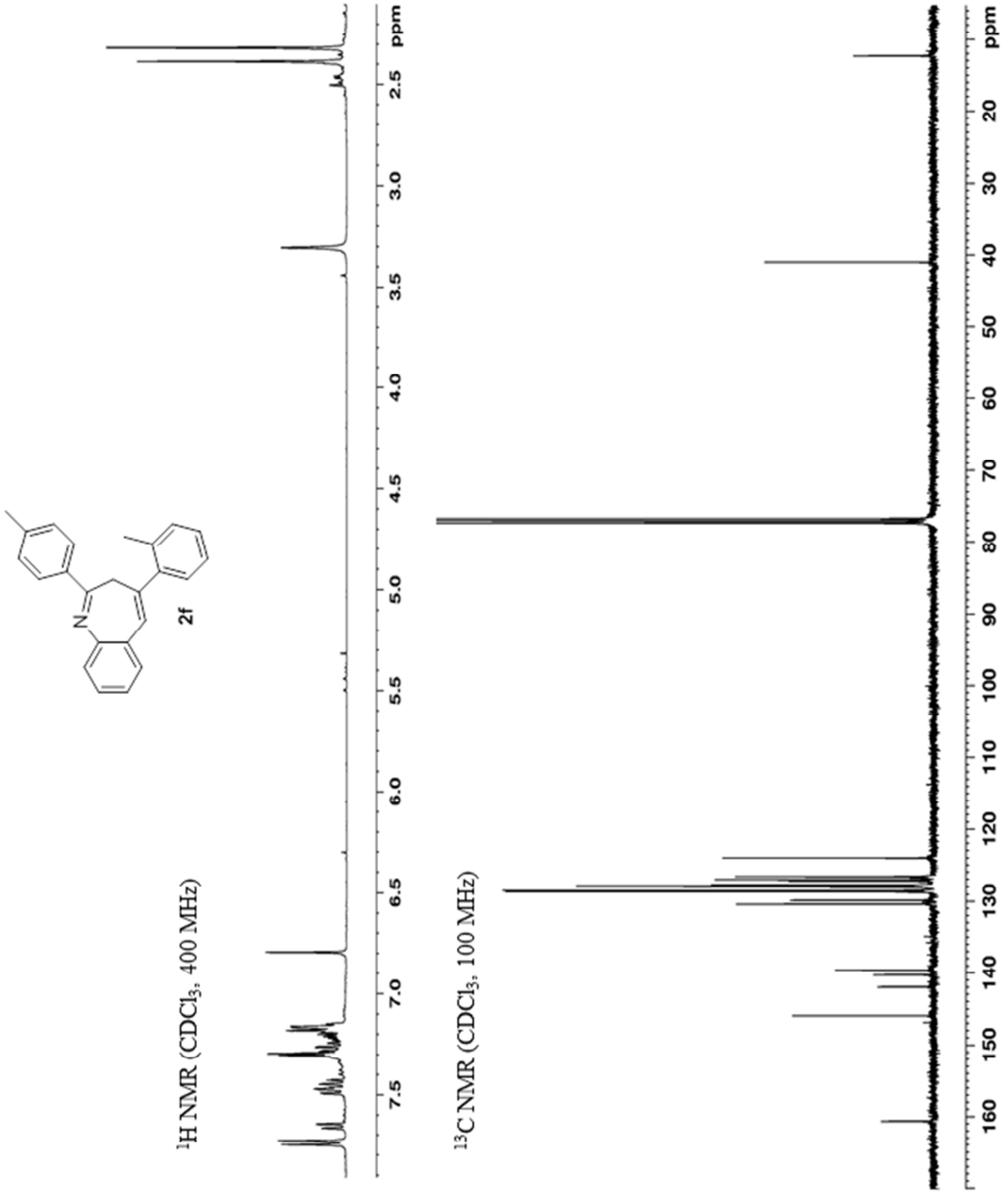
Solvent: DMSO-d_6 NMR: 500 MHz

Temperatures are listed from bottom to top and marked on the spectrum. The 3CH protons is marked with a * at the lowest and highest temperatures. There is hardly any movement of chemical shifts because activation energy is >> 17 kcal/mol.

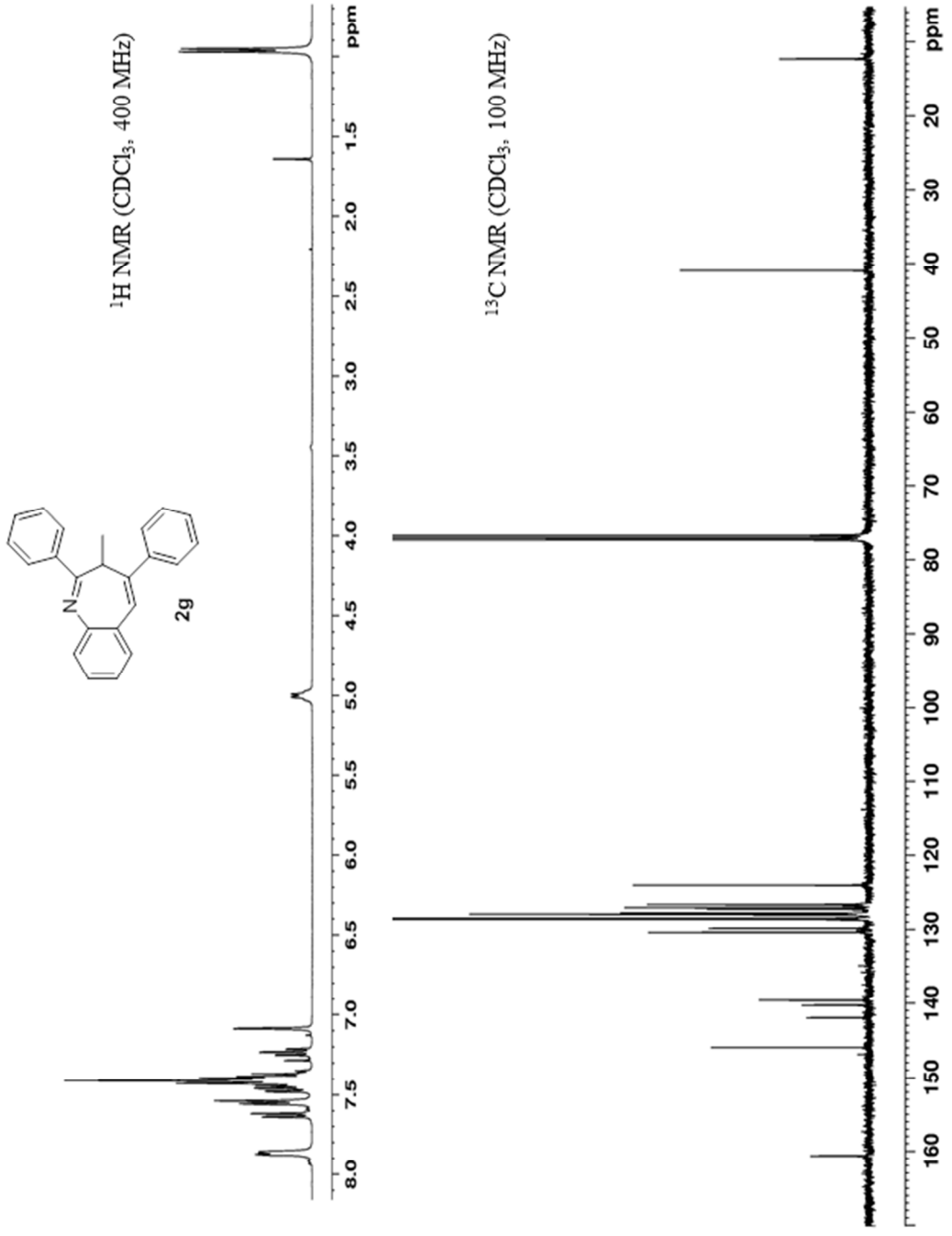
^{1}H and ^{13}C NMR spectra for 2e



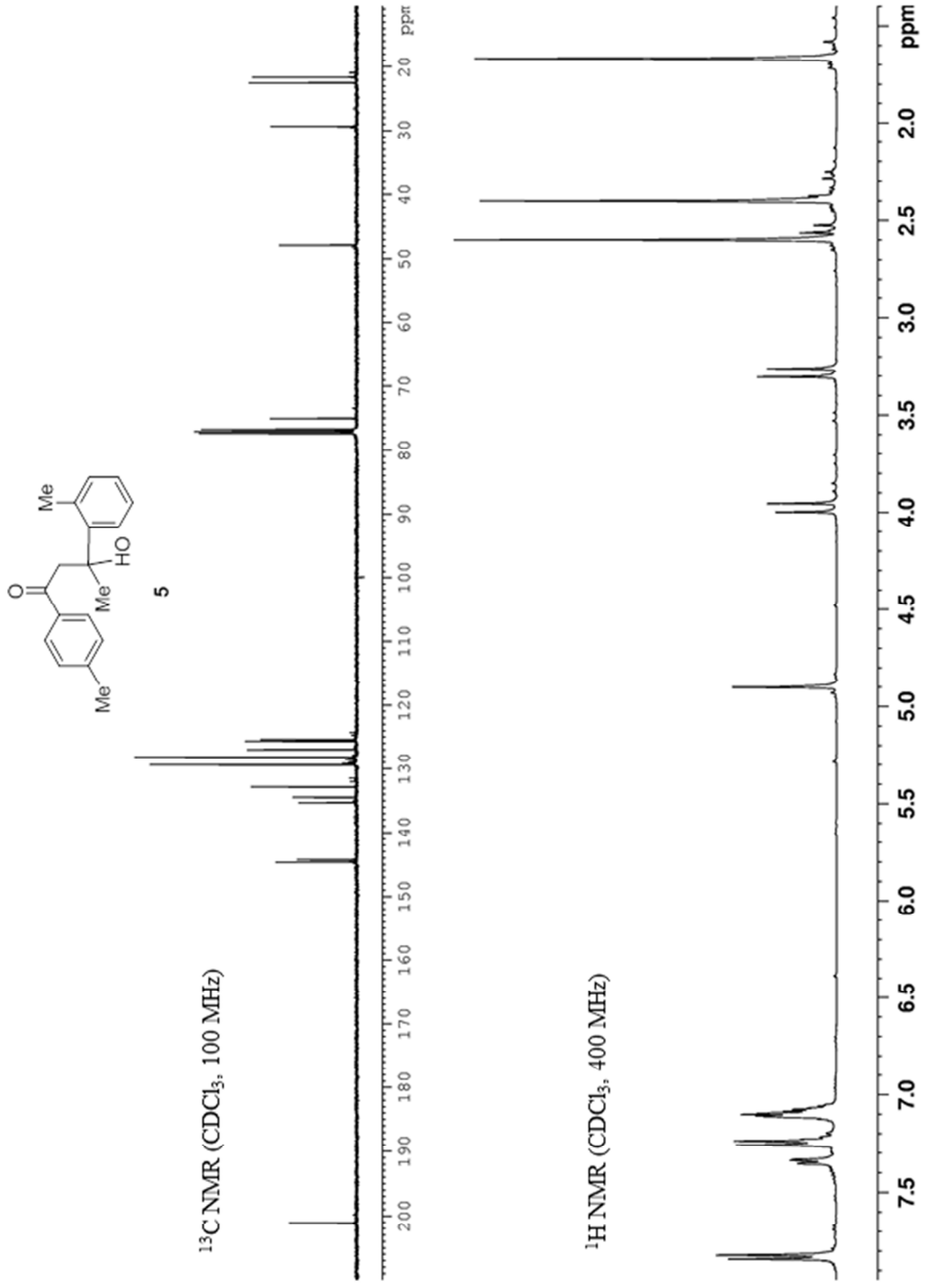
^{1}H and ^{13}C NMR spectra for 2f



^{1}H and ^{13}C NMR spectra for 2g



^{1}H and ^{13}C NMR spectra for 5



^{1}H and ^{13}C NMR spectra for 6

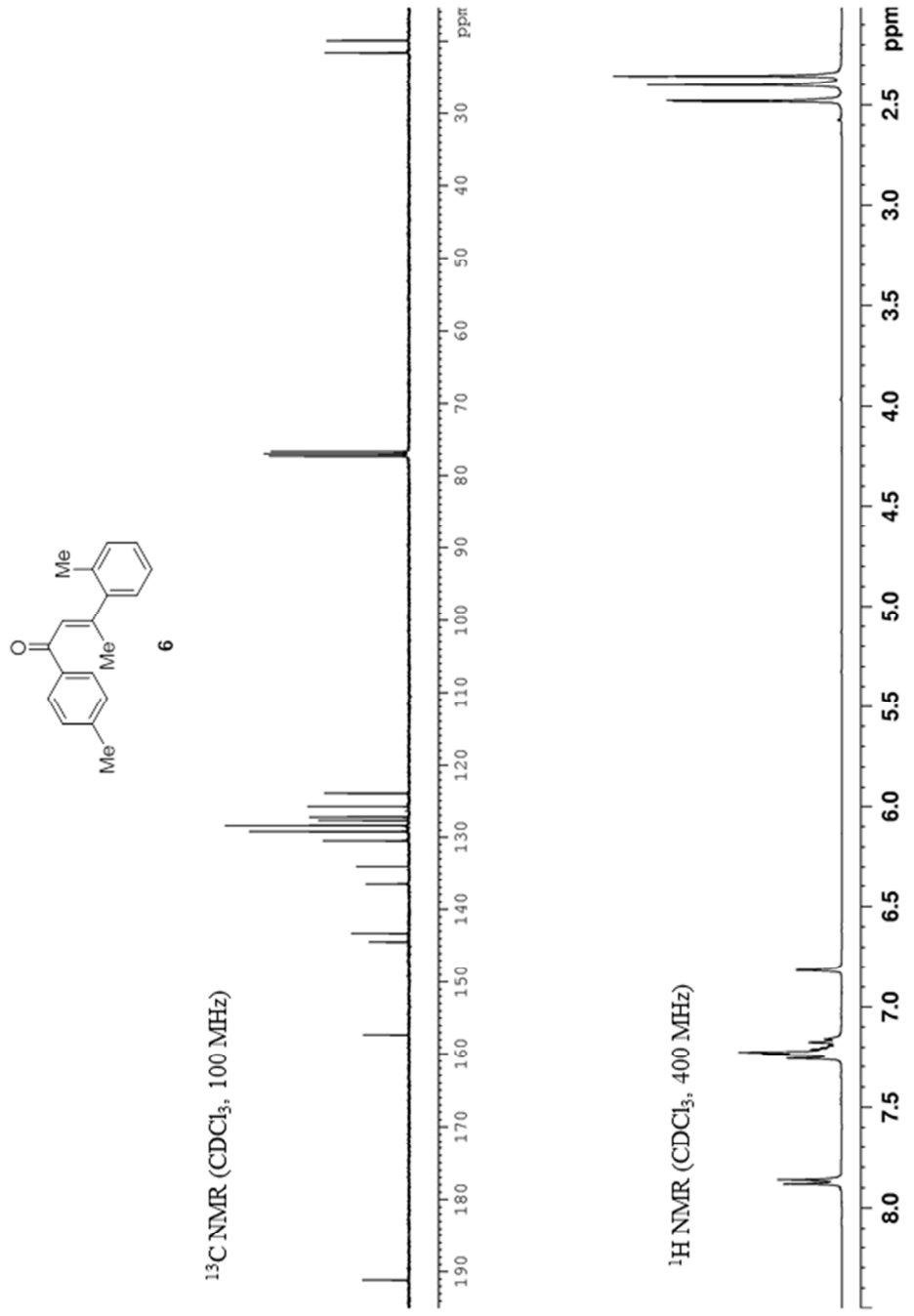
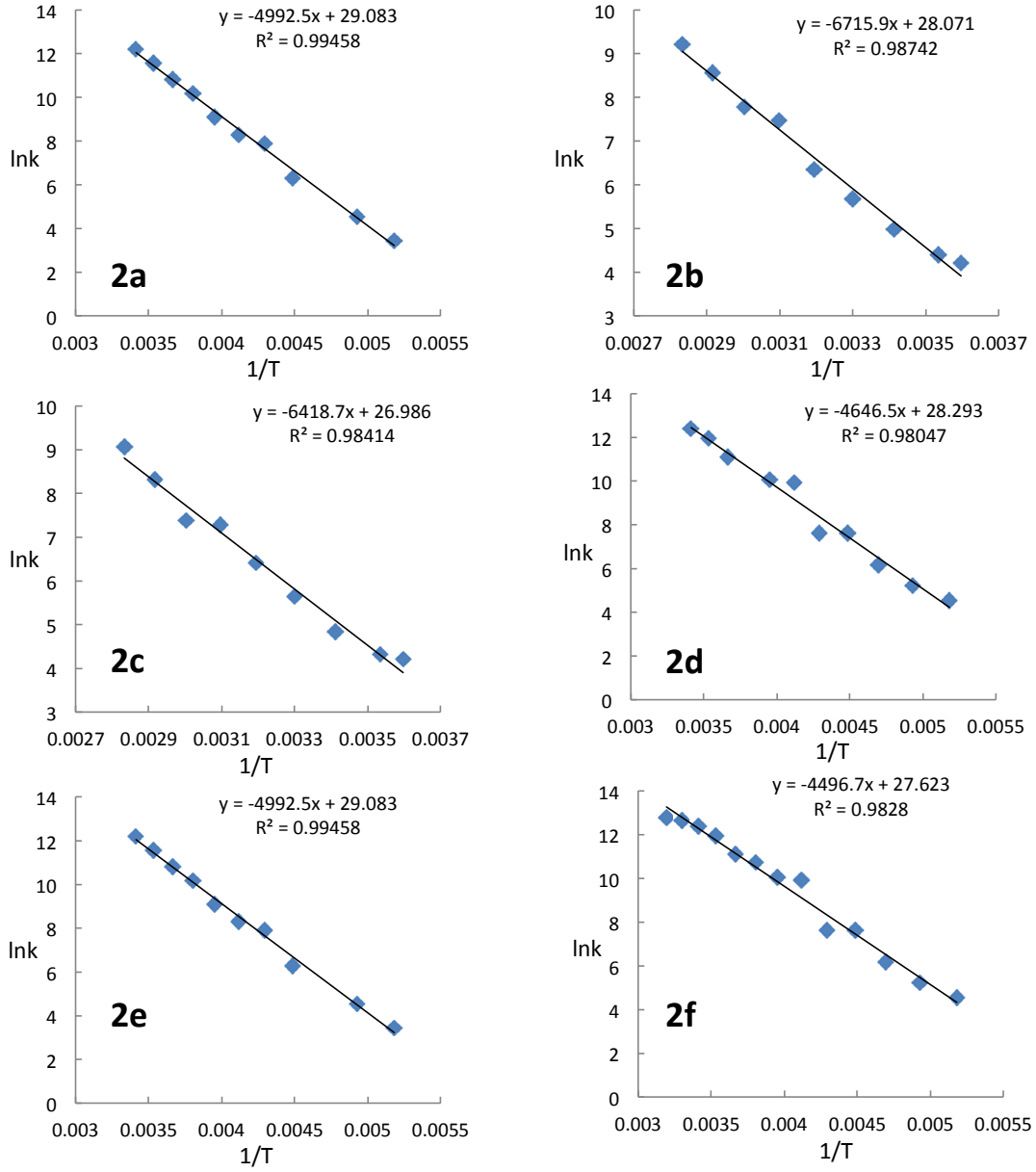


Figure S1: Arrhenius plots of lnk vs 1/T for various benzazepines 2a-2f.



Note: The equation for the linear fit and R^2 values are indicated in each plot.

Figure S2: Eyring plots of ln(k/T) vs 1/T for various benzazepines 2a-2f.

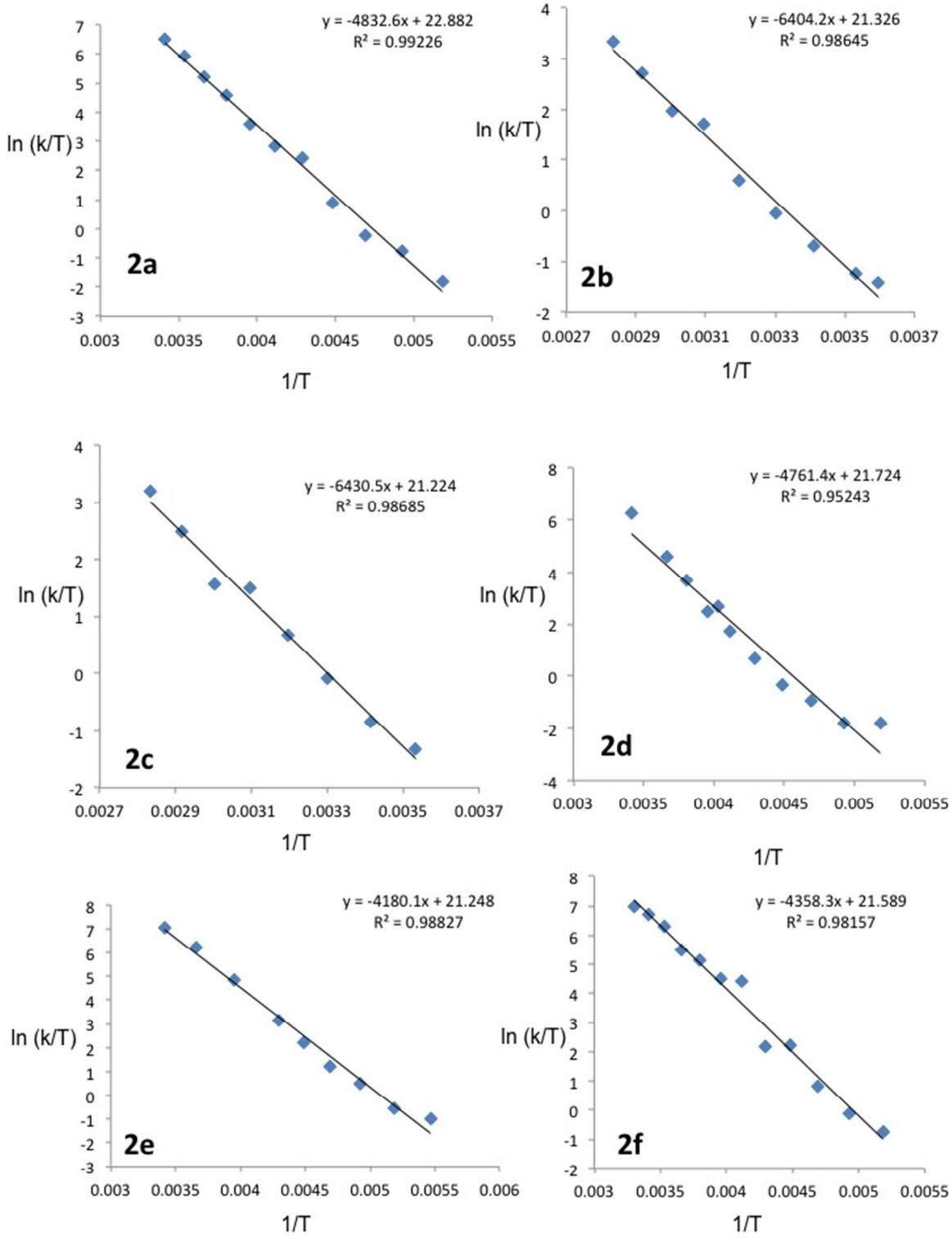


Table S1. Crystal data and structure refinement for 2g.

Identification code	2g
Empirical formula	C23 H19 N
Formula weight	309.39
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Aba2
Unit cell dimensions	a = 13.2591(4) A alpha = 90 deg. b = 25.5247(7) A beta = 90 deg. c = 10.0154(3) A gamma = 90 deg.
Volume	3389.56(17) A^3
Z, Calculated density	8, 1.213 Mg/m^3
Absorption coefficient	0.070 mm^-1
F(000)	1312
Crystal size	.5 x .5 x .4 mm
Theta range for data collection	2.21 to 27.49 deg.
Limiting indices	-17<=h<=16, -33<=k<=33, -13<=l<=12
Reflections collected / unique	16296 / 2057 [R(int) = 0.0373]
Completeness to theta = 27.49	99.8 %
Absorption correction	Multi-scan
Max. and min. transmission	0.7460 and 0.5998
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2057 / 1 / 218
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.0891
R indices (all data)	R1 = 0.0421, wR2 = 0.0943
Absolute structure parameter	0(10)

Largest diff. peak and hole 0.125 and -0.133 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2g.

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	9304(1)	8325(1)	969(2)	52(1)
C(2)	9278(1)	8731(1)	1710(2)	48(1)
C(3)	10204(1)	9053(1)	2085(2)	51(1)
C(4)	10830(1)	8717(1)	3014(2)	48(1)
C(5)	11213(1)	8258(1)	2592(2)	51(1)
C(6)	11058(2)	8011(1)	1304(2)	52(1)
C(7)	10182(2)	8078(1)	521(2)	52(1)
C(21)	8269(2)	8895(1)	2215(2)	51(1)
C(22)	7408(2)	8705(1)	1584(3)	67(1)
C(23)	6460(2)	8851(1)	2005(3)	85(1)
C(24)	6346(2)	9178(1)	3070(3)	84(1)
C(25)	7172(2)	9362(1)	3721(3)	82(1)
C(26)	8134(2)	9223(1)	3300(2)	65(1)
C(41)	11028(1)	8911(1)	4383(2)	49(1)
C(42)	11130(2)	8574(1)	5460(2)	58(1)
C(43)	11339(2)	8761(1)	6724(3)	68(1)
C(44)	11445(2)	9288(1)	6943(2)	70(1)
C(45)	11343(2)	9630(1)	5900(3)	73(1)
C(46)	11142(2)	9446(1)	4631(2)	65(1)
C(31)	10774(2)	9263(1)	868(3)	67(1)
C(13)	11811(2)	7674(1)	816(3)	62(1)
C(14)	11736(2)	7443(1)	-421(3)	67(1)
C(15)	10894(2)	7523(1)	-1200(3)	69(1)
C(16)	10115(2)	7824(1)	-719(2)	62(1)

Table S3. Bond lengths [A] and angles [deg] for 2g.

N(1)-C(2)	1.277(2)
N(1)-C(7)	1.397(3)
C(2)-C(21)	1.490(3)
C(2)-C(3)	1.524(2)
C(3)-C(4)	1.513(3)
C(3)-C(31)	1.532(3)
C(3)-H(3)	0.9800
C(4)-C(5)	1.346(3)
C(4)-C(41)	1.481(3)
C(5)-C(6)	1.451(3)
C(5)-H(5)	0.9300
C(6)-C(13)	1.405(3)
C(6)-C(7)	1.411(3)
C(7)-C(16)	1.404(3)
C(21)-C(26)	1.384(3)
C(21)-C(22)	1.392(3)
C(22)-C(23)	1.377(4)
C(22)-H(22)	0.9300
C(23)-C(24)	1.363(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.358(4)
C(24)-H(24)	0.9300
C(25)-C(26)	1.390(3)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(41)-C(42)	1.386(3)
C(41)-C(46)	1.397(3)
C(42)-C(43)	1.381(3)
C(42)-H(42)	0.9300
C(43)-C(44)	1.372(4)
C(43)-H(43)	0.9300
C(44)-C(45)	1.366(4)
C(44)-H(44)	0.9300
C(45)-C(46)	1.380(4)
C(45)-H(45)	0.9300
C(46)-H(46)	0.9300
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(13)-C(14)	1.377(4)
C(13)-H(13)	0.9300
C(14)-C(15)	1.377(4)
C(14)-H(14)	0.9300
C(15)-C(16)	1.374(3)
C(15)-H(15)	0.9300
C(16)-H(16)	0.9300
C(2)-N(1)-C(7)	125.06(16)
N(1)-C(2)-C(21)	116.67(16)

N(1)-C(2)-C(3)	124.03(17)
C(21)-C(2)-C(3)	119.30(16)
C(4)-C(3)-C(2)	106.75(13)
C(4)-C(3)-C(31)	114.66(17)
C(2)-C(3)-C(31)	113.01(17)
C(4)-C(3)-H(3)	107.4
C(2)-C(3)-H(3)	107.4
C(31)-C(3)-H(3)	107.4
C(5)-C(4)-C(41)	121.01(18)
C(5)-C(4)-C(3)	120.46(18)
C(41)-C(4)-C(3)	118.52(16)
C(4)-C(5)-C(6)	127.24(19)
C(4)-C(5)-H(5)	116.4
C(6)-C(5)-H(5)	116.4
C(13)-C(6)-C(7)	117.85(19)
C(13)-C(6)-C(5)	118.30(19)
C(7)-C(6)-C(5)	123.83(18)
N(1)-C(7)-C(16)	116.05(19)
N(1)-C(7)-C(6)	124.26(18)
C(16)-C(7)-C(6)	119.09(19)
C(26)-C(21)-C(22)	117.5(2)
C(26)-C(21)-C(2)	123.48(18)
C(22)-C(21)-C(2)	119.0(2)
C(23)-C(22)-C(21)	121.1(2)
C(23)-C(22)-H(22)	119.5
C(21)-C(22)-H(22)	119.5
C(24)-C(23)-C(22)	120.4(3)
C(24)-C(23)-H(23)	119.8
C(22)-C(23)-H(23)	119.8
C(25)-C(24)-C(23)	119.9(2)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.4(3)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(21)-C(26)-C(25)	120.8(2)
C(21)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.6
C(42)-C(41)-C(46)	117.2(2)
C(42)-C(41)-C(4)	122.01(16)
C(46)-C(41)-C(4)	120.73(18)
C(43)-C(42)-C(41)	121.3(2)
C(43)-C(42)-H(42)	119.4
C(41)-C(42)-H(42)	119.4
C(44)-C(43)-C(42)	120.3(2)
C(44)-C(43)-H(43)	119.8
C(42)-C(43)-H(43)	119.8
C(45)-C(44)-C(43)	119.6(2)
C(45)-C(44)-H(44)	120.2
C(43)-C(44)-H(44)	120.2
C(44)-C(45)-C(46)	120.5(2)
C(44)-C(45)-H(45)	119.8
C(46)-C(45)-H(45)	119.8

C(45)-C(46)-C(41)	121.1(2)
C(45)-C(46)-H(46)	119.5
C(41)-C(46)-H(46)	119.5
C(3)-C(31)-H(31A)	109.5
C(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(14)-C(13)-C(6)	121.6(2)
C(14)-C(13)-H(13)	119.2
C(6)-C(13)-H(13)	119.2
C(13)-C(14)-C(15)	120.3(2)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	119.6(2)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(15)-C(16)-C(7)	121.4(2)
C(15)-C(16)-H(16)	119.3
C(7)-C(16)-H(16)	119.3

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 2g.

The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	53(1)	47(1)	56(1)	1(1)	-7(1)	-5(1)
C(2)	49(1)	44(1)	50(1)	5(1)	-7(1)	-4(1)
C(3)	51(1)	43(1)	60(1)	3(1)	-10(1)	-3(1)
C(4)	43(1)	46(1)	54(1)	4(1)	-5(1)	-6(1)
C(5)	50(1)	49(1)	55(1)	5(1)	-4(1)	2(1)
C(6)	58(1)	41(1)	56(1)	3(1)	2(1)	-3(1)
C(7)	57(1)	41(1)	57(1)	2(1)	1(1)	-8(1)
C(21)	52(1)	47(1)	54(1)	11(1)	-3(1)	-2(1)
C(22)	55(1)	71(1)	77(1)	-1(1)	-2(1)	-12(1)
C(23)	52(1)	107(2)	96(2)	6(2)	1(1)	-14(1)
C(24)	58(1)	110(2)	83(2)	22(2)	17(1)	10(1)
C(25)	78(2)	97(2)	70(2)	-1(1)	8(1)	16(1)
C(26)	60(1)	73(1)	61(1)	-2(1)	-4(1)	3(1)
C(41)	41(1)	50(1)	55(1)	0(1)	-1(1)	-2(1)
C(42)	52(1)	61(1)	60(1)	5(1)	-3(1)	1(1)
C(43)	62(1)	85(2)	56(1)	11(1)	-1(1)	-2(1)
C(44)	62(1)	95(2)	53(1)	-14(1)	-1(1)	-3(1)
C(45)	84(2)	62(1)	73(2)	-13(1)	-7(1)	-5(1)
C(46)	78(1)	54(1)	61(1)	0(1)	-9(1)	-5(1)
C(31)	67(1)	60(1)	73(1)	19(1)	-11(1)	-17(1)
C(13)	65(1)	48(1)	71(1)	1(1)	3(1)	2(1)
C(14)	80(2)	50(1)	73(1)	-3(1)	17(1)	1(1)
C(15)	92(2)	54(1)	61(1)	-7(1)	9(1)	-12(1)
C(16)	73(1)	53(1)	60(1)	-4(1)	-2(1)	-12(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2g.

	x	y	z	U(eq)
H(3)	9969	9356	2599	62
H(5)	11622	8079	3192	61
H(22)	7474	8477	866	81
H(23)	5893	8725	1561	102
H(24)	5704	9275	3351	101
H(25)	7093	9583	4452	98
H(26)	8694	9351	3753	78
H(42)	11057	8216	5328	69
H(43)	11409	8527	7432	81
H(44)	11585	9413	7795	84
H(45)	11409	9988	6047	88
H(46)	11082	9683	3930	77
H(31A)	11334	9472	1161	100
H(31B)	10329	9474	337	100
H(31C)	11017	8975	342	100
H(13)	12374	7606	1342	74
H(14)	12256	7231	-733	81
H(15)	10852	7375	-2046	83
H(16)	9532	7861	-1225	75

Table S6. Torsion angles [deg] for 2g.

C(7)-N(1)-C(2)-C(21)	-172.66(18)
C(7)-N(1)-C(2)-C(3)	7.9(3)
N(1)-C(2)-C(3)-C(4)	-69.5(2)
C(21)-C(2)-C(3)-C(4)	111.15(19)
N(1)-C(2)-C(3)-C(31)	57.5(2)
C(21)-C(2)-C(3)-C(31)	-121.9(2)
C(2)-C(3)-C(4)-C(5)	61.9(2)
C(31)-C(3)-C(4)-C(5)	-64.1(2)
C(2)-C(3)-C(4)-C(41)	-119.41(17)
C(31)-C(3)-C(4)-C(41)	114.62(19)
C(41)-C(4)-C(5)-C(6)	177.82(17)
C(3)-C(4)-C(5)-C(6)	-3.5(3)
C(4)-C(5)-C(6)-C(13)	152.7(2)
C(4)-C(5)-C(6)-C(7)	-28.8(3)
C(2)-N(1)-C(7)-C(16)	-149.88(19)
C(2)-N(1)-C(7)-C(6)	39.1(3)
C(13)-C(6)-C(7)-N(1)	168.51(17)
C(5)-C(6)-C(7)-N(1)	-10.0(3)
C(13)-C(6)-C(7)-C(16)	-2.2(3)
C(5)-C(6)-C(7)-C(16)	179.32(17)
N(1)-C(2)-C(21)-C(26)	161.0(2)
C(3)-C(2)-C(21)-C(26)	-19.5(3)
N(1)-C(2)-C(21)-C(22)	-18.1(3)
C(3)-C(2)-C(21)-C(22)	161.32(18)
C(26)-C(21)-C(22)-C(23)	1.6(3)
C(2)-C(21)-C(22)-C(23)	-179.2(2)
C(21)-C(22)-C(23)-C(24)	-1.1(4)
C(22)-C(23)-C(24)-C(25)	0.0(4)
C(23)-C(24)-C(25)-C(26)	0.6(4)
C(22)-C(21)-C(26)-C(25)	-1.0(3)
C(2)-C(21)-C(26)-C(25)	179.8(2)
C(24)-C(25)-C(26)-C(21)	0.0(4)
C(5)-C(4)-C(41)-C(42)	-33.5(3)
C(3)-C(4)-C(41)-C(42)	147.83(18)
C(5)-C(4)-C(41)-C(46)	145.1(2)
C(3)-C(4)-C(41)-C(46)	-33.6(3)
C(46)-C(41)-C(42)-C(43)	-0.2(3)
C(4)-C(41)-C(42)-C(43)	178.4(2)
C(41)-C(42)-C(43)-C(44)	0.4(3)
C(42)-C(43)-C(44)-C(45)	-0.1(4)
C(43)-C(44)-C(45)-C(46)	-0.5(4)
C(44)-C(45)-C(46)-C(41)	0.7(4)
C(42)-C(41)-C(46)-C(45)	-0.4(3)
C(4)-C(41)-C(46)-C(45)	-179.0(2)
C(7)-C(6)-C(13)-C(14)	4.2(3)
C(5)-C(6)-C(13)-C(14)	-177.28(18)
C(6)-C(13)-C(14)-C(15)	-2.2(3)
C(13)-C(14)-C(15)-C(16)	-1.9(3)
C(14)-C(15)-C(16)-C(7)	3.8(3)

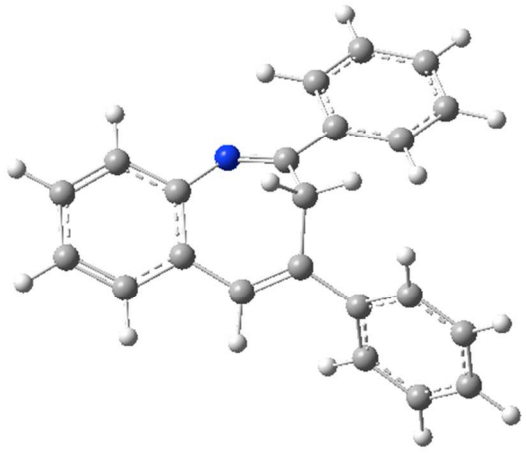
N(1)-C(7)-C(16)-C(15)	-173.19(18)
C(6)-C(7)-C(16)-C(15)	-1.7(3)

Table S7. Proposed Hydrogen Bonds and other close contacts for **(2g)**

D-H···A	D-H, Å	H···A, Å	D···A, Å	□D-H···A, deg
C15-H15···N1[a]	0.93	2.680	3.653	162
C22-H22···C14 [b]	0.93	2.850	3.662	146
C22···C25 [c]			3.368	

[a] 2-x,3/2+y,-1+z [b] -1/2+x,3/2-y, z [c] 3/2-x, y, -1/2+z

Energies, Cartesian Coordinates, and negative frequencies of all structures reported in Figure 1 and 2 (manuscript) at the B3LYP/6-31G(d) level of theory.



2a

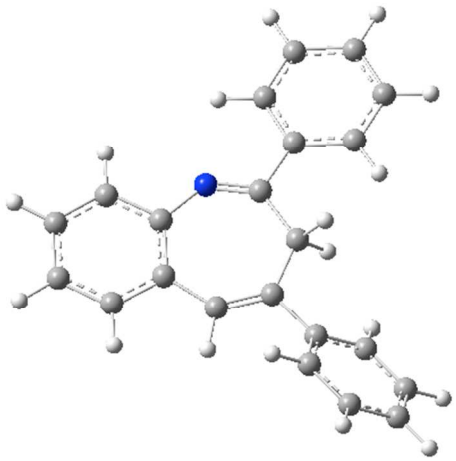
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.326537 (Hartree/Particle)
Thermal correction to Energy= 0.343767
Thermal correction to Enthalpy= 0.344711
Thermal correction to Gibbs Free Energy= 0.280300
Sum of electronic and zero-point Energies= -903.001089
Sum of electronic and thermal Energies= -902.983859
Sum of electronic and thermal Enthalpies= -902.982915
Sum of electronic and thermal Free Energies= -903.047326

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	215.717	71.167	135.564

0 1

C	-2.33366900	-1.18307100	-0.14146300
C	-2.60599600	0.20904400	0.03237100
C	-0.45961000	1.12887600	0.43405100
C	0.12228200	-1.25259000	0.34564900
C	-0.03594700	-0.06784900	1.27505600
H	0.87199900	0.14262100	1.83899200
C	-3.43377400	-2.06206200	-0.27529700
H	-3.22808600	-3.11633200	-0.44740200
C	-3.95096200	0.63575100	0.11086900
C	-5.00229400	-0.26203600	0.04796600
H	-6.02576200	0.09369800	0.13092200
C	-4.74291000	-1.62618900	-0.16148500
H	-5.56269300	-2.33445100	-0.24341400

H	-4.12982200	1.70188300	0.21365600
C	0.49651900	2.22974800	0.14667900
C	1.88155000	2.08312100	0.32936300
C	0.01039700	3.45976500	-0.33465800
C	2.75283500	3.13465600	0.04255100
H	2.29520200	1.13798600	0.66593800
C	0.87933800	4.51042200	-0.60697000
H	-1.05841200	3.56693600	-0.48306500
C	2.25632100	4.35309900	-0.41933800
H	3.82203900	2.99732500	0.17995700
H	0.48396800	5.45637900	-0.96780700
C	-0.99407100	-1.74059900	-0.25310500
N	-1.65355500	1.21918400	-0.03840100
C	1.45594900	-1.85251000	0.11653600
C	2.40911700	-1.93686700	1.14890200
C	1.80368300	-2.37692200	-1.14288200
C	3.65063500	-2.53425800	0.93533000
H	2.16734400	-1.56016500	2.13893200
C	3.04344900	-2.97551600	-1.35589300
H	1.10019700	-2.28606800	-1.96524500
C	3.97402900	-3.05729000	-0.31777400
H	4.36427900	-2.59620700	1.75276300
H	3.28916900	-3.36610700	-2.33996300
H	4.94365100	-3.51803400	-0.48566200
H	2.93520200	5.17411700	-0.63421600
H	-0.91369500	-2.66617700	-0.82059100
H	-0.84090800	-0.26201500	1.99625500



TS-2a

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 37.1i cm-1

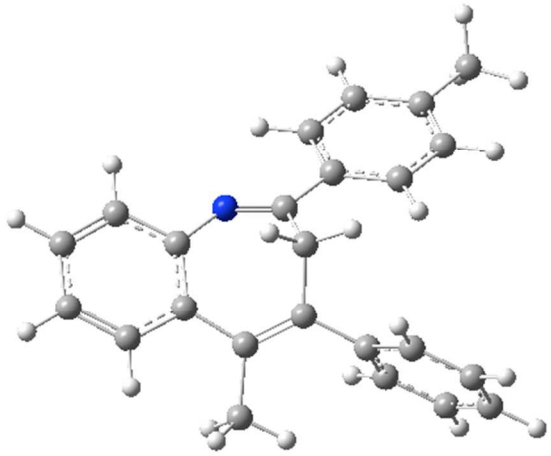
Zero-point correction= 0.326191 (Hartree/Particle)
Thermal correction to Energy= 0.342874
Thermal correction to Enthalpy= 0.343819
Thermal correction to Gibbs Free Energy= 0.280898
Sum of electronic and zero-point Energies= -902.986451
Sum of electronic and thermal Energies= -902.969768
Sum of electronic and thermal Enthalpies= -902.968824
Sum of electronic and thermal Free Energies= -903.031744

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	215.157	69.493	132.427

0 1

C	0.45178000	2.41236800	0.08716000
C	-0.95431000	2.21144900	0.02146000
C	-1.27758600	-0.21323600	-0.03897300
C	1.37507600	0.02129300	0.04233600
C	0.12239000	-0.81640100	-0.06471500
H	0.20217700	-1.41646500	-0.98544200
C	0.92715800	3.73710200	0.13212600
H	2.00188700	3.89410800	0.18823300
C	-1.79485000	3.34072600	-0.00267400
C	-1.29938600	4.63985300	0.03377900
H	-1.98208300	5.48468300	0.01180100
C	0.07932200	4.84008700	0.10433900
H	0.49335000	5.84402000	0.13866300
H	-2.86264200	3.15325800	-0.05036800
C	-2.38315900	-1.23084100	-0.06087400
C	-2.14689900	-2.61225500	-0.18702300
C	-3.72042200	-0.80171500	0.04660700
C	-3.20351400	-3.52470300	-0.20524100
H	-1.13818600	-2.99791500	-0.28006000
C	-4.77160300	-1.71049400	0.03167300
H	-3.90578500	0.26152000	0.14182000
C	-4.51945600	-3.08029200	-0.09461900
H	-2.99166800	-4.58578800	-0.30705100
H	-5.79379500	-1.35126500	0.11916900
C	1.46571400	1.36466900	0.11186600
N	-1.66202600	1.00939300	-0.01067700
C	2.64117000	-0.77143900	0.03206800
C	2.78908200	-1.94778300	0.78926400
C	3.73333800	-0.35888100	-0.75367700
C	3.98452500	-2.66541200	0.78023900

H	1.97517400	-2.29584700	1.41863500
C	4.92707200	-1.07823500	-0.76750300
H	3.63024900	0.52420900	-1.37752900
C	5.05985800	-2.23552600	0.00137400
H	4.07560200	-3.56227200	1.38752500
H	5.75082000	-0.73924000	-1.39037800
H	5.98849600	-2.79959100	-0.01092500
H	-5.34134500	-3.79126800	-0.10672500
H	2.47566000	1.75902400	0.20772200
H	0.14448000	-1.56892500	0.73570100



2b

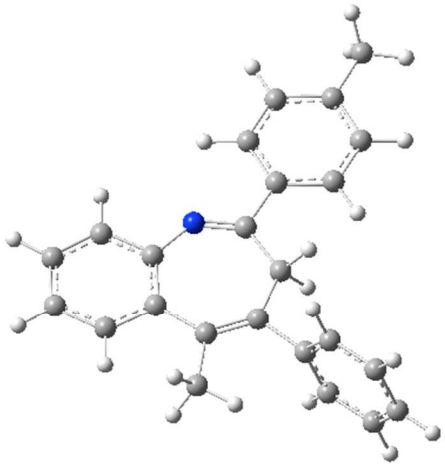
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.381967 (Hartree/Particle)
Thermal correction to Energy= 0.402822
Thermal correction to Enthalpy= 0.403766
Thermal correction to Gibbs Free Energy= 0.329925
Sum of electronic and zero-point Energies= -981.573731
Sum of electronic and thermal Energies= -981.552875
Sum of electronic and thermal Enthalpies= -981.551931
Sum of electronic and thermal Free Energies= -981.625773

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	252.775	82.995	155.413

0 1

C	2.84620900	-0.30704200	-0.09976300
C	2.23784300	-1.59580400	0.03356300
C	-0.01916000	-1.10404400	0.50294700
C	0.89244800	1.14444100	0.36328000

C	0.40166400	0.09129100	1.33972400
H	-0.40940200	0.46808100	1.96266100
C	4.25955700	-0.26448700	-0.15246600
H	4.74992000	0.69590300	-0.27005300
C	3.06019700	-2.74277000	0.11205500
C	4.44036100	-2.65352300	0.11153700
H	5.04561100	-3.55202100	0.19738800
C	5.04736000	-1.39763700	-0.02566300
H	6.13019100	-1.30849800	-0.04223200
H	2.55996500	-3.70447900	0.17492000
C	-1.45028600	-1.42152000	0.27455900
C	-2.48448600	-0.53974000	0.62206500
C	-1.80339100	-2.64872700	-0.32047800
C	-3.81876200	-0.87410600	0.38661700
H	-2.26200900	0.42983600	1.05491800
C	-3.13268200	-2.97781400	-0.54205800
H	-1.00857600	-3.33200900	-0.59882700
C	-4.17026900	-2.09701400	-0.19166000
H	-4.59883900	-0.16648500	0.65780900
H	-3.37662200	-3.93596700	-0.99664700
C	2.07717000	0.94427200	-0.27715600
N	0.87323000	-1.85973100	-0.03865400
C	0.00062200	2.31903500	0.14971500
C	-0.37591600	3.13030900	1.23464900
C	-0.53101200	2.61901700	-1.11620800
C	-1.23419600	4.21506100	1.05705600
H	0.02300200	2.91668500	2.22342500
C	-1.39309700	3.70131500	-1.29456600
H	-0.27444400	1.98499800	-1.96022900
C	-1.74588800	4.50530600	-0.20940700
H	-1.50154100	4.83554100	1.90856800
H	-1.79580300	3.91067200	-2.28216600
H	-2.41780200	5.34807900	-0.34781300
H	1.21490800	-0.23208000	2.00186300
C	2.70269600	2.00943500	-1.15705300
H	2.98606100	1.60385300	-2.13535500
H	2.02942800	2.85236600	-1.31280800
H	3.61766300	2.41045800	-0.70257400
C	-5.61372000	-2.46959600	-0.43098100
H	-6.28713700	-1.64125200	-0.18956300
H	-5.78619300	-2.74967500	-1.47743300
H	-5.91055400	-3.32983900	0.18286900



TS-2b

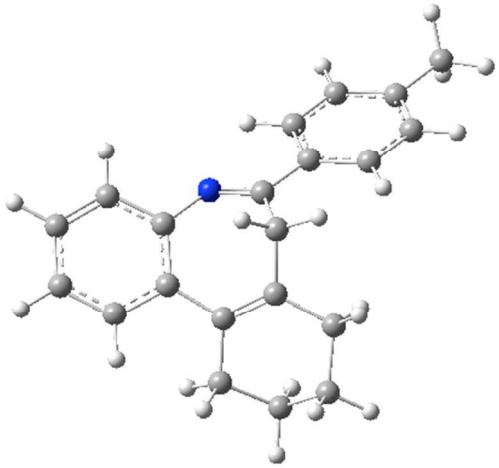
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 43.8i cm-1
Zero-point correction= 0.381684 (Hartree/Particle)
Thermal correction to Energy= 0.401811
Thermal correction to Enthalpy= 0.402756
Thermal correction to Gibbs Free Energy= 0.331293
Sum of electronic and zero-point Energies= -981.553087
Sum of electronic and thermal Energies= -981.532960
Sum of electronic and thermal Enthalpies= -981.532015
Sum of electronic and thermal Free Energies= -981.603478

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	252.140	81.207	150.405

0 1

C	-1.58533200	2.18010100	-0.00000100
C	-0.18881700	2.49017200	-0.00000300
C	1.03088000	0.37302700	-0.00000500
C	-1.53490900	-0.36591400	-0.00000200
C	-0.05531300	-0.68095200	-0.00000200
H	0.13219600	-1.34079000	-0.86250800
H	0.13219800	-1.34078700	0.86250600
C	-2.46503900	3.28433300	0.00000300
H	-3.53189400	3.11108400	0.00000500
C	0.21337700	3.84182700	-0.00000100
C	-0.68370500	4.90104800	0.00000300
H	-0.32540900	5.92670900	0.00000400
C	-2.04390600	4.61198800	0.00000500
H	-2.78412200	5.40756200	0.00000900

H	1.28334200	4.02026800	-0.00000300
C	2.42879200	-0.16663400	-0.00000500
C	2.71797100	-1.54148000	-0.00001500
C	3.52070600	0.72409100	0.00000300
C	4.03613600	-2.00142300	-0.00001500
H	1.92243600	-2.27802000	-0.00002400
C	4.82785200	0.26082800	0.00000400
H	3.30953400	1.78701100	0.00000700
C	5.11546600	-1.11473200	-0.00000300
H	4.22352700	-3.07284600	-0.00002500
H	5.64723500	0.97707300	0.00000900
C	-2.19249400	0.81765100	-0.00000300
N	0.92602500	1.64828500	-0.00000600
C	-2.28217300	-1.67478100	0.00000000
C	-2.59904100	-2.31843600	-1.20564700
C	-2.59905300	-2.31842400	1.20565200
C	-3.23377700	-3.56165400	-1.20639100
H	-2.35478300	-1.83312700	-2.14765900
C	-3.23378900	-3.56164100	1.20640100
H	-2.35480400	-1.83310400	2.14766100
C	-3.55290000	-4.18733800	0.00000700
H	-3.47942300	-4.04067100	-2.15073500
H	-3.47944400	-4.04064800	2.15074900
H	-4.04702100	-5.15520100	0.00001000
C	-3.71573700	0.78535400	-0.00000700
H	-4.09631300	-0.23373400	-0.00001300
H	-4.12677000	1.29020600	0.88268500
H	-4.12676500	1.29021500	-0.88269600
C	6.54258100	-1.60728000	0.00001900
H	6.58986400	-2.70077400	-0.00026200
H	7.08889300	-1.24816400	-0.88129500
H	7.08870800	-1.24863700	0.88164300



2c

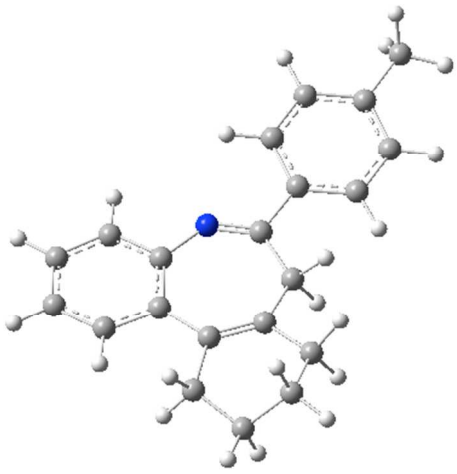
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.366917 (Hartree/Particle)
Thermal correction to Energy= 0.384980
Thermal correction to Enthalpy= 0.385924
Thermal correction to Gibbs Free Energy= 0.319948
Sum of electronic and zero-point Energies= -867.277259
Sum of electronic and thermal Energies= -867.259196
Sum of electronic and thermal Enthalpies= -867.258252
Sum of electronic and thermal Free Energies= -867.324228

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.578	73.270	138.857

0 1

C	2.44441900	-0.53489200	0.00457700
C	1.51464200	-1.61932100	0.04662200
C	-0.53502100	-0.56999900	0.56234700
C	0.97306500	1.34719100	0.65366900
C	3.81827900	-0.85869500	-0.07124500
H	4.54129800	-0.05017300	-0.12268600
C	2.00199100	-2.94546700	0.02631800
C	3.35757600	-3.22342400	0.01026300
H	3.70293700	-4.25382700	0.01893500
C	4.27714800	-2.16693700	-0.04487300
H	5.34467300	-2.36794200	-0.07423000
H	1.26574000	-3.74372900	0.02338000
C	-1.99019600	-0.45635700	0.28657400
C	-2.79187600	0.55989500	0.82746900
C	-2.61074200	-1.39909900	-0.55775700
C	-4.15572400	0.63058300	0.53799900

H	-2.36369600	1.31550400	1.47730900
C	-3.96744000	-1.32665500	-0.83586200
H	-1.99792100	-2.18599100	-0.98328700
C	-4.77073400	-0.30841000	-0.29398400
H	-4.74979300	1.43222500	0.97087900
H	-4.41884200	-2.07178300	-1.48791700
C	2.03849100	0.88459900	-0.04406600
N	0.12970000	-1.49462000	-0.04077300
C	2.87764800	1.82391100	-0.90396600
H	3.79998100	2.09802500	-0.36830300
H	3.20386700	1.29444600	-1.80712500
C	2.12723900	3.10426800	-1.28839200
H	2.81295200	3.80487900	-1.78049300
H	1.34162800	2.86247500	-2.01767600
C	1.49470600	3.74370500	-0.05056600
H	0.99795800	4.68805700	-0.30411600
H	2.28632700	3.98679100	0.67191800
C	0.49164700	2.78103800	0.59810300
H	-0.46395400	2.81010100	0.04901000
H	0.25042200	3.11932600	1.61629500
C	0.17199100	0.38786400	1.50581200
H	-0.51832400	0.91935000	2.16312700
H	0.84092100	-0.20641400	2.14227900
C	-6.24620500	-0.23924400	-0.60647500
H	-6.42125500	-0.13027400	-1.68425500
H	-6.76435300	-1.15318300	-0.28987600
H	-6.72389200	0.60715600	-0.10314800



TS-2c

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

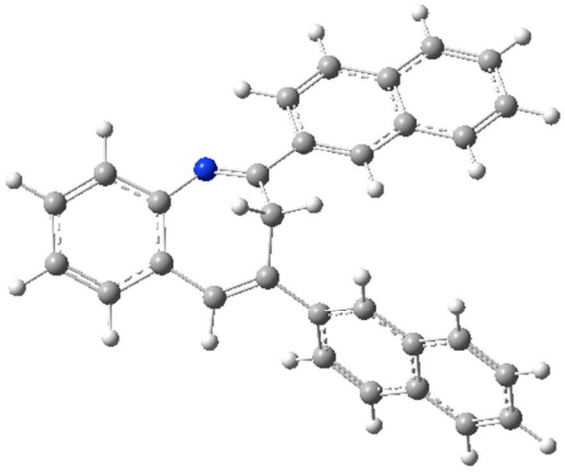
Imag freq = 60.5i cm-1
Zero-point correction= 0.366460 (Hartree/Particle)
Thermal correction to Energy= 0.384000
Thermal correction to Enthalpy= 0.384944
Thermal correction to Gibbs Free Energy= 0.320144
Sum of electronic and zero-point Energies= -867.256330
Sum of electronic and thermal Energies= -867.238790
Sum of electronic and thermal Enthalpies= -867.237845
Sum of electronic and thermal Free Energies= -867.302645

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	240.964	71.622	136.383

0 1

C	-1.84188100	0.99767300	-0.03837800
C	-0.58414500	1.68137900	-0.06020600
C	1.16481800	-0.01724400	-0.09486000
C	-1.09615400	-1.43996300	-0.00883700
C	0.40097600	-1.31816900	-0.19360800
H	0.64205300	-1.76801500	-1.17401400
H	0.87240800	-2.00520400	0.52361600
C	-2.98484700	1.82849700	0.01911800
H	-3.96646100	1.38200200	0.07938100
C	-0.56371300	3.09236000	-0.07250100
C	-1.71172500	3.86981700	-0.04463800
H	-1.64580800	4.95416500	-0.05562800
C	-2.93981000	3.21998900	0.01489500
H	-3.86822500	3.78314200	0.05944800
H	0.41868500	3.55175300	-0.09628900
C	2.65594400	-0.15858200	-0.05755100
C	3.31340800	-1.37856600	-0.28651200
C	3.45811500	0.96950900	0.20472600
C	4.70652500	-1.46465000	-0.25538400
H	2.75187400	-2.28045800	-0.50429300
C	4.84156600	0.87617000	0.24157100
H	2.96209500	1.91737400	0.37844000
C	5.49785900	-0.34492300	0.01190800
H	5.18309100	-2.42426100	-0.44309500
H	5.43033500	1.76679000	0.45271900
C	-2.05431400	-0.48190000	-0.02890500
N	0.71882400	1.18080700	-0.04862300
C	-3.52871700	-0.91000800	-0.03792500
H	-3.99921100	-0.62117600	0.91390200

H	-4.04994500	-0.33841900	-0.81375400
C	-3.79692400	-2.39343300	-0.29804100
H	-4.84957800	-2.61450200	-0.08338200
H	-3.63672100	-2.61938000	-1.36183600
C	-2.85852800	-3.24684900	0.54156200
H	-3.05617800	-4.31791900	0.41261700
H	-3.00512200	-3.01914500	1.60643200
C	-1.42520400	-2.92340100	0.13285100
H	-1.19174800	-3.42531100	-0.82170800
H	-0.72345200	-3.35907200	0.85870500
C	7.00419900	-0.43487300	0.05797400
H	7.46812200	0.26086100	-0.65229500
H	7.38894100	-0.17838500	1.05334100
H	7.35369800	-1.44340900	-0.18435300



2d

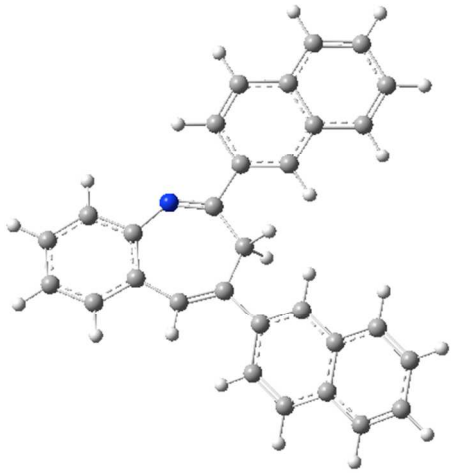
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.420323 (Hartree/Particle)
Thermal correction to Energy= 0.442822
Thermal correction to Enthalpy= 0.443766
Thermal correction to Gibbs Free Energy= 0.367078
Sum of electronic and zero-point Energies= -1210.196541
Sum of electronic and thermal Energies= -1210.174042
Sum of electronic and thermal Enthalpies= -1210.173098
Sum of electronic and thermal Free Energies= -1210.249785

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.875	94.524	161.403

0 1

C	3.46272000	-1.60984700	0.16737700
C	3.84320200	-0.26394400	-0.12775100
C	1.76305000	0.80375900	-0.50821200
C	0.98886400	-1.50413300	-0.21470300
C	1.20571200	-0.41037500	-1.23870500
H	0.29700600	-0.16435900	-1.78593300
C	4.48985800	-2.56937400	0.32594000
H	4.20450000	-3.58533200	0.59020100
C	5.21412400	0.03522400	-0.29615600
C	6.18748500	-0.94440700	-0.20585100
H	7.23212200	-0.68772000	-0.35985200
C	5.82403300	-2.26047200	0.12293400
H	6.58393500	-3.02993200	0.22708500
H	5.47739400	1.07053900	-0.49110700
C	0.91468300	1.99346600	-0.25308300
C	1.53180500	3.20515500	0.18514100
C	-0.46223600	1.96643000	-0.40366700
C	0.78492000	4.32653200	0.43662600
H	2.60866300	3.20951300	0.30839700
C	-1.26345000	3.10702600	-0.13566000
H	-0.97120300	1.05466700	-0.70128100
C	-0.63061600	4.31956400	0.28718100
H	1.27105400	5.24436600	0.75966200
C	2.08816700	-2.03795200	0.37819600
N	2.98359500	0.82760100	-0.09671700
C	-0.37697300	-1.97004500	0.10861100
C	-1.38370800	-2.00042800	-0.84645800
C	-0.69132600	-2.42390000	1.42681200
C	-2.68739700	-2.47596200	-0.55244500
H	-1.17872600	-1.68547700	-1.86659900
C	-1.94339900	-2.88895300	1.74402800
H	0.07309300	-2.36599000	2.19538900
C	-2.98010700	-2.93312600	0.77287100
H	-2.16118000	-3.21743400	2.75770000
H	1.96058600	-2.90689100	1.02125900
H	1.96061800	-0.72687700	-1.97037600
C	-2.67724200	3.08237000	-0.27688800
C	-1.43396300	5.45997600	0.54406400
C	-3.43072100	4.20576400	-0.01820700
C	-2.80306200	5.40598600	0.39486700
H	-3.15556100	2.15793100	-0.59209600
H	-4.51116000	4.17480800	-0.12954500
H	-3.40755900	6.28635000	0.59608700
H	-0.95044600	6.38024000	0.86357600

C	-3.71573600	-2.51759200	-1.53351500
C	-4.97266600	-2.98233900	-1.21809800
C	-5.26195000	-3.42844300	0.09505900
C	-4.28639600	-3.40331000	1.06724500
H	-3.49217000	-2.17476700	-2.54124000
H	-5.74965600	-3.00850800	-1.97732500
H	-6.25809000	-3.79236800	0.33154500
H	-4.50444200	-3.74586300	2.07614500



TS-2d

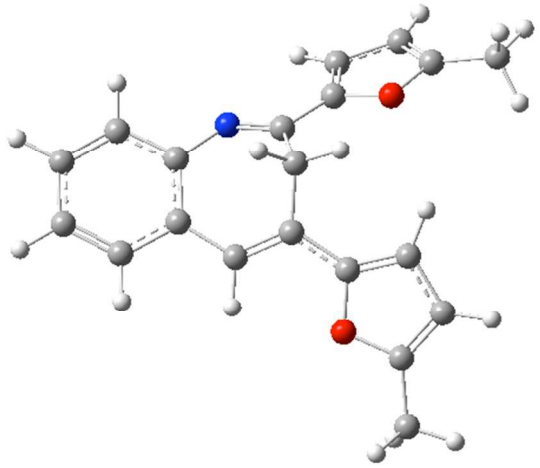
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 37.5i cm-1
Zero-point correction= 0.419876 (Hartree/Particle)
Thermal correction to Energy= 0.441846
Thermal correction to Enthalpy= 0.442790
Thermal correction to Gibbs Free Energy= 0.367849
Sum of electronic and zero-point Energies= -1210.181967
Sum of electronic and thermal Energies= -1210.159997
Sum of electronic and thermal Enthalpies= -1210.159052
Sum of electronic and thermal Free Energies= -1210.233994

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.263	92.895	157.728

C	0.33492500	3.26768200	-0.09257300
C	-1.05082500	2.95207600	-0.04681400
C	-1.16768200	0.51472400	0.11053800
C	1.45935600	0.96849000	0.07970800
C	0.27710300	0.03725400	0.21519100
H	0.37896600	-0.49359800	1.17523000

C	0.69844800	4.62614700	-0.17641800
H	1.75712600	4.87171700	-0.21848600
C	-1.98348000	4.00670600	-0.07952800
C	-1.59777400	5.34072400	-0.15074000
H	-2.34874600	6.12547300	-0.17116700
C	-0.23896600	5.65367600	-0.20245300
H	0.09041100	6.68719400	-0.26416600
H	-3.03257200	3.73113100	-0.04666800
C	-2.18179900	-0.58907100	0.14015700
C	-3.55758800	-0.27509600	-0.08745600
C	-1.84850300	-1.91337300	0.38687800
C	-4.52395700	-1.24633800	-0.06931900
H	-3.81021700	0.76081800	-0.27688000
C	-2.82745000	-2.94171500	0.42051600
H	-0.82166500	-2.20863800	0.57436500
C	-4.19855200	-2.60816900	0.18489100
H	-5.56370600	-0.98324600	-0.25094700
C	1.43323100	2.31070200	-0.05817300
N	-1.65569000	1.69707600	0.01147900
C	2.78761600	0.29035400	0.14126700
C	3.01932000	-0.94543600	-0.44497700
C	3.87536700	0.90962900	0.83248400
C	4.28892400	-1.57755800	-0.40112400
H	2.22911400	-1.45524400	-0.98898500
C	5.11450500	0.32207800	0.89975500
H	3.70216100	1.85241800	1.34183100
C	5.36741400	-0.93319900	0.28495900
H	5.91918500	0.81150800	1.44379600
H	2.40481400	2.78868900	-0.16521500
H	0.38203800	-0.75883400	-0.53391700
C	-2.48536700	-4.29609000	0.68141700
C	-3.45316100	-5.27573500	0.70619700
H	-3.17919200	-6.30784200	0.90725400
C	-4.80929200	-4.94400100	0.47017300
H	-5.56474400	-5.72486100	0.49179400
C	-5.17217500	-3.63891800	0.21522200
H	-1.44268200	-4.54754300	0.86255000
H	-6.21331400	-3.38157900	0.03466600
C	4.52688500	-2.83499600	-1.02075300
C	6.63485900	-1.57020800	0.33204300
C	5.76839800	-3.42694200	-0.96092700
H	5.93659100	-4.38822400	-1.43893200
C	6.83304500	-2.78947200	-0.27725000
H	7.80814400	-3.26724900	-0.23696200

H	3.70885900	-3.32347700	-1.54541000
H	7.44952200	-1.07720900	0.85752100



2e

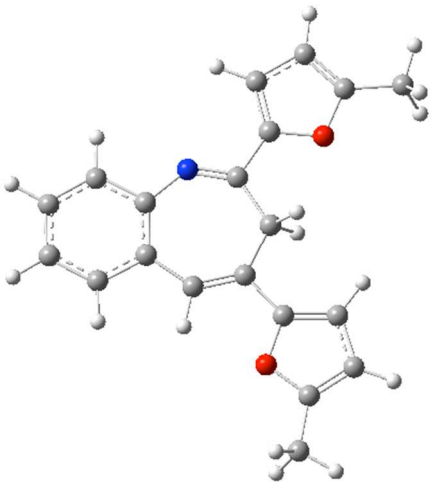
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.321038 (Hartree/Particle)
Thermal correction to Energy= 0.340312
Thermal correction to Enthalpy= 0.341257
Thermal correction to Gibbs Free Energy= 0.272030
Sum of electronic and zero-point Energies= -977.214653
Sum of electronic and thermal Energies= -977.195378
Sum of electronic and thermal Enthalpies= -977.194434
Sum of electronic and thermal Free Energies= -977.263660

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.549	75.425	145.699

0 1

C	-2.58704900	0.66152200	0.00092500
C	-2.64707600	-0.76872500	0.03373300
C	-0.38796000	-1.39737500	-0.27285600
C	-0.16290100	1.03219300	-0.49883900
C	-0.09761200	-0.27598800	-1.25371300
H	0.86348200	-0.42146100	-1.74501100
C	-3.80935300	1.37446800	0.03078700
H	-3.76483200	2.46125400	0.04707100
C	-3.91430400	-1.39530600	0.04731200
C	-5.08960900	-0.66595300	0.00435400
H	-6.04760800	-1.17898600	-0.00372000
C	-5.03811300	0.73731200	0.00859000
H	-5.95476900	1.32071000	0.00491800

H	-3.92932800	-2.47972600	0.10195600
C	-1.35405300	1.42965700	0.02273600
N	-1.56091700	-1.61606400	0.21942500
H	-1.41339800	2.41938700	0.46918700
H	-0.87951000	-0.29055900	-2.02387900
C	0.69387300	-2.27055600	0.14713100
C	0.75929000	-3.30172600	1.04988900
O	1.93145400	-2.09909400	-0.43490200
C	2.09692100	-3.78736500	1.01895100
H	-0.06521400	-3.65182000	1.65312600
C	2.77468100	-3.02522900	0.10495500
H	2.51385400	-4.59716900	1.60210200
C	1.04554200	1.81723900	-0.37318600
C	2.33730600	1.63684900	-0.80627700
O	0.97095000	3.00580300	0.31770600
C	3.08508200	2.76832300	-0.35961000
H	2.71466100	0.78997100	-1.36073000
C	2.21405700	3.57472800	0.31577500
H	4.13707400	2.96161600	-0.51948900
C	4.18174000	-3.01427100	-0.37897700
H	4.66941600	-2.05341300	-0.17165200
H	4.75278900	-3.80189300	0.11976400
H	4.23620200	-3.18396600	-1.46158800
C	2.35081900	4.88345300	1.01021500
H	3.38576300	5.23094200	0.94927200
H	1.70520000	5.64765500	0.55929200
H	2.07572700	4.80674400	2.06959900



TS-2e

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 37.4i cm-1

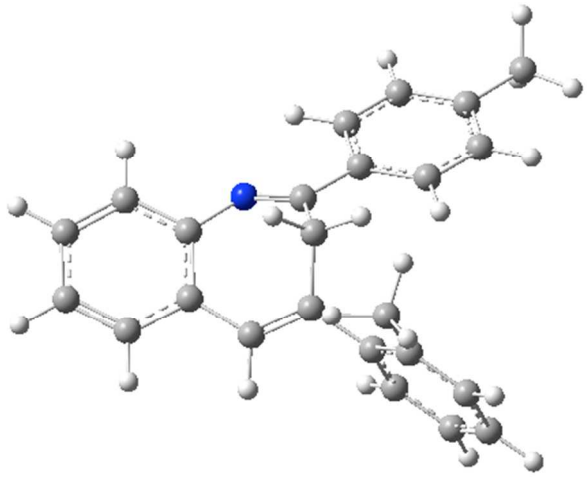
Zero-point correction= 0.320602 (Hartree/Particle)
Thermal correction to Energy= 0.339304
Thermal correction to Enthalpy= 0.340248
Thermal correction to Gibbs Free Energy= 0.272882
Sum of electronic and zero-point Energies= -977.204010
Sum of electronic and thermal Energies= -977.185308
Sum of electronic and thermal Enthalpies= -977.184363
Sum of electronic and thermal Free Energies= -977.251729

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.916	73.707	141.784

0 1

C	0.94414500	2.30925500	-0.00002300
C	-0.46635800	2.51325200	-0.00000800
C	-1.43014800	0.27613400	-0.00004000
C	1.16106100	-0.24343200	-0.00008000
C	-0.27413300	-0.71261500	-0.00023000
H	-0.42363300	-1.37803100	-0.86420900
C	1.77272700	3.45123300	-0.00003200
H	2.84968300	3.29990600	-0.00003400
C	-0.95531700	3.83520700	-0.00001100
C	-0.11474600	4.94171700	-0.00003600
H	-0.53271400	5.94461100	-0.00004000
C	1.26813700	4.74630500	-0.00004400
H	1.94810200	5.59382200	-0.00005500
H	-2.03419600	3.95264000	0.00000900
C	1.62711200	1.02743600	-0.00002000
N	-1.48062700	1.56179300	0.00003700
H	2.71025200	1.11984100	0.00005100
H	-0.42367700	-1.37838800	0.86345900
C	-2.74224200	-0.37103500	0.00004500
C	-4.02241600	0.12477100	0.00016700
O	-2.79364800	-1.74929300	-0.00002400
C	-4.89700700	-0.99798300	0.00017300
H	-4.28048600	1.17291000	0.00023400
C	-4.10738400	-2.11685900	0.00005500
H	-5.97852000	-0.98609400	0.00025200
C	-4.39658000	-3.57660700	0.00004700
H	-3.97414500	-4.07057900	-0.88401700
H	-3.97467300	-4.07050400	0.88440800
H	-5.47740700	-3.74119600	-0.00026300
C	2.10193900	-1.35109500	-0.00008400

C	1.93009200	-2.71558000	-0.00037200
O	3.45072000	-1.07646000	0.00019700
C	3.23367700	-3.29883500	-0.00026600
H	0.98696200	-3.24245400	-0.00064400
C	4.12598200	-2.26546000	0.00008100
H	3.47930600	-4.35200000	-0.00042600
C	5.61187000	-2.18889600	0.00038600
H	5.98684600	-1.65837900	0.88465900
H	6.03649300	-3.19645200	0.00005500
H	5.98715800	-1.65766200	-0.88332300



2f

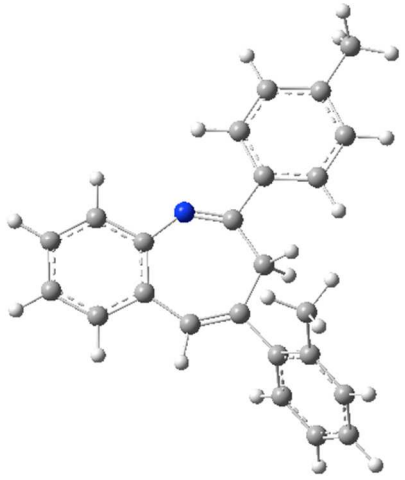
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.381641 (Hartree/Particle)
Thermal correction to Energy= 0.402561
Thermal correction to Enthalpy= 0.403505
Thermal correction to Gibbs Free Energy= 0.329899
Sum of electronic and zero-point Energies= -981.578179
Sum of electronic and thermal Energies= -981.557259
Sum of electronic and thermal Enthalpies= -981.556315
Sum of electronic and thermal Free Energies= -981.629921

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	252.611	83.183	154.916

0 1

C	2.85887200	-0.47147800	-0.33001300
C	2.26495600	-1.72954100	-0.00464900
C	0.01794000	-1.15213500	0.47741600

C	0.96057500	1.08562500	0.14905200
C	0.43710100	0.12260100	1.19580700
H	-0.38348800	0.54857900	1.77114900
C	4.25452500	-0.43248800	-0.55094900
H	4.70083400	0.51718500	-0.83803600
C	3.10054700	-2.86169300	0.12945700
C	4.47328400	-2.77288500	-0.02303400
H	5.09191600	-3.65706700	0.10565500
C	5.05804600	-1.54752400	-0.38110900
H	6.13135400	-1.47514700	-0.53346800
H	2.62152700	-3.81132200	0.34864700
C	-1.41787200	-1.47760500	0.28816100
C	-2.43649400	-0.53230200	0.47986600
C	-1.79035300	-2.77475500	-0.11487700
C	-3.77498100	-0.87260400	0.28017500
H	-2.19661700	0.48963700	0.75507900
C	-3.12424000	-3.10855900	-0.29962600
H	-1.00715900	-3.50752600	-0.27519400
C	-4.14634700	-2.16408400	-0.10461900
H	-4.54247800	-0.11581700	0.42510500
H	-3.38388500	-4.12079900	-0.60309700
C	2.09808700	0.75910500	-0.50995300
N	0.89704700	-1.97675700	0.02313700
C	0.20266800	2.32442100	-0.17521800
C	-0.08338200	3.30954500	0.80104800
C	-0.22857100	2.52827500	-1.49702600
C	-0.79976100	4.44832500	0.41385300
C	-0.94250800	3.66820400	-1.86228300
H	-0.00868100	1.76398400	-2.23692300
C	-1.23475300	4.63203000	-0.89884500
H	-1.00707900	5.21433800	1.15804800
H	-1.26964500	3.79805500	-2.89036900
H	-1.79041900	5.52711900	-1.16585400
H	2.52220700	1.48813700	-1.19901900
H	1.23796000	-0.14495900	1.89817600
C	-5.59489600	-2.54219400	-0.30048200
H	-6.25139900	-1.66994000	-0.22250700
H	-5.75914900	-3.00086600	-1.28314400
H	-5.92112300	-3.27233000	0.45156000
C	0.40431000	3.19101300	2.22888000
H	-0.25768400	2.56807400	2.84451900
H	1.40357700	2.74593000	2.27763300
H	0.44958100	4.17625100	2.70389300



TS-2f

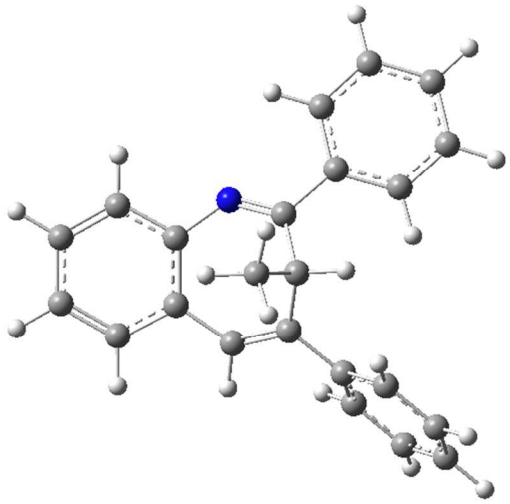
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 28.1i cm-1
Zero-point correction= 0.381071 (Hartree/Particle)
Thermal correction to Energy= 0.401456
Thermal correction to Enthalpy= 0.402400
Thermal correction to Gibbs Free Energy= 0.330197
Sum of electronic and zero-point Energies= -981.564579
Sum of electronic and thermal Energies= -981.544194
Sum of electronic and thermal Enthalpies= -981.543249
Sum of electronic and thermal Free Energies= -981.615452

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	251.918	81.580	151.964

0 1

C	-1.29963400	2.43305400	-0.04720600
C	0.11191000	2.59656900	0.00753400
C	1.05791300	0.33721000	-0.03996700
C	-1.56333700	-0.11091600	-0.09745600
C	-0.13899600	-0.60792300	-0.05023500
H	-0.03309600	-1.27177200	0.82116900
C	-2.10084100	3.58978900	-0.03082100
H	-3.18048100	3.46588600	-0.07538600
C	0.63289100	3.90298100	0.08105400
C	-0.18074700	5.03080400	0.10236400
H	0.26196200	6.02126500	0.16080300
C	-1.56525000	4.87229500	0.04340700
H	-2.22408600	5.73620500	0.05460200

H	1.71346700	3.99543800	0.11922000
C	2.38680200	-0.35741300	-0.06192100
C	2.52055400	-1.75624800	-0.06370100
C	3.57261800	0.40418300	-0.08042100
C	3.77853700	-2.36141400	-0.08330000
H	1.64858200	-2.40022400	-0.04964500
C	4.81928800	-0.20291400	-0.10092000
H	3.48271700	1.48404200	-0.07873300
C	4.95065600	-1.60199700	-0.10289700
H	3.84416400	-3.44710700	-0.08391000
H	5.71364700	0.41700000	-0.11618300
C	-2.00875400	1.15774500	-0.11345600
N	1.10780600	1.61882100	-0.01333600
C	-2.57342800	-1.21826000	-0.19416900
C	-3.20302800	-1.44879700	-1.42710700
C	-2.90072200	-2.03527400	0.91132100
C	-4.13807100	-2.47100800	-1.58522000
H	-2.94774200	-0.81162500	-2.26989400
C	-3.84610800	-3.05391000	0.73499000
C	-4.45866600	-3.28098200	-0.49688800
H	-4.61275000	-2.62928800	-2.54992900
H	-4.11308100	-3.67399400	1.58828800
H	-5.18827500	-4.07978900	-0.60109500
H	-3.09069300	1.27115600	-0.16684700
H	-0.00741600	-1.28664300	-0.90746100
C	-2.28192100	-1.82323600	2.27581400
H	-1.34285600	-2.38165600	2.39068600
H	-2.05909100	-0.76742800	2.45855900
H	-2.95597400	-2.16919100	3.06623800
C	6.31293400	-2.25203700	-0.12592300
H	6.91105700	-1.95697300	0.74548900
H	6.23668200	-3.34386600	-0.12466500
H	6.88101000	-1.95699700	-1.01721100



(*R*p)-2g

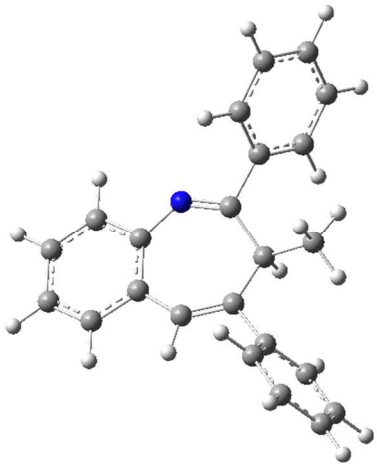
Zero-point correction= 0.354727 (Hartree/Particle)
Thermal correction to Energy= 0.373581
Thermal correction to Enthalpy= 0.374525
Thermal correction to Gibbs Free Energy= 0.306839
Sum of electronic and zero-point Energies= -942.282102
Sum of electronic and thermal Energies= -942.263248
Sum of electronic and thermal Enthalpies= -942.262304
Sum of electronic and thermal Free Energies= -942.329990

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	234.426	76.946	142.457

0 1

C	-2.09379200	-1.44885400	-0.28853100
C	-2.54471000	-0.10644300	-0.11582000
C	-0.52173500	1.09274200	0.32419800
C	0.36329400	-1.20692200	0.24428400
C	0.15609700	-0.00367400	1.15249300
H	1.13441700	0.36780600	1.45745000
C	-3.06647000	-2.45618700	-0.48281100
H	-2.72233700	-3.47424000	-0.65196900
C	-3.93408800	0.14912900	-0.10012900
C	-4.86189100	-0.87135500	-0.22357300
H	-5.92442000	-0.64613500	-0.18939300
C	-4.42463300	-2.18887200	-0.43120800
H	-5.14400800	-2.99276900	-0.55996400
H	-4.24895800	1.18317400	0.00334600
C	0.22049600	2.35469200	0.03579000
C	1.62399400	2.42150400	0.03667500

C	-0.50238400	3.52171900	-0.27448000
C	2.28163100	3.61603900	-0.25986100
H	2.21807900	1.53451100	0.23281500
C	0.15457700	4.71528400	-0.55327100
H	-1.58517900	3.46654200	-0.28759800
C	1.55166100	4.76880800	-0.54757000
H	3.36804000	3.64146200	-0.26711700
H	-0.42349700	5.60811000	-0.77715500
C	-0.69374000	-1.83571900	-0.33220400
N	-1.72637100	1.01372700	-0.12114900
C	1.74376800	-1.69980600	0.01532900
C	2.70915500	-1.67740100	1.03991100
C	2.12801200	-2.21950400	-1.23549600
C	3.99591300	-2.17071100	0.82858000
H	2.44420400	-1.29876800	2.02326100
C	3.41379500	-2.71234900	-1.44727900
H	1.41445900	-2.20749900	-2.05411200
C	4.35486400	-2.69151900	-0.41575800
H	4.71781800	-2.15279000	1.64092300
H	3.68579200	-3.10028700	-2.42548900
H	5.35949900	-3.07059000	-0.58211100
H	2.06509800	5.70091800	-0.76811300
H	-0.49527800	-2.76974900	-0.85562300
C	-0.61682700	-0.30720000	2.45454800
H	-0.69485900	0.59893000	3.06603800
H	-1.62516500	-0.67883600	2.26488500
H	-0.08102100	-1.06628200	3.03505800



(*Sp*)-TS-2g

Temperature 298.150 Kelvin. Pressure 1.00000 Atm
Imag freq = 42.7i cm-1

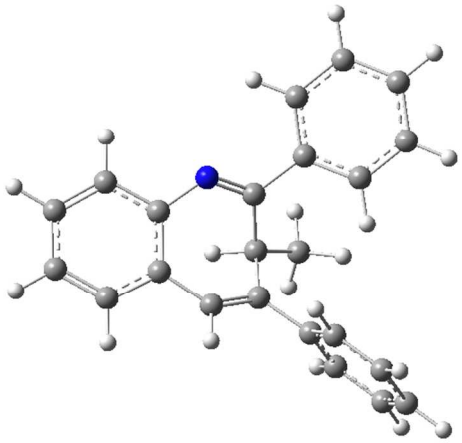
Zero-point correction= 0.353724 (Hartree/Particle)
Thermal correction to Energy= 0.371870
Thermal correction to Enthalpy= 0.372815
Thermal correction to Gibbs Free Energy= 0.307084
Sum of electronic and zero-point Energies= -942.257214
Sum of electronic and thermal Energies= -942.239068
Sum of electronic and thermal Enthalpies= -942.238124
Sum of electronic and thermal Free Energies= -942.303855

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	233.352	75.246	138.343

0 1

C	-1.04348600	-0.46004700	-0.67783700
C	-1.02483800	-1.04400500	0.60963300
C	1.48809000	-1.19156800	1.10683100
C	1.29597500	-0.01008700	-1.21760400
C	2.12816800	-0.91570800	-0.26500200
C	3.55116500	-0.32667800	-0.07608000
C	-2.26479300	-0.36930800	-1.37075000
C	-2.24474700	-1.48637000	1.15775000
C	-3.44103800	-1.40928200	0.45340600
C	-3.44978500	-0.85372300	-0.82906800
C	2.40570600	-1.57125100	2.23237600
C	2.42257700	-0.83320800	3.42520100
C	3.22208200	-2.71285700	2.14710600
C	3.22719800	-1.22025700	4.49884800
C	4.02323100	-3.10255000	3.21880700
C	4.03070400	-2.35582300	4.39996700
N	0.03047100	0.12852300	-1.34519400
C	0.17361300	-1.22277900	1.41633900
C	2.05679200	0.80945800	-2.23113600
C	2.91789700	0.20627500	-3.16037000
C	1.82544400	2.18804300	-2.32658500
C	3.53618500	0.96413500	-4.15498200
C	2.45935000	2.95021600	-3.30730400
C	3.31624200	2.34096000	-4.22597200
H	2.24172800	-1.88443300	-0.78440900
H	3.49829600	0.66134200	0.39525900
H	4.07195200	-0.21403700	-1.02564500
H	4.15747000	-0.96757600	0.56380000
H	-2.24435900	0.10491800	-2.34685800
H	-2.23661800	-1.91301100	2.15826600

H	-4.36060400	-1.77293600	0.90365800
H	-4.37645000	-0.77903500	-1.39134800
H	1.80271000	0.05579000	3.50355800
H	3.21670700	-3.30804700	1.23693700
H	3.22695300	-0.62952800	5.41130700
H	4.63842200	-3.99472400	3.13439200
H	4.65793300	-2.65825800	5.23418400
H	-0.04963900	-1.51089700	2.44243100
H	3.09121400	-0.86658200	-3.12030300
H	1.13641500	2.65392300	-1.62872900
H	4.18798500	0.47734900	-4.87579400
H	2.27721800	4.02054500	-3.35892500
H	3.80461600	2.93324000	-4.99517200



(*Sp*)-2g

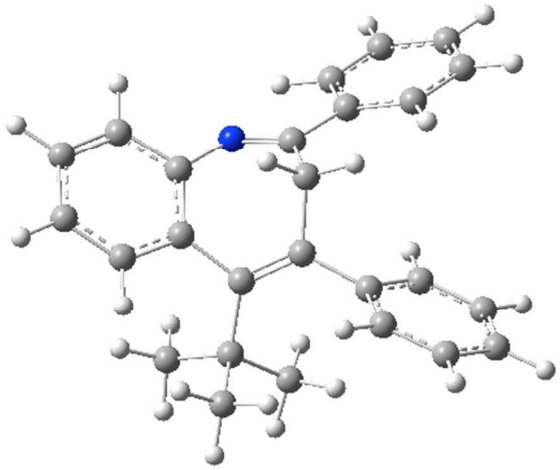
Temperature 298.150 Kelvin. Pressure 1.00000 Atm
Zero-point correction= 0.354552 (Hartree/Particle)
Thermal correction to Energy= 0.373300
Thermal correction to Enthalpy= 0.374244
Thermal correction to Gibbs Free Energy= 0.306903
Sum of electronic and zero-point Energies= -942.275712
Sum of electronic and thermal Energies= -942.256965
Sum of electronic and thermal Enthalpies= -942.256020
Sum of electronic and thermal Free Energies= -942.323361

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	234.249	76.872	141.730

0 1

C	2.34738700	-1.21970200	-0.26670600
C	2.65769600	0.16200800	-0.07697000

C	0.53369100	1.09882900	0.37865100
C	-0.09278000	-1.24730000	0.31641600
C	0.14676900	-0.08499300	1.27764900
C	3.42025800	-2.12213500	-0.45395500
H	3.18403500	-3.16780100	-0.63883100
C	4.01400000	0.55796900	-0.03248600
C	5.03955600	-0.36358300	-0.14544400
H	6.07368100	-0.03448600	-0.08800400
C	4.74157500	-1.71785300	-0.37299800
H	5.54221600	-2.44228100	-0.49380900
H	4.22192600	1.61747400	0.08356900
C	-0.41512600	2.20314400	0.06306500
C	-1.77723600	1.97032200	-0.18553800
C	0.07294700	3.51729700	-0.03546000
C	-2.62814500	3.02571300	-0.51559500
H	-2.16944800	0.95876300	-0.16117400
C	-0.78142100	4.57080700	-0.34878800
H	1.12974800	3.69236300	0.13630600
C	-2.13675600	4.32939100	-0.58931700
H	-3.67662900	2.82509400	-0.71941700
H	-0.38910700	5.58263500	-0.40931500
C	0.98734000	-1.73362300	-0.34830800
N	1.71737900	1.18425700	-0.11979500
C	-1.44063200	-1.81779100	0.04582900
C	-2.25112300	-2.35185500	1.06428900
C	-1.91626800	-1.88061600	-1.27691800
C	-3.48810300	-2.92375100	0.76988500
H	-1.89825800	-2.34697500	2.09023300
C	-3.15526300	-2.45054000	-1.57130200
H	-1.30626600	-1.46394500	-2.07331900
C	-3.94722300	-2.97267800	-0.54806200
H	-4.09150100	-3.33968700	1.57256000
H	-3.50174700	-2.48251600	-2.60097600
H	-4.91323900	-3.41588300	-0.77450800
H	-2.80292500	5.15143400	-0.83751400
H	0.85102700	-2.62028200	-0.96561100
C	-0.90806000	0.21934600	2.34936900
H	-0.90835900	-0.56691400	3.11148700
H	-1.92295600	0.30875000	1.95865100
H	-0.65997600	1.16115600	2.85020400
H	1.07761100	-0.31712500	1.81419700



2h

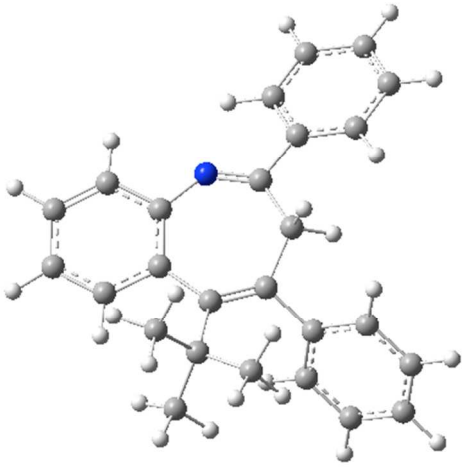
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.439546 (Hartree/Particle)
Thermal correction to Energy= 0.462325
Thermal correction to Enthalpy= 0.463269
Thermal correction to Gibbs Free Energy= 0.387250
Sum of electronic and zero-point Energies= -1060.115510
Sum of electronic and thermal Energies= -1060.092731
Sum of electronic and thermal Enthalpies= -1060.091787
Sum of electronic and thermal Free Energies= -1060.167806

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	290.113	93.013	159.994

0 1

C	-2.15195100	-0.85110600	-0.26059800
C	-1.46462800	-2.09830900	-0.24411500
C	0.77679000	-1.47714100	-0.45860700
C	-0.30443700	0.72575300	-0.51001300
C	0.35010500	-0.34587200	-1.38251300
H	-0.37206100	-0.74982300	-2.10393900
C	-3.51790800	-0.87956300	-0.61704200
H	-4.05892900	0.05754200	-0.68425300
C	-2.17546900	-3.29349800	-0.48674800
C	-3.51486700	-3.28075200	-0.83721400
H	-4.03298000	-4.21205900	-1.04962800
C	-4.18903300	-2.05662200	-0.91946200
H	-5.23497500	-2.02191500	-1.21189500
H	-1.62061900	-4.22419000	-0.41666000
C	2.20276200	-1.70434600	-0.09521500

C	3.26084900	-0.98911800	-0.68059300
C	2.51582300	-2.69187100	0.85943600
C	4.58527400	-1.25310100	-0.32684400
H	3.06548700	-0.21699300	-1.41605400
C	3.83476100	-2.95281000	1.21154800
H	1.69887200	-3.24564600	1.30836800
C	4.87835100	-2.23413500	0.61894500
H	5.38698800	-0.68809800	-0.79478600
H	4.05292500	-3.71869200	1.95126500
C	-1.49263400	0.44729800	0.09161400
N	-0.10928500	-2.26423400	0.04844600
C	0.48201900	1.99840800	-0.45047700
C	1.67828100	2.09401100	0.28023500
C	0.09644900	3.09405500	-1.23891800
C	2.44072100	3.26140700	0.25334300
H	2.00173900	1.25408000	0.88784900
C	0.86063700	4.26279800	-1.26763300
H	-0.80660600	3.02394600	-1.83883300
C	2.03345100	4.35253400	-0.51780500
H	3.35508200	3.31854300	0.83838600
H	0.53878700	5.10072200	-1.88070900
H	2.62830900	5.26173400	-0.53761000
H	5.90968800	-2.43838100	0.89422300
H	1.17927800	0.07575900	-1.94867600
C	-2.20438300	1.36482100	1.14290100
C	-3.09075900	0.52529400	2.09884300
C	-1.18797900	2.08512400	2.06384600
C	-3.07825700	2.44820400	0.46428000
H	-3.93366000	0.04299000	1.60207800
H	-2.50386700	-0.25869500	2.59091200
H	-3.49598200	1.18082300	2.87816300
H	-0.62261200	2.86305200	1.55168700
H	-1.73163700	2.56398500	2.88680400
H	-0.47620500	1.37634400	2.50131300
H	-3.57075500	3.06164500	1.22945200
H	-2.47113000	3.11311000	-0.15676800
H	-3.86393300	2.02106600	-0.16697800



TS-2h

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 82.4i cm-1
Zero-point correction= 0.439413 (Hartree/Particle)
Thermal correction to Energy= 0.461551
Thermal correction to Enthalpy= 0.462495
Thermal correction to Gibbs Free Energy= 0.388688
Sum of electronic and zero-point Energies= -1060.075687
Sum of electronic and thermal Energies= -1060.053549
Sum of electronic and thermal Enthalpies= -1060.052605
Sum of electronic and thermal Free Energies= -1060.126412

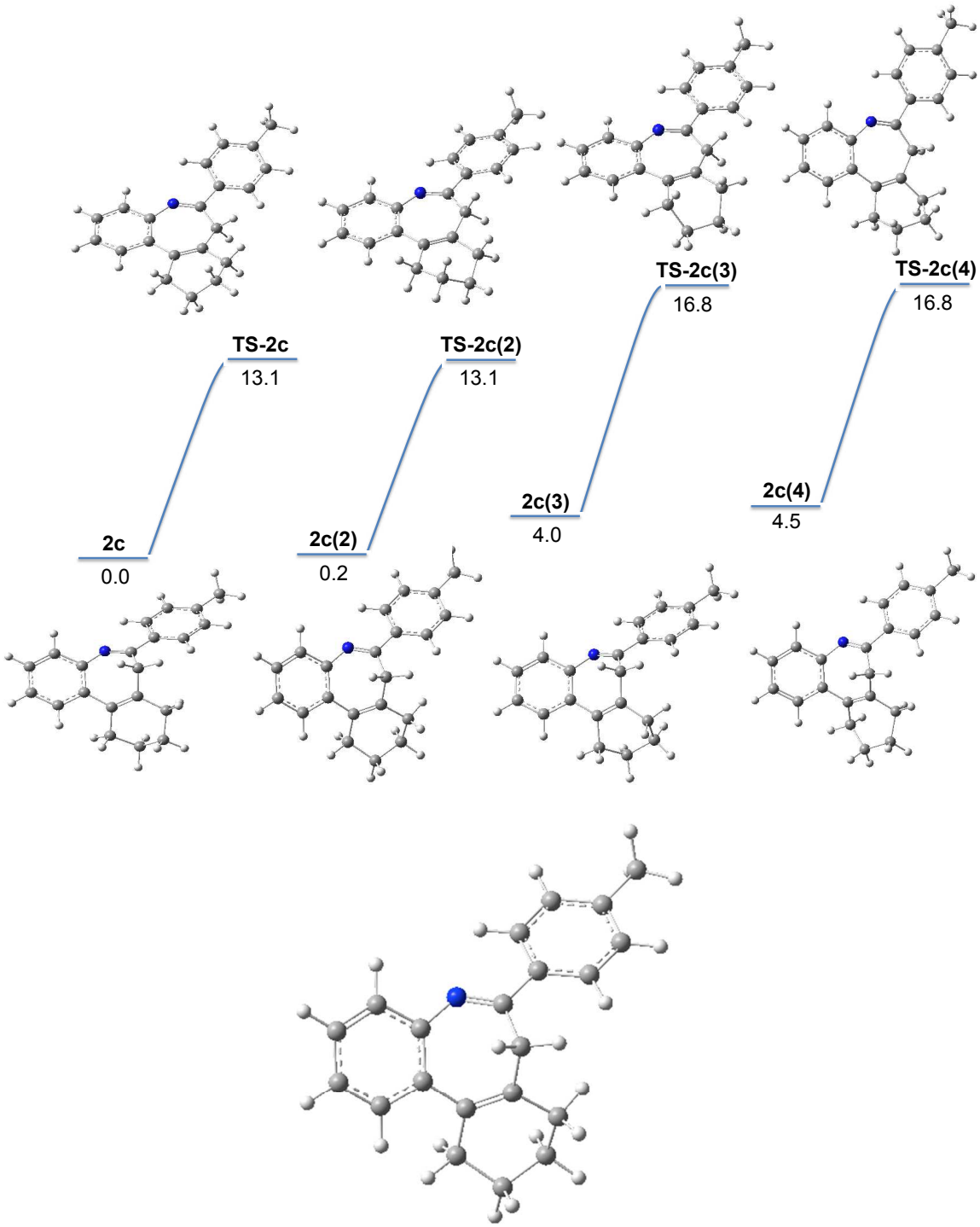
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	289.628	91.281	155.341

0 1

C	0.45246900	2.47372400	0.50760300
C	-0.95411400	2.19616500	0.39674100
C	-1.19598300	-0.10176900	-0.35535200
C	1.43829600	0.22311800	-0.05815000
C	0.23051300	-0.48850700	-0.66432200
H	0.34869200	-0.43935200	-1.76202900
C	0.74709000	3.71078600	1.13311200
H	1.77055800	3.95438000	1.35425400
C	-1.89428800	3.19154100	0.74941200
C	-1.54632900	4.42112400	1.28156900
H	-2.30733700	5.15071300	1.54320900
C	-0.19563300	4.66118000	1.50963200
H	0.13938300	5.58287200	1.97806600
H	-2.93520100	2.92098400	0.60894100

C	-2.22862300	-1.16331400	-0.58120700
C	-1.96326500	-2.33275800	-1.31530900
C	-3.52619200	-0.98766700	-0.06496000
C	-2.95806600	-3.28896700	-1.52636300
H	-0.98263700	-2.50475100	-1.74641100
C	-4.51348900	-1.94565600	-0.26569200
H	-3.73371100	-0.08321500	0.49527500
C	-4.23498100	-3.10326200	-0.99918200
H	-2.73002800	-4.18061100	-2.10444400
H	-5.50529800	-1.79158300	0.15163800
C	1.60314900	1.56557300	0.16546200
N	-1.63324400	1.02921700	0.04471000
C	2.50686600	-0.78952700	0.21555000
C	3.03403300	-0.88639700	1.51455500
C	2.90451900	-1.75531100	-0.72816300
C	3.95749000	-1.87947000	1.84683800
H	2.69493900	-0.18531500	2.27057200
C	3.83220800	-2.74131300	-0.40156200
H	2.50731900	-1.71327800	-1.73902600
C	4.36693000	-2.80619900	0.88827800
H	4.34784500	-1.93325400	2.85983700
H	4.13929500	-3.46203900	-1.15507000
H	5.08589400	-3.57960200	1.14444200
H	-5.00706300	-3.85165800	-1.15712400
H	0.32727900	-1.54964200	-0.42390400
C	3.03755800	2.22606100	-0.00921900
C	3.78862600	2.55641800	1.30960400
C	4.02972100	1.35931200	-0.83503700
C	2.88518200	3.48513100	-0.92544000
H	3.19829200	3.09029900	2.05632300
H	4.13851400	1.63311200	1.78128200
H	4.67329700	3.16688500	1.08867200
H	3.57369400	0.99175700	-1.76020200
H	4.88073900	1.99074300	-1.11523500
H	4.43331000	0.50939000	-0.28879300
H	3.87863400	3.90943600	-1.10978600
H	2.46791400	3.18673600	-1.89438400
H	2.25454600	4.28099400	-0.53690600

Conformational analysis of 2c



2c(2)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.366826 (Hartree/Particle)
Thermal correction to Energy= 0.384929
Thermal correction to Enthalpy= 0.385873

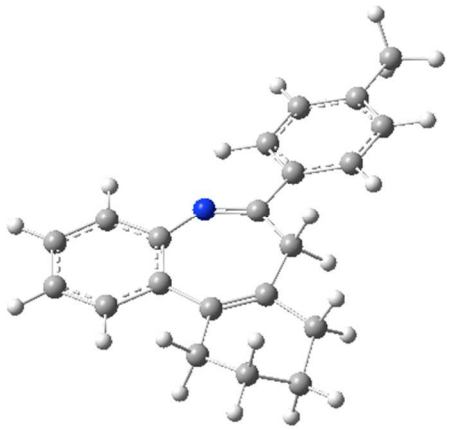
Thermal correction to Gibbs Free Energy= 0.319542
Sum of electronic and zero-point Energies= -867.276947
Sum of electronic and thermal Energies= -867.258844
Sum of electronic and thermal Enthalpies= -867.257900
Sum of electronic and thermal Free Energies= -867.324231

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.546	73.328	139.604

0 1

C	2.46491900	-0.52331600	0.00490300
C	1.52579900	-1.60331300	0.00606500
C	-0.52490700	-0.56952200	0.55148100
C	0.96370300	1.33757400	0.63651000
C	0.18757200	0.37399100	1.50550400
H	-0.49457100	0.90215700	2.17392900
H	0.86711500	-0.22245700	2.12717900
C	3.83686600	-0.86304000	-0.02653500
H	4.57403500	-0.06666100	-0.02220200
C	2.00177800	-2.93327700	-0.03649000
C	3.35409000	-3.22487800	-0.02333900
H	3.68974400	-4.25849200	-0.03118500
C	4.28302900	-2.17587100	-0.01742500
H	5.34936800	-2.38501300	-0.01179600
H	1.25760000	-3.72316600	-0.07354700
C	-1.98286000	-0.45923300	0.28753700
C	-2.80612200	0.48117900	0.92504800
C	-2.58523700	-1.33142300	-0.64172100
C	-4.17205400	0.54885900	0.64446600
H	-2.39511000	1.17504800	1.65021500
C	-3.94364200	-1.26218300	-0.91183100
H	-1.95622200	-2.06090500	-1.13963100
C	-4.76782600	-0.31837200	-0.27465500
H	-4.78292300	1.29057700	1.15393700
H	-4.38001500	-1.95009600	-1.63327200
C	2.05360500	0.89762400	-0.03803400
N	0.14178300	-1.47448500	-0.08042600
C	2.55356500	3.32992700	-0.65380400
H	2.99563300	3.64498200	0.30215900
H	3.01898400	3.94342900	-1.43484200
C	0.42502000	2.74785800	0.53738900
H	-0.66779300	2.70458500	0.42370400
H	0.59679700	3.26226300	1.49763000

C	1.04133200	3.55742400	-0.60819600
H	0.59855700	3.23736700	-1.56144000
H	0.80477900	4.62166800	-0.48890500
C	2.87092500	1.85012400	-0.90191000
H	3.94252200	1.68424200	-0.74568500
H	2.69233500	1.60326700	-1.95982700
C	-6.24534900	-0.25331800	-0.57808800
H	-6.42637300	-0.08464800	-1.64699300
H	-6.74833900	-1.19207900	-0.31344700
H	-6.73384600	0.55442500	-0.02425000



TS-2c(2)

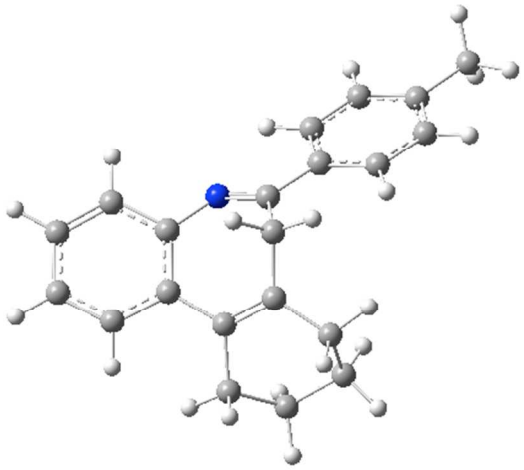
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 61.i cm-1
Zero-point correction= 0.366466 (Hartree/Particle)
Thermal correction to Energy= 0.384005
Thermal correction to Enthalpy= 0.384949
Thermal correction to Gibbs Free Energy= 0.320153
Sum of electronic and zero-point Energies= -867.256327
Sum of electronic and thermal Energies= -867.238788
Sum of electronic and thermal Enthalpies= -867.237844
Sum of electronic and thermal Free Energies= -867.302640

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	240.967	71.619	136.375

0 1

C	1.84480900	0.99754800	-0.03637100
C	0.58871300	1.68442300	-0.05284600
C	-1.16476300	-0.00974800	-0.07399200
C	1.09294500	-1.43805500	0.00287300
C	-0.40476400	-1.31277500	-0.17481100

H	-0.87427300	-1.99756100	0.54578300
H	-0.65192000	-1.76340600	-1.15334300
C	2.99019500	1.82559200	0.01264400
H	3.97101100	1.37676800	0.06857600
C	0.57180500	3.09541700	-0.06864200
C	1.72193000	3.86999800	-0.04925900
H	1.65871800	4.95447900	-0.06267400
C	2.94867100	3.21717800	0.00507700
H	3.87875000	3.77806500	0.04299100
H	-0.40954100	3.55726100	-0.08802500
C	-2.65602800	-0.14713600	-0.02828000
C	-3.31786300	-1.36603100	-0.25061700
C	-3.45382700	0.98325900	0.23713700
C	-4.71089600	-1.44870700	-0.21063200
H	-2.75982800	-2.27012800	-0.46819800
C	-4.83730800	0.89330500	0.28279800
H	-2.95443300	1.92987200	0.40798000
C	-5.49799400	-0.32626000	0.05797900
H	-5.19076100	-2.40790000	-0.39186900
H	-5.42246200	1.78529300	0.49813900
C	2.05347100	-0.48253800	-0.02430600
N	-0.71544700	1.18723400	-0.03255200
C	3.78967200	-2.39928200	-0.29771600
H	3.62345600	-2.62728900	-1.36014700
H	4.84282600	-2.62261800	-0.08790300
C	1.41880900	-2.92200400	0.14654700
H	0.71967500	-3.35398900	0.87711800
H	1.17901000	-3.42562300	-0.80553300
C	2.85336000	-3.24831600	0.54862000
H	3.00602800	-3.01864400	1.61221200
H	3.04752100	-4.32019100	0.42107200
C	3.52667800	-0.91455100	-0.03977500
H	4.04539000	-0.34626800	-0.81969800
H	4.00281900	-0.62458500	0.90889200
C	-7.00485600	-0.41015900	0.09975400
H	-7.40190100	-0.00734200	1.03959100
H	-7.45930500	0.17031700	-0.71361100
H	-7.35204400	-1.44378500	0.00415100



2c(3)

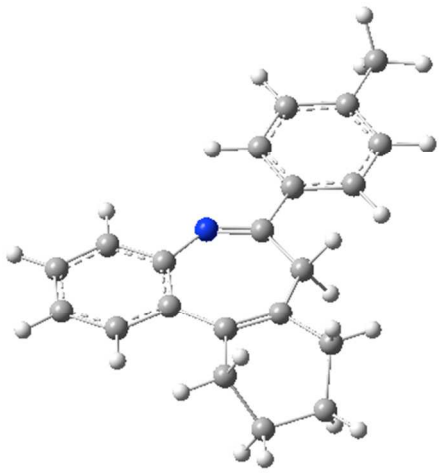
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.366505 (Hartree/Particle)
Thermal correction to Energy= 0.384908
Thermal correction to Enthalpy= 0.385852
Thermal correction to Gibbs Free Energy= 0.318243
Sum of electronic and zero-point Energies= -867.270902
Sum of electronic and thermal Energies= -867.252500
Sum of electronic and thermal Enthalpies= -867.251555
Sum of electronic and thermal Free Energies= -867.319165

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.533	73.537	142.295

0 1

C	2.52036900	-0.41701700	0.04821800
C	1.61751900	-1.52565900	0.01848700
C	-0.47366000	-0.57406400	0.59125100
C	0.97726200	1.36362900	0.82188800
C	3.90314200	-0.69729300	-0.04232000
H	4.60302200	0.13328700	-0.02462500
C	2.14138200	-2.83368000	-0.09376800
C	3.50387900	-3.07290500	-0.12781000
H	3.87656700	-4.09185600	-0.19024000
C	4.39608600	-1.99121000	-0.10655600
H	5.46849600	-2.16220600	-0.14531100
H	1.42750400	-3.64992600	-0.15240900
C	-1.93093000	-0.50247500	0.31003100
C	-2.76948500	0.46914600	0.87598500
C	-2.51514600	-1.44122000	-0.56378700

C	-4.13353000	0.50161400	0.58193500
H	-2.36934200	1.22175800	1.54708900
C	-3.87287800	-1.40829000	-0.84540600
H	-1.87380800	-2.19342600	-1.00950600
C	-4.71301700	-0.43474300	-0.27831000
H	-4.75617700	1.27062500	1.03346900
H	-4.29568800	-2.15003700	-1.52009700
C	2.06918500	0.98013400	0.11612500
N	0.23067800	-1.43317400	-0.06157700
C	2.83523900	2.08140100	-0.59742100
H	3.36614300	2.70542500	0.13810900
H	3.59890900	1.66670700	-1.26157100
C	1.88206300	2.97968100	-1.42123200
H	2.43415700	3.86433600	-1.75987500
H	1.59287400	2.43096400	-2.32435800
C	0.57027100	2.81745400	0.79304500
H	1.25632700	3.39660300	1.43265000
H	-0.42782300	2.95355100	1.22553500
C	0.60766000	3.39660800	-0.63960700
H	-0.28069900	3.04134600	-1.17337000
H	0.52348900	4.48849200	-0.58815300
C	0.18469900	0.34834700	1.60660000
H	0.85399800	-0.26606100	2.22395100
H	-0.53358000	0.82484300	2.27539800
C	-6.18976300	-0.41042300	-0.59145100
H	-6.36791800	-0.32012100	-1.67025500
H	-6.68232100	-1.33442300	-0.26288200
H	-6.69096700	0.42810500	-0.09789300



TS-2c(3)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

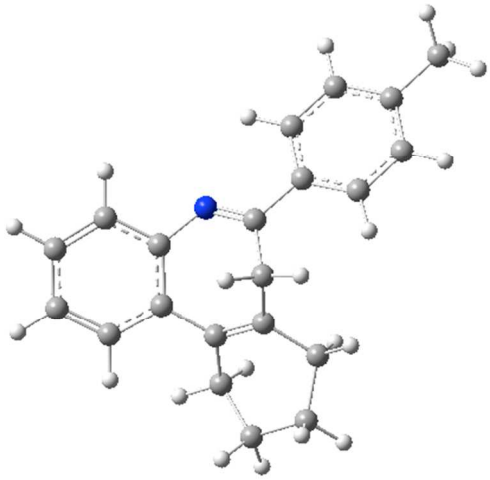
Imag freq = 63.9i cm-1
Zero-point correction= 0.366271 (Hartree/Particle)
Thermal correction to Energy= 0.383989
Thermal correction to Enthalpy= 0.384933
Thermal correction to Gibbs Free Energy= 0.319293
Sum of electronic and zero-point Energies= -867.250540
Sum of electronic and thermal Energies= -867.232823
Sum of electronic and thermal Enthalpies= -867.231879
Sum of electronic and thermal Free Energies= -867.297519

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	240.957	71.822	138.151

0 1

C	1.88232600	0.97612800	-0.11686400
C	0.63041900	1.65816700	0.03130100
C	-1.15246700	-0.02024600	-0.03879400
C	1.07639500	-1.44018500	-0.27922300
C	-0.42057300	-1.33873000	-0.15545100
H	-0.72278600	-1.95774600	0.70700200
H	-0.85433600	-1.87397100	-1.01619800
C	3.02815400	1.80057900	-0.12492200
H	4.00533500	1.35859400	-0.25641200
C	0.62239600	3.06055600	0.18212700
C	1.77566200	3.83208000	0.18669200
H	1.71928100	4.91031700	0.30674700
C	2.99521700	3.18508000	0.02341900
H	3.92681700	3.74451400	0.00824400
H	-0.35368300	3.52061800	0.29289600
C	-2.64660600	-0.12652000	-0.00521900
C	-3.32440100	-1.35690500	-0.01389400
C	-3.43100700	1.04314500	0.03891000
C	-4.71894800	-1.41324100	0.02084500
H	-2.77758200	-2.29270800	-0.04367600
C	-4.81614100	0.98094200	0.07077200
H	-2.91896300	1.99823500	0.04662200
C	-5.49244400	-0.25088800	0.06270700
H	-5.21083500	-2.38336500	0.01485300
H	-5.39068600	1.90470500	0.10215200
C	2.04996100	-0.49676200	-0.26202900
N	-0.67680600	1.16499200	0.04030100
C	3.45531000	-1.08541500	-0.42289300
H	3.56185600	-1.47875100	-1.44477500

H	4.24731800	-0.34911300	-0.31234000
C	3.73096900	-2.22441500	0.58155000
H	4.69911700	-2.68056900	0.34245000
H	3.83039700	-1.78891800	1.58236600
C	1.50886800	-2.89042100	-0.44305800
H	1.89118400	-3.04828700	-1.46368300
H	0.64824200	-3.56045900	-0.33736100
C	2.60385800	-3.28190700	0.56833400
H	2.15040100	-3.36722100	1.56258600
H	2.99383900	-4.27545600	0.31730800
C	-7.00078700	-0.30703400	0.09901400
H	-7.39637700	0.16705100	1.00620800
H	-7.44105700	0.22241700	-0.75532900
H	-7.36427200	-1.33915500	0.07601000



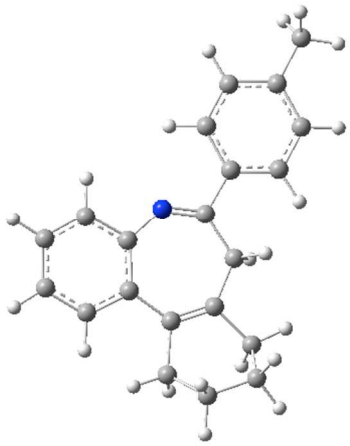
2c(4)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.366457 (Hartree/Particle)
Thermal correction to Energy= 0.384883
Thermal correction to Enthalpy= 0.385827
Thermal correction to Gibbs Free Energy= 0.316829
Sum of electronic and zero-point Energies= -867.270152
Sum of electronic and thermal Energies= -867.251727
Sum of electronic and thermal Enthalpies= -867.250782
Sum of electronic and thermal Free Energies= -867.319780

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	241.518	73.508	145.218

0 1

C	2.35659300	-0.66723000	-0.09628300
C	1.36815400	-1.68744400	0.06797300
C	-0.62026300	-0.48837100	0.52640500
C	0.98370600	1.33431900	0.41450900
C	3.70960700	-1.07277700	-0.15295800
H	4.47627000	-0.31296900	-0.27512400
C	1.78166700	-3.03585800	0.16265700
C	3.11912700	-3.38985500	0.15162500
H	3.40752700	-4.43297300	0.25057900
C	4.09543700	-2.39632700	-0.01073500
H	5.14955100	-2.65945500	-0.03080200
H	1.00329500	-3.78828300	0.24771000
C	-2.07558900	-0.33748100	0.26866500
C	-2.80768000	0.78783400	0.67529800
C	-2.76804700	-1.35637600	-0.41533800
C	-4.17426000	0.89015800	0.41110000
H	-2.32015200	1.60661400	1.19382500
C	-4.12801300	-1.25180600	-0.66780200
H	-2.20912800	-2.22849300	-0.73602700
C	-4.86148500	-0.12418000	-0.26107900
H	-4.71349700	1.77691500	0.73649200
H	-4.63690300	-2.05866100	-1.19141900
C	2.01271900	0.75529200	-0.25061400
N	-0.00916900	-1.49285800	-0.00086000
C	2.79166900	1.65179500	-1.19722000
H	3.69355300	1.16045800	-1.57185700
C	0.67782900	2.78848400	0.14291600
H	-0.06269300	3.17362200	0.85359400
C	3.15457200	3.00671800	-0.54992400
H	3.52825100	3.68421700	-1.32672100
H	3.98594000	2.84703500	0.14651800
C	1.96197900	3.65049900	0.20805400
H	1.74239500	4.64852700	-0.18903400
H	2.22928500	3.78823800	1.26183500
H	0.22805400	2.89550400	-0.85690200
H	2.16743000	1.83860400	-2.08520400
C	0.14523300	0.52146600	1.36899000
H	0.78692400	-0.04561800	2.05710800
H	-0.50920900	1.15204200	1.97247500
C	-6.33872900	-0.01597800	-0.55363300
H	-6.52561700	0.07509400	-1.63156600
H	-6.88058300	-0.90534400	-0.20972700
H	-6.78186400	0.85763800	-0.06536900



TS-2c(4)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 63.9i cm-1
Zero-point correction= 0.366271 (Hartree/Particle)
Thermal correction to Energy= 0.383989
Thermal correction to Enthalpy= 0.384933
Thermal correction to Gibbs Free Energy= 0.319293
Sum of electronic and zero-point Energies= -867.250540
Sum of electronic and thermal Energies= -867.232823
Sum of electronic and thermal Enthalpies= -867.231879
Sum of electronic and thermal Free Energies= -867.297519

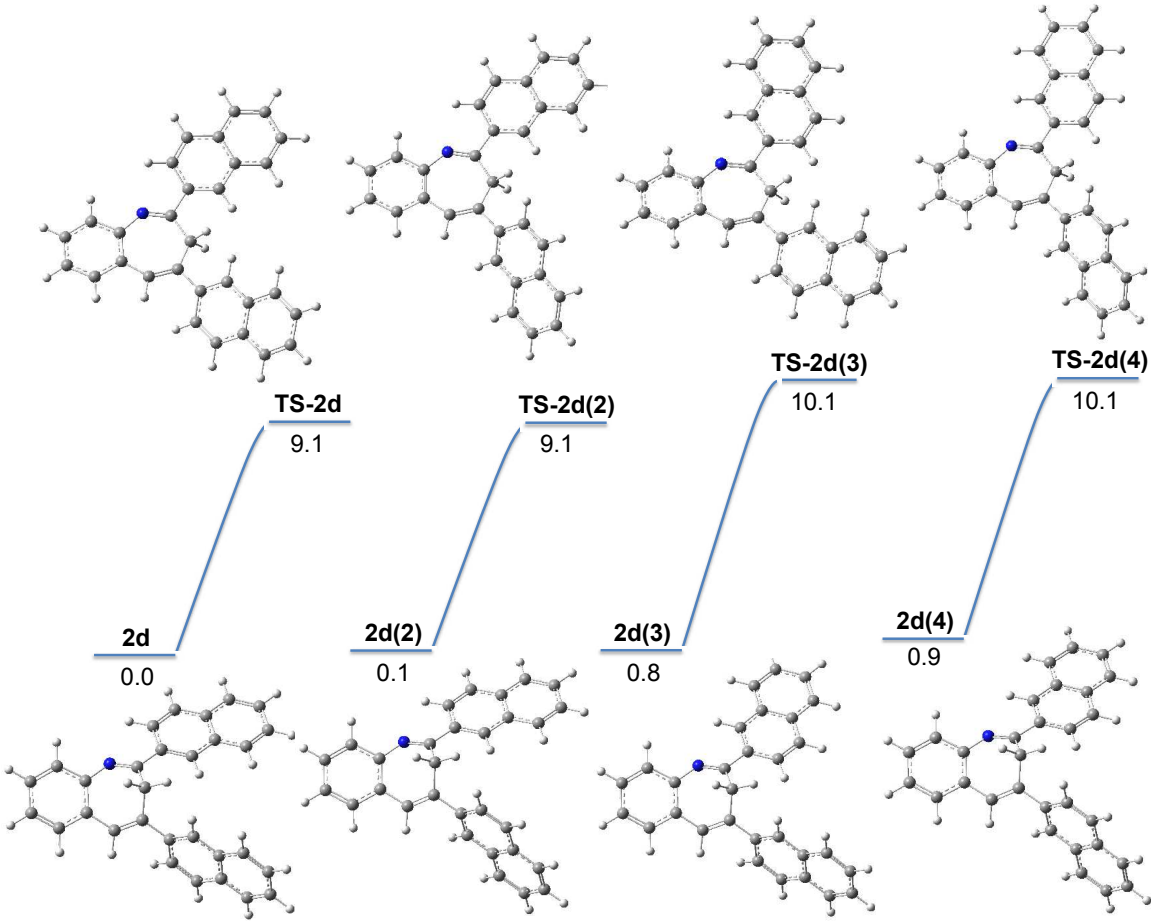
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	240.957	71.822	138.151

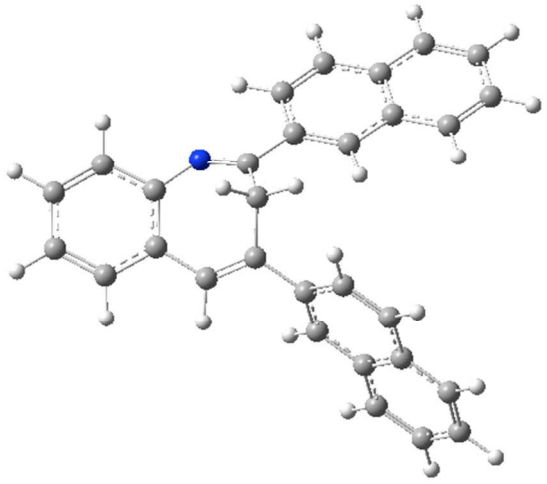
0 1

C	-1.88231800	0.97612300	-0.11680800
C	-0.63040900	1.65815500	0.03137200
C	1.15247200	-0.02026000	-0.03877200
C	-1.07639400	-1.44018800	-0.27923300
C	0.42057500	-1.33874000	-0.15546100
H	0.85433600	-1.87396000	-1.01622100
H	0.72278800	-1.95777800	0.70697600
C	-3.02814500	1.80057700	-0.12484500
H	-4.00532600	1.35859800	-0.25634600
C	-0.62238200	3.06053900	0.18223500
C	-1.77564700	3.83206700	0.18682100
H	-1.71926300	4.91030100	0.30690300
C	-2.99520300	3.18507400	0.02353200
H	-3.92680200	3.74451100	0.00837200
H	0.35369700	3.52059600	0.29301400

C	2.64661200	-0.12653900	-0.00520500
C	3.32440300	-1.35692600	-0.01391000
C	3.43101500	1.04312300	0.03894600
C	4.71895100	-1.41326500	0.02082100
H	2.77758200	-2.29272700	-0.04371000
C	4.81614900	0.98091700	0.07080000
H	2.91897300	1.99821400	0.04668100
C	5.49245000	-0.25091500	0.06270500
H	5.21083500	-2.38339100	0.01480700
H	5.39069700	1.90467800	0.10219700
C	-2.04995800	-0.49676300	-0.26201100
N	0.67681400	1.16497600	0.04035500
C	-3.45530900	-1.08540800	-0.42288600
H	-4.24731400	-0.34910700	-0.31230700
C	-1.50887000	-2.89041900	-0.44310800
H	-0.64824500	-3.56046200	-0.33743200
C	-3.73096600	-2.22443600	0.58152600
H	-4.69911700	-2.68058000	0.34241800
H	-3.83038800	-1.78896700	1.58235500
C	-2.60385900	-3.28193200	0.56827500
H	-2.99384300	-4.27547100	0.31722000
H	-2.15039900	-3.36727700	1.56252400
H	-1.89118900	-3.04825400	-1.46373700
H	-3.56186100	-1.47871400	-1.44477900
C	7.00079300	-0.30706600	0.09900300
H	7.44105900	0.22239400	-0.75533700
H	7.39638900	0.16700900	1.00620000
H	7.36427400	-1.33918700	0.07598500

Conformational analysis of 2d





2d(2)

Zero-point correction= 0.420264 (Hartree/Particle)
Thermal correction to Energy= 0.442767
Thermal correction to Enthalpy= 0.443711
Thermal correction to Gibbs Free Energy= 0.366926
Sum of electronic and zero-point Energies= -1210.196387

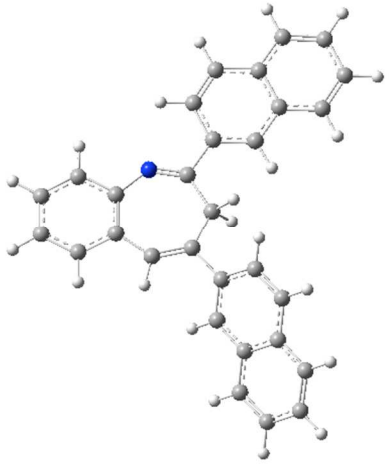
Sum of electronic and thermal Energies= -1210.173884
Sum of electronic and thermal Enthalpies= -1210.172940
Sum of electronic and thermal Free Energies= -1210.249725

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.841	94.529	161.609

0 1

C	-3.26481700	-1.76724300	-0.10350500
C	-3.74875600	-0.42214500	-0.08821400
C	-1.81577700	0.83637100	0.45677300
C	-0.90066500	-1.43003100	0.64917000
C	-1.33363300	-0.21674400	1.44486900
H	-0.53851600	0.16708400	2.08291500
C	-4.20672300	-2.80853500	-0.27498000
H	-3.83598900	-3.82995200	-0.32626100
C	-5.13998300	-0.19755200	-0.19658300
C	-6.03960200	-1.24483700	-0.29128500
H	-7.10524600	-1.04134900	-0.35350800
C	-5.56805000	-2.56652700	-0.34492700
H	-6.26438300	-3.39383800	-0.45012100
H	-5.47782100	0.83434200	-0.21185300
C	-0.99586400	2.03791000	0.16601000
C	-1.59398100	3.13368100	-0.52835100
C	0.33854700	2.12921000	0.52683800
C	-0.87400000	4.26354100	-0.81758300
H	-2.63563900	3.04403100	-0.81423200
C	1.11389300	3.27966100	0.22674000
H	0.83824400	1.30383200	1.02501000
C	0.49711800	4.37811200	-0.45339700
H	-1.34738400	5.09372700	-1.33700500
C	-1.85701100	-2.12541300	-0.01774700
N	-2.94721300	0.71195000	-0.14618700
C	0.52330700	-1.82833000	0.61519100
C	1.09980200	-2.33133500	-0.54219700
C	1.34104800	-1.71945000	1.78137400
C	2.45424800	-2.74741300	-0.58765200
H	0.50943200	-2.38481000	-1.45313100
C	2.65731800	-2.11390900	1.77014200
H	0.90533800	-1.34809100	2.70465500
C	3.25733900	-2.63786100	0.59377800
H	3.25722400	-2.03601700	2.67407000
H	-1.57844500	-3.06897500	-0.48371900

H	-2.18440300	-0.47408700	2.08968700
C	2.48580400	3.37594600	0.58448400
C	1.27230700	5.53073200	-0.74069200
C	3.21301900	4.50778300	0.29015500
C	2.60016200	5.59583800	-0.37744200
H	2.95309500	2.53753100	1.09579500
H	4.26140400	4.56983600	0.56899900
H	3.18362100	6.48410800	-0.60435300
H	0.80034100	6.36425100	-1.25572500
C	3.04793400	-3.26042100	-1.77361900
C	4.36730000	-3.65247200	-1.78841600
C	5.15878000	-3.54741300	-0.61773600
C	4.61486100	-3.05012600	0.54566400
H	2.43903300	-3.33915500	-2.67118000
H	4.80835400	-4.04481400	-2.70074000
H	6.19900200	-3.86052900	-0.64292900
H	5.21966700	-2.96693300	1.44576400



TS-2d(2)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 31.3i cm-1
Zero-point correction= 0.419804 (Hartree/Particle)
Thermal correction to Energy= 0.441771
Thermal correction to Enthalpy= 0.442716
Thermal correction to Gibbs Free Energy= 0.367762
Sum of electronic and zero-point Energies= -1210.181995
Sum of electronic and thermal Energies= -1210.160028
Sum of electronic and thermal Enthalpies= -1210.159083
Sum of electronic and thermal Free Energies= -1210.234037

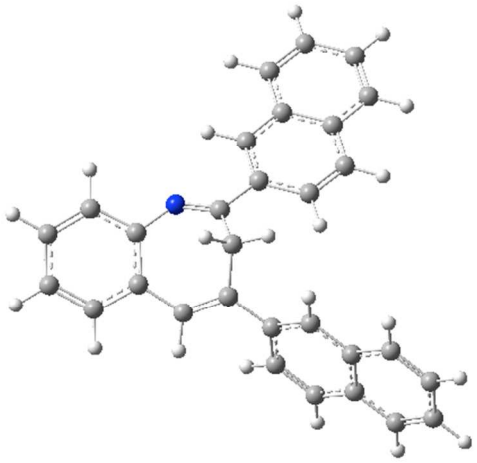
	E (Thermal)	CV	S

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	277.216	92.899	157.754

0 1

C	0.34726900	3.26867400	-0.16923300
C	-1.03763800	2.95120800	-0.10899400
C	-1.15742200	0.51336000	0.08069700
C	1.46515100	0.96973600	-0.00341000
C	0.28889700	0.03306900	0.14163200
H	0.41163700	-0.50806600	1.09370100
C	0.70883000	4.62541400	-0.27619200
H	1.76703500	4.87107900	-0.32786500
C	-1.97172700	4.00417200	-0.15508400
C	-1.58826200	5.33724200	-0.25346500
H	-2.34058700	6.12035400	-0.28467800
C	-0.23035200	5.65126600	-0.31585600
H	0.09718100	6.68405800	-0.39674100
H	-3.02033400	3.72847700	-0.11016300
C	-2.17422200	-0.58492600	0.16454300
C	-3.56219700	-0.25673200	0.06795900
C	-1.83171500	-1.91822500	0.34031100
C	-4.53124100	-1.22243700	0.14351700
H	-3.82191300	0.78585600	-0.06722400
C	-2.81220400	-2.94217300	0.42459600
H	-0.79513500	-2.22563200	0.42698000
C	-4.19602000	-2.59365700	0.32406800
H	-5.58086300	-0.94761200	0.06558900
C	1.44628200	2.31116800	-0.13452200
N	-1.64192700	1.69734900	-0.01672400
C	2.79092100	0.28545100	0.05033000
C	3.79791900	0.76016000	0.87593000
C	3.05825200	-0.87607000	-0.73541400
C	5.07065500	0.13739200	0.94717800
H	3.60652200	1.62313400	1.50865200
C	4.28281600	-1.49861400	-0.69551500
H	2.29250800	-1.25904100	-1.40382100
C	5.32466200	-1.02014400	0.14324900
H	4.47023200	-2.37106700	-1.31740000
H	2.42207400	2.78136200	-0.24173500
H	0.38483900	-0.75598800	-0.61732200
C	-2.45924500	-4.30659200	0.60684300
C	-3.42896800	-5.28152100	0.68510500
H	-3.14659900	-6.32145600	0.82482800
C	-4.79804500	-4.93460000	0.58475000

H	-5.55498900	-5.71174400	0.64809000
C	-5.17153000	-3.61955700	0.40824600
H	-1.40659800	-4.56954200	0.68434700
H	-6.22253100	-3.35076300	0.33125600
C	6.10205000	0.61980200	1.79836800
C	6.59780100	-1.64437000	0.21583300
C	7.32643600	-0.00765800	1.84727200
H	8.10704900	0.37214400	2.50091200
C	7.57766200	-1.15025800	1.04790900
H	8.54849200	-1.63604000	1.09549200
H	5.90713800	1.49681100	2.41124900
H	6.78664100	-2.52184500	-0.39838400



2d(3)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.420249 (Hartree/Particle)
Thermal correction to Energy= 0.442746
Thermal correction to Enthalpy= 0.443691
Thermal correction to Gibbs Free Energy= 0.367100
Sum of electronic and zero-point Energies= -1210.195344
Sum of electronic and thermal Energies= -1210.172847
Sum of electronic and thermal Enthalpies= -1210.171902
Sum of electronic and thermal Free Energies= -1210.248493

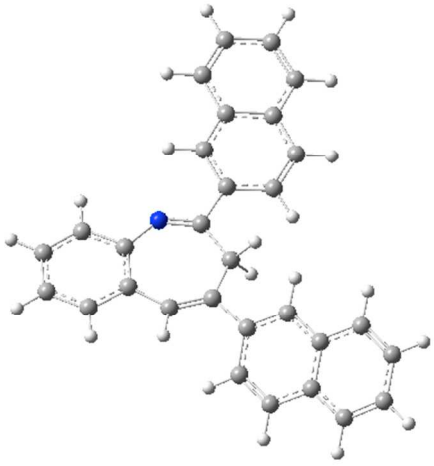
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.828	94.556	161.199

0 1

C	-0.26714500	3.60593000	0.18488100
C	-1.58677000	3.17022500	-0.14877000

C	-1.29479900	0.85622600	-0.56501900
C	1.04600000	1.50582600	-0.20144000
C	0.04407100	1.08361400	-1.25539200
H	0.36380800	0.19792200	-1.80271700
C	-0.05443600	4.99158100	0.37420300
H	0.93994100	5.32110300	0.66759700
C	-2.60071600	4.13932900	-0.32176500
C	-2.33994700	5.49297300	-0.19963800
H	-3.13594700	6.21564500	-0.35786300
C	-1.05495500	5.92554500	0.16625900
H	-0.84815500	6.98431000	0.29511300
H	-3.60039500	3.77932700	-0.54590600
C	-1.81874100	-0.52061700	-0.37034500
C	-0.97533900	-1.66561600	-0.46568700
C	-3.16305500	-0.70862800	-0.08330600
C	-1.47846500	-2.93221200	-0.28275600
H	0.08662900	-1.54374800	-0.65156800
C	-3.71226400	-1.99957200	0.09538400
H	-3.80370400	0.16371800	-0.00107400
C	-2.85462300	-3.14404000	-0.00668300
H	-0.81723100	-3.79326200	-0.34538300
C	0.85432400	2.70576800	0.40548700
N	-2.00704100	1.84578900	-0.15195700
C	2.19881200	0.64057100	0.13056200
C	2.81334000	-0.15751000	-0.82443600
C	2.72920200	0.62423400	1.45775100
C	3.94339600	-0.96002300	-0.52208800
H	2.45434100	-0.15668300	-1.85058900
C	3.82086300	-0.14186800	1.78294600
H	2.23294200	1.20900700	2.22597500
C	4.46540400	-0.95480000	0.81154300
H	4.19849600	-0.14584500	2.80288800
H	1.63129800	3.08006200	1.06958600
H	-0.09726000	1.89356100	-1.98337400
C	-5.09342400	-2.19965100	0.37412700
C	-3.40996700	-4.43850000	0.17372000
C	-5.60086800	-3.46702400	0.54404900
C	-4.75092100	-4.59745200	0.44268000
H	-5.74112100	-1.32972600	0.45164900
H	-6.65702000	-3.60757200	0.75751100
H	-5.16450300	-5.59308500	0.57919100
H	-2.75668200	-5.30451200	0.09618300
C	4.58076600	-1.76789300	-1.50325100
C	5.67638800	-2.53649100	-1.18038700

C	6.18781900	-2.53425700	0.14076700
C	5.59381300	-1.76072100	1.11353300
H	4.18682800	-1.76885400	-2.51704900
H	6.15385700	-3.14974000	-1.93984300
H	7.05269200	-3.14579600	0.38306700
H	5.98389100	-1.75604900	2.12872200



TS-2d(3)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 31.2i cm-1
Zero-point correction= 0.419811 (Hartree/Particle)
Thermal correction to Energy= 0.441796
Thermal correction to Enthalpy= 0.442740
Thermal correction to Gibbs Free Energy= 0.367783
Sum of electronic and zero-point Energies= -1210.180524
Sum of electronic and thermal Energies= -1210.158539
Sum of electronic and thermal Enthalpies= -1210.157595
Sum of electronic and thermal Free Energies= -1210.232552

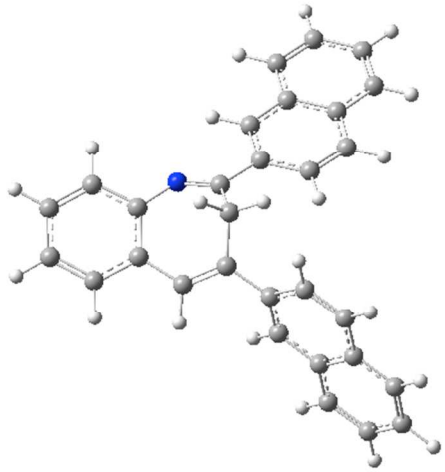
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.231	92.920	157.760

0 1

C	0.34061200	3.30152400	-0.12551700
C	-1.04983400	3.00986900	-0.06711300
C	-1.20691300	0.57738100	0.12388900
C	1.42803900	0.98621400	0.07684700
C	0.22989000	0.07501100	0.21488300
H	0.33010300	-0.46093700	1.17213600
C	0.72677900	4.65158300	-0.23641200

H	1.78933600	4.87810100	-0.28711200
C	-1.96426800	4.07948500	-0.11496800
C	-1.55639500	5.40534000	-0.21487400
H	-2.29434300	6.20202200	-0.24685000
C	-0.19309700	5.69454600	-0.27891400
H	0.15339700	6.72092000	-0.36213900
H	-3.01767500	3.82263600	-0.07037600
C	-2.23751400	-0.51557700	0.16892300
C	-1.90721800	-1.87420200	0.45862200
C	-3.56904300	-0.21144500	-0.08058300
C	-2.87334100	-2.85301100	0.49663100
H	-0.88233800	-2.15840700	0.66664700
C	-4.58381100	-1.19509900	-0.05648700
H	-3.82697000	0.81892600	-0.30055300
C	-4.23568700	-2.55332400	0.24067800
H	-2.59600000	-3.87897800	0.72741600
C	1.42316100	2.32696400	-0.07605600
N	-1.67497600	1.76642600	0.01961800
C	2.74464600	0.28745900	0.15179600
C	2.95514900	-0.96388100	-0.40916600
C	3.84305000	0.90117700	0.83129200
C	4.21375700	-1.61673000	-0.35240800
H	2.15616800	-1.47148400	-0.94220100
C	5.07184200	0.29390900	0.91059300
H	3.68627400	1.85629900	1.32260500
C	5.30328200	-0.97742700	0.32078600
H	5.88469000	0.78001700	1.44540400
H	2.40245200	2.78840200	-0.18549200
H	0.31541500	-0.72135700	-0.53730000
C	-5.94651500	-0.87820600	-0.31949000
C	-6.91496500	-1.85452200	-0.28802800
H	-7.95213500	-1.60096100	-0.48989900
C	-6.56776700	-3.19736600	0.00813300
H	-7.34277200	-3.95885200	0.03029300
C	-5.25894900	-3.53779500	0.26616200
H	-6.20758500	0.15286000	-0.54542600
H	-4.99109800	-4.56718500	0.49314700
C	4.43000600	-2.89021500	-0.94670000
C	6.55959200	-1.63498200	0.38079500
C	5.66126800	-3.50198800	-0.87501700
H	5.81283600	-4.47540500	-1.33364900
C	6.73679200	-2.86935600	-0.20411500
H	7.70358100	-3.36286100	-0.15418800
H	3.60353300	-3.37512300	-1.46135300

H	7.38268700	-1.14563100	0.89648000



2d(4)

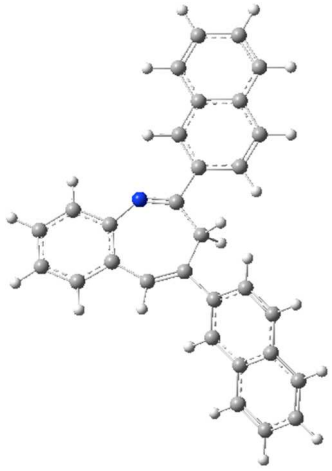
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.420231 (Hartree/Particle)
Thermal correction to Energy= 0.442727
Thermal correction to Enthalpy= 0.443672
Thermal correction to Gibbs Free Energy= 0.367026
Sum of electronic and zero-point Energies= -1210.195184
Sum of electronic and thermal Energies= -1210.172687
Sum of electronic and thermal Enthalpies= -1210.171743
Sum of electronic and thermal Free Energies= -1210.248389

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	277.816	94.539	161.314

0 1

C	-0.20994200	3.51356800	-0.18471400
C	1.19352900	3.27208000	-0.06032700
C	1.28797000	1.00582700	0.62540600
C	-1.14089500	1.33875500	0.63748200
C	0.07133800	1.16296000	1.52796700
H	-0.03192300	0.31926300	2.20973700
C	-0.63339900	4.83388800	-0.46527700
H	-1.69818600	5.01160200	-0.59968100
C	2.08474800	4.36328500	-0.17389700
C	1.62992600	5.65432200	-0.37745800
H	2.33859100	6.47570700	-0.44118900
C	0.25533300	5.89261000	-0.53929400
H	-0.10863200	6.89823000	-0.73063400

H	3.14683900	4.14792500	-0.10463300
C	1.94326900	-0.31822200	0.46529200
C	1.28850600	-1.53034100	0.83091700
C	3.22540800	-0.38935500	-0.05993100
C	1.91066700	-2.74634400	0.67204900
H	0.27229400	-1.50697400	1.21029900
C	3.89632300	-1.62380300	-0.22148700
H	3.72045100	0.53275700	-0.34770600
C	3.22832000	-2.83621800	0.15199800
H	1.39023500	-3.66180100	0.94343800
C	-1.22339100	2.47307200	-0.10415300
N	1.78013500	2.01355300	-0.00697500
C	-2.19378700	0.30080600	0.59478200
C	-2.84156200	-0.01389300	-0.59117800
C	-2.58520900	-0.39404600	1.77987300
C	-3.87702200	-0.98042700	-0.64869600
H	-2.53260000	0.47166200	-1.51315500
C	-3.58474300	-1.33677800	1.75751600
H	-2.10570100	-0.15002900	2.72366600
C	-4.26195800	-1.66164300	0.55159500
H	-3.87637400	-1.84323800	2.67478500
H	-2.14798400	2.66933400	-0.64428100
H	0.22746000	2.06588500	2.13307300
C	5.21692900	-1.70158800	-0.74609000
C	3.90456600	-4.07390800	-0.01404400
C	5.84483800	-2.91653000	-0.89516300
C	5.18221300	-4.11436400	-0.52555100
H	5.72058200	-0.78044100	-1.02910200
H	6.85297700	-2.96361000	-1.29788900
H	5.68945200	-5.06757500	-0.64825100
H	3.39483100	-4.99175700	0.26976000
C	-4.54090700	-1.30583200	-1.86342300
C	-5.54043500	-2.25187600	-1.88870700
C	-5.92272400	-2.92147100	-0.69979700
C	-5.29581500	-2.63267400	0.49196200
H	-4.24527700	-0.79145600	-2.77479200
H	-6.04132200	-2.48964800	-2.82324700
H	-6.71340100	-3.66607800	-0.73329700
H	-5.58581100	-3.14579500	1.40601900



TS-2d(4)

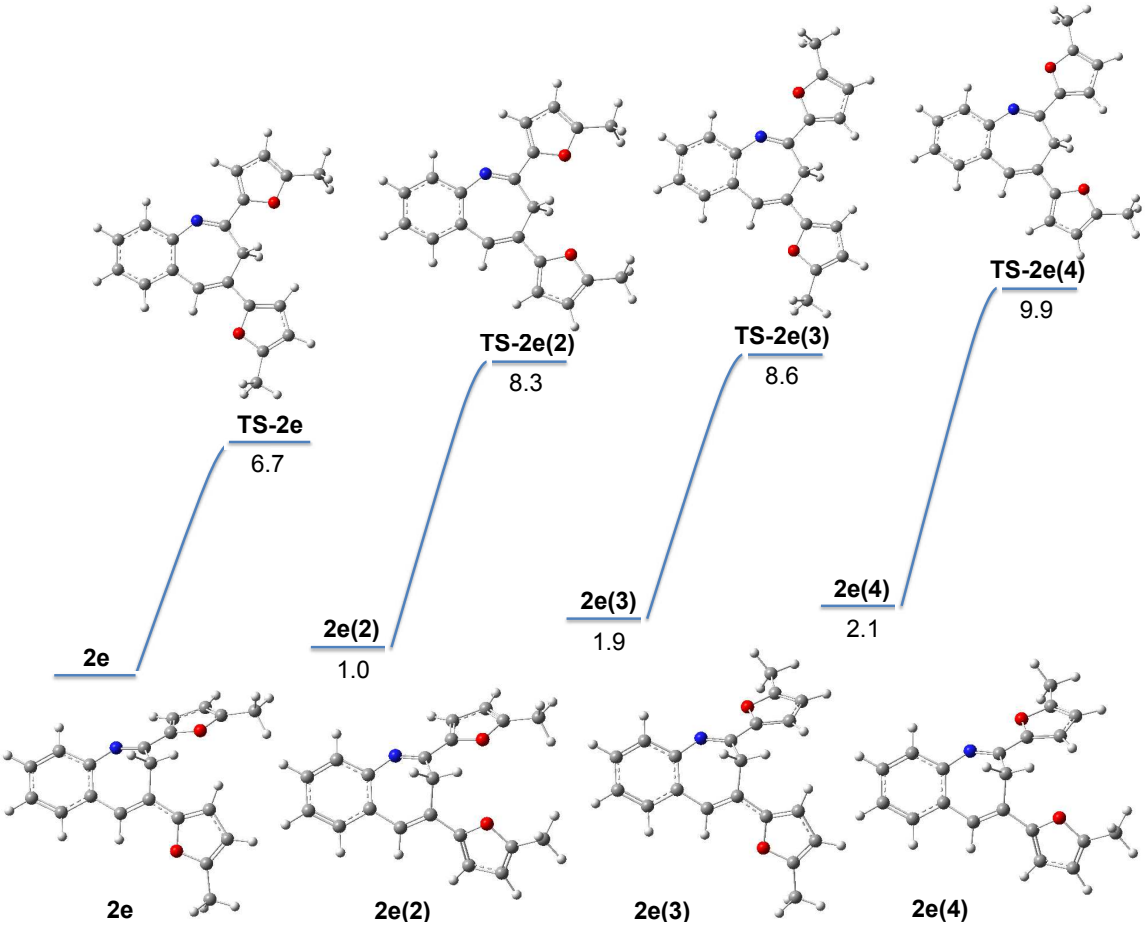
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 27.6i cm-1
Zero-point correction= 0.419753 (Hartree/Particle)
Thermal correction to Energy= 0.441727
Thermal correction to Enthalpy= 0.442671
Thermal correction to Gibbs Free Energy= 0.367793
Sum of electronic and zero-point Energies= -1210.180502
Sum of electronic and thermal Energies= -1210.158527
Sum of electronic and thermal Enthalpies= -1210.157583
Sum of electronic and thermal Free Energies= -1210.232461

0 1

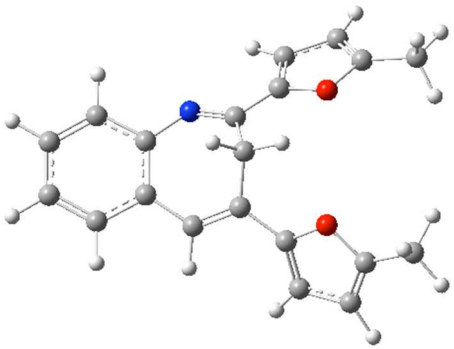
C	0.35673900	3.29807600	-0.20673200
C	-1.03306800	3.00077300	-0.16012000
C	-1.19104000	0.56587200	0.03827900
C	1.43919800	0.98358900	-0.01559400
C	0.24688100	0.06389000	0.11155500
H	0.35191200	-0.48317700	1.06243300
C	0.73957100	4.64831100	-0.31892000
H	1.80187900	4.87788800	-0.35974200
C	-1.95062600	4.06699100	-0.22378100
C	-1.54645500	5.39377400	-0.32782700
H	-2.28701800	6.18739800	-0.37303200
C	-0.18377500	5.68784200	-0.37713300
H	0.15981400	6.71509400	-0.46172300
H	-3.00364300	3.80717700	-0.18810000
C	-2.22351800	-0.52376300	0.11263500
C	-1.88217900	-1.89593500	0.31213800
C	-3.56867400	-0.20282600	-0.01279900
C	-2.84974500	-2.87183300	0.37895300

H	-0.84651100	-2.19486400	0.42270200
C	-4.58605000	-1.18186800	0.04939800
H	-3.83506500	0.83787500	-0.16245200
C	-4.22591100	-2.55458200	0.25005400
H	-2.56264100	-3.90908400	0.53525400
C	1.44119400	2.32458600	-0.15122800
N	-1.65590200	1.75621600	-0.06561600
C	2.75397200	0.28084000	0.06296700
C	3.75521800	0.74722700	0.90036000
C	3.01655800	-0.89061100	-0.70962600
C	5.01767400	0.10709400	0.99552700
H	3.56660400	1.61735400	1.52403700
C	4.23126100	-1.53031800	-0.64629400
H	2.25563700	-1.26828100	-1.38646900
C	5.26717600	-1.06020900	0.20439500
H	4.41528500	-2.41038200	-1.25839200
H	2.42521300	2.78055500	-0.24419900
H	0.33898700	-0.72432700	-0.64925300
C	-5.96338700	-0.84612300	-0.08098500
C	-6.93409700	-1.81844100	-0.01536300
H	-7.98242000	-1.55064500	-0.11569100
C	-6.57463700	-3.17596800	0.18350300
H	-7.35154900	-3.93419100	0.23358600
C	-5.25173700	-3.53464300	0.31284400
H	-6.23351000	0.19602400	-0.23331200
H	-4.97468800	-4.57517600	0.46576500
C	6.04293300	0.58132700	1.85867200
C	6.52996400	-1.70193800	0.30106700
C	7.25730300	-0.06309100	1.93093100
H	8.03333000	0.31063400	2.59348300
C	7.50415800	-1.21537100	1.14416800
H	8.46707200	-1.71457000	1.21022400
H	5.85140100	1.46574200	2.46190200
H	6.71539400	-2.58678100	-0.30354400

Conformational analysis of 2e



Four isomers were considered for **2e** based on the orientation of 5-Me-2-furyl- rings, namely **2e**, **2e(2)**, **2e(3)**, and **2e(4)**. Their structures were optimized at B3LYP/6-31G(d) level of theory. Calculations revealed that **2e** is most stable among considered isomers. Isomers **2e(2)**, **2e(3)**, and **2e(4)** were less stable than **2e** by 1.0 kcal/mol, 1.9 kcal/mol, and 2.1 kcal/mol, respectively. Because **2e** is most stable (therefore most populated at r.t.) we chose to report its E_a, $\Delta G^{\ddagger}$, $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ in the manuscript.



2e(2)

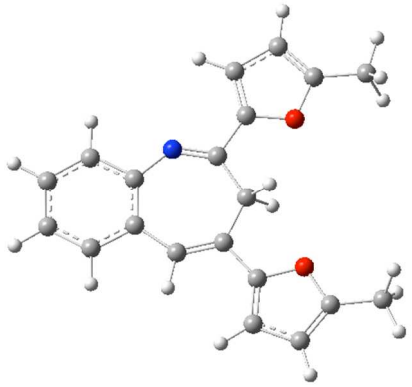
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.320946 (Hartree/Particle)
Thermal correction to Energy= 0.340250
Thermal correction to Enthalpy= 0.341194
Thermal correction to Gibbs Free Energy= 0.271833
Sum of electronic and zero-point Energies= -977.213073
Sum of electronic and thermal Energies= -977.193769
Sum of electronic and thermal Enthalpies= -977.192825
Sum of electronic and thermal Free Energies= -977.262186

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	213.510	75.426	145.984

0 1

C	2.72540900	-0.85598800	0.08737100
C	2.79349700	0.56398800	-0.08279000
C	0.51805300	1.18176200	-0.29822900
C	0.26366900	-1.25057700	-0.16547300
C	0.13107900	-0.05751400	-1.08704100
H	-0.87806200	0.02679700	-1.48643100
C	3.94330700	-1.57702300	0.12463700
H	3.89522600	-2.65072200	0.29337200
C	4.06191300	1.16673200	-0.25014500
C	5.22698500	0.42098900	-0.27674700
H	6.18416400	0.91357700	-0.42575000
C	5.16975500	-0.96785200	-0.07438500
H	6.08093500	-1.55962600	-0.06403800
H	4.08608000	2.24788800	-0.34834500
C	1.49517300	-1.59646900	0.29734800
N	1.72999200	1.44392900	0.06223600
H	1.59607200	-2.53535000	0.83935900
H	0.83389900	-0.15900900	-1.92384200
C	-0.51267700	2.13220400	0.08116300
C	-0.48690800	3.27819200	0.83617000
O	-1.79467200	1.91855100	-0.37382900
C	-1.81400500	3.79226700	0.84237900
H	0.38952600	3.68395400	1.31938000
C	-2.57525700	2.93183900	0.09606400
H	-2.16892100	4.68550400	1.33825900
C	-0.92063800	-2.00169100	0.20141100
C	-1.20878400	-2.88997700	1.20921600
O	-2.03620000	-1.85837700	-0.59496200
C	-2.55530300	-3.31729600	1.01277500

H	-0.54250900	-3.18106100	2.00902600
C	-3.02034500	-2.66120900	-0.09259900
H	-3.11645800	-4.01278200	1.62206900
C	-4.01551000	2.89689700	-0.27656200
H	-4.49962700	1.98001100	0.08228100
H	-4.53470100	3.75305000	0.16240600
H	-4.14982700	2.93448700	-1.36482700
C	-4.32445300	-2.65060200	-0.80929000
H	-5.02748400	-3.32470900	-0.31234500
H	-4.76596100	-1.64603700	-0.82628200
H	-4.21509200	-2.97690900	-1.85124200



TS-2e(2)

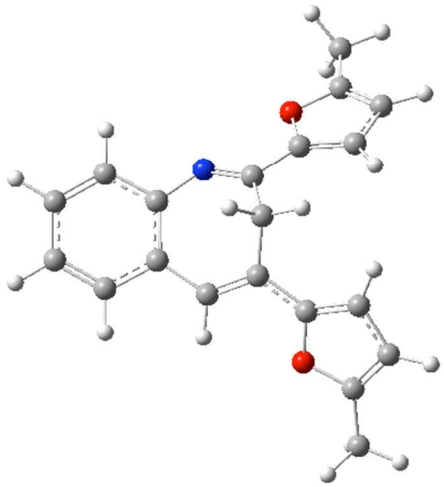
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 52.8i cm-1 and 8.4i cm-1
Zero-point correction= 0.320140 (Hartree/Particle)
Thermal correction to Energy= 0.338102
Thermal correction to Enthalpy= 0.339046
Thermal correction to Gibbs Free Energy= 0.273590
Sum of electronic and zero-point Energies= -977.201458
Sum of electronic and thermal Energies= -977.183496
Sum of electronic and thermal Enthalpies= -977.182552
Sum of electronic and thermal Free Energies= -977.248008

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.162	71.911	137.764

0 1

C	-2.46317200	-1.24738700	-0.00000300
C	-2.71253400	0.15555600	0.00001600
C	-0.50639000	1.18609800	0.00002600
C	0.09924700	-1.38764100	0.00005800
C	0.52079800	0.06310100	0.00029900

H	1.18575100	0.23354100	0.85902800
C	-3.57787900	-2.11217200	0.00001800
H	-3.39349000	-3.18412600	-0.00001100
C	-4.04921000	0.60129300	0.00007000
C	-5.12862400	-0.27431700	0.00011500
H	-6.14434300	0.11136900	0.00016000
C	-4.88880800	-1.64990700	0.00008400
H	-5.71365000	-2.35717400	0.00010500
H	-4.20095500	1.67588200	0.00007000
C	-1.15910400	-1.88691800	-0.00005600
N	-1.79316300	1.19913600	-0.00005900
H	-1.22984100	-2.97308700	-0.00018100
H	1.18628700	0.23364300	-0.85798400
C	0.09765200	2.51880600	-0.00009600
C	-0.44189100	3.78154300	-0.00027100
O	1.47279100	2.61762300	-0.00000200
C	0.65004000	4.69396100	-0.00028900
H	-1.49829000	4.00329600	-0.00036800
C	1.79518700	3.94250900	-0.00012300
H	0.60136300	5.77446100	-0.00040900
C	3.24422500	4.28129300	-0.00009000
H	3.75193100	3.87545700	0.88390600
H	3.75192100	3.87573500	-0.88422300
H	3.37196700	5.36711100	0.00007300
C	1.21786000	-2.32473200	-0.00001700
C	1.33542300	-3.69579400	-0.00026100
O	2.48340200	-1.77877100	0.00019900
C	2.72865700	-3.99471400	-0.00018400
H	0.52493900	-4.41056500	-0.00047700
C	3.39143800	-2.79935600	0.00009900
H	3.18536900	-4.97518000	-0.00032600
C	4.82947300	-2.41738100	0.00032700
H	5.08843300	-1.82134000	0.88461900
H	5.45233100	-3.31610200	0.00006400
H	5.08854300	-1.82074000	-0.88352700



2e(3)

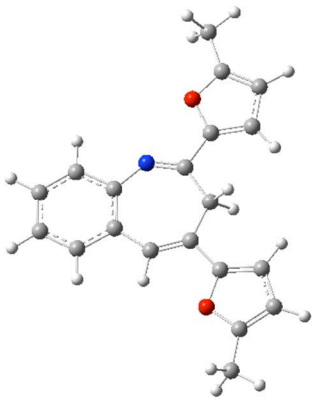
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.320947 (Hartree/Particle)
Thermal correction to Energy= 0.340221
Thermal correction to Enthalpy= 0.341165
Thermal correction to Gibbs Free Energy= 0.271880
Sum of electronic and zero-point Energies= -977.211588
Sum of electronic and thermal Energies= -977.192314
Sum of electronic and thermal Enthalpies= -977.191369
Sum of electronic and thermal Free Energies= -977.260655

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.492	75.462	145.823

0 1

C	-0.05878200	2.54091700	0.08487700
C	-1.41832100	2.11776400	-0.06193200
C	-1.20954600	-0.17873700	-0.59010600
C	1.16523300	0.44993100	-0.54379700
C	0.02971600	0.02818300	-1.44765300
H	0.27395100	-0.86525600	-2.02308500
C	0.18662600	3.91957500	0.29133100
H	1.21570200	4.23683800	0.44551900
C	-2.43933300	3.09583800	-0.04481200
C	-2.15558500	4.44386800	0.08573100
H	-2.96208300	5.17224400	0.07624400
C	-0.82727400	4.86156600	0.26969000
H	-0.59625800	5.91463700	0.40484800
H	-3.46296700	2.74318700	-0.12725900
C	1.07958700	1.63974700	0.10920100

N	-1.85505900	0.79964200	-0.05317800
H	1.94720000	1.97809500	0.67056700
H	-0.18947900	0.83163800	-2.16272500
C	-1.67451200	-1.53737800	-0.37592900
C	-1.23604400	-2.76124100	-0.82679000
O	-2.76340300	-1.72656300	0.43840500
C	-2.09959900	-3.74188400	-0.26072800
H	-0.39305900	-2.94499100	-1.47660400
C	-3.01309000	-3.06171300	0.49915100
H	-2.05354200	-4.81356300	-0.39687100
C	2.31293000	-0.42203800	-0.41971900
C	2.70677900	-1.56807200	-1.06898700
O	3.26608000	-0.09688400	0.51866400
C	3.95759200	-1.95833100	-0.50167500
H	2.18081700	-2.06852100	-1.86927400
C	4.25925800	-1.03447400	0.45751100
H	4.55866300	-2.81598100	-0.77108400
C	-4.16863000	-3.48827700	1.33414100
H	-5.10552600	-3.04763100	0.97202200
H	-4.26693000	-4.57683000	1.30973800
H	-4.04215300	-3.17495000	2.37757100
C	5.39728000	-0.86442500	1.40062700
H	6.12048800	-1.67259100	1.26142600
H	5.91392500	0.09010500	1.23947400
H	5.05953400	-0.88127000	2.44440200



TS-2e(3)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 42.7i cm-1
Zero-point correction= 0.320571 (Hartree/Particle)
Thermal correction to Energy= 0.339284
Thermal correction to Enthalpy= 0.340228
Thermal correction to Gibbs Free Energy= 0.272819
Sum of electronic and zero-point Energies= -977.200984

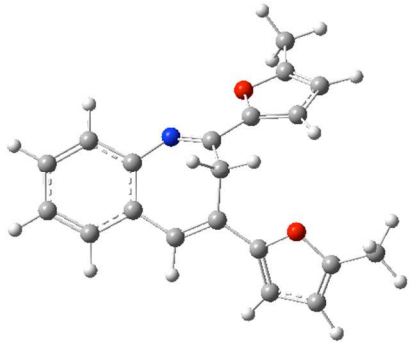
Sum of electronic and thermal Energies= -977.182272
Sum of electronic and thermal Enthalpies= -977.181328
Sum of electronic and thermal Free Energies= -977.248736

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.904	73.698	141.873

0 1

C	0.60101400	2.24110200	-0.00005900
C	-0.82005700	2.13432400	-0.00003900
C	-1.28291000	-0.25549000	-0.00007500
C	1.36424200	-0.20414400	-0.00019200
C	0.06387000	-0.97110400	-0.00041600
H	0.06584500	-1.64757900	-0.86958700
C	1.16303000	3.53559400	-0.00007400
H	2.24720300	3.62146400	-0.00007400
C	-1.58467600	3.31870000	-0.00005100
C	-1.00353800	4.58078600	-0.00009300
H	-1.62855700	5.46954500	-0.00010600
C	0.38914700	4.68978600	-0.00010000
H	0.86888900	5.66474600	-0.00012000
H	-2.66296100	3.19691500	-0.00002000
C	1.54422200	1.13772500	-0.00005300
N	-1.60624400	0.98768700	0.00004200
H	2.58195800	1.46137500	0.00005100
H	0.06593700	-1.64816400	0.86829200
C	-2.39530100	-1.20612300	0.00006300
C	-2.44843000	-2.58214300	-0.00003200
O	-3.67566800	-0.71322500	0.00032100
C	-3.82645100	-2.94257600	0.00019100
H	-1.60546800	-3.25815600	-0.00023500
C	-4.53194100	-1.76952000	0.00040000
H	-4.24485900	-3.93973400	0.00019700
C	-5.98570900	-1.45104400	0.00065000
H	-6.26464700	-0.86388400	0.88416400
H	-6.26504700	-0.86424600	-0.88298400
H	-6.57137300	-2.37424000	0.00096400
C	2.52419400	-1.08039900	-0.00018700
C	2.65733100	-2.44918600	-0.00037200
O	3.77966900	-0.51638100	0.00001700
C	4.05722300	-2.73173200	-0.00027100
H	1.85493000	-3.17244600	-0.00056800
C	4.70023000	-1.52747900	-0.00003500

H	4.52813400	-3.70521800	-0.00036500
C	6.13277100	-1.12568400	0.00018900
H	6.38170000	-0.52553200	0.88439000
H	6.76863100	-2.01514000	-0.00002400
H	6.38182200	-0.52501600	-0.88362500



2e(4)

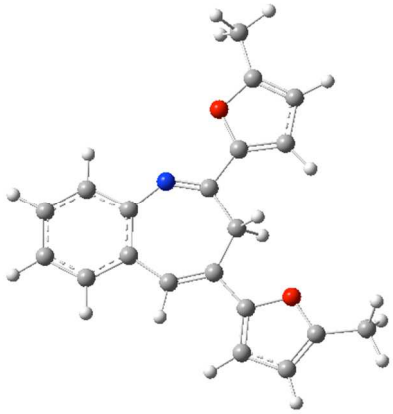
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.320934 (Hartree/Particle)
Thermal correction to Energy= 0.340207
Thermal correction to Enthalpy= 0.341151
Thermal correction to Gibbs Free Energy= 0.271900
Sum of electronic and zero-point Energies= -977.211234
Sum of electronic and thermal Energies= -977.191961
Sum of electronic and thermal Enthalpies= -977.191017
Sum of electronic and thermal Free Energies= -977.260268

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	213.483	75.428	145.751

0 1

C	2.36810400	-1.38646500	0.17429200
C	2.65346500	-0.02293900	-0.15962800
C	0.50858600	0.89438900	-0.53992000
C	-0.11344000	-1.44065800	-0.14549100
C	-0.01818800	-0.36661300	-1.20463500
H	-0.97591500	-0.20172800	-1.69592500
C	3.46195300	-2.26854800	0.34770900
H	3.24857600	-3.29414100	0.64156700
C	4.00174700	0.36012100	-0.34876300
C	5.04049400	-0.54735000	-0.24103600
H	6.06406600	-0.22388300	-0.41059800
C	4.77017500	-1.87627900	0.12528200
H	5.58120200	-2.58966600	0.24303200

H	4.19109300	1.40565300	-0.57228000
C	1.03443300	-1.90626400	0.41675400
N	1.73331800	1.01669900	-0.15452700
H	0.97483100	-2.76953700	1.07772400
H	0.70776800	-0.66871400	-1.97004700
C	-0.42081700	1.98959400	-0.33258800
C	-1.76055600	2.13786500	-0.60837500
O	0.04238600	3.13320000	0.26918500
C	-2.13093600	3.43553900	-0.15340800
H	-2.40757900	1.39918300	-1.05914400
C	-0.99898500	4.00209600	0.36888900
H	-3.10853400	3.89477800	-0.20505100
C	-1.41649300	-1.93869200	0.24748900
C	-1.87162700	-2.68756400	1.30534400
O	-2.48241600	-1.64916400	-0.57987800
C	-3.27182700	-2.87618700	1.10961100
H	-1.27689500	-3.04330500	2.13481100
C	-3.60172100	-2.22460300	-0.04519800
H	-3.95453200	-3.41643300	1.75134700
C	-0.70950900	5.32332400	0.98939600
H	0.05016400	5.87282500	0.42004600
H	-1.61926800	5.92866600	1.02414100
H	-0.33087700	5.20775300	2.01223600
C	-4.87674100	-2.02735500	-0.78655800
H	-5.69058000	-2.54147500	-0.26801600
H	-5.13945200	-0.96448300	-0.86423800
H	-4.81574200	-2.42512000	-1.80737400



TS-2e(4)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Imag freq = 50.6i cm-1
Zero-point correction= 0.320324 (Hartree/Particle)
Thermal correction to Energy= 0.339143

Thermal correction to Enthalpy= 0.340087
Thermal correction to Gibbs Free Energy= 0.271290
Sum of electronic and zero-point Energies= -977.198832
Sum of electronic and thermal Energies= -977.180013
Sum of electronic and thermal Enthalpies= -977.179069
Sum of electronic and thermal Free Energies= -977.247866

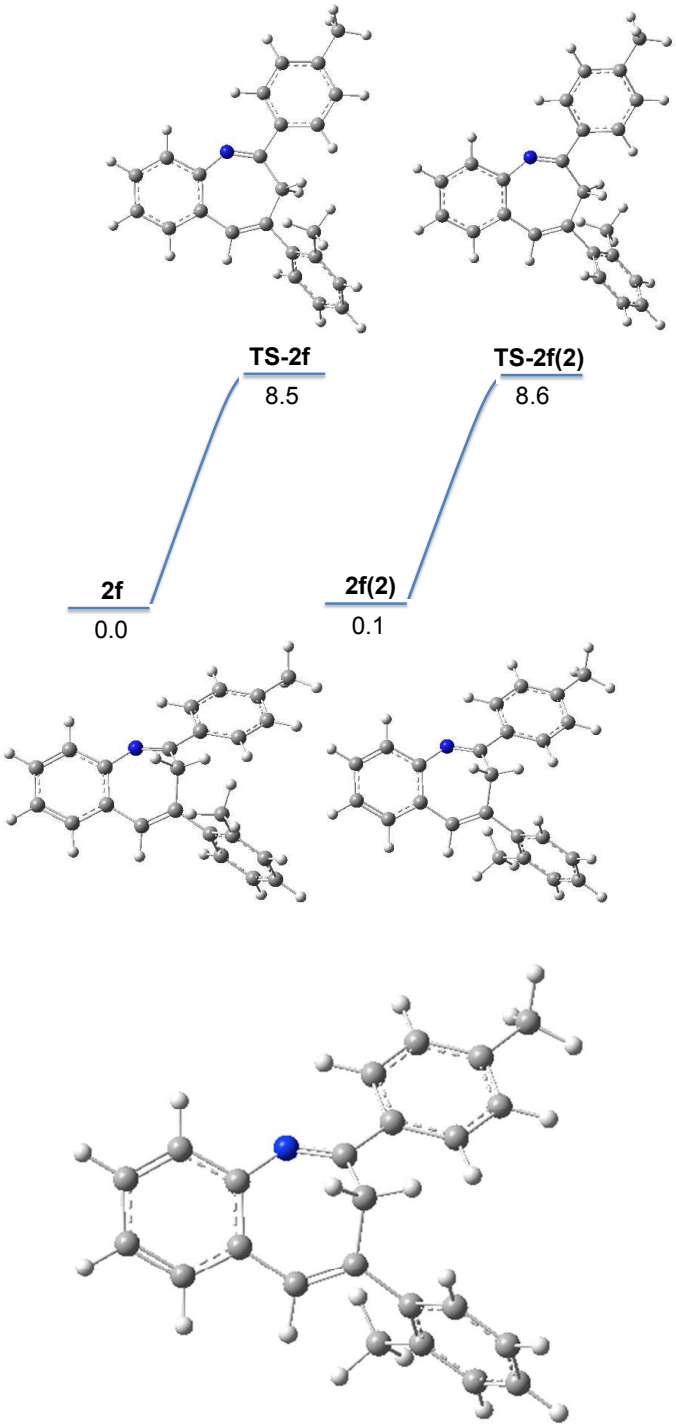
	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	212.815	73.810	144.795

0 1

C	-0.02036200	2.60282500	0.00003000
C	1.30795100	2.08695300	0.00007900
C	1.05038700	-0.33218100	0.00011100
C	-1.46896100	0.48583400	0.00009500
C	-0.44672500	-0.62496800	0.00042100
H	-0.64826900	-1.27463700	0.86479400
C	-0.18067500	4.00484900	0.00004500
H	-1.19253400	4.40397300	-0.00001000
C	2.38381100	2.99721400	0.00015800
C	2.19591600	4.37417100	0.00020300
H	3.05283600	5.04213200	0.00027000
C	0.89562900	4.88404100	0.00014000
H	0.72022100	5.95636900	0.00015800
H	3.37974600	2.56632300	0.00017700
C	-1.24341100	1.82084400	-0.00005000
N	1.72612600	0.76049900	0.00000500
H	-2.13575700	2.44418500	-0.00022400
H	-0.64847000	-1.27526700	-0.86342100
C	1.83334200	-1.56817000	-0.00003700
C	1.47704400	-2.89833200	0.00005000
O	3.20248700	-1.47560100	-0.00029400
C	2.68705100	-3.64975100	-0.00015600
H	0.47154500	-3.29392200	0.00024800
C	3.70801700	-2.73771700	-0.00036500
H	2.79187300	-4.72607700	-0.00015600
C	5.19095800	-2.86351200	-0.00060900
H	5.63114000	-2.38512700	-0.88410500
H	5.63141100	-2.38549300	0.88295400
H	5.47751100	-3.91860600	-0.00086500
C	-2.84926400	0.01302000	-0.00000800
C	-4.08340400	0.62089600	-0.00029100
O	-3.03613200	-1.35373400	0.00024000

C	-5.05979400	-0.41717700	-0.00022400
H	-4.27601600	1.68423100	-0.00053200
C	-4.37982700	-1.60255400	0.00010300
H	-6.13510100	-0.30078700	-0.00039800
C	-4.79769000	-3.03058700	0.00034700
H	-4.42261300	-3.56107700	0.88481000
H	-5.88904800	-3.09772600	0.00007900
H	-4.42214900	-3.56150600	-0.88366100

Conformational analysis of 2f



2f(2)

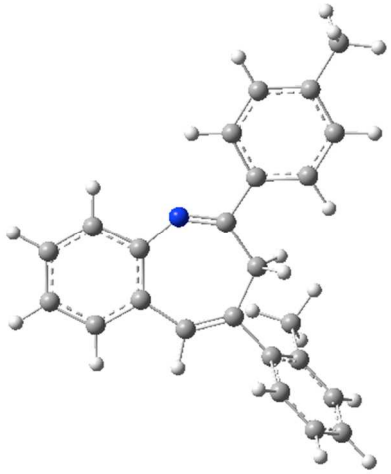
Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.381804 (Hartree/Particle)
Thermal correction to Energy= 0.402659

Thermal correction to Enthalpy= 0.403603
Thermal correction to Gibbs Free Energy= 0.329845
Sum of electronic and zero-point Energies= -981.577946
Sum of electronic and thermal Energies= -981.557092
Sum of electronic and thermal Enthalpies= -981.556148
Sum of electronic and thermal Free Energies= -981.629905

0 1

C	-2.87655100	-0.35729700	0.11023300
C	-2.30426900	-1.65161200	-0.08916200
C	-0.03536200	-1.16388600	-0.56383400
C	-0.92595800	1.11371500	-0.43106300
C	-0.41206900	0.05731800	-1.38960300
H	0.42607500	0.41778000	-1.98519100
C	-4.27684400	-0.27087900	0.28799800
H	-4.70896400	0.70911900	0.47887700
C	-3.16221400	-2.77352700	-0.14618400
C	-4.53586500	-2.64363500	-0.03947000
H	-5.17123800	-3.52265600	-0.10740700
C	-5.10102400	-1.37936900	0.19351900
H	-6.17597200	-1.27134200	0.30871600
H	-2.69937300	-3.74818800	-0.26911400
C	1.38880200	-1.50192300	-0.31821500
C	2.43070600	-0.59506400	-0.56514000
C	1.72564400	-2.76871600	0.19654500
C	3.75726400	-0.94371600	-0.30972200
H	2.21769200	0.40517300	-0.92863400
C	3.04867700	-3.11220100	0.43552800
H	0.92434200	-3.47051700	0.40023200
C	4.09387900	-2.20717100	0.18541500
H	4.54316100	-0.21600000	-0.49849700
H	3.28118300	-4.10082400	0.82621300
C	-2.09526600	0.86815000	0.20842200
N	-0.94245400	-1.92945900	-0.06254300
C	-0.16084300	2.37659400	-0.26059000
C	0.16873400	2.91702400	1.00737300
C	0.25584600	3.06220500	-1.41808700
C	0.88023100	4.12459200	1.05384000
C	0.95179100	4.26507800	-1.34904000
H	0.00121000	2.65134300	-2.39183800
C	1.26534700	4.80250200	-0.10053000
H	1.14562700	4.53418500	2.02601000
H	1.24565100	4.77697600	-2.26142200
H	1.81535100	5.73677700	-0.02459300

H	-2.53663000	1.66301200	0.80652600
H	-1.21064100	-0.24717600	-2.07926400
C	5.53095300	-2.59819800	0.43344100
H	6.19549500	-1.72918300	0.39763200
H	5.65226400	-3.07717500	1.41218200
H	5.88360800	-3.31516600	-0.31982500
C	-0.18042900	2.23460600	2.31244300
H	-1.18940700	2.49524800	2.65650600
H	-0.14525600	1.14515300	2.22646200
H	0.51592000	2.54211600	3.09953200



TS-2f(2)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.381194 (Hartree/Particle)
Thermal correction to Energy= 0.401519
Thermal correction to Enthalpy= 0.402463
Thermal correction to Gibbs Free Energy= 0.330829
Sum of electronic and zero-point Energies= -981.564452
Sum of electronic and thermal Energies= -981.544128
Sum of electronic and thermal Enthalpies= -981.543183
Sum of electronic and thermal Free Energies= -981.614817

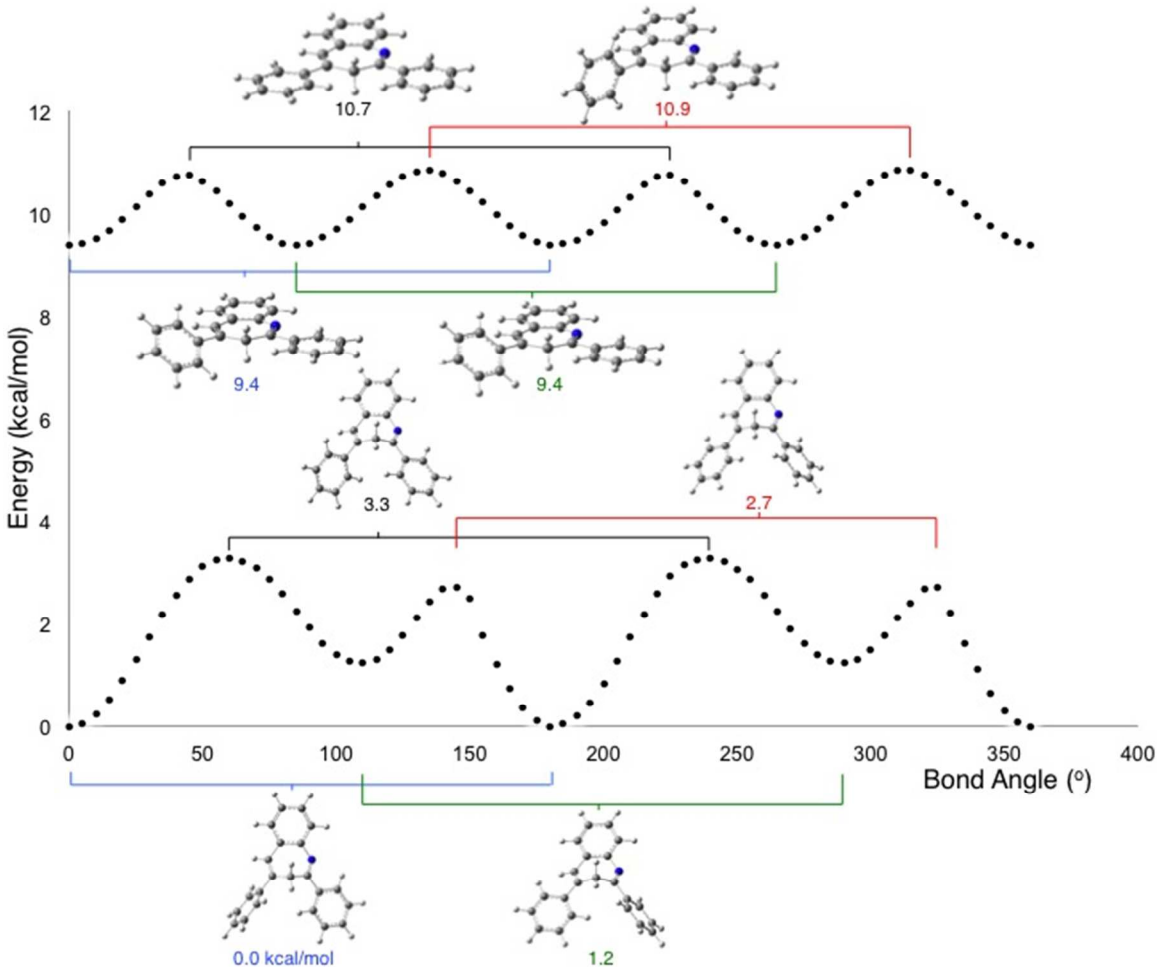
	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	251.957	81.548	150.765

0 1

C	-1.31818300	2.50766000	0.12690000
C	0.09591100	2.65670500	0.13868200

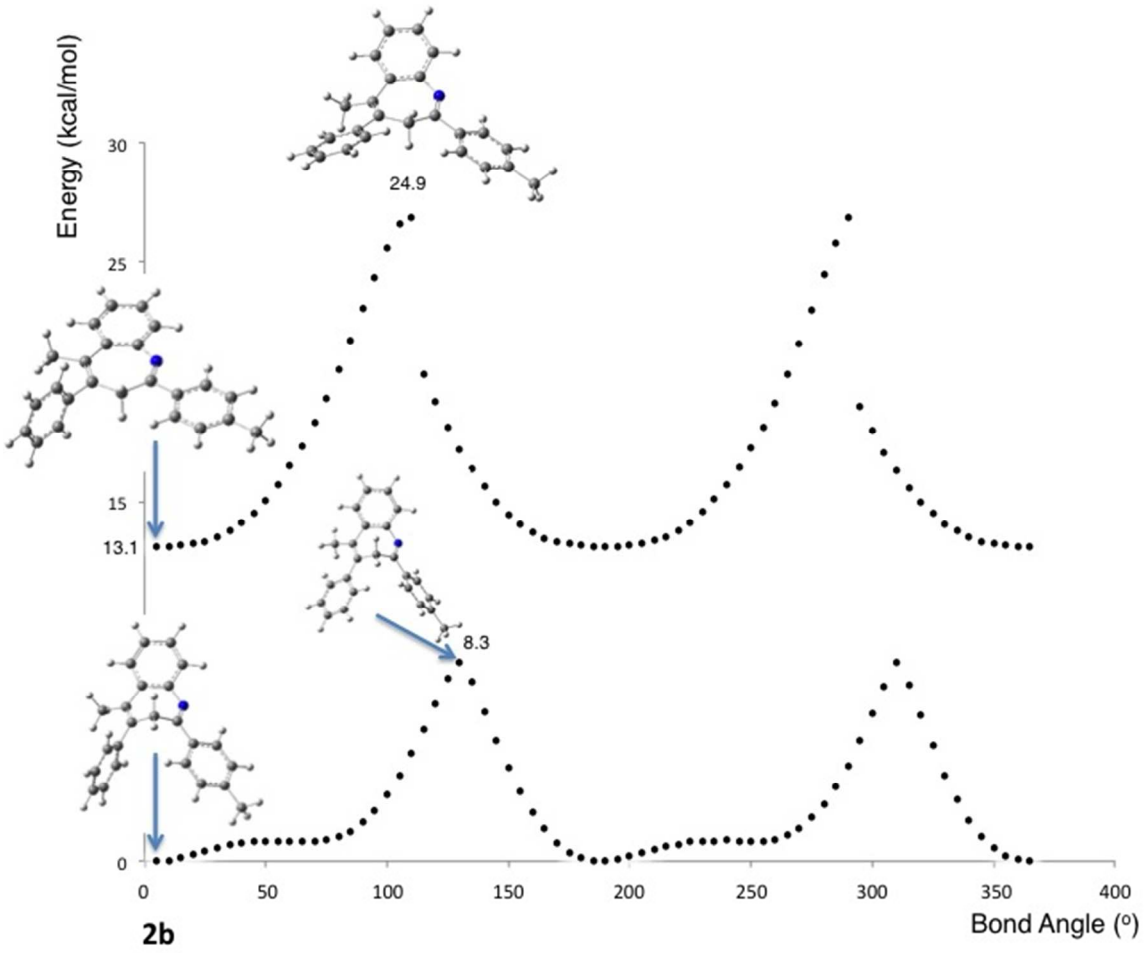
C	1.01693600	0.40082400	-0.11715500
C	-1.60920600	-0.01428000	-0.19031600
C	-0.18923500	-0.51929000	-0.27536100
H	-0.08644700	-1.31822900	0.47567100
C	-2.10679400	3.66643300	0.25183000
H	-3.18850500	3.55318400	0.24541100
C	0.63224200	3.95220400	0.27120800
C	-0.16889400	5.08313300	0.38804600
H	0.28545900	6.06503500	0.48733400
C	-1.55613400	4.93827400	0.37965100
H	-2.20545600	5.80448300	0.47229100
H	1.71436400	4.03344000	0.27954300
C	2.33824500	-0.30697100	-0.16457100
C	2.45994000	-1.69061700	-0.37753900
C	3.52957900	0.42712200	0.00389700
C	3.71170400	-2.30730400	-0.42096600
H	1.58320000	-2.31293000	-0.51586400
C	4.76997400	-0.19154000	-0.03843900
H	3.44915300	1.49532500	0.16708200
C	4.88930800	-1.57529500	-0.25205900
H	3.76805300	-3.38028900	-0.58992400
H	5.66884700	0.40709900	0.09572600
C	-2.04151700	1.24581400	-0.00696400
N	1.08033800	1.67172700	0.04556300
C	-2.63378600	-1.10938600	-0.27224100
C	-2.94093900	-1.76278800	-1.48689000
C	-3.29920900	-1.49609400	0.90141100
C	-3.90282600	-2.78123800	-1.47533600
C	-4.25023900	-2.51577000	0.89472100
C	-4.55089800	-3.16483700	-0.30177700
H	-4.15412200	-3.27468900	-2.41191400
H	-4.75260100	-2.79671400	1.81654100
H	-5.29255700	-3.95895700	-0.32594500
H	-3.12324500	1.36575900	0.03563100
H	-0.06725600	-1.04947500	-1.23205900
C	6.24462700	-2.23907900	-0.29060800
H	6.75441600	-2.16104100	0.67832600
H	6.16429800	-3.30189000	-0.53951400
H	6.89922700	-1.76795600	-1.03423100
H	-3.05917700	-0.98387800	1.82954300
C	-2.28405300	-1.37492100	-2.79368200
H	-2.05116700	-0.30599000	-2.82667000
H	-1.34485100	-1.92063500	-2.95796600
H	-2.93797500	-1.60570700	-3.64097300

Figure S3. Scan for the rotation of the Ph at C4 in benzazepine 2a in its equilibrium energy vs. scan for the rotation of the Ph at C4 in the transition state for the racemization of TS-2a.



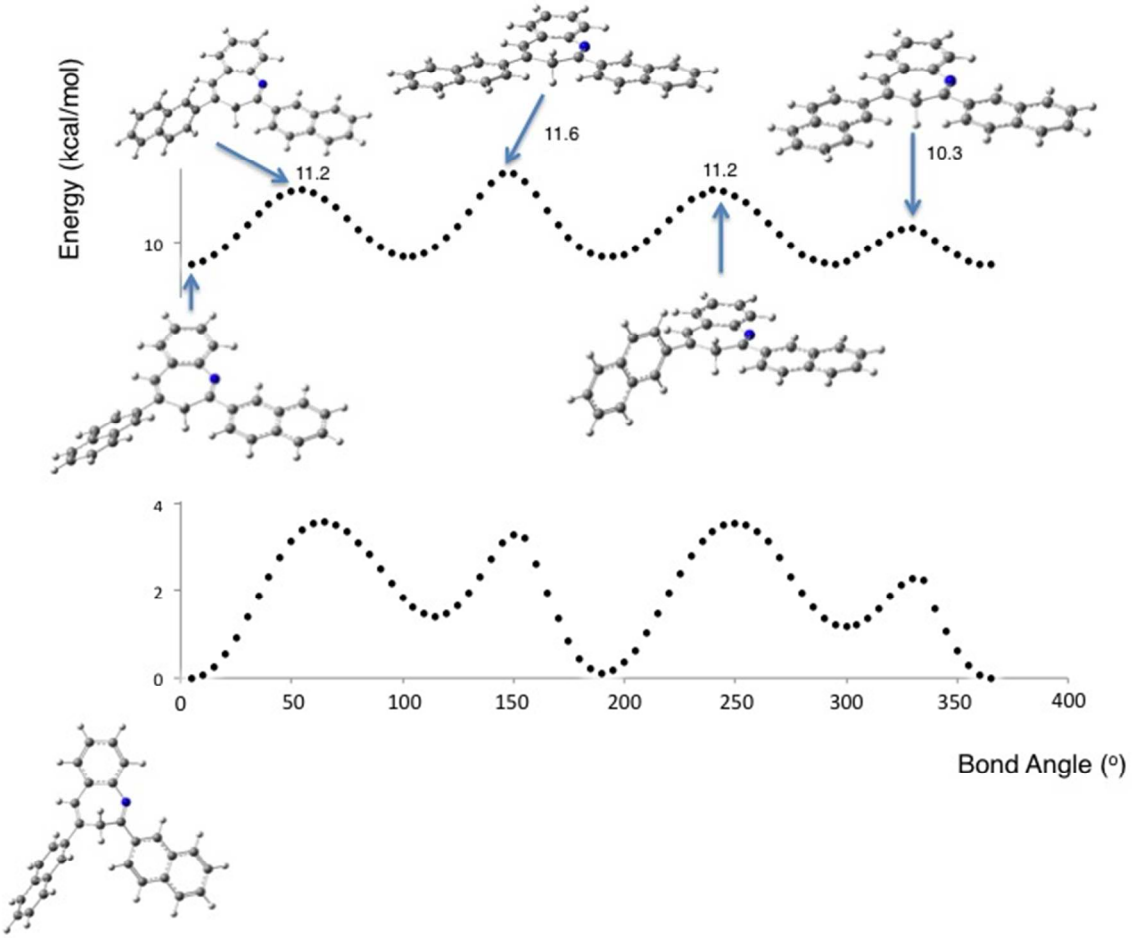
This analysis helped us to confirm that the barriers observed experimentally correspond to the ring-flip (racemization of benzazepin) rather than the rotation of the phenyl group at C4. The rotation costs less than the ring flip.

Figure S4. Scan for the rotation of the Ph at C4 in benzazepine 2b in its equilibrium energy vs. scan for the rotation of the Ph at C4 in the transition state for the racemization of TS-2b.



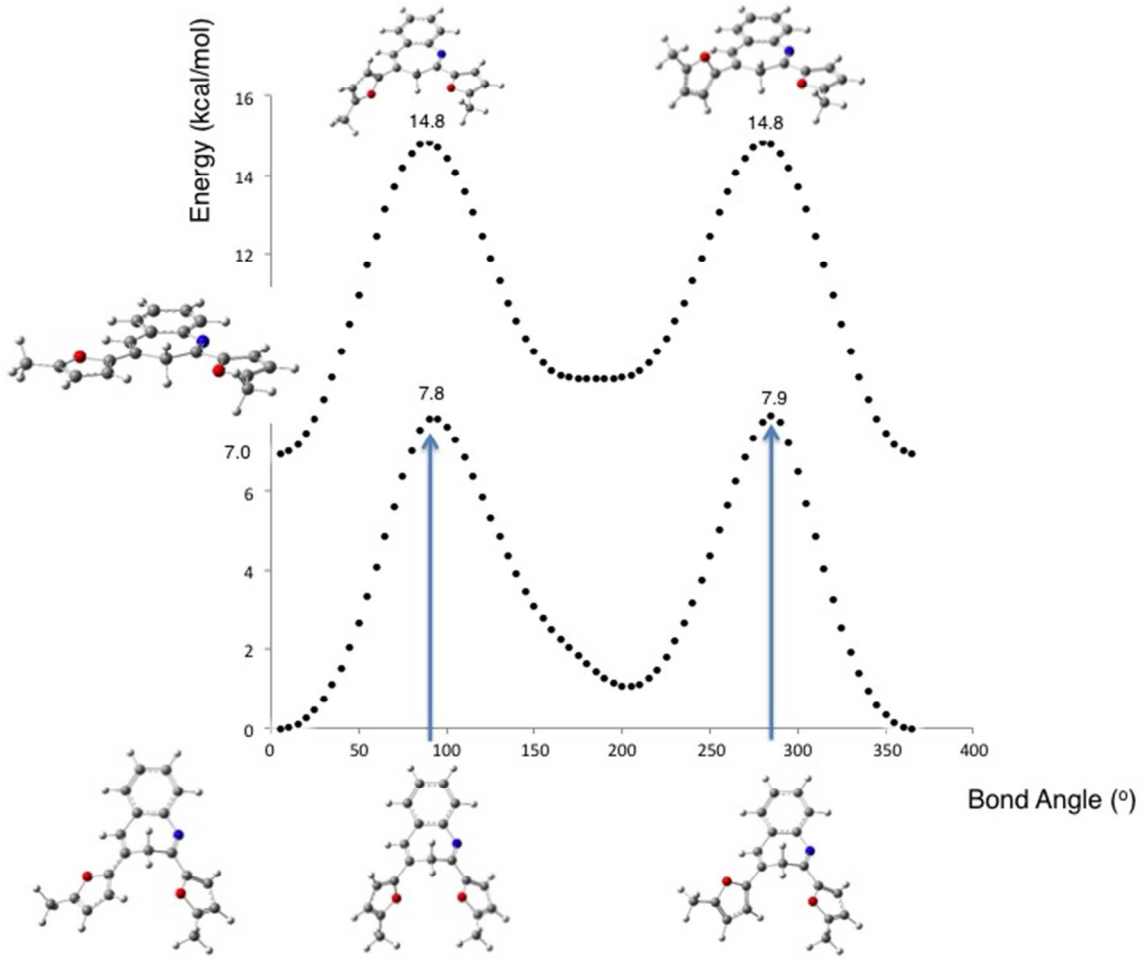
The analysis provided evidence that the barriers observed experimentally correspond to the ring-flip (racemization of benzazepine) of **2b** rather than the rotation of the phenyl group at C4. The rotation requires less energy than the ring flip.

Figure S5. Scan for the rotation of the naphthyl group at C4 in benzazepine 2d in its equilibrium energy vs. scan for the rotation of the naphthyl group at C4 in the transition state for the racemization of TS-2d.



The analysis provided evidence that the barriers observed experimentally correspond to the ring-flip (racemization of benzazepine) in **2d** rather than the rotation of the naphthyl group at C4. The rotation requires less energy than the ring flip.

Figure S6. Scan for the rotation of the 2-methyl-furyl group at C4 in benzazepine 2e in its equilibrium energy vs. scan for the rotation of the 2-methyl-furyl group at C4 in the transition state for the racemization of TS-2e.



This the only instance where the rotation of the 2-methyl-furyl group interferes with the ring flip.

Figure S7. Scan for the rotation of the *ortho*-methyl-phenyl group at C4 in benzazepine 2f in its equilibrium energy vs. scan for the rotation of the *ortho*-methyl-phenyl group at C4 in the transition state for the racemization of TS-2f.