Room temperature tandem hydroamination and hydrosilation/protodesilation catalysis by a tricarbonylchromium-bound iridacycle.

Wissam Iali, Frédéric La Paglia, Xavier-Frédéric Le Goff, Dušan Sredojević, Michel Pfeffer and Jean-Pierre Djukic*

Electronic Supporting Information

Content

1. Crystallographic data for compound 2a.

Table 1. Crystal data for **2a**

Compound	**2a**
Molecular formula	$C_{39}H_{40}IrN_2,CH_2Cl_2,Cl$
Molecular weight	849.31
Crystal habit	Red Block
Crystal dimensions(mm)	0.40x0.22x0.14
Crystal system	triclinic
Space group	P-1
a(Å)	10.572(1)
b(Å)	12.130(1)
c(Å)	14.836(1)
α(°)	101.006(1)
β(°)	103.841(1)
γ(°)	98.418(1)
V(Å^3)	1776.1(3)
Z	2
d(g-cm^{-3})	1.588
F(000)	848
μ(cm^{-1})	4.015
Absorption corrections	multi-scan ; 0.2965 min, 0.6033 max
Diffractometer	KappaCCD
X-ray source	MoKα
λ(Å)	0.71069
Monochromator	graphite
T (K)	150.0(1)
Scan mode	phi and omega scans
Maximum θ	30.02
HKL ranges	-14 14 ; -17 17 ; -18 20
Reflections measured	18121
Unique data	10172
Rint	0.0319
Reflections used	9843
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	mixed
Parameters refined	435
Reflections / parameter	22
wR2	0.0611
R1	0.0249
Weights a, b	0.0219 ; 3.1388
GoF	1.046
difference peak / hole (e Å^{-3})	1.353(0.106) / -1.944(0.106)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 2a

atom	x	y	z	U(eq)
Ir(1)	5172(1)	6690(1)	3276(1)	15(1)
N(1)	4372(2)	5116(2)	2269(2)	19(1)
N(2)	3471(3)	8789(2)	-456(2)	36(1)
Cl(1)	4277(1)	614(1)	2858(1)	28(1)
C(1)	4416(3)	4141(2)	2581(2)	24(1)
C(2)	3823(3)	3065(2)	2019(2)	28(1)
C(3)	3119(3)	2974(2)	1079(2)	29(1)
C(4)	3087(3)	3954(2)	741(2)	24(1)
C(5)	3742(2)	5038(2)	1333(2)	18(1)
C(6)	3712(2)	6055(2)	931(2)	18(1)
C(7)	3764(2)	5938(2)	-20(2)	22(1)
C(8)	3712(3)	6823(2)	-479(2)	23(1)
C(9)	3575(3)	7905(2)	-6(2)	23(1)
C(10)	3562(2)	8045(2)	956(2)	20(1)
C(11)	3633(2)	7151(2)	1420(2)	17(1)
C(12)	3715(2)	7446(2)	2447(2)	17(1)
C(13)	3025(2)	6754(2)	2939(2)	17(1)
C(14)	3661(2)	6936(2)	3926(2)	19(1)
C(15)	3448(2)	7234(2)	4777(2)	21(1)
C(16)	2277(2)	7669(2)	4947(2)	20(1)
C(17)	1329(3)	7946(2)	4232(2)	25(1)
C(18)	268(3)	8388(3)	4437(2)	30(1)
C(19)	113(3)	8557(3)	5355(2)	33(1)
C(20)	1036(3)	8282(3)	6065(2)	32(1)
C(21)	2110(3)	7847(2)	5866(2)	27(1)
C(22)	3371(4)	8601(3)	-1467(2)	38(1)
C(23)	3199(4)	9855(3)	4(2)	40(1)
C(24)	1887(2)	5767(2)	2469(2)	18(1)
C(25)	989(2)	5758(2)	1608(2)	23(1)
C(26)	-99(3)	4855(3)	1193(2)	28(1)
C(27)	-297(3)	3963(3)	1629(2)	36(1)
C(28)	563(3)	3979(3)	2501(3)	37(1)
C(29)	1651(3)	4875(2)	2919(2)	27(1)
C(30)	6609(2)	8198(2)	4201(2)	19(1)
C(31)	6855(2)	7220(2)	4606(2)	19(1)
C(32)	7192(2)	6414(2)	3927(2)	22(1)
C(33)	7220(2)	6897(2)	3103(2)	20(1)
C(34)	6904(2)	7998(2)	3292(2)	19(1)
C(35)	6336(3)	9289(2)	4706(2)	24(1)
C(36)	6837(3)	7118(3)	5597(2)	27(1)
C(37)	7657(3)	5333(3)	4081(2)	32(1)
C(38)	7625(3)	6347(3)	2254(2)	31(1)
C(39)	6877(3)	8822(2)	2653(2)	25(1)
Cl(2A)	-22(3)	8534(2)	1569(3)	93(1)
Cl(3A)	457(3)	10998(2)	1735(2)	61(1)
C(40A)	859(6)	9841(5)	2184(5)	64(2)
Cl(2B)	10(10)	8520(6)	1010(10)	93(1)
Cl(3B)	470(10)	10889(7)	1409(6)	61(1)
C(40B)	1060(20)	9730(10)	1650(10)	64(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3. Bond lengths (A) and angles (deg) for complex 2a

Ir(1)-C(14)	2.082(2)	Ir(1)-N(1)	2.103(2)
Ir(1)-C(12)	2.160(2)	Ir(1)-C(30)	2.184(2)
Ir(1)-C(13)	2.221(2)	Ir(1)-C(33)	2.224(2)
Ir(1)-C(32)	2.226(2)	Ir(1)-C(31)	2.231(2)
Ir(1)-C(34)	2.233(2)	N(1)-C(1)	1.353(3)
N(1)-C(5)	1.366(3)	N(2)-C(9)	1.372(3)
N(2)-C(23)	1.445(4)	N(2)-C(22)	1.449(4)
C(1)-C(2)	1.373(4)	C(1)-H(1)	0.9500
C(2)-C(3)	1.390(4)	C(2)-H(2)	0.9500
C(3)-C(4)	1.378(4)	C(3)-H(3)	0.9500
C(4)-C(5)	1.408(3)	C(4)-H(4)	0.9500
C(5)-C(6)	1.471(3)	C(6)-C(7)	1.405(3)
C(6)-C(11)	1.412(3)	C(7)-C(8)	1.378(4)
C(7)-H(7)	0.9500	C(8)-C(9)	1.410(4)
C(8)-H(8)	0.9500	C(9)-C(10)	1.408(3)
C(10)-C(11)	1.392(3)	C(10)-H(10)	0.9500
C(11)-C(12)	1.476(3)	C(12)-C(13)	1.441(3)
C(12)-H(12)	0.95(3)	C(13)-C(14)	1.417(3)
C(13)-C(24)	1.492(3)	C(14)-C(15)	1.328(3)
C(15)-C(16)	1.471(3)	C(15)-H(15)	0.9500
C(16)-C(21)	1.396(3)	C(16)-C(17)	1.404(3)
C(17)-C(18)	1.384(4)	C(17)-H(17)	0.9500
C(18)-C(19)	1.389(4)	C(18)-H(18)	0.9500
C(19)-C(20)	1.382(5)	C(19)-H(19)	0.9500
C(20)-C(21)	1.390(4)	C(20)-H(20)	0.9500
C(21)-H(21)	0.9500	C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800	C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800	C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800	C(24)-C(25)	1.394(3)
C(24)-C(29)	1.399(3)	C(25)-C(26)	1.392(4)
C(25)-H(25)	0.9500	C(26)-C(27)	1.377(4)
C(26)-H(26)	0.9500	C(27)-C(28)	1.387(5)
C(27)-H(27)	0.9500	C(28)-C(29)	1.387(4)
C(28)-H(28)	0.9500	C(29)-H(29)	0.9500
C(30)-C(34)	1.439(3)	C(30)-C(31)	1.457(3)
C(30)-C(35)	1.495(3)	C(31)-C(32)	1.413(3)
C(31)-C(36)	1.502(3)	C(32)-C(33)	1.458(3)
C(32)-C(37)	1.503(4)	C(33)-C(34)	1.417(3)
C(33)-C(38)	1.497(3)	C(34)-C(39)	1.503(3)
C(35)-H(35A)	0.9800	C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800	C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800	C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800	C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800	C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800	C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800	C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800	Cl(2A)-C(40A)	1.680(6)
Cl(3A)-C(40A)	1.729(6)	C(40A)-H(40A)	0.9900
C(40A)-H(40B)	0.9900	Cl(2B)-C(40B)	1.67(1)
Cl(3B)-C(40B)	1.68(1)	C(40B)-H(40C)	0.9900
C(40B)-H(40D)	0.9900		

C(14)-Ir(1)-N(1)	103.3(1)	C(14)-Ir(1)-C(12)	68.9(1)
N(1)-Ir(1)-C(12)	88.91(8)	C(14)-Ir(1)-C(30)	95.5(1)
N(1)-Ir(1)-C(30)	160.6(1)	C(12)-Ir(1)-C(30)	102.2(1)
C(14)-Ir(1)-C(13)	38.28(8)	N(1)-Ir(1)-C(13)	79.88(8)
C(12)-Ir(1)-C(13)	38.39(8)	C(30)-Ir(1)-C(13)	118.6(1)
C(14)-Ir(1)-C(33)	158.0(1)	N(1)-Ir(1)-C(33)	97.28(8)
C(12)-Ir(1)-C(33)	119.7(1)	C(30)-Ir(1)-C(33)	63.5(1)
C(13)-Ir(1)-C(33)	157.4(1)	C(14)-Ir(1)-C(32)	128.2(1)
N(1)-Ir(1)-C(32)	100.3(1)	C(12)-Ir(1)-C(32)	156.6(1)
C(30)-Ir(1)-C(32)	63.6(1)	C(13)-Ir(1)-C(32)	164.4(1)
C(33)-Ir(1)-C(32)	38.2(1)	C(14)-Ir(1)-C(31)	96.9(1)
N(1)-Ir(1)-C(31)	132.45(8)	C(12)-Ir(1)-C(31)	138.6(1)

C(30)-Ir(1)-C(31)	38.5(1)	C(13)-Ir(1)-C(31)	134.41(8)
C(33)-Ir(1)-C(31)	62.8(1)	C(32)-Ir(1)-C(31)	37.0(1)
C(14)-Ir(1)-C(34)	127.7(1)	N(1)-Ir(1)-C(34)	126.38(8)
C(12)-Ir(1)-C(34)	94.36(8)	C(30)-Ir(1)-C(34)	38.0(1)
C(13)-Ir(1)-C(34)	129.50(8)	C(33)-Ir(1)-C(34)	37.1(1)
C(32)-Ir(1)-C(34)	62.8(1)	C(31)-Ir(1)-C(34)	62.9(1)
C(1)-N(1)-C(5)	118.8(2)	C(1)-N(1)-Ir(1)	118.0(2)
C(5)-N(1)-Ir(1)	123.1(2)	C(9)-N(2)-C(23)	121.2(2)
C(9)-N(2)-C(22)	120.4(3)	C(23)-N(2)-C(22)	117.4(2)
N(1)-C(1)-C(2)	123.9(2)	N(1)-C(1)-H(1)	118.1
C(2)-C(1)-H(1)	118.1	C(1)-C(2)-C(3)	118.1(2)
C(1)-C(2)-H(2)	121.0	C(3)-C(2)-H(2)	121.0
C(4)-C(3)-C(2)	119.0(2)	C(4)-C(3)-H(3)	120.5
C(2)-C(3)-H(3)	120.5	C(3)-C(4)-C(5)	121.1(2)
C(3)-C(4)-H(4)	119.5	C(5)-C(4)-H(4)	119.5
N(1)-C(5)-C(4)	119.1(2)	N(1)-C(5)-C(6)	121.9(2)
C(4)-C(5)-C(6)	119.0(2)	C(7)-C(6)-C(11)	116.6(2)
C(7)-C(6)-C(5)	117.9(2)	C(11)-C(6)-C(5)	125.4(2)
C(8)-C(7)-C(6)	123.1(2)	C(8)-C(7)-H(7)	118.4
C(6)-C(7)-H(7)	118.4	C(7)-C(8)-C(9)	120.4(2)
C(7)-C(8)-H(8)	119.8	C(9)-C(8)-H(8)	119.8
N(2)-C(9)-C(10)	121.2(2)	N(2)-C(9)-C(8)	121.7(2)
C(10)-C(9)-C(8)	117.1(2)	C(11)-C(10)-C(9)	122.1(2)
C(11)-C(10)-H(10)	118.9	C(9)-C(10)-H(10)	118.9
C(10)-C(11)-C(6)	120.6(2)	C(10)-C(11)-C(12)	116.1(2)
C(6)-C(11)-C(12)	123.2(2)	C(13)-C(12)-C(11)	125.7(2)
C(13)-C(12)-Ir(1)	73.1(1)	C(11)-C(12)-Ir(1)	112.2(2)
C(13)-C(12)-H(12)	116(2)	C(11)-C(12)-H(12)	113(2)
Ir(1)-C(12)-H(12)	107(2)	C(14)-C(13)-C(12)	114.3(2)
C(14)-C(13)-C(24)	119.5(2)	C(12)-C(13)-C(24)	125.3(2)
C(14)-C(13)-Ir(1)	65.6(1)	C(12)-C(13)-Ir(1)	68.5(1)
C(24)-C(13)-Ir(1)	126.6(2)	C(15)-C(14)-C(13)	141.4(2)
C(15)-C(14)-Ir(1)	141.9(2)	C(13)-C(14)-Ir(1)	76.2(1)
C(14)-C(15)-C(16)	124.8(2)	C(14)-C(15)-H(15)	117.6
C(16)-C(15)-H(15)	117.6	C(21)-C(16)-C(17)	117.9(2)
C(21)-C(16)-C(15)	119.0(2)	C(17)-C(16)-C(15)	123.0(2)
C(18)-C(17)-C(16)	120.7(3)	C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6	C(17)-C(18)-C(19)	120.7(3)
C(17)-C(18)-H(18)	119.7	C(19)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	119.2(3)	C(20)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4	C(19)-C(20)-C(21)	120.5(3)
C(19)-C(20)-H(20)	119.8	C(21)-C(20)-H(20)	119.8
C(20)-C(21)-C(16)	121.0(3)	C(20)-C(21)-H(21)	119.5
C(16)-C(21)-H(21)	119.5	N(2)-C(22)-H(22A)	109.5
N(2)-C(22)-H(22B)	109.5	H(22A)-C(22)-H(22B)	109.5
N(2)-C(22)-H(22C)	109.5	H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5	N(2)-C(23)-H(23A)	109.5
N(2)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23B)	109.5
N(2)-C(23)-H(23C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5	C(25)-C(24)-C(29)	118.9(2)
C(25)-C(24)-C(13)	120.5(2)	C(29)-C(24)-C(13)	120.4(2)
C(26)-C(25)-C(24)	120.2(2)	C(26)-C(25)-H(25)	119.9
C(24)-C(25)-H(25)	119.9	C(27)-C(26)-C(25)	120.3(3)
C(27)-C(26)-H(26)	119.8	C(25)-C(26)-H(26)	119.8
C(26)-C(27)-C(28)	120.1(3)	C(26)-C(27)-H(27)	119.9
C(28)-C(27)-H(27)	119.9	C(29)-C(28)-C(27)	119.9(3)
C(29)-C(28)-H(28)	120.0	C(27)-C(28)-H(28)	120.0
C(28)-C(29)-C(24)	120.5(3)	C(28)-C(29)-H(29)	119.8
C(24)-C(29)-H(29)	119.8	C(34)-C(30)-C(31)	107.1(2)
C(34)-C(30)-C(35)	126.0(2)	C(31)-C(30)-C(35)	126.1(2)
C(34)-C(30)-Ir(1)	72.9(1)	C(31)-C(30)-Ir(1)	72.5(1)
C(35)-C(30)-Ir(1)	128.0(2)	C(32)-C(31)-C(30)	108.2(2)
C(32)-C(31)-C(36)	125.8(2)	C(30)-C(31)-C(36)	125.9(2)
C(32)-C(31)-Ir(1)	71.3(1)	C(30)-C(31)-Ir(1)	69.0(1)
C(36)-C(31)-Ir(1)	128.1(2)	C(31)-C(32)-C(33)	108.0(2)
C(31)-C(32)-C(37)	126.2(2)	C(33)-C(32)-C(37)	125.1(2)
C(31)-C(32)-Ir(1)	71.7(1)	C(33)-C(32)-Ir(1)	70.8(1)
C(37)-C(32)-Ir(1)	130.4(2)	C(34)-C(33)-C(32)	107.9(2)

C(34)-C(33)-C(38)	127.0(2)	C(32)-C(33)-C(38)	124.9(2)
C(34)-C(33)-Ir(1)	71.8(1)	C(32)-C(33)-Ir(1)	70.9(1)
C(38)-C(33)-Ir(1)	126.6(2)	C(33)-C(34)-C(30)	108.6(2)
C(33)-C(34)-C(39)	125.9(2)	C(30)-C(34)-C(39)	125.5(2)
C(33)-C(34)-Ir(1)	71.2(1)	C(30)-C(34)-Ir(1)	69.1(1)
C(39)-C(34)-Ir(1)	125.5(2)	C(30)-C(35)-H(35A)	109.5
C(30)-C(35)-H(35B)	109.5	H(35A)-C(35)-H(35B)	109.5
C(30)-C(35)-H(35C)	109.5	H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5	C(31)-C(36)-H(36A)	109.5
C(31)-C(36)-H(36B)	109.5	H(36A)-C(36)-H(36B)	109.5
C(31)-C(36)-H(36C)	109.5	H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5	C(32)-C(37)-H(37A)	109.5
C(32)-C(37)-H(37B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(32)-C(37)-H(37C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5	C(33)-C(38)-H(38A)	109.5
C(33)-C(38)-H(38B)	109.5	H(38A)-C(38)-H(38B)	109.5
C(33)-C(38)-H(38C)	109.5	H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5	C(34)-C(39)-H(39A)	109.5
C(34)-C(39)-H(39B)	109.5	H(39A)-C(39)-H(39B)	109.5
C(34)-C(39)-H(39C)	109.5	H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5	Cl(2A)-C(40A)-Cl(3A)	117.2(4)
Cl(2A)-C(40A)-H(40A)	108.0	Cl(3A)-C(40A)-H(40A)	108.0
Cl(2A)-C(40A)-H(40B)	108.0	Cl(3A)-C(40A)-H(40B)	108.0
H(40A)-C(40A)-H(40B)	107.2	Cl(2B)-C(40B)-Cl(3B)	111.2(8)
Cl(2B)-C(40B)-H(40C)	109.4	Cl(3B)-C(40B)-H(40C)	109.4
Cl(2B)-C(40B)-H(40D)	109.4	Cl(3B)-C(40B)-H(40D)	109.4
H(40C)-C(40B)-H(40D)	108.0		

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for complex 2a

atom	U11	U22	U33	U23	U13	U12
Ir(1)	17(1)	15(1)	15(1)	5(1)	4(1)	4(1)
N(1)	20(1)	16(1)	21(1)	4(1)	6(1)	4(1)
N(2)	57(2)	34(1)	26(1)	19(1)	16(1)	17(1)
Cl(1)	38(1)	24(1)	26(1)	8(1)	9(1)	12(1)
C(1)	28(1)	20(1)	27(1)	11(1)	11(1)	7(1)
C(2)	34(1)	16(1)	38(1)	9(1)	14(1)	6(1)
C(3)	35(1)	15(1)	35(1)	1(1)	12(1)	2(1)
C(4)	27(1)	19(1)	24(1)	2(1)	7(1)	3(1)
C(5)	19(1)	17(1)	20(1)	4(1)	6(1)	5(1)
C(6)	20(1)	16(1)	17(1)	4(1)	5(1)	4(1)
C(7)	22(1)	25(1)	19(1)	2(1)	6(1)	6(1)
C(8)	24(1)	30(1)	17(1)	7(1)	8(1)	6(1)
C(9)	23(1)	26(1)	22(1)	11(1)	8(1)	6(1)
C(10)	22(1)	20(1)	19(1)	8(1)	5(1)	4(1)
C(11)	17(1)	18(1)	17(1)	5(1)	5(1)	3(1)
C(12)	18(1)	15(1)	16(1)	5(1)	4(1)	5(1)
C(13)	19(1)	18(1)	16(1)	5(1)	5(1)	7(1)
C(14)	20(1)	19(1)	18(1)	6(1)	7(1)	4(1)
C(15)	19(1)	25(1)	18(1)	8(1)	4(1)	5(1)
C(16)	18(1)	22(1)	20(1)	5(1)	7(1)	3(1)
C(17)	23(1)	29(1)	22(1)	4(1)	4(1)	5(1)
C(18)	21(1)	33(1)	32(1)	3(1)	2(1)	7(1)
C(19)	22(1)	34(1)	41(2)	0(1)	14(1)	4(1)
C(20)	34(1)	36(2)	30(1)	2(1)	17(1)	5(1)
C(21)	27(1)	32(1)	23(1)	7(1)	10(1)	7(1)
C(22)	55(2)	43(2)	25(1)	20(1)	16(1)	13(1)
C(23)	61(2)	29(2)	33(2)	16(1)	11(1)	16(1)
C(24)	16(1)	20(1)	19(1)	3(1)	5(1)	4(1)
C(25)	19(1)	28(1)	21(1)	6(1)	6(1)	6(1)
C(26)	18(1)	35(1)	26(1)	4(1)	0(1)	3(1)
C(27)	23(1)	33(2)	43(2)	5(1)	2(1)	-4(1)
C(28)	30(1)	29(1)	48(2)	16(1)	6(1)	-3(1)
C(29)	24(1)	24(1)	31(1)	12(1)	4(1)	0(1)
C(30)	18(1)	17(1)	19(1)	3(1)	4(1)	2(1)
C(31)	16(1)	24(1)	18(1)	7(1)	2(1)	6(1)
C(32)	18(1)	22(1)	25(1)	6(1)	5(1)	6(1)
C(33)	16(1)	23(1)	21(1)	4(1)	7(1)	4(1)
C(34)	16(1)	20(1)	19(1)	7(1)	3(1)	3(1)
C(35)	27(1)	19(1)	24(1)	1(1)	5(1)	6(1)
C(36)	28(1)	36(1)	19(1)	12(1)	5(1)	10(1)
C(37)	32(1)	28(1)	41(2)	12(1)	9(1)	16(1)
C(38)	32(1)	32(1)	29(1)	1(1)	16(1)	7(1)
C(39)	25(1)	25(1)	27(1)	13(1)	8(1)	2(1)
Cl(2A)	88(1)	46(1)	146(3)	32(1)	33(2)	3(1)
Cl(3A)	67(1)	45(1)	76(2)	10(1)	32(1)	16(1)
C(40A)	49(3)	69(4)	87(5)	35(4)	29(3)	14(3)
Cl(2B)	88(1)	46(1)	146(3)	32(1)	33(2)	3(1)
Cl(3B)	67(1)	45(1)	76(2)	10(1)	32(1)	16(1)
C(40B)	49(3)	69(4)	87(5)	35(4)	29(3)	14(3)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

Table 5. Hydrogen Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex 2a

atom	x	y	z	U(eq)
H(1)	4886	4204	3226	28
H(2)	3890	2402	2266	34
H(3)	2667	2247	675	35
H(4)	2615	3898	97	29
H(7)	3838	5215	-361	26
H(8)	3768	6703	-1119	28
H(10)	3503	8773	1300	24
H(12)	3940(30)	8250(30)	2720(20)	20
H(15)	4099	7161	5316	25
H(17)	1416	7829	3600	30
H(18)	-361	8578	3946	36
H(19)	-618	8859	5492	39
H(20)	935	8391	6693	39
H(21)	2740	7668	6363	32
H(22A)	4182	8377	-1584	57
H(22B)	3262	9310	-1676	57
H(22C)	2601	7990	-1826.0001	57
H(23A)	2278	9732	41	59
H(23B)	3328	10427	-368	59
H(23C)	3805	10129	649	59
H(25)	1121	6370	1304	27
H(26)	-708	4854	607	34
H(27)	-1024	3336	1331	43
H(28)	408	3376	2811	44
H(29)	2239	4883	3516	32
H(35A)	7174	9844	5006	36
H(35B)	5904	9136	5197	36
H(35C)	5750	9602	4246	36
H(36A)	6370	6348	5570	40
H(36B)	6377	7689	5865	40
H(36C)	7752	7251	6000	40
H(37A)	8622	5509	4366	48
H(37B)	7438	4775	3467	48
H(37C)	7215	5013	4511	48
H(38A)	7262	6666	1710	46
H(38B)	7281	5518	2091	46
H(38C)	8598	6497	2402	46
H(39A)	7774	9273	2775	38
H(39B)	6276	9338	2782	38
H(39C)	6560	8394	1984	38
H(40A)	1808	9843	2232	77
H(40B)	761	9962	2841	77
H(40C)	1927	9747	1506	77
H(40D)	1204	9758	2340	77

2. Experimental Part

2.1. Main literature references for the products quoted in the manuscript

All the compounds refered to herein were found to fit the spectral and analytical features reported in the following papers. Any new compound was fully characterised; the corresponding data are provided in the following sections.

4a, 4c: J. S. M. Samec, J-E. Bäckvall, *Chem. Eur. J.* **2002**, *8,* 2955-2961.

4b: Y. Kuninobu, P. Yu, K. Takai, *Org. Lett.,* **2010**, *12*, 4274-4276.

4d, 4e, 6d: A. Lühl , H. P. Nayek , S. Blechert, P. W. Roesky *Chem. Commun.*, **2011**,*47*, 8280-8282

4h: K. Takaki, S. Koizumi, Y. Yamamoto, K. Komeyama, *Tetrahedron Lett.,* **2006**, *47*, 7335-7337.

6a: D. W. Stephan, S. Greenberg, T. W. Graham, P. Chase, J. J. Hastie, S. J. Geier, J. M. Farrell, C. C. Brown, Z. M. Heiden, G. C. Welch, M. Ullrich, *Inorg. Chem.* **2011**, *50*, 12338–12348

6b: S. Zhou, S. Fleischer, K. Junge and M. Beller, *Angew. Chem., Int. Ed.* **2011**, *50*, 5120-5124.

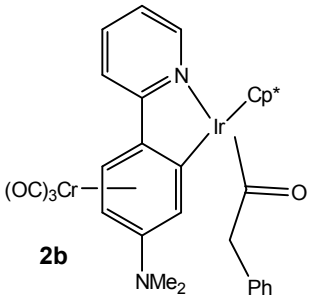
6c : W.-J. Lu, Y.-W. Chen and X.-L. Hou, *Adv. Synth. Catal.* **2010**, *352*, 103-107.

6e : M. Kawatsura and J. F. Hartwig, *J. Am. Chem. Soc.* **2000**, *122*, 9546-9547.

6i : G. M. Coppola, *J. Heterocycl. Chem.* **1991**, *28*, 1769-1772.

7f: W. Zhan, Z. Liang, A. Zhu, S. Kurtkaya, H. Shim, J.P. Snyder, D. C. Liotta, *J. Med. Chem.* **2007,** *50,* 5655-5664.

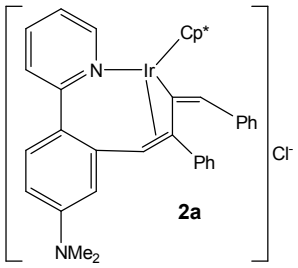
2.2. **Procedures**



2b

Synthesis of compound 2b.

A mixture of **1b** compound (200 mg, 0.287 mmol) and phenylacetylene (117,35 mg, 1.149 mmol) in MeOH (8 mL) with one drop of water was stirred at room temperature (25 °C) for 3 h under argon. The heterogeneous orange yellow solution was turned to dark orange homogenous solution after 30 minutes. The resulting dark orange solution was evaporated to dryness under reduced pressure. The resulting oil was dissolved in CH_2Cl_2, and silica gel was added. After evaporation of the solvent under reduced pressure, the coated silica gel was loaded on the top of a SiO_2 column packed in a pentane/ dichloromethane (50/50) mixture. Complex acyl-iridium **2b** was eluted with pentane/dichloromethane (80/20). The solvent was removed under vacuum to afford a orange powder in 64 % yield (143.2 mg). Anal. Calcd for $C_{34}H_{35}N_2O_4CrIr\bullet H_2O$ ¼(CH_2Cl_2): C, 50.22; H, 4.61; N, 3.41. Found: C, 50.29; H, 4.60; N, 3.10. IR ν(C=O): 1925 (Cr-*C*=*O*), 1829 (Cr-*C*=*O*) and 1605 (Ir-*C*=*O*) cm^{-1}. ^1H NMR ($CDCl_3$): δ 1.74 (s, 15 H, C_5Me_5), 2.97 (s, 6 H, NMe_2), 3.13 (s, 1 H, $CH_{benzyl.}$), 3.15 (s, 1 H, $CH_{benzyl.}$), 4.74 (dd, 1 H, ^2J = 2.5, ^3J = 7.0 Hz), 5.62 (d, 1 H, ^3J = 2.4 Hz), 6.11 (d, 1 H, ^3J = 7.1 Hz), 6.66 (dd, 2 H, ^2J = 1.8, ^3J = 7.2 Hz), 7.04 (m, 5 H, C_6H_5), 7.31 (d, 1 H, ^3J = 8.1 Hz), 7.59 (dd, 1 H, ^3J = 7.4, ^3J = 8.1 Hz), 8.57 (d, 1 H, ^3J = 5.8 Hz). ^{13}C NMR ($CDCl_3$): δ 235.63 (Cr(*C*O)3, 220.59(Ir-*C*(O)), 166.02, 151.81, 136.40, 136.03, 134.59, 129.18, 127.77, 125.51, 122.16, 118.07, 102.42, 93.12, 93.33, 92.38, 87.60, 71.45, 62.65, 40.1, 8.75.



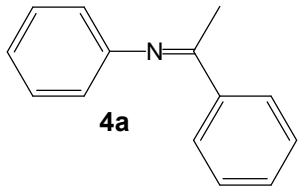
2a

Synthesis of compound 2a.

A mixture of **1a** compound (200 mg, 0.357 mmol) and phenylacetylene (146.01 mg, 1.42 mmol) were stirred a room temperature in 8 ml of methanol for 3 h. The solution turned dark red homogenous within 15 minutes. The red solution was evaporated under reduced pressure. The resulting red solid was purified by a SiO_2 column packed in a pentane/ dichloromethane (50/50) mixture. Insertion complex **2a** was eluted with dichloromethane / methanol (95/5). The solvent was removed under vacuum to afford a red dark solid in 80 % yield (176 mg). Anal. Calcd for $C_{39}H_{40}N_2ClIr\bullet\ C_3H_6O$ ¼(CH_2Cl_2): C, 60.14; H, 5.55; N, 3.32. Found: C, 60.27; H, 5.69; N, 2.98. ^{1}H NMR ($CDCl_3$): δ 1.65 (s, 15 H, C_5Me_5), 3.16 (s, 6 H, NMe_2), 4.28 (s, 1 H, CH_{vinyl}), 6.22 (s, 1 H, CH_{vinyl}), 6.57 (dd, 1 H, ^4J = 2.8, ^3J = 8.96 Hz), 6.85 (d, 1 H, ^3J = 7.3 Hz), 6.9 (d, 1 H, ^4J = 2.7 Hz), 7.01 (m, 6 H, C_6H_5), 7.12 (t, 2 H, ^3J = 7.9 Hz), 7.22 (d, 1 H, ^3J = 9.1 Hz), 7.31 (m, 2 H), 8.63 (dd, 1 H, ^4J = 1.4, ^3J = 5.9 Hz). ^{13}C NMR ($CDCl_3$): δ 157.22, 156.83, 154.61, 151.37, 138.48, 136.17, 133.83, 132.83, 130.11, 128.42, 127.10, 127.00, 125.11, 124.87, 123.34, 122.02, 118.62, 111.11, 110.80, 100.87, 95.32, 77.24, 51.80, 40.20, 29.64, 8.69.

General procedure for hydroamination of terminal alkynes catalyzed by iridium(III) complex.

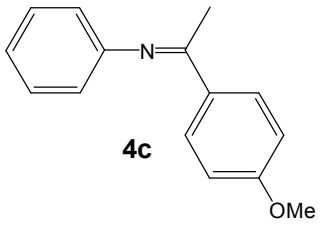
A solution of terminal alkyne and aniline in MeOH was added the **1b** complex. The resulting solution was left to stir for 2-3 h at room temperature under argon atmosphere. The yield in imine product was determined by integration of the product resonances relative to the substrate peaks in the ^{1}H NMR spectrum.



4a

Hydroamination of phenylacetylene.

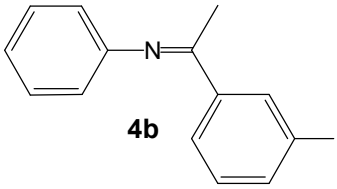
Phenylacetylene (102.1 mg, 1 mmol), aniline (93.1 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent, gave the imine corresponding **4a** after 2 h in 95 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 2.24 (s, 3 H, Me), 6.81 (d, 2 H, ^{3}J = 7.71 Hz), 7.09 (t, 1 H, ^{3}J = 7.5 Hz), 7.34 (dd, 2 H, ^{3}J = 7.4, 8.0 Hz), 7.45 (m, 3 H), 7.98 (dd, 2 H, ^{4}J = 1.4, ^{4}J = 1.8, ^{4}J = 2.3, ^{3}J = 6.7 Hz).



4c

Hydroamination of 4-ethynylanisole.

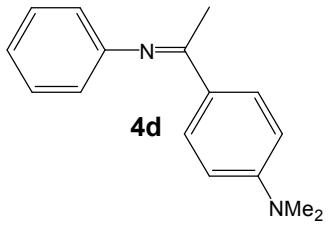
4-Ethynylanisole (133.1 mg, 1 mmol), aniline (93.1 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent, gave the imine corresponding **4c** after 2 h in 100 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 2.18 (s, 3 H, Me), 3.85 (s, 3 H, OMe), 6.77 (d, 2 H, ^{3}J = 7.7 Hz), 6.93 (d, 2 H, ^{3}J = 8.9 Hz), 7.05 (t, 1 H, ^{3}J = 7.4 Hz), 7.32 (t, 2 H, ^{3}J = 7.8 Hz), 7.92 (d, 2 H, ^{3}J = 8.9 Hz).



4b

Hydroamination of 3-ethynyltoluene.

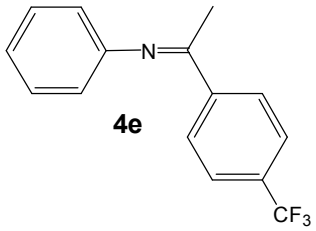
3-ethynyltoluene (116.1 mg, 1 mmol), aniline (93.1 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent, gave the corresponding imine **4b** after 2 h in 95 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 2.20 (s, 3 H, Me), 2.40 (s, 3 H, Me), 6.77 (d, 2 H, ^{3}J = 7.8 Hz), 7.06 (t, 1 H, ^{3}J = 7.6 Hz), 7.32 (m, 4 H), 7.71 (d, 1 H, ^{3}J = 7.7 Hz), 7.81 (s, 1 H).



4d

Hydroamination of 4-ethynyl-*N,N*-dimethylaniline.

4-ethynyl-*N,N*-dimethylaniline (145.2, 1 mmol), aniline (93.1 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent, gave the corresponding imine **4d** after 1.45 h in 95 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 2.18 (s, 3 H, Me), 3.03 (s, 6 H, NMe_2), 6.72 (d, 2 H, ^{3}J = 8.8 Hz), 6.79 (d, 2 H, ^{3}J = 7.8 Hz), 7.04 (t, 1 H, ^{3}J = 7.4 Hz), 7.32 (dd, 2 H, ^{3}J = 7.3, 7.9 Hz), 7.89 (d, 2 H, ^{3}J = 8.7 Hz).



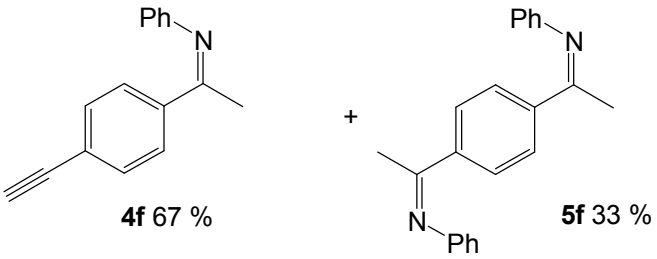
4e

Hydroamination of 1-ethynyl-4-(trifluoromethyl)benzene.

1-ethynyl-4-(trifluoromethyl)benzene (170.1 mg, 1 mmol), aniline (93.1 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent, gave the corresponding imine **4e** after 3 h in 95 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 2.24 (s, 3 H, Me), 6.78 (d, 2 H, ^{3}J = 7.8 Hz), 7.09 (t, 1 H, ^{3}J = 7.3 Hz), 7.35 (t, 2 H, ^{3}J = 7.9 Hz), 7.68 (d, 2 H, ^{3}J = 8.2 Hz), 8.06 (d, 2 H, ^{3}J = 8.2 Hz).

Competitive hydroamination reaction.

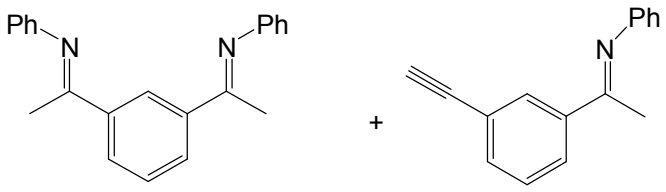
Phenylacetylene (102.1 mg, 1 mmol), 4-ethynyl-*N,N*-dimethylaniline (145.2, 1 mmol), 1-ethynyl-4-(trifluoromethyl)benzene (170.1 mg, 1 mmol), aniline (93.1 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent. The progress of the reaction was monitored by NMR.



4f 67 % **5f** 33 %

Hydroamination of 1,4-diethynylbenzene.

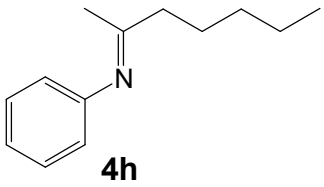
1,4-diethynylbenzene (300 mg, 2.37 mmol), aniline (664.4 mg, 7.13 mmol), **1b** complex (41.7 mg, 0.06 mmol) and MeOH 10 mL as solvent, gave the two corresponding imines **4f** and **5f** after 3 h in 67 and 33 % yield (NMR) respectively. Product **4f** was isolated as a yellow solid by a second recrystallization of the reaction mixture. The resulting yellow precipitate washed with pentane three times to remove unreated aniline. For **4f** ESI(+) MS (m/z) : 220.112 $[MH]^+$**.** ^{1}H NMR ($CDCl_3$): δ 2.03 (s, 3 H, Me), 2.99 (s, 1H, CH), 6.59 (dd, 2 H, ^4J = 1.3, ^3J = 7.8 Hz), 6.9 (t, 1 H, ^3J = 7.5 Hz), 7.16 (t, 2 H, ^3J = 7.6 Hz), 7.37 (d, 2 H, ^3J = 8.1 Hz), 7.74 (d, 2 H, ^3J = 8.4 Hz). ^{13}C NMR ($CDCl_3$): δ 164.63, 151.42, 139.60, 132.10, 132.01, 128.99, 127.11, 123.42, 119.29, 79.01, 78.95, 17.30. MS (m/z) 220.112 $[M]^+$. For **5f** ^{1}H NMR ($CDCl_3$): δ 2.27 (s, 6 H, Me), 6.82 (d, 4H, ^3J = 7.8 Hz), 7.1 (t, 2 H, ^3J = 7.4 Hz), 7.37 (t, 4 H, ^3J = 7.5 Hz), 8.05 (s, 4 H).



5g 50 % **4g** 50 %

Hydroamination of 1,3-diethynylbenzene.

1,4-Diethynylbenzene (200 mg, 1.58 mmol), aniline (443 mg, 4.75 mmol), **1b** (27.5 mg, 0.039 mmol) and MeOH (10 mL) as solvent, gave the two corresponding imines **5g** and **4g** after 3 h in 50 and 50 % yield respectively. The diimine product **5g** was isolated as an orange solid by precipitation of the reaction mixture. The resulting liquor was concentrated and cooled to -70 °C. The resulting yellow precipitate, identified as imine **4g**, was washed with pentane three times to remove unreacted aniline. For **5g:** ESI(+) MS (m/z) 313.168 $[MH]^+$. ^{1}H NMR ($CDCl_3$): δ 2.27 (s, 6 H, Me), 6.79 (d,4 H, ^3J = 7.8 Hz), 7.09 (t, 2 H, ^3J = 7.3 Hz), 7.34 (t, 4 H, ^3J = 7.7 Hz), 7.51 (t, 1 H, ^3J = 7.9 Hz), 8.05 (dd, 2 H, ^4J = 1.72, ^3J = 7.9 Hz), 8.55 (s, 1 H). ^{13}C NMR ($CDCl_3$): δ 165.42, 151.57, 139.79, 129.20, 129.00, 128.46, 126.00, 123.38, 119.39, 17.30. For **4g:** ESI(+) MS (m/z) for $C_{16}H_{13}NNa$: 242.094 $[MNa]^+$. ^{1}H NMR ($CDCl_3$): δ 2.21 (s, 3 H, Me), 3.09 (s, 1 H, C≡CH), 6.77 (d, 2 H, ^3J = 7.8 Hz), 7.08 (t, 1 H, ^3J = 7.4 Hz), 7.36 (m, 3 H), 7.57 (d, 1 H, ^3J = 7.6 Hz), 7.96 (d, 1 H, ^3J = 7.9 Hz), 8.07 (s, 1 H). ^{13}C NMR ($CDCl_3$): δ 164.60, 151.34, 139.64, 133.87, 131.00, 129.00, 128.71, 128.43, 127.53, 123.43, 122.34, 119.30, 83.27, 78.26, 17.70.



4h

Hydroamination of 1-hexyne.

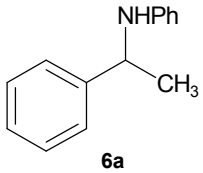
1-Hexyne (82.14 mg, 1 mmol), aniline (93.13 mg, 1 mmol), **1b** complex (7 mg, 0.01 mmol) and MeOH (7 mL) as solvent, gave the corresponding imine **4h** after 2 h in 50 % yield (NMR).^{1}H NMR ($CDCl_3$): δ 0.96 (t, 3 H, ^{3}J = 7.5 Hz), 1.2 (sext, 2 H, ^{3}J = 7.5 Hz), 1.66 (m, 2 H), 2.41 (t, 2 H, ^{3}J = 7.5 Hz), 6.69 (d, 2 H, ^{3}J = 7.6 Hz), 7.04 (t, 1 H, ^{3}J = 6.9 Hz), 7.29 (d, 2 H, ^{3}J = 7.7 Hz).

An alternative synthesis of imine 4a.

A mixture of phenylacetylene (102.1 mg, 1 mmol), aniline (111.7 mg, 1.2 mmol), **1b** (7.0 mg, 0.01 mmol), and $NaBAr^{F}_{4}$ (17.7 mg, 0.02 mmol) in toluene (10 mL) under argon was heated to reflux for 12 h. Upon cooling, the resulting solution was filtered through Celite. The solvent was evaporated under reduced pressure and the outcome of the reaction was monitored by ^{1}H NMR: yield 30 %

General procedure for hydrosilylation of imines catalyzed by iridium(III) complex.

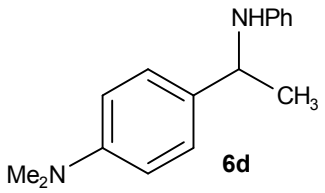
The imine was introduced with **1b** complex in 7 mL of distilled MeOH as solvent. Triethylsilane was then added and the mixture was stirred at room temperature under argon for 2-3 h. The crude reaction mixture was hydrolyzed with water and the organic phase was extracted with dichloromethane. The solvent was evaporated under vacuum to give the amine product, which was washed thrice with cool pentane to remove the impurities.



6a

Hydrosilylation of *N*-(1-phenylethylidene)benzenamine (4a).

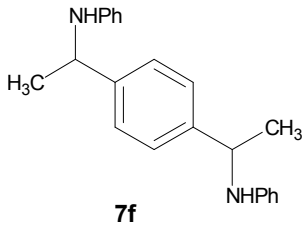
N-(1-phenylethylidene)benzenamine (50 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** complex (4.8 mg, 0.007 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **6a** after 2 h in 100 % yield (50 mg). ^{1}H NMR ($CDCl_3$): δ 1.51 (d, 3 H, ^{3}J = 6.75 Hz), 4.12 (s, 1 H, NH), 4.47 (q, 1 H, ^{3}J = 6.7 Hz), 6.51 (d, 2 H, ^{3}J = 7.9 Hz), 6.64 (t, 1 H, ^{3}J = 7.3 Hz), 7. 07 (t, 2 H, ^{3}J = 7.7 Hz), 7.20 (m, 1 H), 7.32 (m, 4 H).



6d

Hydrosilation of *N*,*N*-dimethyl-4-[1-(phenylimino)ethyl]aniline (4d).

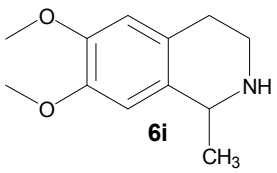
(**4d**) *N*,*N*-dimethyl-4-[1-(phenylimino)ethyl]aniline (60.9 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** complex (4.8 mg, 0.007 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **6d** after 2 h in 100 % yield (70 mg).



7f

Hydrosilylation of *N*,*N*-(1,4-phenylenediethylidyne)bis-benzenamine (5f).

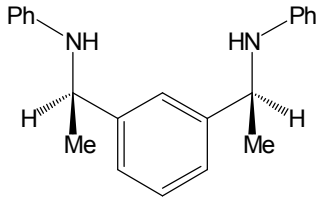
(**5f**) *N*,*N*-(1,4-phenylenediethylidyne)bis-benzenamine (79.9 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** (4.8 mg, 0.007 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **7f** after 2 h in 100 % yield (80 mg). ^{1}H NMR ($CDCl_3$): δ 1.47 (d, 6 H, ^{3}J = 6.7 Hz), 4.00 (s, 2 H, NH), 4.45 (q, 2 H, ^{3}J = 6.9 Hz), 6.49 (d, 4 H, ^{3}J = 8.0 Hz), 6.62 (t, 2 H, ^{3}J = 7.4 Hz), 7.08 (t, 4 H, ^{3}J = 8.0 Hz), 7.29 (s, 4H).



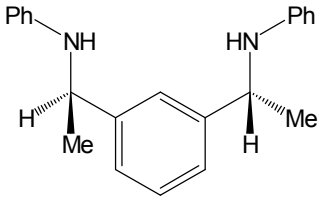
6i

Hydrosilylation of 6,7-diméthoxy-1-méthyl-3,4-dihydroisoquinoline (4i).

(**4i**) 6,7-dimethoxy-1-methyl-3,4-dihydroisoquinoline (52.5 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** complex (4.8 mg, 0.007 mmol) and MeOH 7 mL as solvent, gave the corresponding amine **6i** after 3 h in 100 % yield (51 mg). ^{1}H NMR ($CDCl_3$): δ 1.42 (d, 3 H, ^{3}J = 6.6 Hz), 2.61 (m, 1H), 2.77 (m, 1H), 2.98 (m, 1 H), 3,22 (m, 1 H), 3.82 (s, 3 H, OMe), 3.83 (s, 3 H, OMe), 4.03 (q, 1 H, ^{3}J = 6.7 Hz), 6.55 (s, 1 H), 6.61 (s, 1 H).



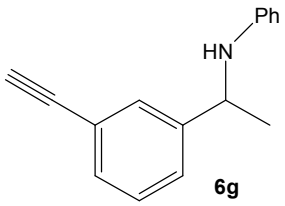
7g, meso isomer



7g , homochiral isomer

Hydrosilation of *N*,*N*-(1,3-phenylenediethylidyne)bis-benzenamine (5g).

(**5g**) *N*,*N*-(1,3-phenylenediethylidyne)bis-benzenamine (50 mg, 0.160 mmol), triethylsilane (37.21 mg, 0.32 mmol), **1b** (2.8 mg, 0.004 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **7g** as a mixture of diastereomers after 2 h in 100 % yield (50 mg). Anal. Calcd for $C_{22}H_{24}N_2 \bullet$ ½ (CH_2Cl_2): C, 75.30; H, 7.02; N, 7.80. Found: C, 75.52; H, 6.75; N, 7.50. ^{1}H NMR ($CDCl_3$): δ 1.47 (d, 6 H, ^3J = 6.7 Hz), 3.97 (s, 2 H, NH), 4.44 (q, 2 H, ^3J = 6.6 Hz), 6.46 (t, 4 H, ^3J = 8.9 Hz), 6.62 (t, 2 H, ^3J = 7.8 Hz), 7.06 (dt, 3 H, ^3J = 5.4, ^3J = 7.1 Hz), 7.23 (d, 4 H), 7.33 (s, 1 H). ^{13}C NMR ($CDCl_3$): δ 147.11, 145.64, 145.46, 129.6, 128.96, 124.40, 124.35, 123.88, 123.65, 124.40, 117.25, 113.38, 53.43, 53.56, 24.90, 24.56.



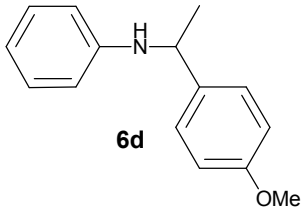
6g

Hydrosilation of 4g.

4g (50.0 mg, 0.23 mmol), triethylsilane (32.2 mg, 0.276 mmol), **1b** (4.0 mg, 0.006 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **6g** after 2 h in 100 % yield (50 mg). Anal. Calcd for $C_{16}H_{14}N$: C, 86.84; H, 6.83; N, 6.33. Found: C, 86.60; H, 6.50; N, 6.31. ^{1}H NMR ($CDCl_3$): δ 1.48 (d, 3 H, ^{3}J = 6.9 Hz), 3.04 (s, 1 H, C≡CH), 4.43 (q, 1 H, ^{3}J = 6.8 Hz), 6.47 (d, 2 H, ^{3}J = 7.9 Hz), 6.63 (t, 1 H, ^{3}J = 7.3 Hz), 7.07 (t, 2 H, ^{3}J = 7.6 Hz), 7.24 (t, 1 H), 7.34 (d,2 H, ^{3}J = 7.3 Hz), 7.49 (s, 1 H). ^{13}C NMR ($CDCl_3$): δ 147.15, 145.80, 130.86, 129.76, 129.26, 128.82, 126.56, 122.32, 117.59, 113.44, 83.93, 77.35, 50.81, 25.16.

General procedure for hydroamination, hydrosilylation in « one pot ».

The terminal alkyne was introduced with aniline in 7 mL of distilled MeOH. Catalyst **1b** was subsequently added. The mixture was stirred a few seconds before triethylsilane was injected. The resulting solution was stirred at room temperature under argon for 3-5 h. The progress of the reaction was monitored by ^{1}H NMR. The crude reaction mixture was hydrolyzed and the organic phase was extracted with dichloromethane. The solvent was evaporated under vacuum to give the amine product, which was washed thrice with cool pentane cooling to remove the impurities.



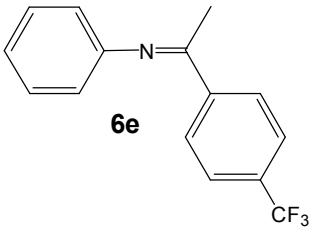
6d

Synthesis of 6d amine product by one pot reaction.

1-Ethynyl-4-methoxybenzene (34.0 mg, 0.256 mmol), aniline (23.8 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1a** (4.8 mg, 0.007 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **6d** after 4 h in 80 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 1.48 (d, 3 H, ^{3}J = 6.65 Hz), 3.76 (s, 3 H, OMe), 4.43 (q, 1 H, ^{3}J = 6.6 Hz), 6.51 (d, 2 H, ^{3}J = 8.0 Hz), 6.64 (t, 1 H, ^{3}J = 7.7 Hz), 6.84 (d, 2 H, ^{3}J = 8.7 Hz), 7.09 (t, 2 H, ^{3}J = 7.6 Hz), 7.36 (d, 2 H, ^{3}J = 8.7 Hz).

An alternative synthesis of 6a amine product by one pot reaction.

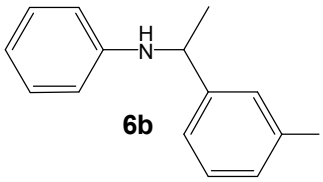
Phenyacetylene (26.1 mg, 0.256 mmol), aniline (23.8 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** complex (4.8 mg, 0.007 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **6a** after 4 h in 90 % yield (^{1}H NMR).



6e

Synthesis of 6e amine product by one pot reaction.

1-Ethynyl-4-(trifluoromethyl)benzene (43.5 mg, 0.256 mmol), aniline (23.8 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** complex (4.8 mg, 0.007 mmol) and MeOH (7 mL) as solvent, gave the corresponding amine **6e** after 4 h in 90 % yield (^{1}H NMR). ^{1}H NMR ($CDCl_3$): δ 1.51 (d, 3 H, ^3J = 6.75 Hz), 4.05 (s, 1 H, NH), 4.51 (q, 1 H, ^3J = 6.7 Hz), 6.45 (d, 2 H, ^3J = 8.0 Hz), 6.65 (t, 1 H, ^3J = 7.5 Hz), 7.08 (t, 2 H, ^3J = 7.1 Hz), 7.47 (d, 2 H, ^3J = 8.1Hz), 7.55 (d, 2 H, J = 8.0 Hz).

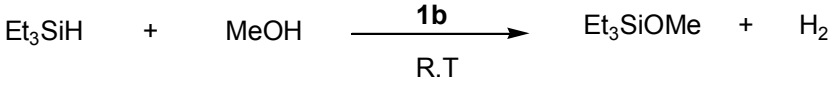


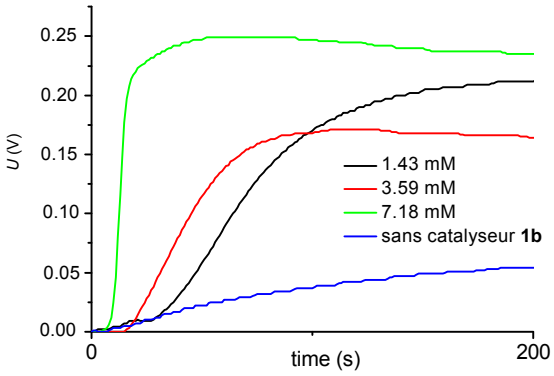
6b

Synthesis of 6b amine product by one pot reaction.

3-Ethynyltoluene (30 mg, 0.256 mmol), aniline (23.8 mg, 0.256 mmol), triethylsilane (38.4 mg, 0.33 mmol), **1b** complex (4.8 mg, 0.007 mmol) and MeOH 7 mL as solvent, gave the corresponding amine **6b** after 5 h in 50 % yield (NMR). ^{1}H NMR ($CDCl_3$): δ 1.53 (d, 3 H, ^{3}J = 7.3, CH_3), 2.36 (s, 3 H, CH_3), 4.03 (bs, 1 H, NH), 4.47 (q, ^{3}J = 6.9, 1 H, CH), 6.55 (d, 2 H, ^{3}J = 8.7,), 6.67 (t, 1 H, ^{3}J = 7.6), 7.06-7.25 (m, 6 H).

3. Catalytic H_2 release monitored by fuel-cell's response to partial H_2 pressure variation





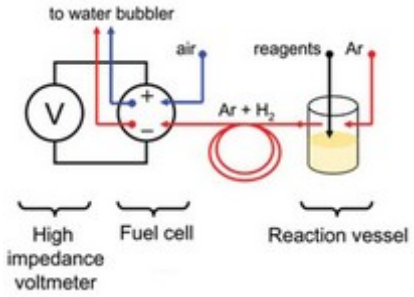


Figure 1. The release of H_2 was monitored by capturing the variation of potential at the plugs of a single stack fuel-cell: MeOH (V = 2 mL), Et_3SiH (V = 80 µL, c= 250 mM); injection of Et_3SiH occurs at t= 0 s.

General procedure. The complex **1b** was introduced in the clean and dry vessel. A volume of methanol (2.0 mL) was injected in this vessel through which a steady stream 11.5 mL min^{-1} of argon, used here as a carried gas, was flowed in the hydrogen compartment of a LightFC-1U fuel-cell (http://www.h2economy.com) *via* a 95 cm long 1.5 mm inner diameter coiled Teflon hose. Standard settings implied the concomitant steady flow of air in the fuel-cell's oxygencompartment at a value of 21.5 mL min^{-1}. The fuel-cell's electrodes were preliminary plugged to an ADC 42 Picotechnologies™ analogic-logic signal converter connected to a computer in order to acquire the variations of potential over time with a sampling frequency of 10 Hz. The experiment was started immediately after injection of triethylsilane by micro-syringe in the vessel. The experiment was repeated with different concentrations of **1b** complex (Table 1).

Table 1

Concentration of **1b** (mM)	Concentration of Et_3SiH (mM)	MeOH (mL)
0	250	2
1.43	250	2
3.59	250	2
7.18	250	2

4. Spectra

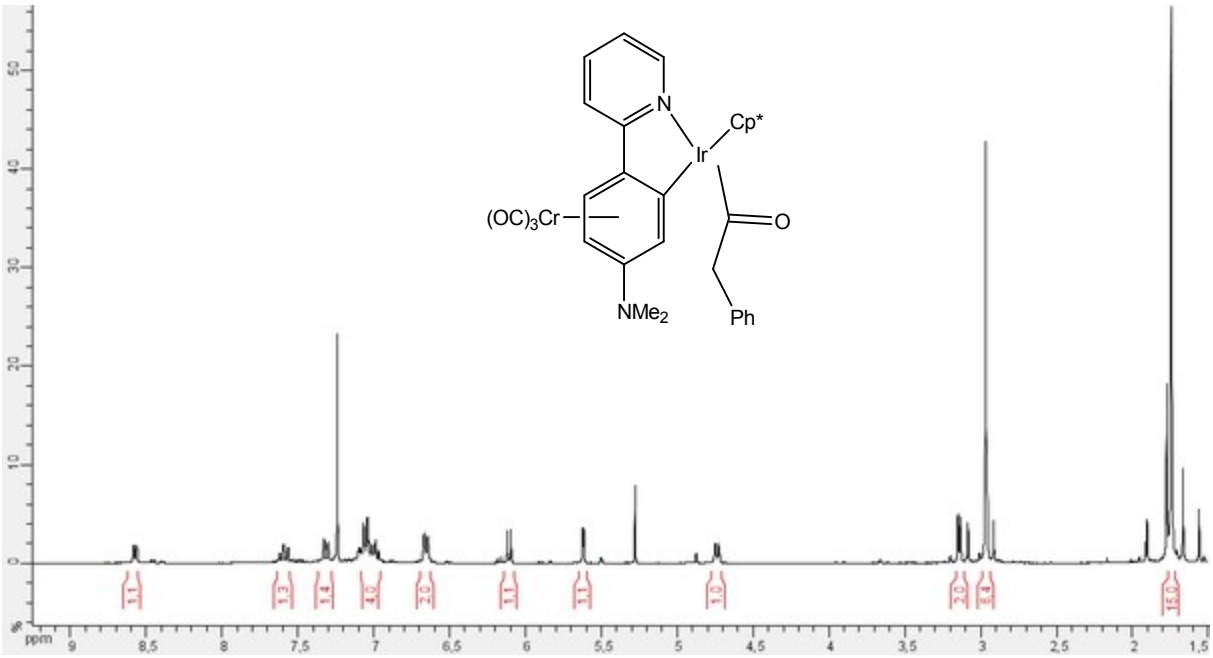


Figure 2. ^{1}H NMR in $CDCl_3$

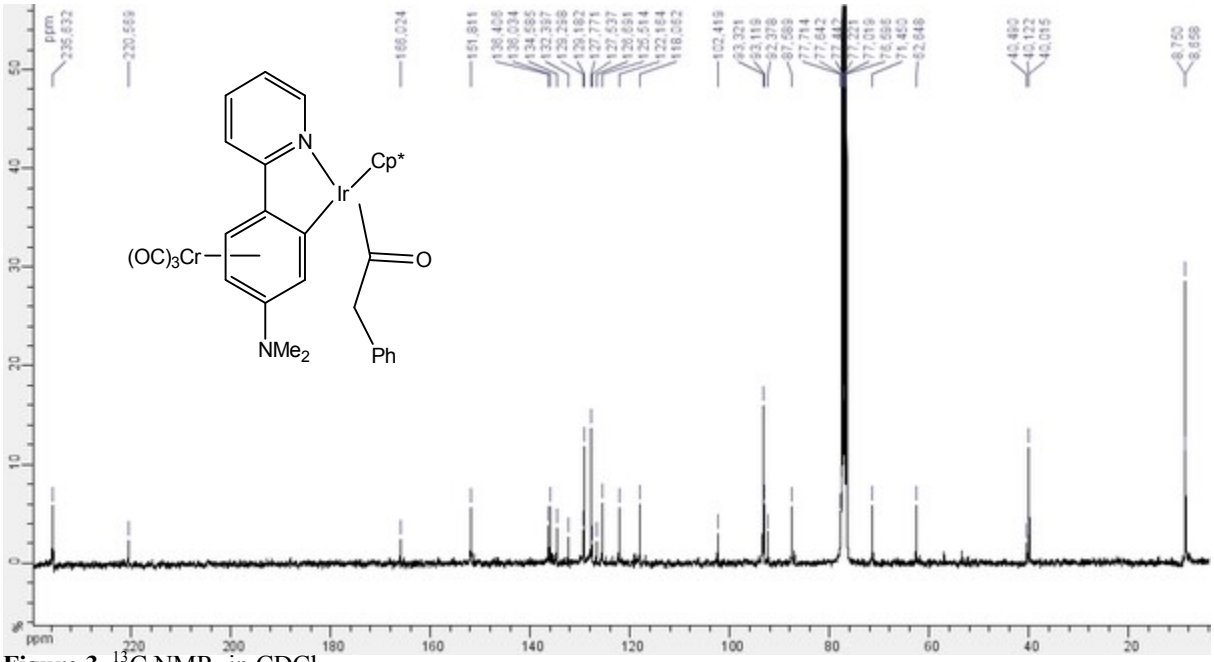


Figure 3. ^{13}C NMR in $CDCl_3$

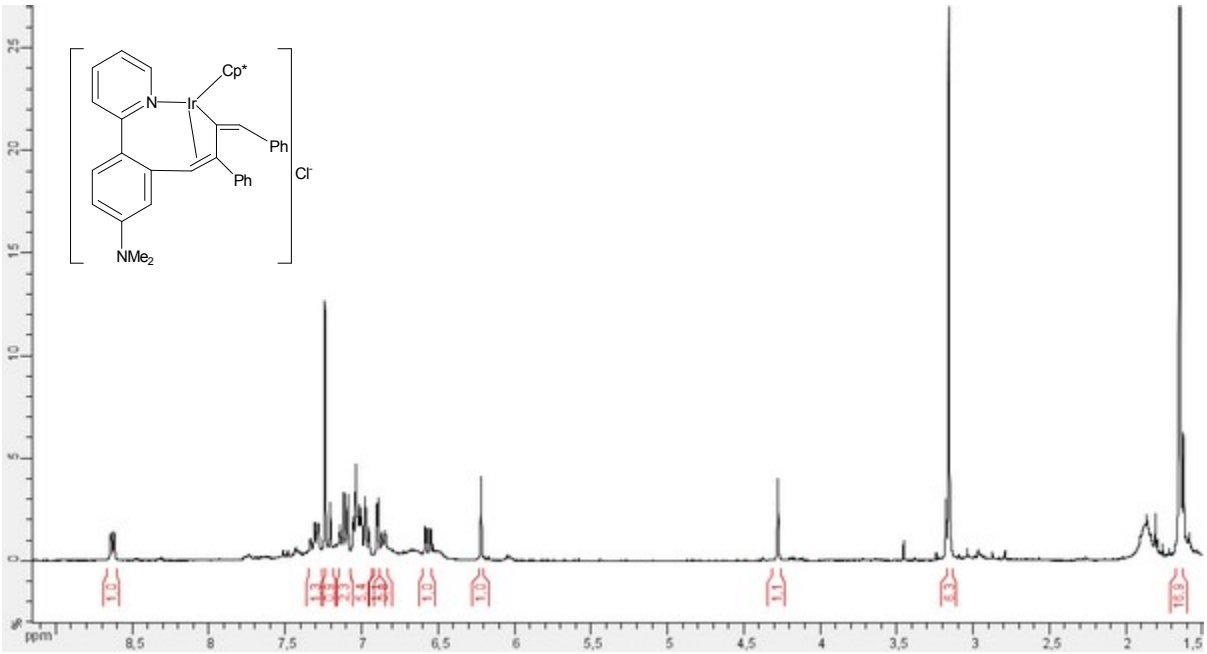


Figure 4. ^{1}H NMR in $CDCl_3$

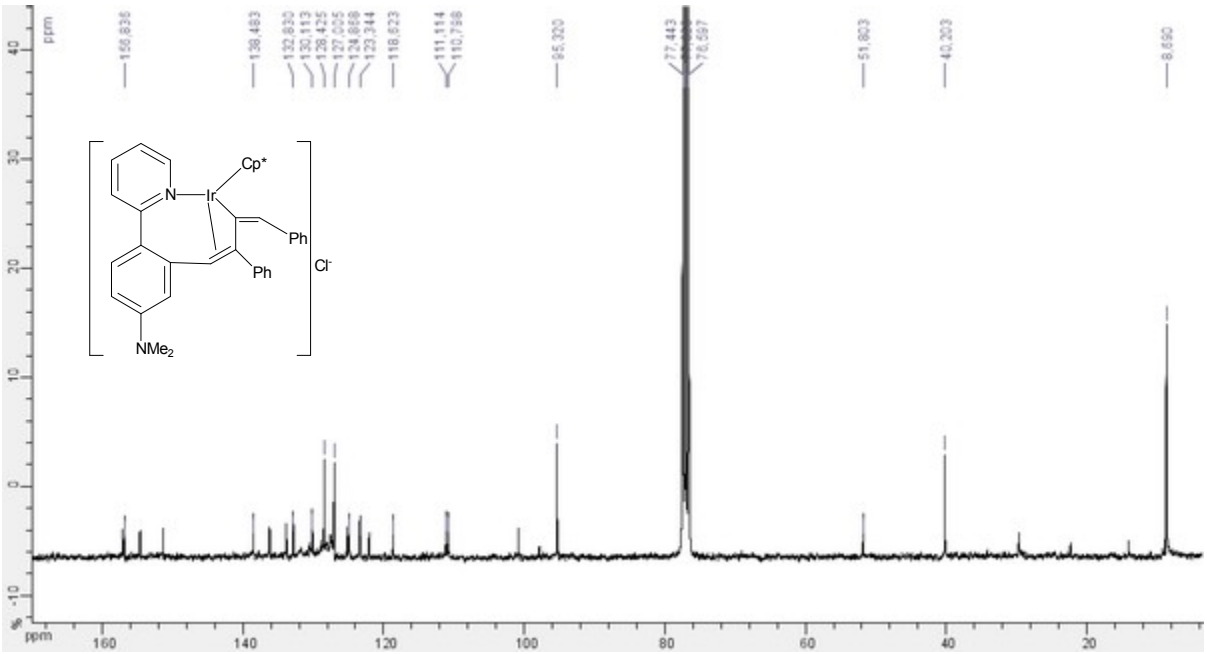


Figure 5. ^{13}C NMR in $CDCl_3$

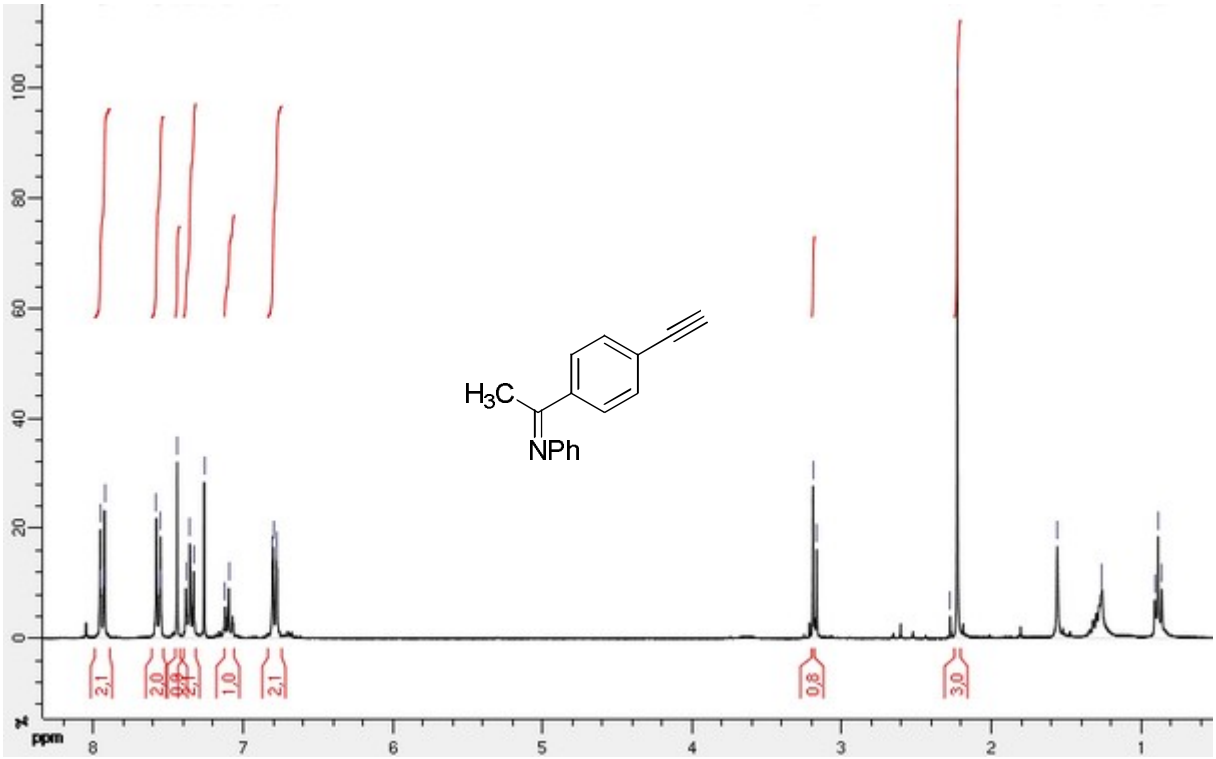


Figure 6. ^{1}H NMR in $CDCl_3$

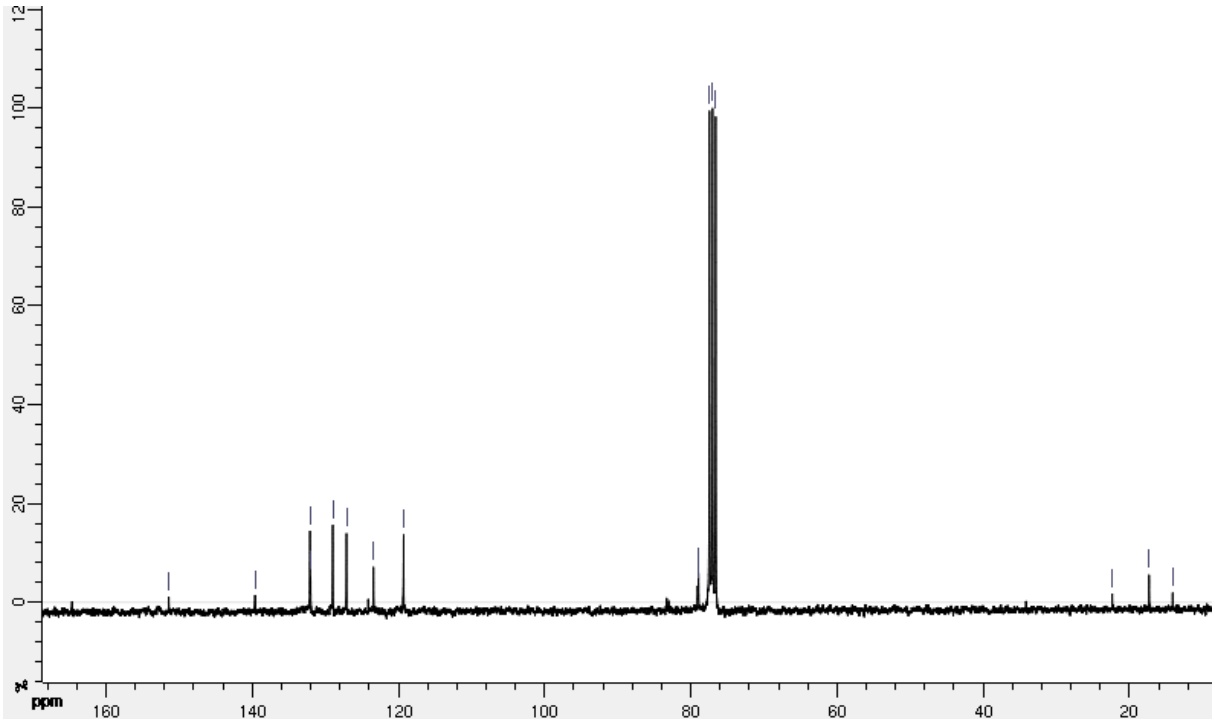


Figure 7. ^{13}C NMR in $CDCl_3$

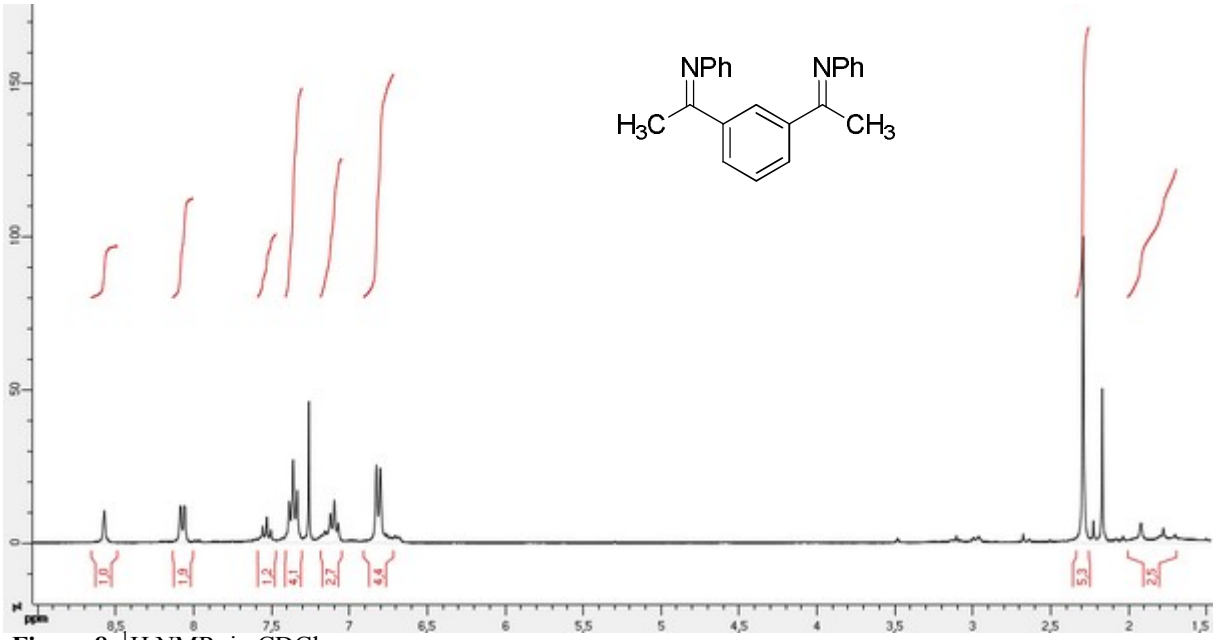


Figure 8. ^{1}H NMR in $CDCl_3$

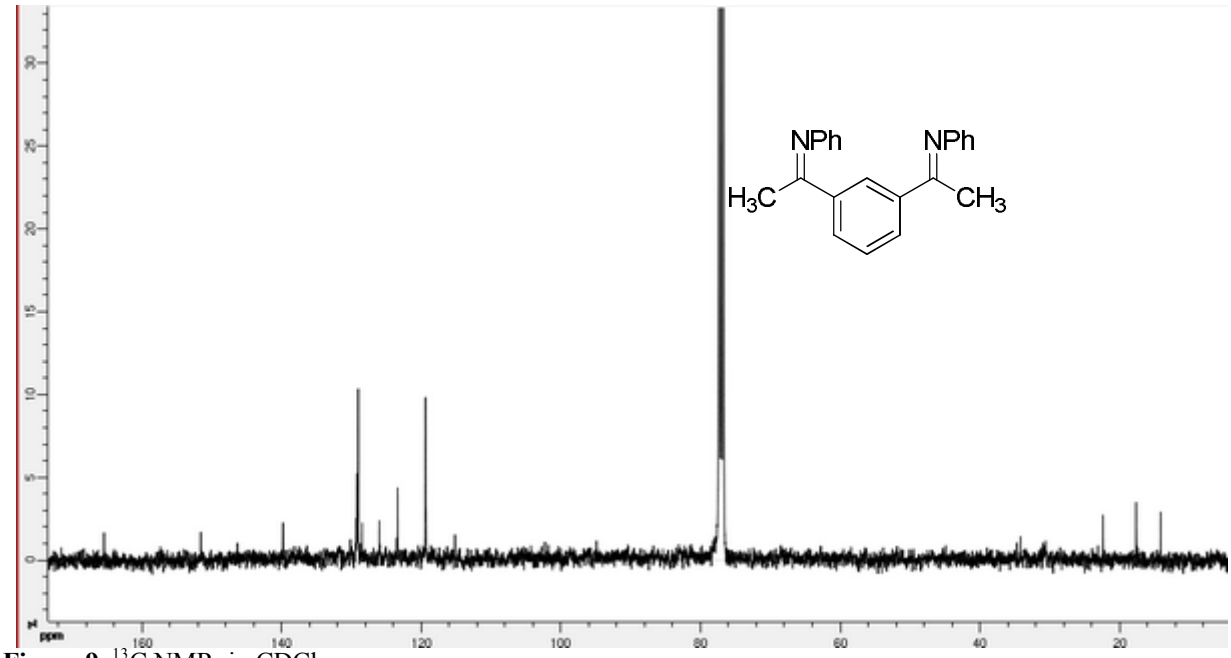


Figure 9. ^{13}C NMR in $CDCl_3$

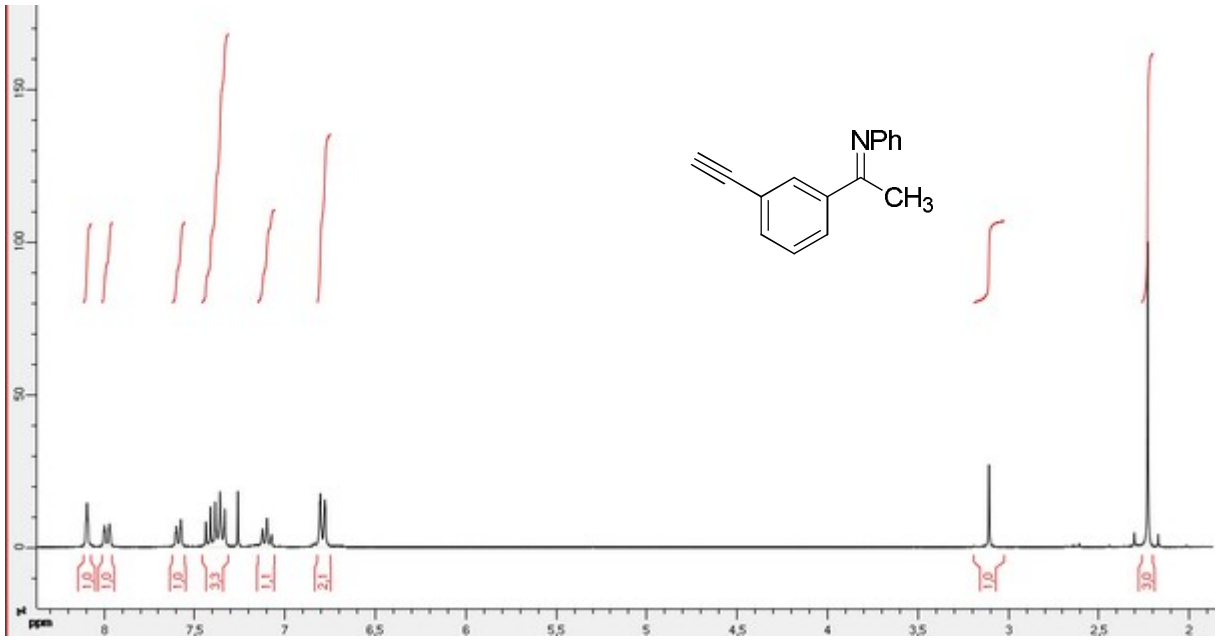


Figure 10. ^{1}H NMR in $CDCl_3$

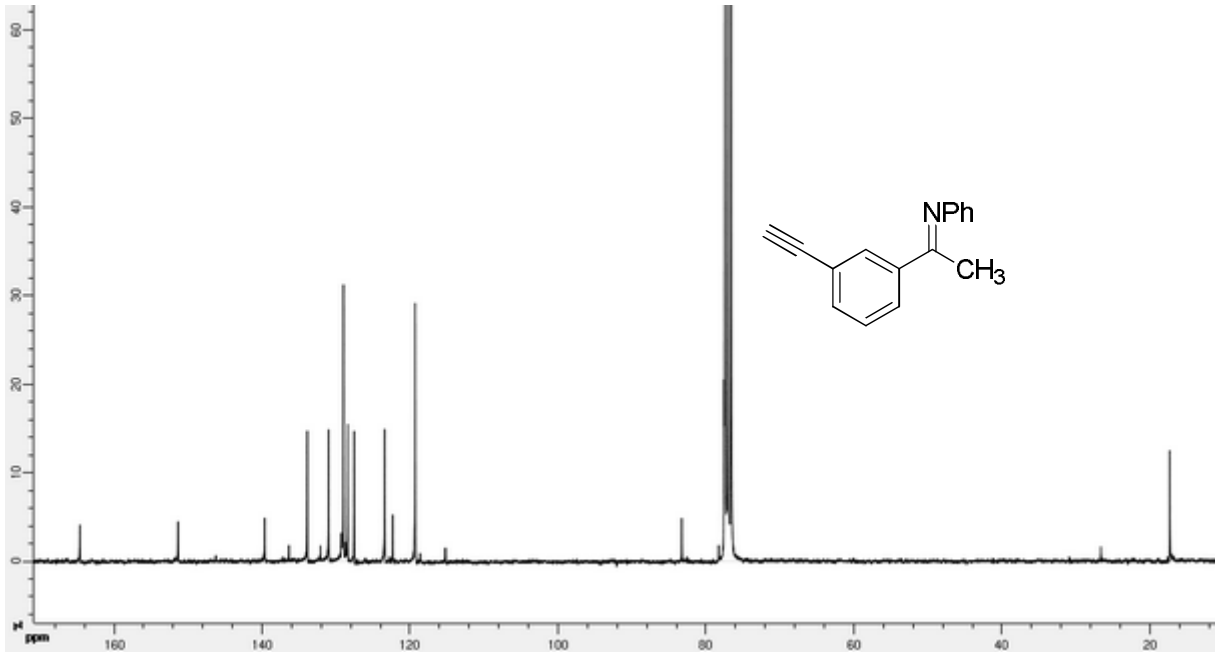


Figure 11. ^{13}C NMR in $CDCl_3$

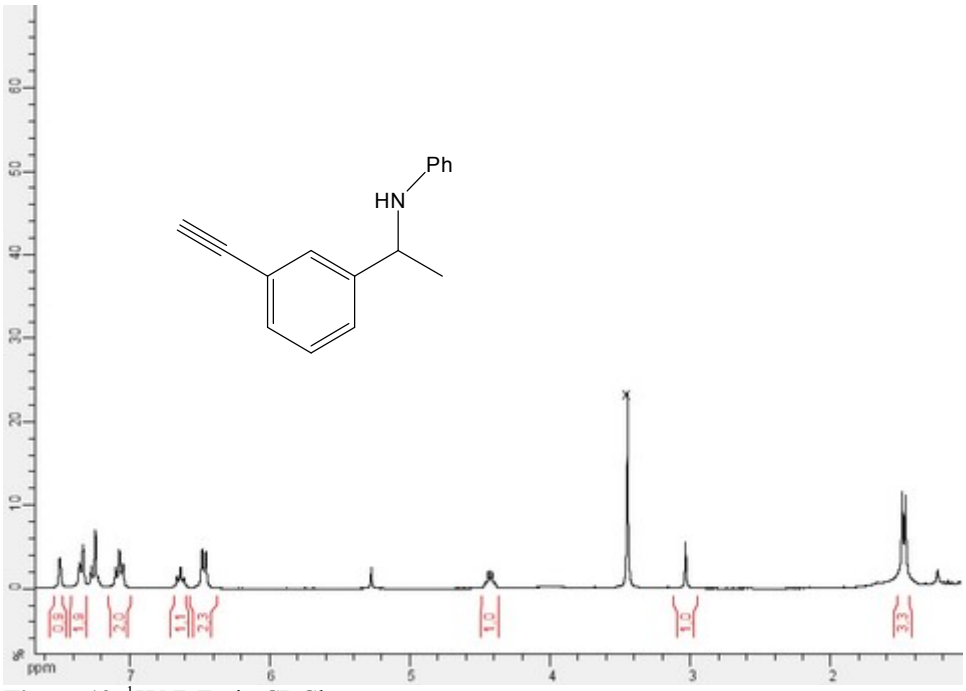


Figure 12. ^{1}H NMR in $CDCl_3$

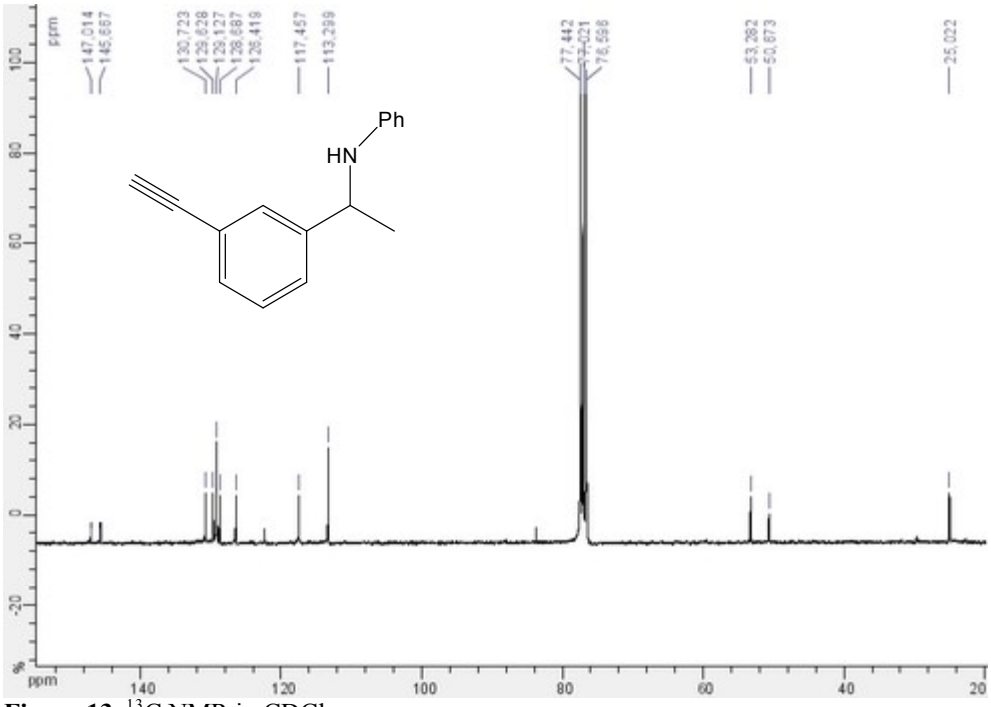


Figure 13. ^{13}C NMR in $CDCl_3$

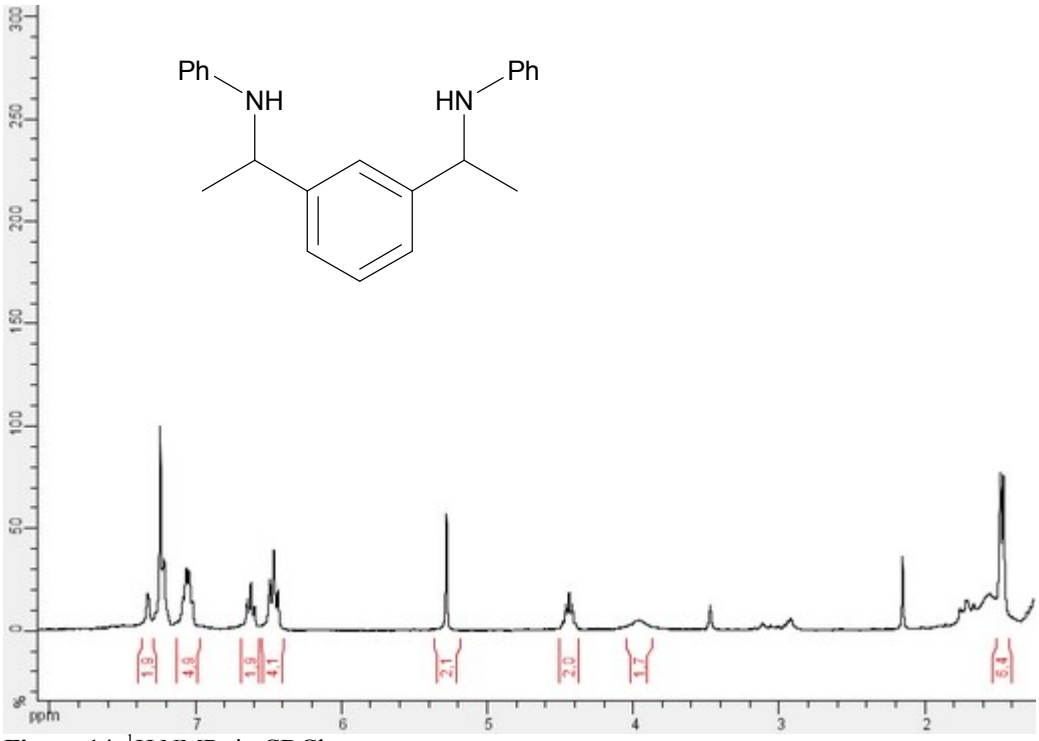


Figure 14. ^{1}H NMR in $CDCl_3$

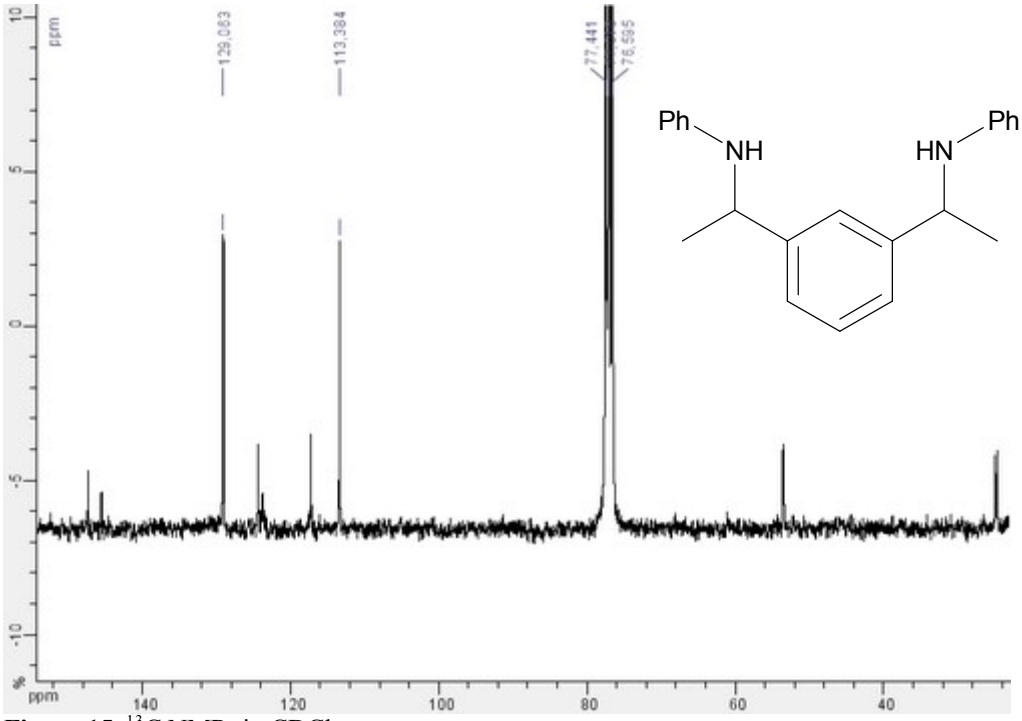


Figure 15. ^{13}C NMR in $CDCl_3$

The dehydrogenative methxylation of Et_3SiH in methanol

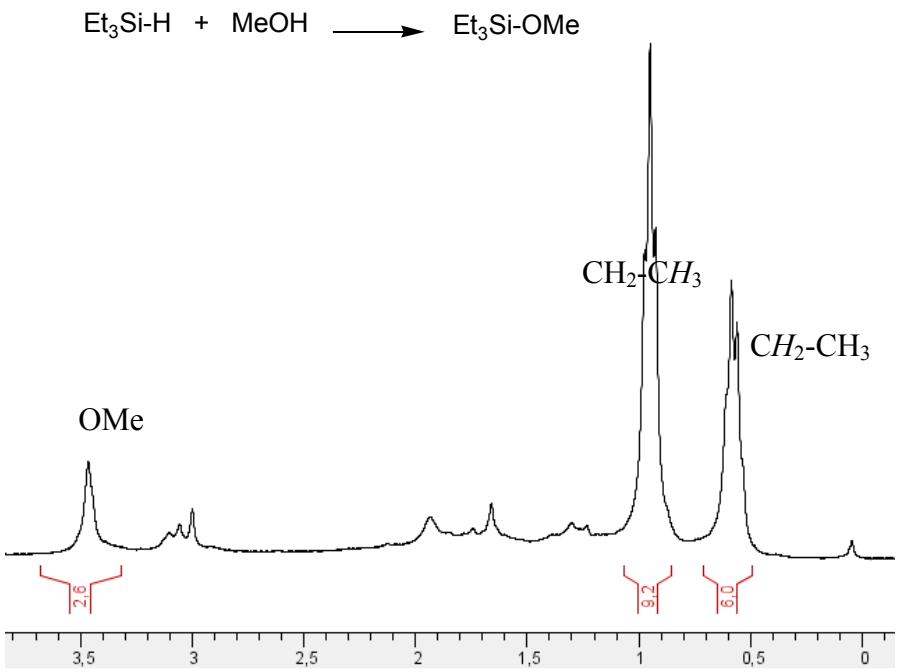


Figure 16. ^1H NMR in $CDCl_3$ of the crude reaction mixture resulting from the treatment of Et_3SiH with MeOH in the presence of **1b** (W. Caseri and P. S. Pregosin, *Organometallics* **1988**, *7*, 1373-1380).

Reaction of Et_3SiH with DMAP mediated by 1b.

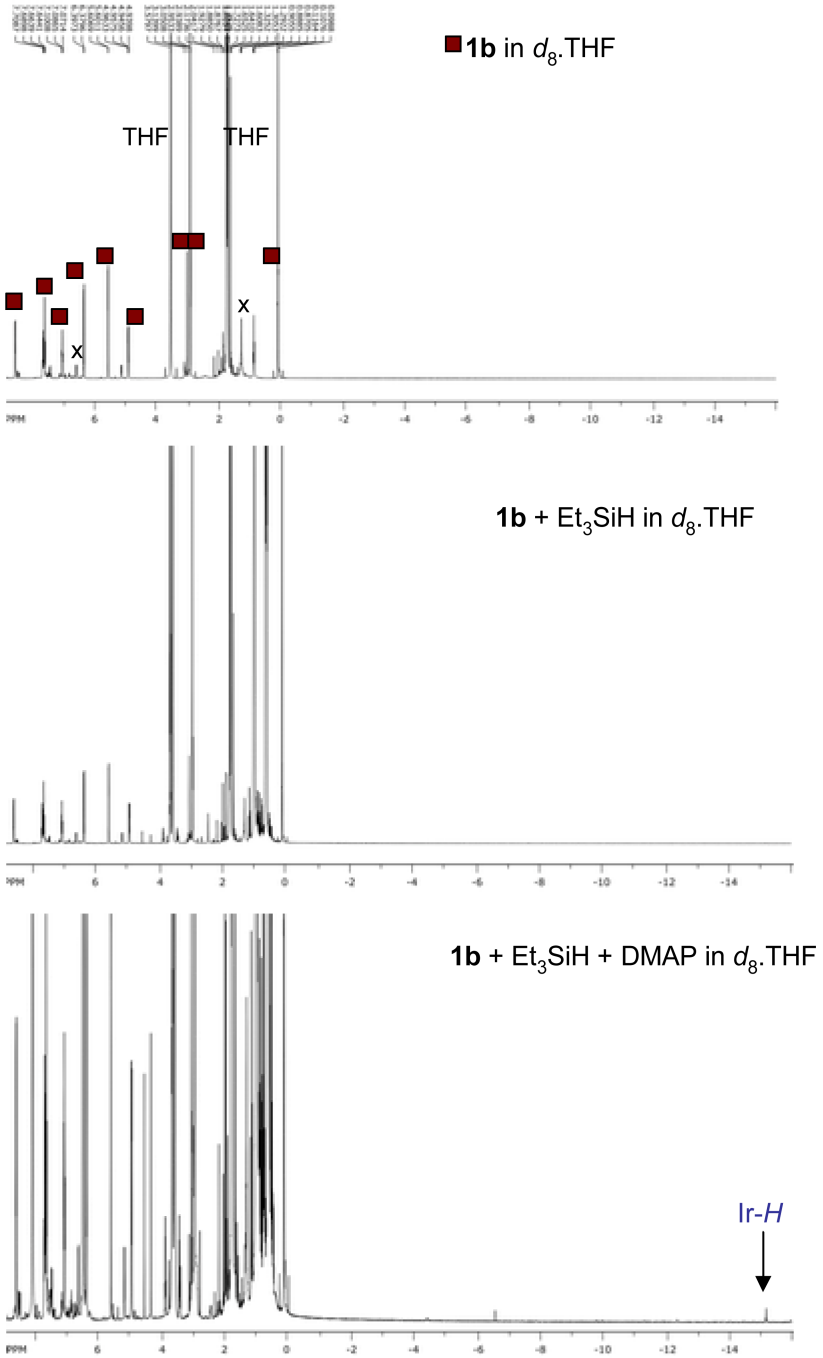


Figure 17. Et_3Si-H (c = 6.44 mM, V = 15 µL); **1b** (c = 12.08 mM, 14.3 mg); DMAP (c = 9.60 mM, 2 mg); THF[D8] (V = 1.7 mL)

5. High resolution mass spectra for new organic compounds

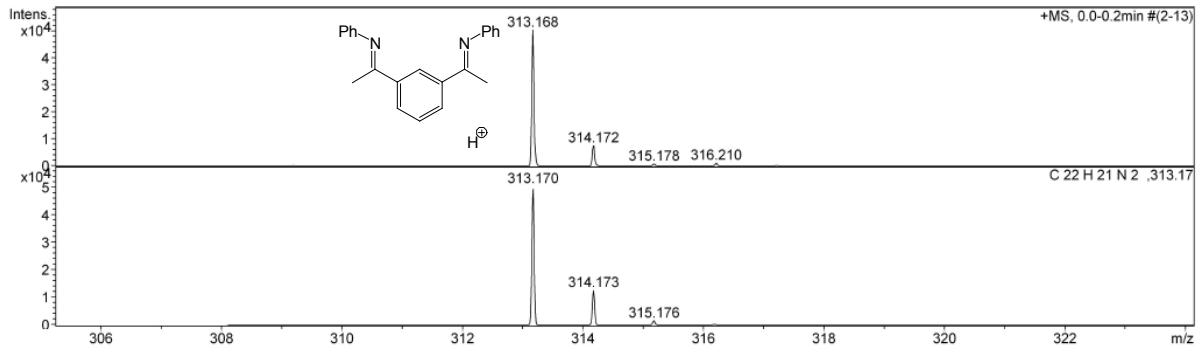


Figure 18. High resolution electrospray (ES+) mass spectrum of **5g**

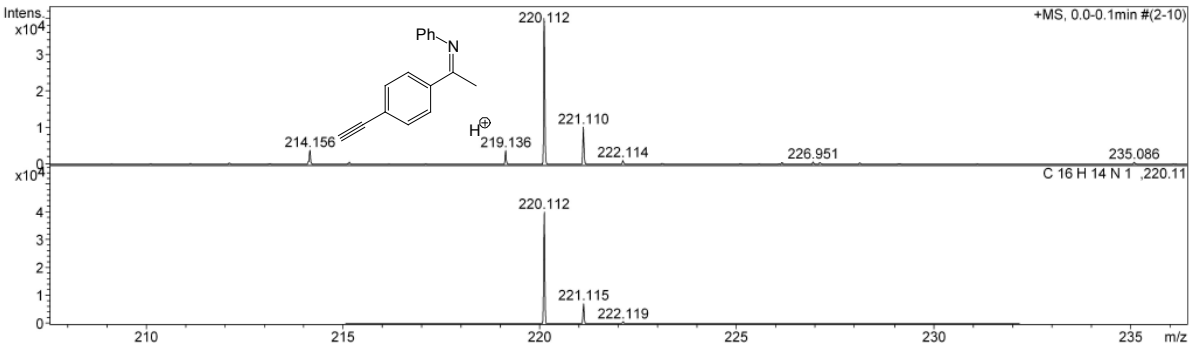


Figure 19. High resolution electrospray (ES+) mass spectrum of **4f**

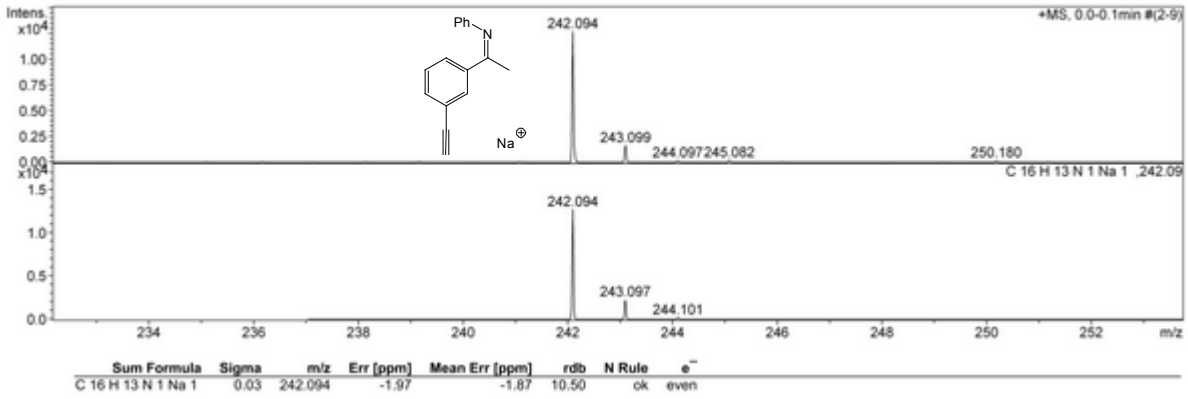


Figure 20. High resolution electrospray (ES+) mass spectrum of **4g**.

6. Computational details

Geometry optimizations and ground state electronic structure determination have been performed by DFT methods using the *Amsterdam Density Functional*[1, 2] package (*ADF2012*) using the *Perdew-Burke-Ernzerhof* [3] GGA functional (*PBE*x-*PBE*c). Within the *PBE* scheme electron correlation was treated within the local density approximation (LDA) in the *PW92* parametrization [4]. Electronic configurations of atoms were described by a triple-ζ *Slater*-type orbital (STO) basis set for H 1*s*, C 2*s* and 2*p*, N 2*s* and 2*p*, O 2*s* and 2*p*, Cl 3*s* and 3*p* augmented with a 3*d* single-ζ polarization for N, O and C atoms, with a 2*p* single-ζ polarization for H [5]. A triple-ζ (TZP STO) basis set was used for Mn 3d and 4*s* augmented with a 4*p* single-ζ polarization function. The *PBE*-D3(0) functional (the "3" suffix designates the so-called zero-damped third generation [6] of Grimme-type semi-empirical dispersion-corrected functionals), implemented in ADF2012.01 (LDA: *PW92*), was used in this study to include the contribution of dispersion interactions according to Grimme's recommendations [6]. The treatment of dispersion includes long-range electron correlations by adding an atom-pair wise dispersion corrections to the standard functionals of the form C_6R^{-6}, where R are interatomic distances and C_6 are the dispersion coefficients. Solvation by methanol was accounted for using the COSMO procedure with Klamt's values of *van der Waals* radii. Geometry optimizations were carried out in all cases with an integration grid of 5.5 and an energy gradient convergence criterion of 10^{-3} au. Counterpoise correction for basis set superposition error (*BSSE*) was neglected in all calculations due to the exclusive use of triple-ζ basis sets [7]. Vibrational modes were computed with optimized geometries using ADF subroutines: the analytical second derivative [8-10] method was applied exclusively for gas-phase structures. Thermodynamic data were computed by standard procedures. Representations of molecular structures and orbitals were drawn using *ADFview* v12.

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Intermediate A, gas phase.

```
============================
 G E O M E T R Y   U P D A T E  ***  99  ***
 ============================

 *** Using NEW gradient routines ***

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                  X         Y         Z
 ------------------------------------------
     1 C     0.000061 -0.000037  0.000013
     2 H     0.000014 -0.000055  0.000073
     3 C    -0.000090  0.000019  0.000020
     4 H     0.000005 -0.000032  0.000001
     5 C    -0.000011 -0.000083 -0.000120
     6 H    -0.000124  0.000027 -0.000080
     7 C    -0.000114  0.000035 -0.000027
     8 H    -0.000120 -0.000026 -0.000077
     9 C    -0.000005 -0.000036  0.000050
    10 C    -0.000081 -0.000051 -0.000082
    11 C    -0.000168 -0.000086  0.000100
    12 C     0.000043 -0.000054  0.000134
    13 H     0.000023  0.000050  0.000007
    14 C     0.000031  0.000032  0.000007
    15 N    -0.000045 -0.000026 -0.000001
    16 C     0.000005  0.000162  0.000096
    17 H     0.000041  0.000007  0.000102
    18 C     0.000283  0.000104  0.000296
    19 H     0.000078 -0.000001  0.000091
    20 C     0.000096  0.000034  0.000173
    21 C     0.000529 -0.000110 -0.000205
    22 C     0.000396  0.000341 -0.000543
    23 C     0.000001 -0.000020  0.000021
    24 C     0.000016 -0.000046 -0.000061
    25 C     0.000096 -0.000131 -0.000103
    26 C     0.000053 -0.000016 -0.000158
    27 C    -0.000045 -0.000048 -0.000182
    28 H    -0.000080 -0.000098 -0.000048
    29 H     0.000058 -0.000014 -0.000027
    30 H     0.000143  0.000034 -0.000108
    31 H     0.000050 -0.000001 -0.000124
    32 H    -0.000056 -0.000055 -0.000095
    33 N    -0.000018 -0.000082 -0.000055
    34 Ir    0.000560  0.000472  0.000299
    35 O     0.000079  0.000243 -0.000006
    36 O    -0.000371  0.000266  0.000174
    37 O    -0.000212  0.000104  0.000715
    38 Cr   -0.000042 -0.000573 -0.000615
    39 C    -0.000301  0.000278  0.000055
    40 C     0.000011  0.000028 -0.000033
    41 H     0.000009  0.000011 -0.000043
    42 H    -0.000061  0.000038 -0.000013
    43 H    -0.000056  0.000011 -0.000077
    44 C    -0.000055  0.000041 -0.000061
    45 H    -0.000036 -0.000029 -0.000085
    46 H    -0.000079 -0.000006 -0.000120
    47 H    -0.000089  0.000074 -0.000052
    48 C    -0.000012 -0.000882  0.000216
    49 C    -0.000096  0.000215 -0.000223
    50 C    -0.000245 -0.000098  0.000036
    51 C    -0.000173 -0.000133  0.000175
    52 C    -0.000035  0.000143 -0.000003
    53 C     0.000024  0.000095  0.000272
    54 C     0.000172  0.000001 -0.000015
    55 H    -0.000325 -0.000167 -0.000014
    56 H    -0.000318  0.000019 -0.000040
    57 H    -0.000004  0.000100  0.000116
    58 H     0.000290  0.000045  0.000087
    59 H     0.000194 -0.000006  0.000120
    60 H     0.000104 -0.000023  0.000048
 ------------------------------------------


 ==========================
 Geometry Convergence Tests
 ==========================

 Energy  old :        -14.51879529
         new :        -14.51881330

 Convergence tests:
 (Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

       Item               Value          Criterion    Conv.         Ratio
 ------------------------------------------------------------------------
 change in energy      -0.00001801     0.00100000     YES         0.87261317
 gradient max           0.00085426     0.00100000     YES         0.83903986
 gradient rms           0.00017576     0.00066667     YES         0.84308308
 cart. step max         0.01000000     0.01000000     YES         1.00000000
 cart. step rms         0.00240902     0.00666667     YES         1.00032734

 prediction dE :       -0.00003046
```

```
 ***************************************************************************************************
                              Geometry CONVERGED
 ***************************************************************************************************

                                          ********************
                                          *  Final Geometry  *
                                          ********************

                                      hartree             eV         kcal/mol          kJ/mol
                                 --------------------  -----------  ----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):            165.064984851232140    4491.6468    103579.85     433378.06
  Delta V^Pauli Coulomb:          -83.891898469609785   -2282.8147    -52642.97    -220258.15
  Delta V^Pauli LDA-XC:           -20.733087084004516    -564.1760    -13010.21     -54434.71
  Delta V^Pauli GGA-Exchange:       1.020831161232962      27.7782       640.58       2680.19
  Delta V^Pauli GGA-Correlation:   -0.232277095397782      -6.3206      -145.76       -609.84
                                 --------------------  -----------  ----------  -----------
  Total Pauli Repulsion:          61.228553363453017    1666.1137     38421.50     160755.54
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 61.228553363453017    1666.1137     38421.50     160755.54
  Electrostatic Interaction:      -13.047987233853629    -355.0538     -8187.74     -34257.49
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                 --------------------  -----------  ----------  -----------
  Total Steric Interaction:       48.180566129599384    1311.0599     30233.76     126498.06
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -62.635615740226505   -1704.4018    -39304.45    -164449.79
                                 --------------------  -----------  ----------  -----------
  Total Orbital Interactions:     -62.643671363313594   -1704.6210    -39309.50    -164470.94

Alternative Decomposition Orb.Int.
  Kinetic:                       -150.625002874663835   -4098.7149    -94518.63    -395465.89
  Coulomb:                         81.028067680960930    2204.8859     50845.89     212739.16
  XC:                               6.953263830389305     189.2079      4363.24      18255.79
                                 --------------------  -----------  ----------  -----------
  Total Orbital Interactions:     -62.643671363313601   -1704.6210    -39309.50    -164470.94

  Residu (E=Steric+OrbInt+Res):     0.000012889245879       0.0004         0.01         0.03
  Dispersion Energy:               -0.055737363865468      -1.5167       -34.98       -146.34

Total Bonding Energy:              -14.518829708333799    -395.0775    -9110.70     -38119.18


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
=============================================================================================

  Electrostatic Energy:            -13.047987233853629    -355.0538     -8187.74     -34257.49
  Kinetic Energy:                   14.439981976568305     392.9319      9061.23      37912.17
  Coulomb (Steric+OrbInt) Energy:   -2.863817899402974     -77.9285     -1797.07      -7518.95
  XC Energy:                       -12.991269187780032    -353.5104     -8152.15     -34108.57
  Dispersion Energy:               -0.055737363865468      -1.5167       -34.98       -146.34
                                 --------------------  -----------  ----------  -----------
  Total Bonding Energy:            -14.518829708333799    -395.0775    -9110.70     -38119.18


List of All Frequencies:


 Intensities
 ===========

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2                km/mole
             ----------       ----------             ----------
              13.616605          0.000000               0.000000
              22.355406         55.343674               0.310119
              39.361362        145.834969               1.438831
              59.880606        272.999456               4.097567
              62.699885         42.532870               0.668451
              65.496764         49.694589               0.815844
              72.498245         49.273456               0.895403
              75.891324         46.447162               0.883546
              77.219538        153.253420               2.966303
              81.145016         59.270188               1.205525
              87.007147         15.474581               0.337483
              95.429023         25.852955               0.618399
              98.162469         21.970415               0.540582
             120.712697        129.053942               3.904831
             125.112954         85.217139               2.672436
             130.600725        204.428881               6.692154
             136.340048         70.827492               2.420490
             148.571132        137.498155               5.120465
             161.633918        233.759761               9.470662
             170.833597        135.191424               5.788959
             174.865541          4.386646               0.192271
             180.570448         63.456928               2.872128
             187.489317         54.458253               2.559283
             201.361476        187.012754               9.438993
             237.029372        105.934935               6.293894
             242.159243         49.359310               2.996044
             253.644998        143.511232               9.124105
             287.598448         16.924777               1.220078
             291.455523         16.341801               1.193851
             299.469603        234.949609              17.636221
             304.703631        247.075581              18.870592
             326.603901        240.350911              19.676380
```

333.957814	68.827685	5.761464
342.681723	65.001192	5.583292
361.971094	99.201676	9.000590
388.303417	15.211074	1.480503
398.466609	11.677086	1.166284
416.302345	18.263755	1.905799
433.974505	129.913425	14.131762
437.614728	14.597829	1.601247
454.637496	100.863116	11.494119
459.929523	207.869370	23.964030
471.777591	27.496375	3.251553
475.873019	258.058750	30.781356
480.898473	54.352213	6.551620
487.341691	11.697856	1.428953
497.610029	160.499263	20.018901
511.997448	74.452547	9.554884
513.011426	37.875297	4.870361
516.318925	194.289034	25.144581
529.751451	22.596908	3.000539
538.200654	204.612599	27.602897
547.079018	117.445723	16.105171
563.068508	25.715010	3.629326
565.876822	21.562330	3.058410
570.403996	30.804077	4.404218
590.379517	20.806109	3.078933
617.083220	11.106781	1.717948
630.613278	248.947295	39.350349
637.930206	570.214679	91.177909
644.233887	61.624556	9.951200
657.802259	143.962446	23.736826
665.462026	33.419822	5.574494
679.114363	70.221832	11.953447
685.816968	251.955783	43.312238
687.347670	313.784018	54.061159
715.914155	45.008339	8.076664
731.239038	60.112691	11.018021
746.840477	121.915880	22.822657
753.920719	35.154865	6.643381
756.491111	186.662707	35.394800
786.146437	72.925380	14.370114
796.370316	4.584966	0.915228
804.562020	7.878454	1.588834
810.443856	72.170957	14.660996
814.051990	1.668181	0.340387
825.371139	120.368661	24.902376
828.354272	7.940080	1.648614
830.410350	104.684245	21.789745
850.021488	40.503923	8.629886
851.337170	11.674029	2.491153
861.425296	51.219340	11.059352
892.200400	8.025930	1.794882
906.862986	13.127453	2.984010
914.258558	13.984592	3.204770
917.352893	18.348020	4.218944
935.799942	1.269795	0.297848
937.163334	88.765263	20.851457
959.375566	3.337882	0.802671
972.668768	0.036290	0.008848
979.926098	0.857108	0.210527
988.796285	13.039373	3.231779
990.881198	26.798060	6.655842
992.519324	35.777987	8.900880
996.079670	28.164258	7.031864
1013.661303	55.799905	14.177655
1020.913769	22.212873	5.684233
1039.378228	58.932417	15.353448
1044.010070	42.844770	11.211935
1044.364149	25.048560	6.557115
1054.531007	21.303959	5.631158
1058.604218	17.266334	4.581544
1075.311301	18.002751	4.852339
1086.474075	2.083426	0.567382
1098.343553	7.200713	1.982402
1107.341343	144.722414	40.169404
1108.585916	4.490082	1.247676
1126.320177	3.981556	1.124069
1155.873245	51.975117	15.058571
1158.714912	64.661564	18.780228
1159.814992	29.928872	8.700759
1160.152959	10.800066	3.140651
1181.256809	14.854442	4.398238
1217.449841	36.663199	11.188182
1221.343398	74.795032	22.897529
1238.158673	1.253385	0.388990
1271.215569	5.485142	1.747773
1288.657674	0.133107	0.042995
1295.607244	20.667416	6.711778
1314.187643	74.551493	24.557932
1332.228080	0.146358	0.048874
1335.624027	19.009500	6.364041
1338.216726	210.076364	70.466340
1342.249746	3.463497	1.165269
1353.833360	14.338303	4.865652
1381.713201	15.113400	5.234294
1397.952599	5.926280	2.076599
1402.100637	16.846403	5.920582
1402.483318	65.997791	23.200918
1404.233535	46.090029	16.222747
1426.721417	34.092476	12.192024
1431.301854	11.413250	4.094667
1441.853397	9.233123	3.336935
1445.216558	6.968532	2.524366
1452.981511	120.485862	43.880771

1457.829247	101.165093	36.967103
1461.972577	17.637539	6.463314
1469.109370	9.505224	3.500214
1481.076689	121.358493	45.053215
1498.450649	226.227055	84.969890
1539.424377	1162.539709	448.584461
1548.556947	85.906440	33.345019
1560.087397	3.921451	1.533465
1587.196433	14.694788	5.846178
1599.528924	203.141261	81.445729
1884.909926	1337.753310	632.040206
1911.568000	1561.556532	748.213489
1915.194952	24.870003	11.938971
1956.876466	2807.636882	1377.153719
2938.521484	33.787588	24.886517
2946.426627	41.597333	30.721271
3017.129206	14.066814	10.638189
3028.308105	12.817991	9.729670
3077.896266	1.398908	1.079248
3084.898264	13.696719	10.590963
3106.067998	1.057369	0.823219
3110.297716	2.251358	1.755192
3119.538865	2.824661	2.208690
3121.204059	2.543878	1.990199
3126.580318	1.261921	0.988962
3127.015310	0.385461	0.302126
3135.227995	7.019161	5.516103
3136.539955	3.304163	2.597708
3142.161124	2.751475	2.167066
3155.136546	1.839078	1.454442
3157.373533	1.975373	1.563339
3161.556251	0.947346	0.750737
3166.983475	1.387079	1.101096
3171.768354	1.549890	1.232198
3175.913310	10.889543	8.668748
3182.160206	12.738740	10.160769
3191.679086	4.980210	3.984235
3231.808164	45.718485	37.035266

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

       9843.8715      24277.6301      26643.5700
-----------------------------------------------------
         -0.2430          0.3932         -0.8868
         -0.0480         -0.9179         -0.3938
          0.9688          0.0531         -0.2419


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.

    Temp                                                  Transl     Rotat    Vibrat     Total
    ----                                                  ------     -----    ------     -----

    298.15   Entropy (cal/mole-K):                        45.488    37.097   121.185   203.770
             Internal Energy (Kcal/mole):                  0.889     0.889   297.432   299.209
             Constant Volume Heat Capacity (cal/mole-K):   2.981     2.981   123.838   129.799


*****************************************************************************************************


=====================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
=====================================================================
```

Intermediate B, gas phase

```
============================
G E O M E T R Y   U P D A T E  ***  120  ***
============================

*** Using NEW gradient routines ***

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X          Y          Z
------------------------------------------
    1 C    -0.000019 -0.000014 -0.000013
    2 H    -0.000053 -0.000053 -0.000072
    3 C    -0.000050 -0.000067 -0.000120
    4 H    -0.000049 -0.000027 -0.000036
    5 C    -0.000019 -0.000036  0.000000
    6 H     0.000008 -0.000029  0.000009
    7 C    -0.000058 -0.000086 -0.000115
    8 H     0.000008 -0.000018  0.000005
    9 C    -0.000030 -0.000006 -0.000084
   10 C     0.000099  0.000051  0.000149
   11 C    -0.000029 -0.000092  0.000136
   12 C    -0.000061 -0.000011 -0.000012
   13 H     0.000036 -0.000018  0.000056
   14 C    -0.000048  0.000014  0.000012
   15 N    -0.000035 -0.000020 -0.000012
   16 C    -0.000035 -0.000094  0.000014
   17 H    -0.000026 -0.000045 -0.000079
   18 C    -0.000189 -0.000089 -0.000230
   19 H    -0.000066 -0.000022 -0.000053
   20 C    -0.000122  0.000247 -0.000031
   21 C     0.000320 -0.000194 -0.000303
   22 C     0.000241  0.000579 -0.000247
   23 C    -0.000069 -0.000248  0.000089
   24 C    -0.000007 -0.000064  0.000108
   25 C    -0.000014  0.000044 -0.000043
   26 C    -0.000031  0.000153 -0.000010
   27 C    -0.000031  0.000069  0.000262
   28 H    -0.000026  0.000086  0.000255
   29 H    -0.000066 -0.000077  0.000148
   30 H     0.000015  0.000002 -0.000005
   31 H     0.000118  0.000146 -0.000039
   32 H     0.000085  0.000203  0.000088
   33 N     0.000064  0.000135  0.000043
   34 Ir    0.000137  0.000228 -0.000066
   35 O    -0.000122 -0.000062 -0.000167
   36 O    -0.000100  0.000090  0.000282
   37 O     0.000075 -0.000167  0.000078
   38 Cr    0.000181 -0.000188  0.000091
   39 C    -0.000484 -0.000277 -0.000868
   40 C     0.000009 -0.000041 -0.000039
   41 H    -0.000062 -0.000063 -0.000046
   42 H    -0.000027  0.000000 -0.000051
   43 H    -0.000021 -0.000035 -0.000015
   44 C     0.000086 -0.000042  0.000072
   45 H     0.000076 -0.000056  0.000079
   46 H     0.000058 -0.000008  0.000103
   47 H     0.000049  0.000031  0.000071
   48 C     0.000678 -0.000153  0.000736
   49 C    -0.000133 -0.000029  0.000105
   50 C     0.000244  0.000158  0.000085
   51 C     0.000244  0.000118  0.000207
   52 C    -0.000027  0.000160 -0.000029
   53 C    -0.000234 -0.000198 -0.000160
   54 C    -0.000195 -0.000090 -0.000176
   55 H     0.000258  0.000382  0.000146
   56 H     0.000233  0.000495 -0.000005
   57 H    -0.000001  0.000057 -0.000115
   58 H    -0.000284 -0.000324 -0.000208
   59 H    -0.000309 -0.000445 -0.000095
   60 H    -0.000185  0.000039  0.000114
------------------------------------------


==========================
Geometry Convergence Tests
==========================

Energy  old :        -14.52203141
        new :        -14.52205418

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00002277     0.00100000    YES        6.27722645
gradient max           0.00088000     0.00100000    YES        0.61795003
gradient rms           0.00017474     0.00066667    YES        0.60931719
cart. step max         0.01000000     0.01000000    YES        2.15869055
cart. step rms         0.00241211     0.00666667    YES        2.59575860
```

prediction dE : -0.00004076

****
Geometry CONVERGED
****

****
* Final Geometry *
****

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	164.864143669050890	4486.1816	103453.82	432850.75
Delta V^Pauli Coulomb:	-84.028842415596898	-2286.5411	-52728.90	-220617.69
Delta V^Pauli LDA-XC:	-20.644777796550660	-561.7730	-12954.80	-54202.86
Delta V^Pauli GGA-Exchange:	1.013865372823261	27.5887	636.21	2661.90
Delta V^Pauli GGA-Correlation:	-0.229879033463405	-6.2553	-144.25	-603.55
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	60.974509796263192	1659.2008	38262.09	160088.55
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	60.974509796263192	1659.2008	38262.09	160088.55
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-13.018994288869935	-354.2649	-8169.54	-34181.36
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	47.955515507393258	1304.9360	30092.54	125907.19
Orbital Interactions				
A:	-62.421596678779260	-1698.5781	-39170.15	-163887.88
Total Orbital Interactions:	-62.424661364356758	-1698.6615	-39172.07	-163895.93
Alternative Decomposition Orb.Int.				
Kinetic:	-150.428014924025121	-4093.3546	-94395.01	-394948.70
Coulomb:	81.087098857136581	2206.4922	50882.93	212894.15
XC:	6.916254702531760	188.2009	4340.02	18158.62
Total Orbital Interactions:	-62.424661364356780	-1698.6615	-39172.07	-163895.93
Residu (E=Steric+OrbInt+Res):	0.000002661192863	0.0001	0.00	0.01
Dispersion Energy:	-0.052959762308176	-1.4411	-33.23	-139.05
Total Bonding Energy:	-14.522102958078813	-395.1665	-9112.76	-38127.78

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.018994288869935	-354.2649	-8169.54	-34181.36
Kinetic Energy:	14.436128745025769	392.8271	9058.81	37902.05
Coulomb (Steric+OrbInt) Energy:	-2.941740897267451	-80.0488	-1845.97	-7723.54
XC Energy:	-12.944536754659044	-352.2388	-8122.82	-33985.88
Dispersion Energy:	-0.052959762308176	-1.4411	-33.23	-139.05
Total Bonding Energy:	-14.522102958078836	-395.1665	-9112.76	-38127.78

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
15.263930	0.000000	0.000000
33.643544	207.749961	1.751946
50.728406	10.399502	0.132234
52.924088	405.187390	5.375110
56.761396	34.277592	0.487687
60.749625	26.451376	0.402782
66.193530	20.301830	0.336844
70.018715	28.645648	0.502749
73.241686	98.964093	1.816829
80.666157	26.235832	0.530474
86.143357	24.906845	0.537797
91.765022	4.394048	0.101069
99.324481	60.884423	1.515795
114.619631	71.511196	2.054524
118.799637	32.240009	0.960038
131.519761	157.528055	5.193104
138.100284	112.301029	3.887374
159.654224	55.294908	2.212807
175.570252	30.980479	1.363381
180.237111	8.665392	0.391481
192.708856	18.726120	0.904540
204.292542	75.004199	3.840751
222.984085	37.059010	2.071313

242.023207	19.782589	1.200102
246.123735	65.899827	4.065518
277.467470	71.548691	4.976131
286.501924	57.481265	4.127926
289.982303	25.911807	1.883420
294.660172	96.348656	7.116151
298.511374	15.689982	1.173982
320.397274	291.115132	23.379309
330.201459	34.786004	2.879132
349.564677	53.429749	4.681540
380.830134	11.709774	1.117784
385.631679	45.850531	4.431953
396.908957	2.820633	0.280618
406.327206	64.781390	6.597877
416.213699	2.551105	0.266148
435.696106	3.590088	0.392073
438.143580	35.940461	3.947100
456.318363	30.678279	3.508949
459.681700	77.855034	8.970610
470.375397	11.661031	1.374864
479.684241	72.631940	8.732954
486.805914	21.050084	2.568548
492.023203	191.203976	23.580911
508.574640	89.475661	11.406113
527.403676	9.762284	1.290544
536.751959	173.799535	23.383005
544.079942	115.938025	15.811267
563.215409	9.429663	1.331217
564.733719	104.327628	14.767981
570.698420	14.416564	2.062275
579.478919	130.318665	18.928767
585.724721	16.768358	2.461853
614.943792	1.266610	0.195234
629.668594	242.374926	38.254083
636.206135	441.872098	70.464845
644.410515	70.870081	11.447315
650.743610	58.903166	9.607859
656.791917	129.962859	21.395632
664.865367	92.117024	15.351531
681.940375	36.416632	6.224783
686.532454	114.617092	19.723706
687.469567	646.001913	111.317989
715.796251	41.182083	7.388832
730.531430	45.357842	8.305568
752.684706	247.508538	46.696179
755.233619	88.196806	16.695993
790.531458	25.746687	5.101743
802.731447	36.170808	7.277908
804.815665	50.891514	10.266440
811.117774	14.072554	2.861112
812.759700	41.946444	8.545459
818.201184	5.301122	1.087191
820.161275	21.531483	4.426406
832.282754	306.915263	64.027634
840.834780	39.627786	8.351963
848.240255	71.077938	15.112342
851.498204	3.254182	0.694550
893.018572	16.959751	3.796278
897.027024	4.909457	1.103868
903.650665	10.319237	2.337363
921.114494	10.319044	2.382490
937.002743	3.122423	0.733349
941.520895	56.462529	13.325035
947.173772	0.238319	0.056580
972.474365	0.140630	0.034279
974.888084	0.260792	0.063728
987.315790	17.380775	4.301335
989.542228	46.619978	11.563371
990.720368	39.094281	9.708282
1001.330679	14.732962	3.697819
1015.479315	46.394348	11.809030
1023.344771	23.216375	5.955174
1038.907359	49.582242	12.911629
1044.966814	0.670679	0.175669
1047.490000	46.913097	12.317485
1054.678918	26.089278	6.897003
1057.376879	13.356440	3.539962
1069.037293	20.181639	5.407884
1087.888843	0.828723	0.225981
1100.361690	0.513367	0.141593
1104.198799	94.975736	26.286817
1110.789147	8.087770	2.251845
1118.520768	24.828116	6.960908
1127.935203	4.228189	1.195409
1155.301777	1.342104	0.388651
1157.433361	41.682682	12.092880
1161.281444	26.934785	7.840235
1169.311845	14.520625	4.255923
1200.974115	4.357053	1.311609
1220.560495	47.493995	14.530350
1225.195230	76.693428	23.552744
1239.749076	0.457324	0.142114
1270.025572	5.963371	1.898377
1298.849731	16.947313	5.517443
1300.112582	5.182678	1.688936
1316.646219	71.365362	23.552371
1332.217592	0.321882	0.107485
1336.193827	4.174662	1.398199
1341.651168	19.509426	6.560881
1344.719506	208.543242	70.291999
1356.431222	12.550278	4.267064
1390.007588	12.633812	4.401793
1398.474024	12.167404	4.265112

1399.446639	5.114263	1.793979
1405.681467	75.314330	26.536437
1419.981608	11.244007	4.002044
1427.228166	25.081730	8.972820
1434.849011	18.439001	6.631651
1444.383170	7.056142	2.554629
1447.293143	4.632050	1.680381
1455.972891	102.792015	37.513772
1458.843990	100.498548	36.749100
1464.131332	35.428498	13.002021
1476.930767	27.996668	10.364409
1482.666012	118.148413	43.908570
1501.994246	248.903630	93.708195
1545.239779	775.953875	300.545241
1552.000542	294.386214	114.521600
1568.887219	4.183132	1.645021
1586.524656	83.604748	33.247258
1600.843542	204.012875	81.862412
1701.278614	705.230696	300.735516
1881.566924	1239.060285	584.373047
1913.718632	1556.093646	746.434811
1957.021684	2822.717978	1384.653785
2938.737603	36.380686	26.798456
2948.320959	42.236515	31.213388
3006.818786	12.284513	9.258556
3021.666556	8.729758	6.611908
3037.733029	38.470575	29.292494
3079.180765	0.252677	0.195020
3086.276278	6.331053	4.897662
3086.640075	9.642770	7.460464
3097.623525	0.732918	0.569065
3104.581338	1.391892	1.083145
3112.950822	6.622836	5.167665
3122.078783	1.957795	1.532107
3126.897963	6.684394	5.239065
3127.002006	1.232193	0.965795
3138.700221	2.798797	2.201909
3143.189435	3.740332	2.946855
3157.013460	1.398884	1.106971
3158.321916	2.069357	1.638211
3166.069662	0.374114	0.296895
3167.815113	1.790179	1.421459
3170.056580	0.293187	0.232965
3178.797067	9.846287	7.845368
3181.985373	13.036251	10.397501
3193.015154	3.473193	2.779764

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

      16785.4498      17394.6219      23336.0559
-------------------------------------------------
          0.8639         -0.3265          0.3835
          0.4646          0.2231         -0.8569
          0.1942          0.9185          0.3444


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.

    Temp                                                    Transl     Rotat    Vibrat     Total
    ----                                                    ------     -----    ------     -----

    298.15   Entropy (cal/mole-K):                          45.488    37.164   117.423   200.075
             Internal Energy (Kcal/mole):                    0.889     0.889   296.908   298.685
             Constant Volume Heat Capacity (cal/mole-K):     2.981     2.981   121.147   127.109


*****************************************************************************************************


=====================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
=====================================================================
```

TSAB, gas phase

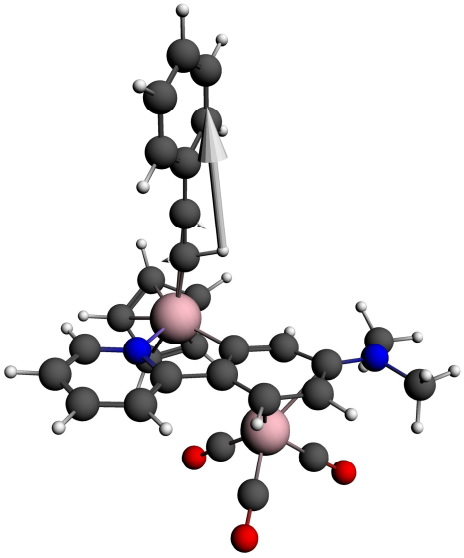

Figure 21 Displacement vectors for $\mathbf{TS_{AB}}$ at the imaginary vibrational mode (530.1*i* cm^{-1})

```
Geometry CYCLE 133
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom       Cartesian (a.u./angstrom)
                  X          Y          Z
 ----------------------------------------
     1 C      0.000017   0.000030   0.000069
     2 H     -0.000005  -0.000001   0.000001
     3 C      0.000054  -0.000004   0.000098
     4 H     -0.000008  -0.000004  -0.000009
     5 C     -0.000007   0.000011   0.000009
     6 H     -0.000008  -0.000007  -0.000011
     7 C      0.000026   0.000007   0.000045
     8 H      0.000004  -0.000002   0.000013
     9 C     -0.000084  -0.000007  -0.000076
    10 C      0.000006  -0.000036  -0.000045
    11 C      0.000237  -0.000024   0.000203
    12 C     -0.000096  -0.000032  -0.000123
    13 H      0.000000  -0.000005   0.000008
    14 C     -0.000053  -0.000060  -0.000044
    15 N      0.000112   0.000049   0.000097
    16 C      0.000047   0.000027   0.000035
    17 H     -0.000001   0.000003   0.000015
    18 C     -0.000016   0.000016  -0.000009
    19 H      0.000009  -0.000004   0.000000
    20 C     -0.000230   0.000463  -0.000376
    21 C      0.000154   0.000101   0.000030
    22 C     -0.000085   0.000028   0.000086
    23 C      0.000039   0.000005  -0.000020
    24 C     -0.000014   0.000024   0.000006
    25 C     -0.000035  -0.000034   0.000017
    26 C     -0.000080   0.000083   0.000020
    27 C      0.000026  -0.000022  -0.000018
    28 H      0.000016   0.000006   0.000003
    29 H     -0.000001  -0.000003  -0.000016
    30 H     -0.000031   0.000024  -0.000012
    31 H     -0.000037   0.000008   0.000035
    32 H      0.000006  -0.000002   0.000020
    33 N     -0.000114   0.000002  -0.000159
    34 Ir     0.000437  -0.000121  -0.000220
    35 O      0.000222  -0.000520   0.000401
    36 O     -0.000147  -0.000136  -0.000072
    37 O      0.000057  -0.000064  -0.000091
    38 Cr    -0.000013   0.000138   0.000086
    39 C     -0.000397  -0.000015   0.000090
    40 C     -0.000083  -0.000027  -0.000090
    41 H      0.000013  -0.000011   0.000012
    42 H     -0.000005   0.000015   0.000010
    43 H     -0.000013  -0.000013  -0.000017
    44 C     -0.000007  -0.000001   0.000014
    45 H     -0.000045   0.000001  -0.000010
    46 H      0.000016  -0.000006   0.000054
    47 H      0.000026   0.000000  -0.000030
    48 C      0.000092   0.000050  -0.000180
    49 C     -0.000048   0.000038   0.000066
```

```
    50 C     0.000034  0.000013 -0.000015
    51 C     0.000021 -0.000005 -0.000020
    52 C    -0.000049  0.000007 -0.000015
    53 C     0.000036 -0.000018 -0.000064
    54 C     0.000031 -0.000030  0.000010
    55 H     0.000001  0.000000  0.000005
    56 H    -0.000009 -0.000002  0.000005
    57 H     0.000002  0.000003 -0.000006
    58 H    -0.000022  0.000002  0.000008
    59 H    -0.000006  0.000005  0.000004
    60 H     0.000005  0.000058  0.000173
 ----------------------------------------
Hessian eigenvector     1 has overlap with TSRC:    0.30023E+00
Hessian eigenvector     2 has overlap with TSRC:    0.88799E-01
Hessian eigenvector     1 has the largest overlap with TSRC:  0.30023

------------------------------------------------------------
Geometry Convergence after Step 133       ** CONVERGED **
------------------------------------------------------------
current energy                          -14.48859559 Hartree
energy change                 0.00006581     0.00100000    T
constrained gradient max      0.00051980     0.00100000    T
constrained gradient rms      0.00010092     0.00066667    T
gradient max                  0.00051960
gradient rms                  0.00010092
cart. step max                0.00878826     0.01000000    T
cart. step rms                0.00268562     0.00666667    T
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	164.839054348504362	4485.4989	103438.08	432784.88
Delta V^Pauli Coulomb:	-83.867247695265888	-2282.1439	-52627.50	-220193.43
Delta V^Pauli LDA-XC:	-20.655490966040251	-562.0645	-12961.52	-54230.98
Delta V^Pauli GGA-Exchange:	1.010471058615153	27.4963	634.08	2652.99
Delta V^Pauli GGA-Correlation:	-0.227870587006967	-6.2007	-142.99	-598.27
Total Pauli Repulsion:	61.098916158806411	1662.5861	38340.15	160415.18
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	61.098916158806411	1662.5861	38340.15	160415.18
Electrostatic Interaction:	-13.037637110080187	-354.7722	-8181.24	-34230.31
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	48.061279048726220	1307.8139	30158.91	126184.87
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-62.494340781582906	-1700.5575	-39215.80	-164078.87
Total Orbital Interactions:	-62.499781444182524	-1700.7056	-39219.21	-164093.15
Alternative Decomposition Orb.Int.				
Kinetic:	-150.472272542561171	-4094.5589	-94422.79	-395064.90
Coulomb:	81.057232473925723	2205.6795	50864.19	212815.73
XC:	6.915258624452912	188.1738	4339.39	18156.01
Total Orbital Interactions:	-62.499781444182538	-1700.7056	-39219.21	-164093.15
Residu (E=Steric+OrbInt+Res):	0.000000090171530	0.0000	0.00	0.00
Dispersion Energy:	-0.050093282815237	-1.3631	-31.43	-131.52
Total Bonding Energy:	-14.488595588100010	-394.2547	-9091.73	-38039.80

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.037637110080187	-354.7722	-8181.24	-34230.31
Kinetic Energy:	14.366781805943191	390.9400	9015.29	37719.98
Coulomb (Steric+OrbInt) Energy:	-2.810015131168640	-76.4644	-1763.31	-7377.69
XC Energy:	-12.957631869979155	-352.5951	-8131.04	-34020.26
Dispersion Energy:	-0.050093282815237	-1.3631	-31.43	-131.52
Total Bonding Energy:	-14.488595588100027	-394.2547	-9091.73	-38039.80

List of All Frequencies:

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-530.383170	5414.268170	-719.792915
13.428726	0.000000	0.000000
14.918092	0.000000	0.000000
35.874371	150.985040	1.357676
47.262762	6.132987	0.072656
56.750430	240.506509	3.421165
59.975003	66.213597	0.995395
66.757743	27.283760	0.456545
69.537429	89.062069	1.552349
73.831284	187.930827	3.477895
80.215637	23.258787	0.467653

87.517928	4.979382	0.109232
88.602111	11.367429	0.252455
93.484019	18.554715	0.434780
104.728032	31.797443	0.834705
116.276376	78.269698	2.281199
124.149912	59.494097	1.851392
131.662803	82.457844	2.721279
142.984795	116.565307	4.177700
156.128276	62.622026	2.450681
176.123156	5.087066	0.224575
181.824696	50.816089	2.315966
197.302710	48.147562	2.381143
200.566788	44.618634	2.243124
229.754245	47.427110	2.731293
242.041258	4.737759	0.287436
248.037562	11.359591	0.706250
274.831350	27.533413	1.896725
284.523090	39.218155	2.796937
289.188068	87.472034	6.340561
290.113441	53.189091	3.867840
299.710598	32.737649	2.459391
313.082768	53.471192	4.196209
324.402911	191.219748	15.548753
333.046142	53.163493	4.438089
351.982660	15.324304	1.352011
382.399427	11.172766	1.070917
385.057523	66.848171	6.451983
406.217477	10.471641	1.066231
417.727473	4.708298	0.492987
436.621533	70.938923	7.763683
438.811900	21.198366	2.331626
452.360356	54.660302	6.197758
457.199466	28.384586	3.252867
470.116899	14.753584	1.738527
478.128424	13.466723	1.613929
480.653884	64.818664	7.809273
487.146219	7.166675	0.875095
494.680440	201.859709	25.029516
512.614853	129.488849	16.638019
528.435868	6.134511	0.812550
536.405981	223.949126	30.110714
545.154978	114.120876	15.594202
551.906221	138.688681	19.185997
567.850624	89.158925	12.690449
570.341290	47.690606	6.817823
571.762283	22.213012	3.183472
589.205369	15.143019	2.236440
614.406434	2.900483	0.446688
625.964028	51.926106	8.147291
629.693252	253.114864	39.950734
637.147250	502.968511	80.326469
645.223927	56.467484	9.132443
658.489033	189.058349	31.204877
665.751726	27.005562	4.506544
676.848871	148.284200	25.157336
687.456225	457.332007	78.805171
716.202750	36.626498	6.575207
732.624530	72.778471	13.364800
757.137390	156.512438	29.703089
757.838378	106.382747	20.208118
785.942516	77.344047	15.236869
792.214495	62.864762	12.483263
797.186059	12.863881	2.570454
805.858869	66.391118	13.410564
810.079847	47.159655	9.575832
814.892222	17.022225	3.476919
823.457163	62.041594	12.805662
826.979901	0.351375	0.072836
832.648780	149.595934	31.221927
844.756563	88.035790	18.640987
852.515622	5.868122	1.253948
890.138905	6.347487	1.416243
899.915402	15.081970	3.402027
908.660871	4.361068	0.993282
922.186118	0.014412	0.003331
936.523681	1.936751	0.454643
938.441802	71.133814	16.732526
962.267946	0.041167	0.009929
972.813337	0.115967	0.028278
978.984446	9.597555	2.355128
986.578325	0.448206	0.110838
989.763036	28.953283	7.183021
993.603787	71.608427	17.834274
1000.408656	19.717581	4.944349
1013.942721	51.991189	13.213603
1020.199941	24.712494	6.319460
1038.018859	50.381252	13.108478
1043.380497	1.359116	0.355449
1044.412066	57.689781	15.102500
1053.714162	23.157119	6.116253
1055.738005	21.393572	5.661318
1076.698307	21.443908	5.787301
1086.376288	1.836235	0.500019
1097.585191	10.005543	2.752688
1106.209410	137.394958	38.096600
1108.649501	5.269448	1.464325
1126.848034	4.207961	1.188544
1155.702448	44.065736	12.765127
1159.225782	33.420099	9.710774
1163.321530	5.112679	1.490824
1165.906671	125.075369	36.552211
1200.897175	149.147832	44.895296
1219.231147	19.659190	6.007997

1221.146003	94.966385	29.068028
1237.330849	0.517105	0.160377
1269.922365	2.808949	0.894127
1291.244825	0.264769	0.085695
1295.116610	12.950119	4.203980
1313.521042	80.353440	26.455720
1334.667986	24.441539	8.176734
1337.573297	161.101135	54.012498
1337.663918	68.199387	22.866808
1341.800602	2.265629	0.762000
1353.300377	16.805585	5.700670
1380.466401	15.911291	5.505659
1396.268485	17.851644	6.247773
1396.642516	3.231183	1.131162
1402.521735	98.552918	34.646324
1417.454302	13.022171	4.626691
1426.212122	29.139494	10.417037
1433.317615	22.706593	8.157789
1441.311048	6.314640	2.281310
1445.448272	5.859159	2.122833
1453.256174	127.233016	46.346833
1457.558286	96.825169	35.374659
1462.586512	21.975079	8.056197
1471.714756	0.030149	0.011122
1481.305002	122.680379	45.550974
1498.205565	230.090916	86.407005
1539.527449	1133.058299	437.237863
1550.565240	36.709670	14.267523
1561.112612	1.451300	0.567897
1588.504982	45.496565	18.115289
1599.735699	196.903746	78.955117
1883.478708	1357.952691	641.096529
1904.627316	1598.113551	762.949360
1951.114235	2903.896139	1420.174946
1984.930506	16.305571	8.112587
2305.470238	88.658586	51.234015
2939.844599	36.825454	27.136295
2946.402535	42.659294	31.505314
3014.149651	14.284828	10.792397
3026.976666	12.411071	9.416650
3077.249896	0.788162	0.607934
3084.108731	14.507576	11.215086
3110.488586	0.121626	0.094827
3116.605459	1.460400	1.140859
3119.877714	2.784495	2.177520
3121.821682	0.650869	0.509307
3125.036235	0.248472	0.194631
3130.615536	0.063486	0.049818
3136.581556	1.425686	1.120879
3138.231259	7.781253	6.120862
3141.629396	2.530186	1.992441
3156.780715	2.283361	1.806746
3157.505300	2.077324	1.644093
3162.173456	0.292151	0.231564
3169.577532	0.749781	0.595681
3170.179388	1.141383	0.906970
3177.166002	5.431050	4.325156
3183.515220	8.327645	6.645187
3194.706601	7.107365	5.691381

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

      14065.0718      24716.1599      27237.1474
-------------------------------------------------
         -0.0515         -0.9986          0.0146
         -0.0415         -0.0124         -0.9991
          0.9978         -0.0520         -0.0408


    Temp                                                  Transl     Rotat    Vibrat     Total
    ----                                                  ------     -----    ------     -----

    298.15   Entropy (cal/mole-K):                        45.488    37.491   116.813   199.792
             Internal Energy (Kcal/mole):                  0.889     0.889   294.303   296.080
             Constant Volume Heat Capacity (cal/mole-K):   2.981     2.981   121.564   127.525


*****************************************************************************************************


=====================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
=====================================================================
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Intermediate A, COSMO MeOH

```
============================
 G E O M E T R Y   U P D A T E  ***  16  ***
 ============================

 *** Using NEW gradient routines ***

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 C     0.000141  0.000044  0.000077
     2 H     0.000060  0.000007  0.000164
     3 C     0.000109 -0.000077  0.000216
     4 H     0.000167 -0.000022  0.000246
     5 C     0.000149 -0.000009  0.000127
     6 H     0.000081  0.000013  0.000182
     7 C    -0.000206 -0.000003  0.000131
     8 H     0.000029  0.000063 -0.000009
     9 C     0.000137 -0.000066  0.000019
    10 C    -0.000190  0.000183 -0.000114
    11 C    -0.000179  0.000060  0.000063
    12 C    -0.000238  0.000014 -0.000473
    13 H    -0.000016  0.000003  0.000004
    14 C     0.000278  0.000052  0.000329
    15 N    -0.000114 -0.000010 -0.000202
    16 C    -0.000300  0.000063 -0.000322
    17 H    -0.000047 -0.000027 -0.000004
    18 C     0.000008  0.000099 -0.000003
    19 H    -0.000097 -0.000054 -0.000116
    20 C    -0.000974 -0.000758  0.000500
    21 C     0.000043 -0.000618 -0.000694
    22 C    -0.000911 -0.000779  0.000820
    23 C    -0.000074  0.000101  0.000042
    24 C    -0.000059 -0.000044  0.000183
    25 C     0.000164  0.000038  0.000049
    26 C     0.000087 -0.000047 -0.000133
    27 C    -0.000093 -0.000094 -0.000094
    28 H    -0.000024 -0.000047 -0.000008
    29 H    -0.000007 -0.000003 -0.000044
    30 H    -0.000072 -0.000061 -0.000007
    31 H    -0.000035 -0.000052 -0.000002
    32 H     0.000061 -0.000022  0.000006
    33 N    -0.000292 -0.000219  0.000061
    34 Ir    0.000180  0.000165 -0.000285
    35 O     0.000550  0.000092 -0.000249
    36 O    -0.000085  0.000385  0.000305
    37 O     0.000427  0.000766 -0.000399
    38 Cr   -0.000222  0.000611 -0.000538
    39 C    -0.000234  0.000467 -0.000485
    40 C     0.000085  0.000029  0.000055
    41 H     0.000061  0.000077  0.000162
    42 H     0.000175  0.000011  0.000029
    43 H     0.000138  0.000051  0.000192
    44 C     0.000046  0.000083  0.000076
    45 H     0.000041  0.000098  0.000090
    46 H     0.000088  0.000044  0.000117
    47 H     0.000076 -0.000067  0.000087
    48 C     0.000041 -0.000836  0.000181
    49 C     0.000134  0.000347 -0.000042
    50 C    -0.000075 -0.000032 -0.000043
    51 C    -0.000049  0.000008 -0.000045
    52 C     0.000104  0.000030 -0.000063
    53 C     0.000247  0.000026  0.000004
    54 C     0.000209 -0.000040 -0.000009
    55 H    -0.000202 -0.000087 -0.000080
    56 H    -0.000151 -0.000052 -0.000083
    57 H     0.000108  0.000046 -0.000018
    58 H     0.000353  0.000095  0.000043
    59 H     0.000315  0.000075  0.000046
    60 H     0.000055 -0.000120 -0.000045
 ----------------------------------------


 ==========================
 Geometry Convergence Tests
 ==========================

 Energy  old :        -14.60166566
         new :        -14.60167029

 Convergence tests:
 (Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

       Item               Value         Criterion    Conv.        Ratio
 ------------------------------------------------------------------------
 change in energy      -0.00000463     0.00100000    YES        0.09338821
 gradient max           0.00093941     0.00100000    YES        0.80728787
 gradient rms           0.00024387     0.00066667    YES        0.88992119
 cart. step max         0.01000000     0.01000000    YES        1.00000000
 cart. step rms         0.00297982     0.00666667    YES        0.97602032

 prediction dE :       -0.00004300
```

```
*****************************************************************************************************
                          Geometry CONVERGED
*****************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	164.778403706667262	4483.8485	103400.02	432625.64
Delta V^Pauli Coulomb:	-83.813620536014184	-2280.6847	-52593.85	-220052.63
Delta V^Pauli LDA-XC:	-20.695438918811991	-563.1515	-12986.59	-54335.87
Delta V^Pauli GGA-Exchange:	1.018425949542483	27.7128	639.07	2673.88
Delta V^Pauli GGA-Correlation:	-0.231272785055486	-6.2933	-145.13	-607.21
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	61.056497416328085	1661.4318	38313.53	160303.81
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	61.056497416328085	1661.4318	38313.53	160303.81
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-13.012881280641613	-354.0985	-8165.71	-34165.31
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	48.043616135686470	1307.3333	30147.83	126138.50
Orbital Interactions				
A:	-62.492159084485337	-1700.4982	-39214.43	-164073.14
Total Orbital Interactions:	-62.497040210457477	-1700.6310	-39217.49	-164085.96
Alternative Decomposition Orb.Int.				
Kinetic:	-150.338293452491712	-4090.9131	-94338.71	-394713.13
Coulomb:	80.917115172396180	2201.8667	50776.26	212447.86
XC:	6.924138069638043	188.4154	4344.96	18179.32
Total Orbital Interactions:	-62.497040210457492	-1700.6310	-39217.49	-164085.96
Residu (E=Steric+OrbInt+Res):	0.000001134054604	0.0000	0.00	0.00
Solvation Energy (el):	-0.092942275360742	-2.5291	-58.32	-244.02
Dispersion Energy:	-0.055375773464441	-1.5069	-34.75	-145.39
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.000000000000000	0.0000	0.00	0.00
Total Bonding Energy:	**-14.601740989541584**	**-397.3336**	**-9162.73**	**-38336.87**

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-13.012881280641613	-354.0985	-8165.71	-34165.31
Kinetic Energy:	14.440110254175551	392.9354	9061.31	37912.50
Coulomb (Steric+OrbInt) Energy:	-2.896504229563405	-78.8179	-1817.58	-7604.77
XC Energy:	-12.984147684686954	-353.3166	-8147.68	-34089.87
Solvation:	-0.092942275360742	-2.5291	-58.32	-244.02
Dispersion Energy:	-0.055375773464441	-1.5069	-34.75	-145.39
Total Bonding Energy:	-14.601740989541605	-397.3336	-9162.73	-38336.87

List of All Frequencies:

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
6.953185	0.000000	0.000000
29.446742	242.932243	1.793083
44.918129	578.795482	6.516657
52.692943	846.010961	11.173945
59.111299	347.205647	5.144407
60.366944	458.192339	6.933062
69.459731	401.242035	6.985823
77.386886	159.984547	3.103298
81.495475	193.816876	3.959161
85.914660	97.748695	2.105020
90.989594	11.505942	0.262417
110.383190	281.079516	7.776966
112.829629	114.915620	3.249977
121.468777	315.376824	9.602239
122.873139	677.941714	20.879850
128.530033	19.752235	0.636354
140.246739	194.738027	6.845759
148.717374	195.150231	7.274595

156.195204	442.367651	17.319252
165.229879	186.398438	7.719851
170.528285	205.946230	8.802952
195.800736	387.273189	19.006836
229.146778	266.387950	15.300527
235.022547	102.565950	6.042140
242.760948	350.527721	21.329431
279.274503	104.177007	7.292581
285.865747	84.473873	6.052887
299.197219	337.252966	25.292479
305.435213	415.537506	31.813203
309.377848	1092.740664	84.739206
329.923101	190.926761	15.789108
342.075575	61.552126	5.277682
360.881372	221.108301	20.000810
379.459928	125.620119	11.948219
395.370573	32.164594	3.187576
424.569779	34.933713	3.717679
431.837664	255.982522	27.708238
436.233207	28.335212	3.098298
449.113692	265.043951	29.836801
454.682163	204.403570	23.295630
469.449263	87.079320	10.246647
471.874821	593.541411	70.203037
483.937695	198.595322	24.089985
495.352051	18.984380	2.357157
507.027603	34.128865	4.337420
507.680980	187.961924	23.918770
509.818995	447.144227	57.140194
515.207008	218.853629	28.262696
527.762568	29.790163	3.940847
544.404948	359.479142	49.053933
546.559938	417.573549	57.206957
563.870641	111.387549	15.743243
566.617657	110.251341	15.658568
567.455604	63.526832	9.035811
588.142511	35.345204	5.210641
611.265243	11.763782	1.802415
633.472494	689.726828	109.517356
639.891529	156.862714	25.159625
642.533286	1073.212166	172.845982
656.830975	326.026818	53.676603
665.699397	172.360057	28.760264
666.657570	128.783721	21.519980
680.317582	544.462784	92.844881
687.894591	1077.242767	185.743469
712.388828	59.936994	10.702621
729.625102	281.103169	51.409524
740.550670	278.754762	51.743422
748.898267	91.224524	17.124287
754.183682	414.777228	78.409757
788.979253	45.809308	9.059357
799.796843	149.525782	29.976011
806.130185	48.472846	9.794489
808.566115	13.246767	2.684748
822.146697	91.891289	18.936588
826.070369	78.592195	16.273259
827.340183	753.618906	156.283804
830.736780	63.391127	13.199880
843.850162	87.649904	18.539365
854.175918	25.796773	5.523200
858.833919	71.967093	15.492490
905.607198	10.771421	2.445068
909.930909	16.749375	3.820191
914.683965	75.935398	17.409785
920.977667	52.220499	12.055027
932.895660	138.706279	32.434504
938.079399	6.414532	1.508282
956.514951	6.981684	1.673902
973.001270	0.628831	0.153365
975.285586	0.997390	0.243823
976.707357	59.828168	14.646985
980.982183	50.910133	12.518244
983.010380	18.968982	4.673909
990.617018	216.592750	53.780864
1011.744057	69.174952	17.542747
1014.481910	40.064237	10.187773
1021.441050	8.124885	2.080217
1033.516462	45.486633	11.783634
1037.994781	25.447632	6.620955
1039.560460	198.667745	51.767261
1053.258801	41.304578	10.904641
1067.245749	74.324257	19.882596
1075.771928	3.367969	0.908168
1094.952407	4.203528	1.153685
1098.118760	264.274860	72.741664
1099.763582	16.669298	4.595097
1116.908653	7.146169	2.000640
1135.367418	1.054035	0.299964
1136.076212	49.695149	14.151404
1151.398141	76.890018	22.190831
1153.385256	99.321698	28.714192
1168.638402	58.604479	17.166788
1211.341737	178.786896	54.285074
1220.548590	182.936011	55.967041
1225.548201	5.437716	1.670417
1271.044805	4.126967	1.314831
1284.279914	0.722516	0.232587
1293.131646	30.859695	10.002589
1306.828212	162.527261	53.238129
1325.146774	5.085689	1.689242
1328.055249	22.600009	7.523204
1335.074901	20.686073	6.922481

1340.664975	356.634023	119.845328
1351.614239	22.401107	7.589275
1381.957929	31.335049	10.854336
1390.019467	17.150758	5.975610
1392.064385	113.912986	39.747574
1394.994422	102.121312	35.708115
1400.047998	331.953370	116.492530
1415.533837	105.467168	37.421019
1419.655273	45.278264	16.112048
1425.425345	31.591644	11.287422
1429.400642	148.071354	53.052163
1438.335430	8.700960	3.136934
1440.452353	29.020554	10.478103
1452.740546	343.601200	125.118290
1460.309770	31.009990	11.350753
1464.301074	372.152094	136.593149
1498.556848	373.778094	140.399363
1534.845249	2389.026797	919.101946
1545.740660	154.618016	59.906617
1552.758789	9.147731	3.560373
1578.885071	12.695419	5.024301
1594.583332	302.609492	120.950547
1800.134435	4572.784053	2063.306292
1809.399522	4615.701366	2093.390475
1894.013335	6350.208805	3014.734760
1909.153508	50.951077	24.382166
2939.499662	56.732422	41.800628
2944.712776	60.749937	44.840128
3024.917317	19.033359	14.431352
3030.776861	17.175765	13.048125
3085.584893	1.034863	0.800384
3090.752927	10.358699	8.025047
3106.611317	1.016505	0.791543
3112.435489	1.757700	1.371270
3119.370859	1.021921	0.799029
3125.680635	0.938437	0.735238
3125.926707	2.754203	2.158007
3132.595632	9.685730	7.605273
3137.203869	3.224629	2.535715
3140.375516	5.493444	4.324186
3145.016890	4.963425	3.912753
3158.827100	6.753695	5.347434
3165.393812	0.912379	0.723904
3165.705066	6.499808	5.157617
3166.604225	1.379094	1.094626
3168.921144	9.192282	7.301512
3176.916136	29.710628	23.658960
3183.580042	40.458428	32.285153
3191.373911	2.214822	1.771718
3227.266262	102.524887	82.935825

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                 1.000000 atm.
Temperature:            298.150000 K
```

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.488	37.114	116.292	198.894
	Internal Energy (Kcal/mole):	0.889	0.889	295.181	296.958
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	120.599	126.561

Intermediate B, COSMO MeOH

```
============================
G E O M E T R Y   U P D A T E  ***  18  ***
============================

*** Using NEW gradient routines ***

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
------------------------------------------
    1 C    -0.000103 -0.000120 -0.000056
    2 H    -0.000022  0.000024  0.000018
    3 C     0.000065  0.000082 -0.000003
    4 H     0.000020  0.000021  0.000012
    5 C    -0.000062 -0.000006  0.000031
    6 H     0.000054  0.000009  0.000020
    7 C     0.000081 -0.000051 -0.000076
    8 H    -0.000012 -0.000014 -0.000066
    9 C    -0.000271 -0.000040  0.000021
   10 C     0.000159 -0.000024  0.000046
   11 C    -0.000250 -0.000102 -0.000511
   12 C    -0.000227 -0.000194  0.000027
   13 H    -0.000080 -0.000068 -0.000098
   14 C     0.000137  0.000038  0.000112
   15 N    -0.000075  0.000050 -0.000091
   16 C    -0.000248  0.000053 -0.000117
   17 H    -0.000038 -0.000058 -0.000102
   18 C    -0.000105 -0.000102 -0.000050
   19 H    -0.000086 -0.000088 -0.000124
   20 C     0.000154 -0.000074 -0.000589
   21 C     0.000107  0.000232  0.000382
   22 C     0.000441  0.000943 -0.000587
   23 C    -0.000023  0.000067  0.000112
   24 C    -0.000103 -0.000024  0.000003
   25 C     0.000099 -0.000064 -0.000063
   26 C     0.000088  0.000108  0.000023
   27 C     0.000001  0.000165  0.000008
   28 H    -0.000016  0.000010  0.000189
   29 H    -0.000045 -0.000015  0.000048
   30 H    -0.000035  0.000092 -0.000075
   31 H     0.000101  0.000080 -0.000030
   32 H     0.000093  0.000052  0.000144
   33 N    -0.000075  0.000067 -0.000133
   34 Ir    0.000610 -0.000268  0.000669
   35 O    -0.000200  0.000194  0.000196
   36 O    -0.000069  0.000020  0.000038
   37 O     0.000042 -0.000512  0.000233
   38 Cr   -0.000861 -0.000648 -0.000869
   39 C     0.000006 -0.000170 -0.000420
   40 C     0.000088 -0.000007  0.000050
   41 H     0.000085 -0.000033  0.000134
   42 H    -0.000037  0.000032  0.000106
   43 H     0.000110 -0.000011  0.000134
   44 C     0.000091 -0.000058  0.000179
   45 H     0.000172 -0.000096  0.000113
   46 H     0.000213 -0.000002  0.000190
   47 H     0.000053  0.000126  0.000194
   48 C    -0.000270  0.000059  0.000186
   49 C     0.000027 -0.000026  0.000141
   50 C     0.000181  0.000347 -0.000024
   51 C     0.000128  0.000403  0.000131
   52 C     0.000077  0.000023 -0.000091
   53 C    -0.000142 -0.000266  0.000062
   54 C    -0.000150 -0.000327 -0.000019
   55 H     0.000320  0.000487  0.000152
   56 H     0.000345  0.000566  0.000096
   57 H     0.000034  0.000077  0.000033
   58 H    -0.000273 -0.000448 -0.000032
   59 H    -0.000295 -0.000465 -0.000013
   60 H    -0.000006 -0.000045  0.000002
------------------------------------------


=========================
Geometry Convergence Tests
=========================

Energy  old :        -14.60935425
        new :        -14.60939940

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00004515     0.00100000    YES        2.18187962
gradient max           0.00094744     0.00100000    YES        0.80890892
gradient rms           0.00022248     0.00066667    YES        0.95267321
cart. step max         0.01000000     0.01000000    YES        1.00000000
cart. step rms         0.00200235     0.00666667    YES        0.96168095
```

prediction dE : -0.00004290

****
Geometry CONVERGED
****

****
* Final Geometry *
****

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	164.691640254039612	4481.4876	103345.58	432397.84
Delta V^Pauli Coulomb:	-84.029403803503570	-2286.5564	-52729.25	-220619.17
Delta V^Pauli LDA-XC:	-20.624674096822915	-561.2259	-12942.18	-54150.07
Delta V^Pauli GGA-Exchange:	1.013227435906117	27.5713	635.81	2660.23
Delta V^Pauli GGA-Correlation:	-0.230000745194763	-6.2586	-144.33	-603.87
Total Pauli Repulsion:	60.820789044424480	1655.0179	38165.63	159684.96
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	60.820789044424480	1655.0179	38165.63	159684.96
Electrostatic Interaction:	-12.995717149994924	-353.6315	-8154.94	-34120.25
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	47.825071894429556	1301.3864	30010.69	125564.71
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-62.280525374077456	-1694.7393	-39081.62	-163517.50
Total Orbital Interactions:	-62.283973651935412	-1694.8332	-39083.79	-163526.55
Alternative Decomposition Orb.Int.				
Kinetic:	-150.275698642862551	-4089.2098	-94299.43	-394548.79
Coulomb:	81.089890563737384	2206.5682	50884.68	212901.48
XC:	6.901834427189731	187.8085	4330.97	18120.76
Total Orbital Interactions:	-62.283973651935433	-1694.8332	-39083.79	-163526.55
Residu (E=Steric+OrbInt+Res):	0.000001431449790	0.0000	0.00	0.00
Solvation Energy (el):	-0.097656265566700	-2.6574	-61.28	-256.40
Dispersion Energy:	-0.052894522708185	-1.4393	-33.19	-138.87
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.000000000000000	0.0000	0.00	0.00
Total Bonding Energy:	-14.609451114330950	-397.5434	-9167.57	-38357.11

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-12.995717149994924	-353.6315	-8154.94	-34120.25
Kinetic Energy:	14.415941611177061	392.2777	9046.14	37849.05
Coulomb (Steric+OrbInt) Energy:	-2.939511808316396	-79.9882	-1844.57	-7717.69
XC Energy:	-12.939612978921829	-352.1048	-8119.73	-33972.95
Solvation:	-0.097656265566700	-2.6574	-61.28	-256.40
Dispersion Energy:	-0.052894522708185	-1.4393	-33.19	-138.87
Total Bonding Energy:	-14.609451114330973	-397.5434	-9167.57	-38357.11

List of All Frequencies:

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
13.827713	0.000000	0.000000
30.813845	293.995212	2.270723
43.233744	204.700655	2.218299
48.495506	1246.859294	15.156433
54.447549	141.418827	1.930028
57.675478	67.791595	0.980043
68.030526	658.900460	11.235741
77.146407	172.790111	3.341278
81.664303	120.201281	2.460478
88.327704	42.882667	0.949417
92.731292	191.298815	4.446483
100.600144	135.700512	3.421828
107.899944	103.873791	2.809346
113.712746	408.945764	11.656091
117.235639	162.032785	4.761465
133.449605	158.574054	5.304293

145.509969	219.337444	7.999882
156.125016	77.821853	3.045455
188.468437	96.023768	4.536234
198.844025	177.790075	8.861314
218.621874	133.407082	7.310559
230.013399	97.689743	5.632227
235.061838	149.502758	8.808651
272.945450	60.008066	4.105476
282.391192	29.370930	2.078964
283.701576	113.711332	8.086183
288.148694	328.632658	23.735886
301.408815	88.853284	6.712859
308.776489	862.913772	66.786655
325.939845	129.843272	10.608036
352.694844	142.227997	12.573676
374.263505	62.157700	5.831100
387.422796	104.632402	10.160836
399.001165	8.790800	0.879186
413.237411	124.614077	12.907579
424.592302	12.205852	1.299027
434.144485	5.425794	0.590440
440.654673	51.105950	5.644792
452.333193	31.933273	3.620595
461.439901	343.026636	39.675377
470.208770	4.874889	0.574558
482.588764	224.707385	27.181450
494.914703	29.943649	3.714609
504.369355	252.836222	31.964363
509.659469	274.928502	35.121894
526.376319	26.410374	3.484568
543.783180	303.136588	41.318277
546.595671	382.788636	52.444904
561.683597	209.543856	29.501544
565.266373	53.707143	7.609625
567.986816	105.747222	15.055157
577.256297	177.362808	25.663111
585.006683	16.430892	2.409351
609.860316	6.288887	0.961352
633.476630	665.554613	105.679893
640.645275	756.051209	121.407890
640.895917	366.119904	58.815110
650.728242	13.505513	2.202870
658.364490	405.284979	66.881342
663.321438	75.114674	12.488978
681.896096	556.167702	95.060926
683.576177	446.364169	76.481133
687.739505	1144.249810	197.252670
713.417352	51.664034	9.238683
728.987288	265.823435	48.572593
748.004535	487.741226	91.447485
752.019871	285.192603	53.758314
789.630030	50.203445	9.936541
800.300305	184.959394	37.102865
801.573370	74.984516	15.065826
809.306709	51.229224	10.392236
814.453900	33.666854	6.873012
818.398159	4.206923	0.862993
824.717565	1021.323548	211.128402
829.569056	27.815059	5.783764
842.491500	52.058547	10.993491
852.775567	6.408118	1.369756
856.686214	162.984941	34.998331
891.131468	60.948589	13.613930
908.333785	18.700749	4.257773
911.880487	7.971162	1.821955
916.630214	26.152325	6.008728
935.891831	105.595862	24.771404
937.636204	8.800180	2.068254
947.401860	2.535513	0.602113
966.941152	1.574392	0.381585
973.187468	70.440217	17.182853
974.384672	0.607540	0.148383
983.448741	16.226270	3.999894
984.958330	30.254277	7.469348
988.819515	225.227762	55.823495
1013.332562	73.231965	18.600763
1016.002954	52.028672	13.249997
1020.272429	3.060861	0.782777
1037.333836	37.078059	9.640812
1038.220817	31.831530	8.283718
1040.674670	146.927226	38.326162
1053.806438	46.153105	12.191014
1059.839381	87.249178	23.178187
1077.145753	1.909156	0.515459
1095.454333	2.438766	0.669642
1096.573526	196.421388	53.988915
1100.203630	37.511814	10.344731
1110.130196	79.461721	22.111080
1117.275678	10.518027	2.945593
1132.826868	0.528665	0.150114
1136.067254	43.943780	12.513521
1155.074674	94.156643	27.260831
1155.534370	8.751725	2.534864
1200.852715	23.109184	6.955885
1216.197777	158.422879	48.294778
1221.480148	209.491688	64.140343
1226.621993	0.898986	0.276402
1271.159175	8.580794	2.734044
1294.357406	52.823525	17.137981
1296.026704	19.669188	6.389670
1308.551093	162.243913	53.215380
1326.608414	2.703453	0.898958
1327.103805	4.367636	1.452879

1333.673088	24.754400	8.275226
1345.822453	320.432289	108.094131
1352.692874	17.570952	5.957617
1387.319276	25.397712	8.831797
1388.088380	93.331476	32.473068
1396.216042	74.702984	26.143796
1401.955097	265.450251	93.281455
1411.156401	57.343426	20.283218
1418.880058	57.651248	20.503711
1423.970601	33.683223	12.022443
1425.076923	71.307695	25.471398
1429.360135	149.204904	53.456785
1440.895953	10.482581	3.785985
1441.612223	18.120725	6.547901
1454.230834	427.623908	155.873898
1467.806609	387.712127	142.644915
1468.204096	56.147970	20.663247
1501.789431	440.970938	165.995793
1542.032101	1771.847004	684.853537
1548.994699	588.895060	228.647214
1559.953224	18.810189	7.355002
1578.941235	253.076233	100.160250
1594.591847	356.045252	142.309145
1690.937400	1823.833120	773.019943
1800.925918	4379.947528	1977.164601
1811.557143	4634.333278	2104.347076
1895.514037	6263.002515	2975.689833
2942.183635	57.155040	42.150466
2947.846432	62.594729	46.250954
3019.132587	18.948750	14.339725
3027.089246	15.704634	11.916017
3038.659496	106.613353	81.202932
3086.951529	1.223360	0.946590
3092.901932	10.883204	8.437251
3094.865329	3.383464	2.624710
3096.777651	0.507717	0.394103
3105.388518	1.886254	1.468230
3111.381371	10.980906	8.563859
3122.669408	13.570490	10.621836
3126.687422	1.699201	1.331702
3138.718204	2.738768	2.154694
3141.989403	7.179297	5.654116
3146.715919	7.264871	5.730117
3162.327926	13.486230	10.689947
3166.200454	5.825209	4.623044
3168.741817	1.857386	1.475255
3169.412953	11.463088	9.106647
3169.739263	1.299045	1.032110
3179.279013	35.088293	27.962047
3181.857688	48.787868	38.910845
3190.659438	1.147169	0.917458

==========
Statistical Thermal Analysis *** ideal gas assumed ***
==========

Pressure: 1.000000 atm.
Temperature: 298.150000 K

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.488	37.174	112.874	195.537
	Internal Energy (Kcal/mole):	0.889	0.889	294.745	296.522
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	117.738	123.700

TSAB, COSMO MeOH

```
Geometry CYCLE 208
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 C    -0.000025  0.000001 -0.000018
     2 H     0.000006  0.000021  0.000011
     3 C     0.000099  0.000018  0.000167
     4 H    -0.000022 -0.000005 -0.000040
     5 C    -0.000018 -0.000006 -0.000065
     6 H    -0.000009 -0.000002 -0.000013
     7 C     0.000015 -0.000013  0.000053
     8 H     0.000017  0.000041  0.000027
     9 C    -0.000039 -0.000046 -0.000111
    10 C     0.000079 -0.000052  0.000149
    11 C    -0.000151  0.000025 -0.000130
    12 C     0.000123  0.000021  0.000026
    13 H     0.000034 -0.000001 -0.000012
    14 C    -0.000020 -0.000076 -0.000162
    15 N    -0.000005  0.000033  0.000039
    16 C    -0.000047  0.000146  0.000003
    17 H     0.000003 -0.000144  0.000116
    18 C    -0.000018  0.000002 -0.000056
    19 H    -0.000028 -0.000015 -0.000032
    20 C     0.000178  0.000075 -0.000196
    21 C    -0.000048  0.000135  0.000010
    22 C    -0.000168  0.000063  0.000294
    23 C    -0.000083 -0.000040 -0.000077
    24 C    -0.000044  0.000011  0.000277
    25 C     0.000071 -0.000047  0.000011
    26 C     0.000017  0.000003  0.000032
    27 C    -0.000001  0.000118 -0.000017
    28 H    -0.000072  0.000024  0.000001
    29 H    -0.000028 -0.000026  0.000074
    30 H     0.000019 -0.000003 -0.000002
    31 H     0.000095 -0.000107 -0.000126
    32 H    -0.000021 -0.000046 -0.000051
    33 N    -0.000101 -0.000033  0.000360
    34 Ir    0.000025  0.000061 -0.000512
    35 O     0.000031 -0.000084  0.000056
    36 O    -0.000005 -0.000007  0.000008
    37 O     0.000109 -0.000141 -0.000234
    38 Cr   -0.000259 -0.000031  0.000118
    39 C     0.000523  0.000025 -0.000003
    40 C     0.000078  0.000058  0.000034
    41 H     0.000031  0.000061  0.000024
    42 H    -0.000019  0.000081  0.000015
    43 H    -0.000064 -0.000074 -0.000118
    44 C     0.000039  0.000042  0.000089
    45 H    -0.000015 -0.000012 -0.000005
    46 H     0.000001 -0.000009 -0.000011
    47 H     0.000005 -0.000005  0.000001
    48 C    -0.000327  0.000281  0.000401
    49 C     0.000078 -0.000114 -0.000077
    50 C     0.000070 -0.000019 -0.000027
    51 C    -0.000011  0.000020  0.000011
    52 C     0.000002 -0.000011 -0.000010
    53 C    -0.000025  0.000041  0.000017
    54 C    -0.000070  0.000033  0.000021
    55 H     0.000014  0.000014  0.000003
    56 H    -0.000018 -0.000002  0.000005
    57 H     0.000003 -0.000006 -0.000006
    58 H     0.000016 -0.000010 -0.000014
    59 H     0.000037 -0.000009 -0.000017
    60 H    -0.000056 -0.000260 -0.000314
 ----------------------------------------
Hessian eigenvector     1 has overlap with TSRC:    0.24064E+00
Hessian eigenvector     2 has overlap with TSRC:    0.24926E+00
Hessian eigenvector     3 has overlap with TSRC:    0.31812E-01
Hessian eigenvector     2 has the largest overlap with TSRC:  0.24926

------------------------------------------------------------
Geometry Convergence after Step 208       ** CONVERGED **
------------------------------------------------------------
current energy                          -14.57101334 Hartree
energy change                0.00000546     0.00100000    T
constrained gradient max     0.00052341     0.00100000    T
constrained gradient rms     0.00010856     0.00066667    T
gradient max                 0.00052341
gradient rms                 0.00010856
cart. step max               0.00751946     0.01000000    T
cart. step rms               0.00197681     0.00666667    T

                                    hartree          eV        kcal/mol         kJ/mol
                                ---------------  ----------  ----------  ----------

Pauli Repulsion
  Kinetic (Delta T^0):          164.642637666723942    4480.1541     103314.83      432269.18
  Delta V^Pauli Coulomb:        -83.838891402422419   -2281.3723     -52609.70     -220118.98
  Delta V^Pauli LDA-XC:         -20.626514435432767    -561.2760     -12943.33      -54154.91
  Delta V^Pauli GGA-Exchange:     1.008763982393063      27.4499        633.01        2648.51
  Delta V^Pauli GGA-Correlation:   -0.227357669851479      -6.1867       -142.67        -596.93
                                ---------------  ----------  ----------  ----------
  Total Pauli Repulsion:        60.958638141410340    1658.7689      38252.13      160046.88
```

```
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  60.958638141410340       1658.7689         38252.13        160046.88
  Electrostatic Interaction:       -13.010944822643278       -354.0458         -8164.49        -34160.23
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------       ----------      -----------
  Total Steric Interaction:         47.947693318767065       1304.7231         30087.63        125886.65
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -62.369536353549776      -1697.1614        -39137.48       -163751.19
                                   --------------------     -----------       ----------      -----------
  Total Orbital Interactions:      -62.374993457704001      -1697.3099        -39140.90       -163765.52

Alternative Decomposition Orb.Int.
  Kinetic:                        -150.272347200367591      -4089.1186        -94297.33       -394539.99
  Coulomb:                          81.007838681820715       2204.3354         50833.19        212686.05
  XC:                                6.889515060842918        187.4732          4323.24         18088.42
                                   --------------------     -----------       ----------      -----------
  Total Orbital Interactions:      -62.374993457703958      -1697.3099        -39140.90       -163765.52

  Residu (E=Steric+OrbInt+Res):      0.000000205437424          0.0000             0.00            0.00


  Solvation Energy (el):            -0.094038799996357         -2.5589           -59.01          -246.90
  Dispersion Energy:                -0.049674614288689         -1.3517           -31.17          -130.42

Post-SCF Solvation Energies
  Solvation Energy (cd):             0.000000000000000          0.0000             0.00            0.00

Total Bonding Energy:              -14.571013347784557        -396.4974         -9143.45        -38256.19


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================================

  Electrostatic Energy:            -13.010944822643278        -354.0458         -8164.49        -34160.23
  Kinetic Energy:                   14.370290466356352         391.0355          9017.49         37729.19
  Coulomb (Steric+OrbInt) Energy:   -2.831052515164274         -77.0369         -1776.51         -7432.93
  XC Energy:                       -12.955593062048266        -352.5396         -8129.76        -34014.90
  Solvation:                        -0.094038799996357         -2.5589           -59.01          -246.90
  Dispersion Energy:                -0.049674614288689         -1.3517           -31.17          -130.42
                                   --------------------     -----------       ----------      -----------
  Total Bonding Energy:            -14.571013347784511        -396.4974         -9143.45        -38256.19

List of All Frequencies:


 Intensities
 ===========

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2               km/mole
             ----------       ----------             ----------
           -543.255775         8314.205056        -1132.147869
             11.560815            0.000000            0.000000
             32.564842          295.239261            2.409912
             50.144944         1234.882780           15.521402
             54.474049          185.566983            2.533777
             56.655613          370.447133            5.260745
             66.683844          345.168070            5.769382
             71.862234          192.068890            3.459679
             80.601009          130.579244            2.638109
             82.369431           98.561236            2.034934
             87.800519           87.663148            1.929266
             92.329955           72.672307            1.681859
            100.896129          168.059479            4.250261
            114.237414          237.610359            6.803804
            116.536393          183.832703            5.369853
            120.865429          213.766961            6.476207
            133.341219           43.956407            1.469145
            143.832933          380.659531           13.723760
            151.095294           69.618065            2.636641
            189.339506          496.753293           23.575454
            190.837294          460.623339           22.033691
            194.913253          439.108778           21.453174
            225.981308          113.363137            6.421292
            233.438441           39.980174            2.339350
            237.173914           46.206547            2.746936
            273.734344          126.279428            8.664429
            277.526485           37.391688            2.601103
            285.091072           79.066879            5.650102
            294.686145          119.131296            8.799615
            308.770409          260.292639           20.145388
            316.877473          453.678711           36.034445
            328.461197          132.230112           10.886606
            355.833155           71.161310            6.346999
            374.776637           56.833611            5.338950
            385.020499          140.693576           13.578012
            394.761651           10.917527            1.080282
            425.787849            6.089925            0.649955
            433.502347          149.975734           16.296357
            438.540677           65.992171            7.254047
            447.598565           98.609509           11.063322
            454.029612           79.675111            9.067445
            469.870618           16.870428            1.986930
            482.965270          174.235512           21.092626
            484.602456          120.038345           14.580878
            495.933577           40.517175            5.036638
```

509.616965	150.908113	19.276782
515.031667	339.500506	43.828078
526.360175	20.030717	2.642759
545.581358	405.058949	55.393120
546.378187	295.590957	40.482056
547.519117	273.908821	37.590956
566.946619	175.904367	24.997516
568.808290	91.120764	12.991561
573.358530	84.805816	12.187931
589.868894	20.235568	2.991913
606.715158	155.692191	23.677167
609.001857	7.234674	1.104373
634.320920	667.282134	106.095412
640.839982	242.948235	39.024866
643.172487	936.804373	151.026945
657.659197	355.623746	58.623227
668.366644	137.935522	23.108351
668.907551	468.651856	78.576831
688.836860	1150.259724	198.605084
712.841627	44.230819	7.903075
730.167878	348.933076	63.862061
750.905525	272.770173	51.340518
755.491483	362.204093	68.590031
785.688451	117.542666	23.148560
790.772423	39.075143	7.745156
799.086369	164.396598	32.927944
804.524970	127.171844	25.645346
810.290258	18.741851	3.806547
819.406845	1.974973	0.405638
821.539713	576.014696	118.615159
827.471491	53.974589	11.194906
833.303274	364.678244	76.171238
839.305449	82.559743	17.368665
853.819189	10.517022	2.250799
907.073134	5.473161	1.244396
908.281128	15.583588	3.547855
909.210649	48.657847	11.089079
916.375693	9.063977	2.081951
933.593218	123.448110	28.888181
937.691451	7.259042	1.706150
957.592689	0.010011	0.002403
962.857254	61.556067	14.856306
971.908248	0.221286	0.053908
980.494794	0.281969	0.069299
982.993831	43.325990	10.675233
984.968332	54.537339	13.464626
991.461905	230.096362	57.182594
1011.477341	81.877965	20.758753
1012.111690	31.888819	8.089933
1020.632555	0.551666	0.141132
1029.235294	36.677542	9.462218
1036.564744	73.436540	19.080366
1040.675531	141.349535	36.871245
1052.735299	45.485292	12.002404
1067.042404	72.666718	19.435481
1075.535232	4.421858	1.192086
1090.834774	12.551065	3.431766
1098.347376	30.245843	8.326903
1098.667827	281.928945	77.639753
1116.792618	6.644726	1.860063
1135.456428	38.168684	10.863149
1137.078450	1.310133	0.373408
1150.215678	87.398267	25.197658
1153.325955	132.323659	38.253188
1195.318139	348.408352	104.387894
1211.916419	165.845836	50.379669
1219.006605	204.691158	62.543648
1223.566551	2.156349	0.661340
1270.426645	6.241813	1.987643
1285.416732	1.017590	0.327865
1291.000489	17.800355	5.760141
1305.722122	154.963650	50.717597
1325.806189	8.062986	2.679502
1330.694718	36.535017	12.186130
1332.377337	9.852318	3.290362
1339.671712	385.955950	129.602744
1350.298950	24.077635	8.149328
1379.314909	38.456096	13.295562
1384.469299	72.539707	25.173129
1389.808239	27.667356	9.638304
1398.295364	366.492559	128.452378
1407.835060	61.893140	21.840992
1415.577896	108.554106	38.517500
1420.986251	79.733856	28.399501
1425.956128	21.234744	7.589816
1428.717025	151.230203	54.158026
1437.653820	12.072999	4.350584
1438.872667	42.311667	15.260212
1452.388878	334.396638	121.737082
1461.342410	1.065373	0.390240
1463.224370	390.851889	143.351160
1498.429919	391.990510	147.227880
1534.697412	2380.565627	915.758565
1547.452346	97.815319	37.940428
1552.780883	2.591329	1.008581
1578.961789	91.722745	36.301681
1594.472456	300.023971	119.908797
1794.700616	4741.136758	2132.811948
1804.512941	4589.072058	2075.692175
1890.831545	6443.002799	3053.649798
1989.922695	41.452342	20.675849
2354.134060	148.189096	87.443093
2939.364966	57.437783	42.318401

2944.696129	70.386441	51.952633
3024.003021	20.111005	15.243829
3031.517962	16.508516	12.544294
3083.649830	1.440575	1.113472
3088.928304	10.485649	8.118601
3110.393858	0.054889	0.042794
3117.528733	0.943269	0.737096
3122.452522	0.372567	0.291594
3124.028435	2.326074	1.821447
3129.861121	0.213656	0.167617
3135.422951	9.351567	7.349514
3135.777396	3.080943	2.421625
3139.604940	3.227277	2.539741
3144.292603	3.808012	3.001230
3160.008740	10.691717	8.468643
3164.561908	3.533463	2.802801
3164.601528	2.068801	1.641027
3167.390905	1.271891	1.009787
3170.875251	8.801358	6.995309
3177.261655	23.238810	18.507379
3181.311139	24.503152	19.539172
3190.251961	2.978687	2.381924

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                  1.000000 atm.
Temperature:             298.150000 K
```

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.488	37.494	113.124	196.106
	Internal Energy (Kcal/mole):	0.889	0.889	292.042	293.819
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	118.441	124.403