Supplementary Material (ESI) for Chemical Communications

Charge-induced facial selectivity in the formation of new cationic planar chiral iridacycles derived from aniline.

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ESI

Figure S1

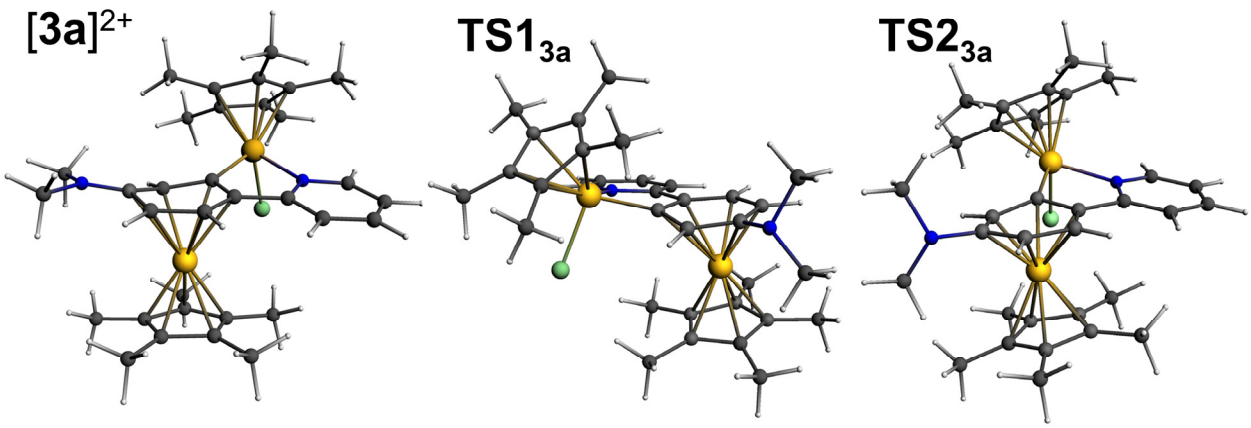


Fig. S1 Singlet ground state geometry for [*endo*-**3a**]$^{2+}$ and singlet transition state geometries **TS1$_{3a}$** and **TS2$_{3a}$** computed at the COSMO (acetone) ZORA-PBE/all electron TZP(Ir),DZP(H,C,N,Cl) level. **TS1$_{3a}$**, 105*i* cm^{-1}; **TS2$_{3a}$**, 95*i* cm^{-1}. Atoms are colored as follows: yellow, Ir; green, Cl; blue, N; grey, C; white, H. Selected interatomic distances and angle for [*endo*-**3a**]$^{2+}$: d_M, 2.476 Å; d_N, 1.337 Å; d_{Cl}, 2.420 Å; α, 114.1 deg; C_{ipso}-N-C_{Me}, 120.9-120.5 deg. *wbi* (C_{Ar}-N)= 1.30. Selected interatomic distances and angle for **TS1$_{3a}$**(identical values are found for **TS2$_{3a}$**): d_M, 2.318 Å;d_N, 1.425 Å; d_{Cl}, 2.424 Å; α, 118.4 deg; C_{ipso}-N-$C_{Me\ endo}$, 115.9 deg; C_{ipso}-N-$C_{Me\ exo}$, 110.9 deg. *wbi* (C_{Ar}-N) = 1.01.

Crystal Data (succinct form)

Crystal data for **2a**: $C_{23}H_{28}ClIrN_2$, *M*r = 560.12 g/mol, 0.38×0.30×0.20 mm^3, monoclinic, $P2_1/c$, a = 16.5371(6), b = 7.5131(3), c = 20.9885(6) Å, β = 128.903(2)1, V = 2029.35(12) Å^3, Z = 4, ρ_{calcd} = 1.833 g cm^{-3}, μ = 6.72 mm^{-1}, T=173(2)K, θ_{max}=32.1, 20707 reflections measured, 7014 independent reflections, R_{int}=0.017, R=0.023, wR^2=0.052, CCDC 805113. [*endo*-**3a**][PF_6]$_2$: $C_{33}H_{43}ClIr_2N_2$•2(F_6P)•C_3H_6O, *M*r = 1235.56 g/mol, 0.28×0.12×0.10 mm^3, monoclinic, $P2_1/c$, a = 13.019(1), b = 20.090(1), c = 17.132(1) Å , β = 108.824(1)°, V = 4241.2(5) Å^3, Z = 4, ρ_{calcd} = 1.935 g cm^{-3}, μ = 6.492 mm^{-1}, T=150(2)K, θ_{max}= 30.02, 30593 reflections measured, 12327 independent reflections, R_{int}=0.0464, R=0.0440, wR^2= 0.1312, CCDC 805114. [*endo*-**4a**][PF_6]: $C_{33}H_{43}ClIrN_2Ru,F_6P$, *M*r = 941.38 g/mol, 0.24×0.18×0.12 mm^3, monoclinic, $P2_1/c$, a = 8.671(1), b = 13.989(1), c = 28.862(1) Å , β = 105.194(2)°, V = 3378.5(5) Å^3, Z = 4, ρ_{calcd} = 1.851 g cm^{-3}, μ = 4.568 mm^{-1}, T=150(2)K, θ_{max}= 30.02, 29565 reflections measured, 9531 independent reflections, R_{int}=0.0298, R=0.0314, wR^2= 0.0704, CCDC 805115. [*exo*-**5b**]^0: $C_{30}H_{36}ClCrIrN_2O_3,C_3H_6O$, *M*r = 810.34 g/mol, 0.34×0.04×0.02 mm^3, monoclinic, $P2_1/c$, a = 10.649(1), b = 15.812(1), c = 21.131(1) Å , β = 107.397(3)°, V = 3395.3(4) Å^3, Z = 4, ρ_{calcd} = 1.585 g cm^{-3}, μ = 4.351 mm^{-1}, T=150(2)K, θ_{max}= 29.95, 26792 reflections measured, 9667 independent reflections, R_{int}=0.0494, R=0.0495, wR^2= 0.0624, CCDC 805116. For all structures Mo Kα radiation (0.71073 Å).

Experimental procedures

All experiments were carried out under a dry argon atmosphere using the standard Schlenk technique or in an argon filled glove-box when necessary. Anhydrous THF was distilled from purple solutions of Na/benzophenone under argon. All other solvents were distilled over sodium or CaH_2 under argon. Deuterated solvents were dried over sodium or CaH_2 and purified by trap-to-trap techniques, degassed by freeze-pump-thaw cycles and stored under argon. ^{1}H, ^{13}C NMR spectra were obtained on Bruker DPX 300, 400 or Avance 500 spectrometers. Chemical shifts were referenced against solvent peaks or external references.

Complex **2a**

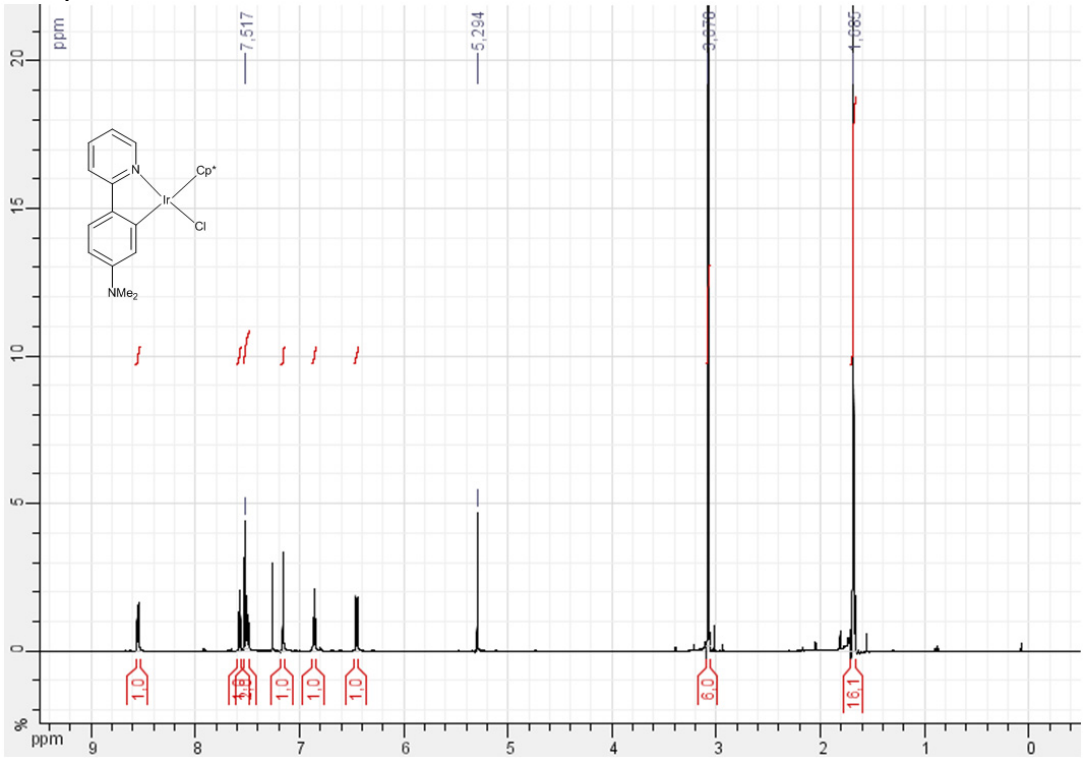


Figure 2 NMR ^{1}H in $CDCl_3$

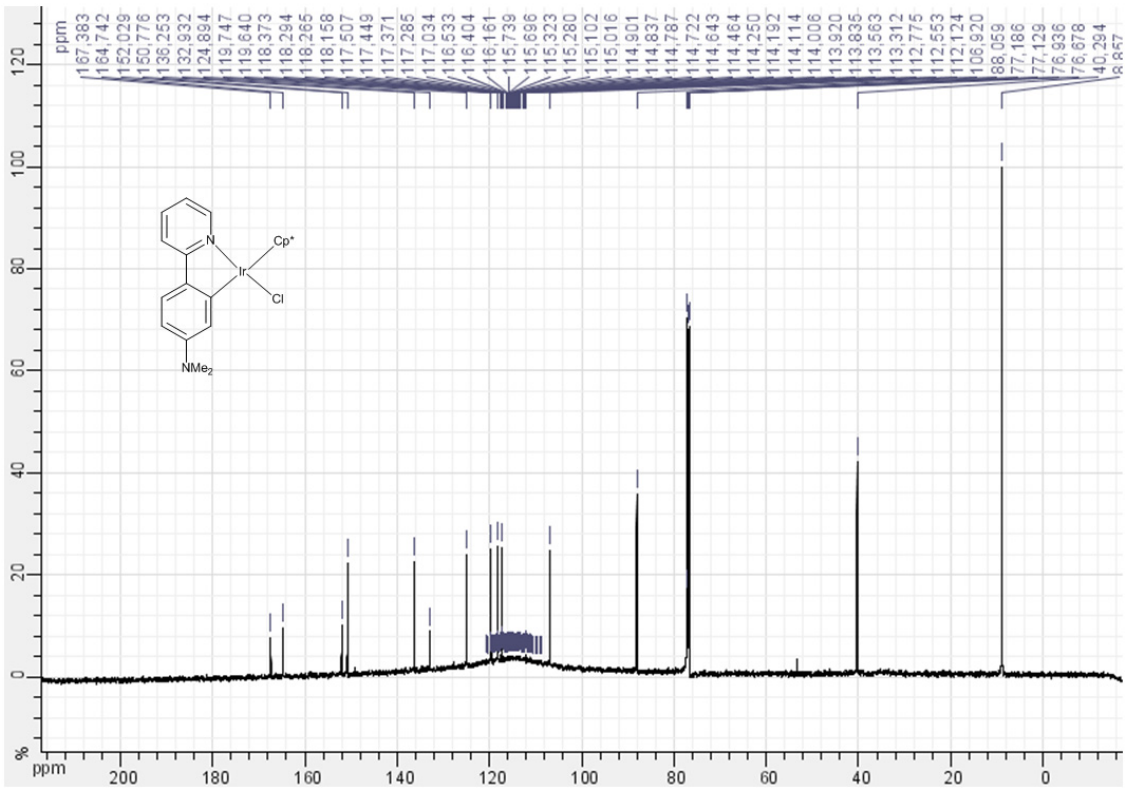


Figure 3 NMR ^{13}C in $CDCl_3$

A mixture $[Cp^*IrCl_2]_2$ (500 mg, 0.628 mmol), NaOAc (307 mg, 3.75 mmol) and **1a** (251 mg, 1.25

mmol) was stirred in 15 mL of CH_2Cl_2 at room temperature for 24h. Cyclometalated compound **2a** was isolated as a yellow-orange solid upon recrystallization in 80% yield (559.5 mg). Anal. Calcd for $C_{23}H_{28}ClIrN_2$. 1/4 CH_2Cl_2: C, 48.03; H, 4.94; N, 4.82. Found: C, 48.04; H, 4.743; N, 4.717. ^{1}H NMR ($CDCl_3$): δ 1.68 (s,15 H, C_5Me_5), 3.08 (s, 6 H, NMe_2), 6.45 (dd, 1 H, ^4J = 2.6, ^3J = 8.6 Hz), 6.86 (ddd,1 H, ^4J = 1.5, ^3J =5.7, ^3J =7.2 Hz), 7.16 (d,1 H, ^4J = 2.5 Hz), 7.50(m,1 H, ^4J = 1.3, ^4J =2.6, ^3J =7.5 Hz), 7.53 (d, 1 H, ^3J = 8.5 Hz), 7.58 (dd, ^2J = 1.41, ^3J =8.12 Hz), 8.55 (d, 1 H, ^3J = 5.8 Hz). ^{13}C NMR($CDCl_3$): δ 167.4, 164.7, 152.0, 150.7, 136.2, 132.9, 124.8, 119.6, 118.1, 117.3, 106.9, 88.0, 40.29, 8.8.

Complex **2b**

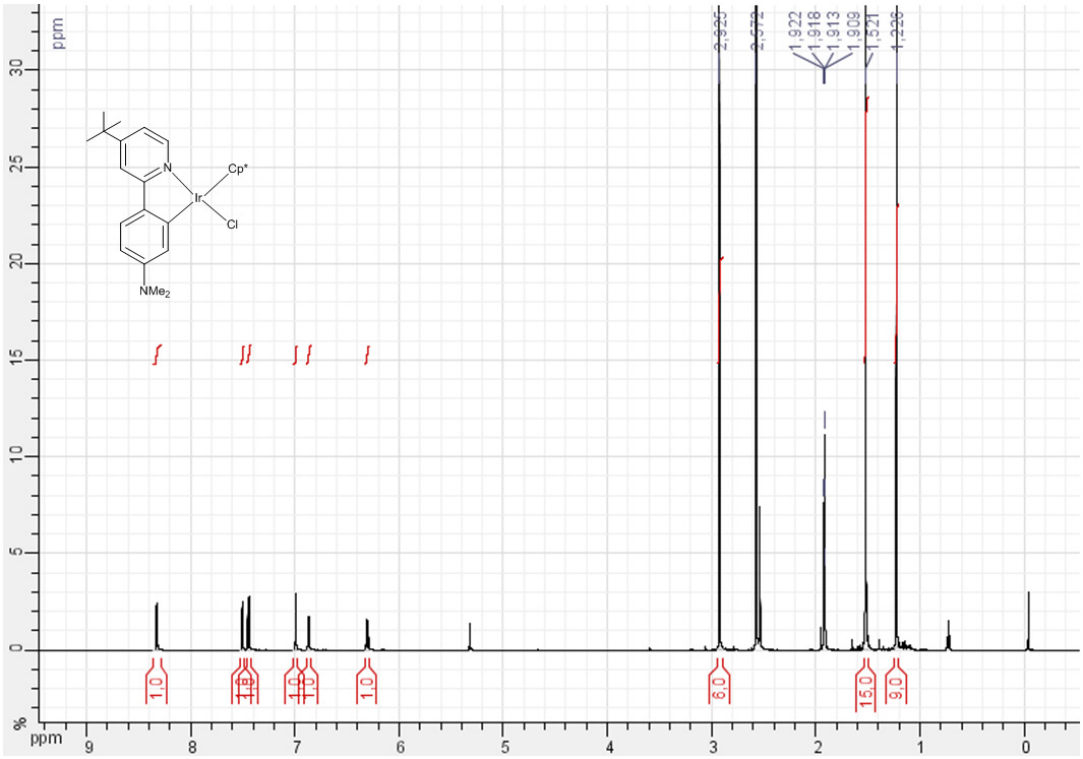


Figure 4 NMR (^{1}H) in CD_2Cl_2 with sight contamination by acetone

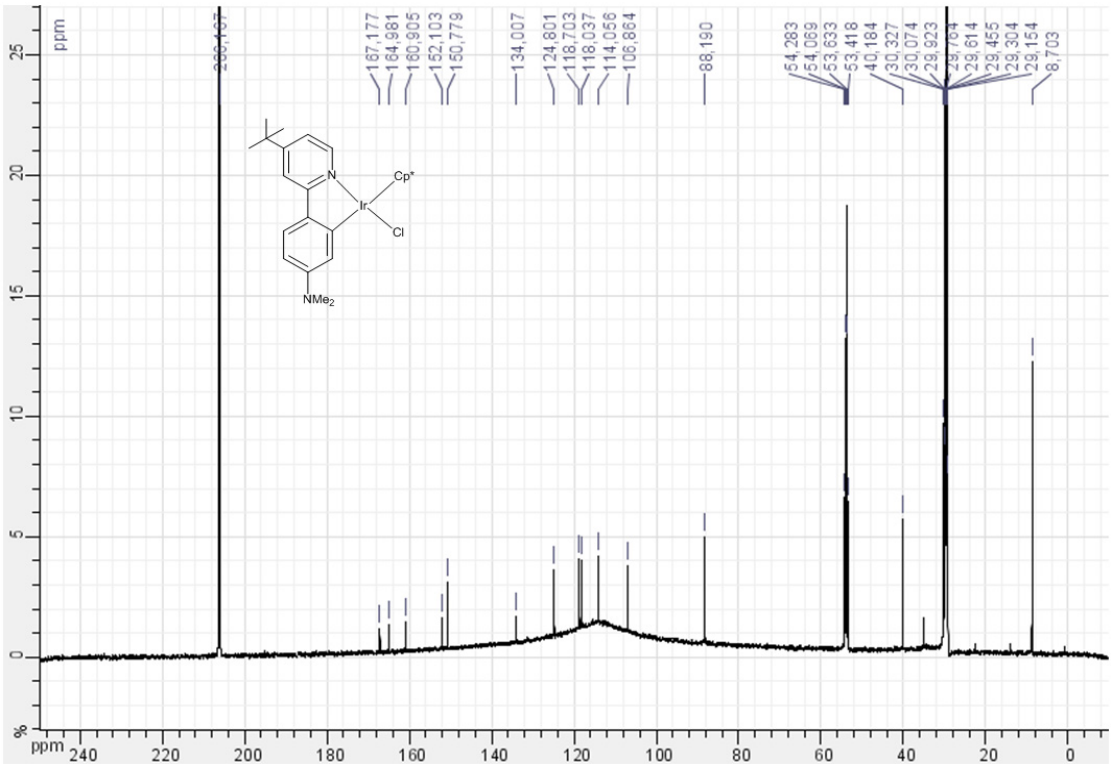


Figure 5 NMR ^{13}C in CD_2Cl_2 with sight contamination by acetone

Similar procedure was applied for the synthesis of complex **2b**: $[Cp^*IrCl_2]_2$ (800 mg, 1 mmol), **1b** (510

mg, 2 mmol) and NaOAc (350 mg, 4.26 mmol) in 20 mL of CH_2Cl_2. yield is 80% (986.4 mg). Anal. Calcd for $C_{27}H_{36}ClIrN_2$: C, 52.6; H, 5.89; N, 4.55. Found: C, 52.52; H, 5.812; N, 4.433. ^{1}H NMR (CD_2Cl_2): δ 1.23 (s, 9 H, tBu), 1.52 (s, 15 H, C_5Me_5), 2.92 (s, 6 H, NMe_2), 6.30 (dd, 1 H, ^4J = 2.6, ^3J =8.6 Hz), 6.87 (dd, 1 H, ^4J = 2.1, ^3J =6.2 Hz), 6.99 (d, 1 H, ^4J = 2.6 Hz), 7.44 (d, 1 H, ^3J = 8.6 Hz), 7.50 (d, 1 H, ^4J = 2.1 Hz), 8.33 (d, 1 H, J = 6.2 Hz). ^{13}C NMR(CD_2Cl_2): δ 167.17, 164.9, 160.9, 152.1, 150.8, 134.0, 124.8, 118.7, 118.0, 114.0, 106.8, 88.2, 40.2, 30.3, 8.7.

Complex **1c**

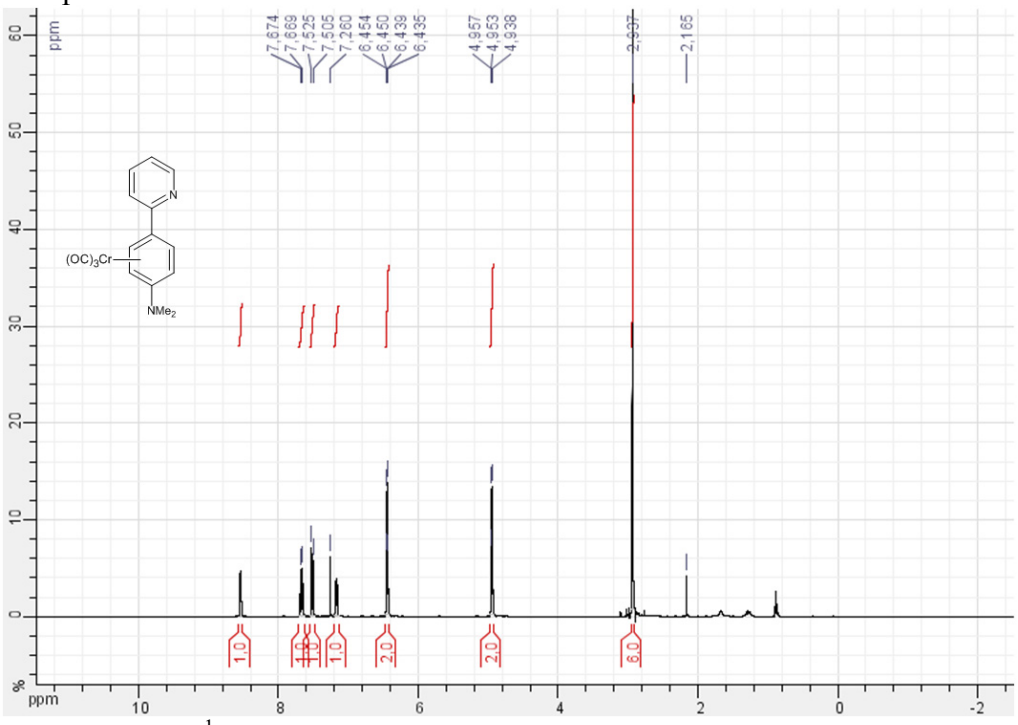


Figure 6 NMR ^{1}H in $CDCl_3$

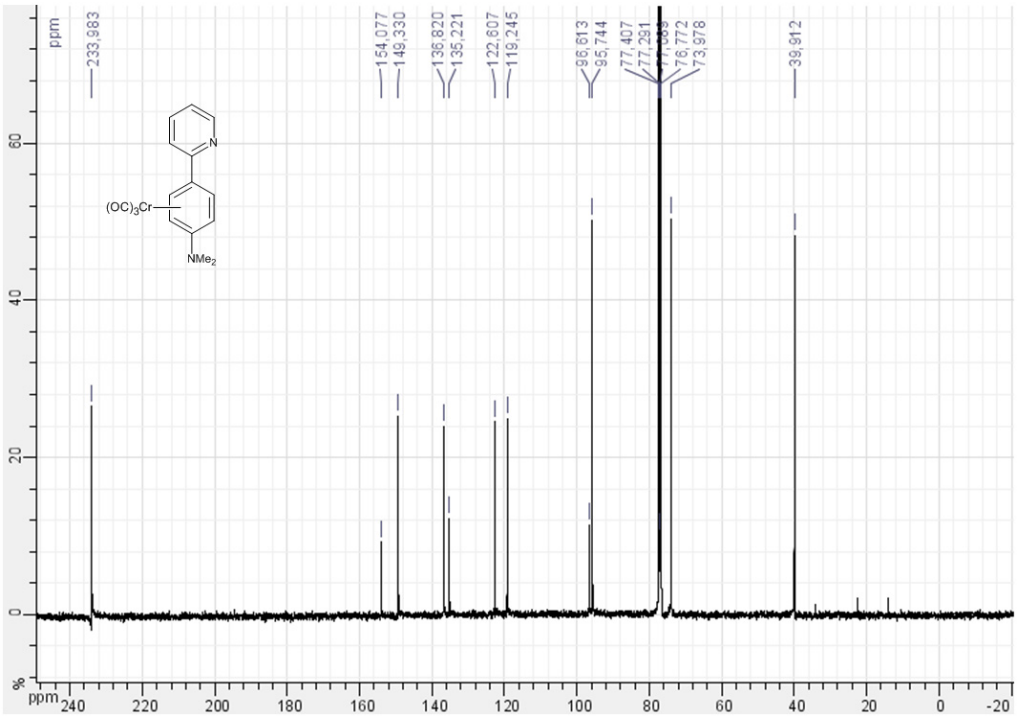


Figure 7 NMR ^{13}C in $CDCl_3$

A mixture of **1a** (1.335 g, 6.74 mmol) and $Cr(CO)_6$ (1.63 g, 7.416 mmol) was dissolved in *n*-Bu_2O (150 mL), and THF (10 mL) was added to the resulting mixture. The suspension was gently refluxed for 7

days under argon. The resulting yellow solution was cooled to room temperature and filtered through Celite. The filtrate was evaporated under reduced pressure, the resulting oil dissolved in CH_2Cl_2, and silica gel 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 mixture pentane/ acetone (95/5). Complex **1c** was eluted with pentane/acetone (85/15), the polarity was increased. The solvent was removed under vacuum and the bright yellow solid. The yield is 76% (1.7 g). Anal. Calcd for $C_{16}H_{14}CrN_2O_3$: C, 57.47; H, 4.22; N, 8.38. Found: C, 57.47; H, 4.188; N, 8.248. (IR) υ= 1936(s), 1835(vs) (C=O). ^{1}H NMR ($CDCl_3$): δ 2.94 (s, 6 H, NMe_2), 4.95 (d, 2 H, ^3J = 7.4 Hz), 6.44 (d, 2 H, ^3J = 7.3 Hz), 7.17 (dd, 1 H, ^3J = 4.89, ^3J =7.4 Hz), 7.51 (d, 1 H, ^3J = 8.1 Hz), 7.67 (dd, 1 H, ^4J = 1.66, ^3J =6 Hz), 8.54 (d, 1 H, ^3J = 5.0 Hz). ^{13}C NMR ($CDCl_3$): δ 233.9, 154.0, 136.8, 135.2, 122.6, 119.2, 96.6, 95.7, 73.9, 39.9.

Complex **1d**

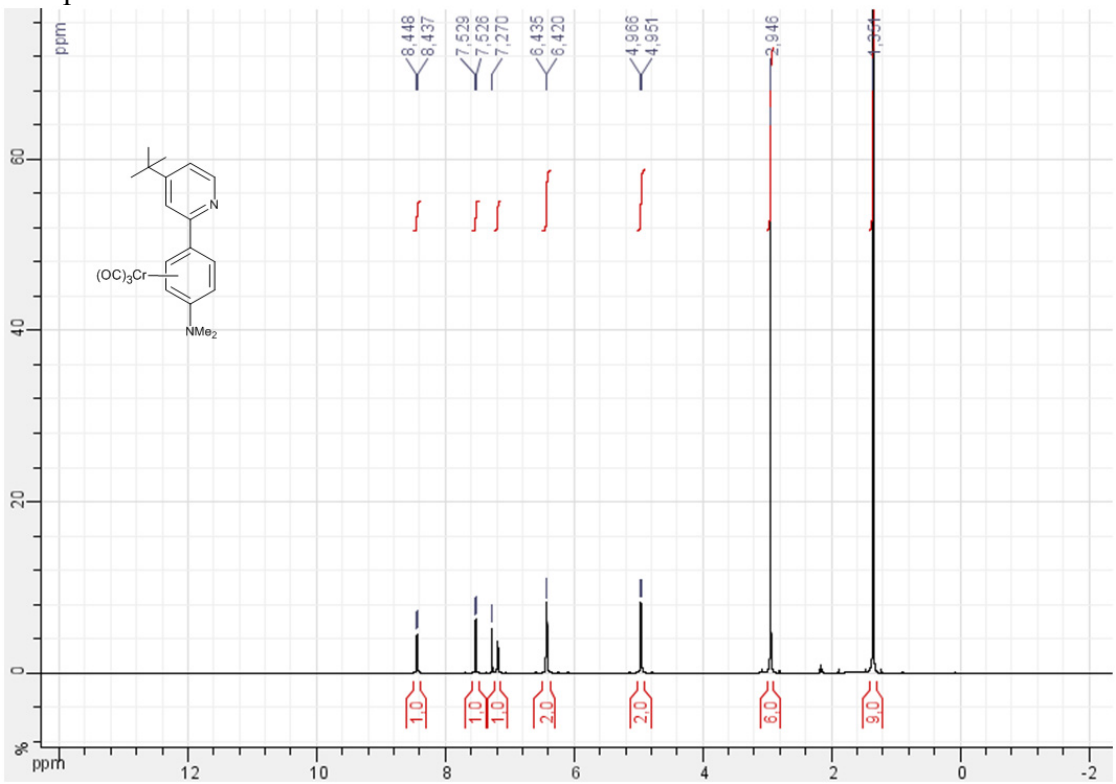


Figure 8 NMR ^{1}H in $CDCl_3$

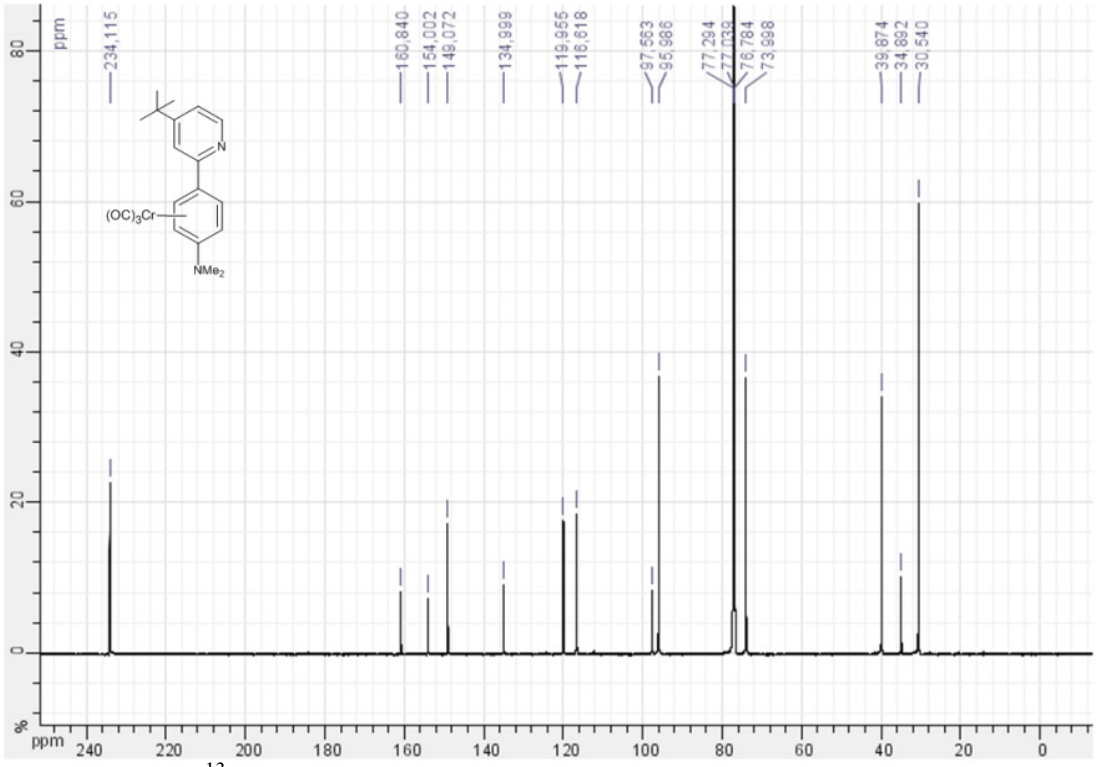


Figure 9 NMR ^{13}C in $CDCl_3$

A similar procedure was applied for the synthesis of complex **1d**: **1a** (2 g, 7.84 mmol) and $Cr(CO)_6$ (1.9 g, 8.62 mmol). The yield is 71.8 % (2.2 g). Anal. Calcd for $C_{20}H_{22}CrN_2O_3$: C, 61.51; H, 5.68; N, 7.18. Found: C, 61.35; H, 5.82; N, 7.04. (IR) υ= 1936, 1840 (C=O).^{1}H NMR ($CDCl_3$): δ 1.35 (s, 9 H, tBu), 2.94 (s, 6 H, NMe_2), 4.96 (d, 2 H, ^3J = 7.3 Hz), 6.43 (d, 2 H, ^3J = 7.3 Hz), 7.19 (dd, 1 H, ^4J = 1.8, ^3J =5.3 Hz), 7.53 (d, 1 H, ^4J = 1.9 Hz), 8.44 (d, 1 H, ^3J = 5.3 Hz). ^{13}C NMR ($CDCl_3$): δ 234.1, 160.8, 154.0, 149.0, 13, 1, 116.6, 97.5, 96, 7, 39.8, 34.8, 30.5.

Complex endo-**3a**

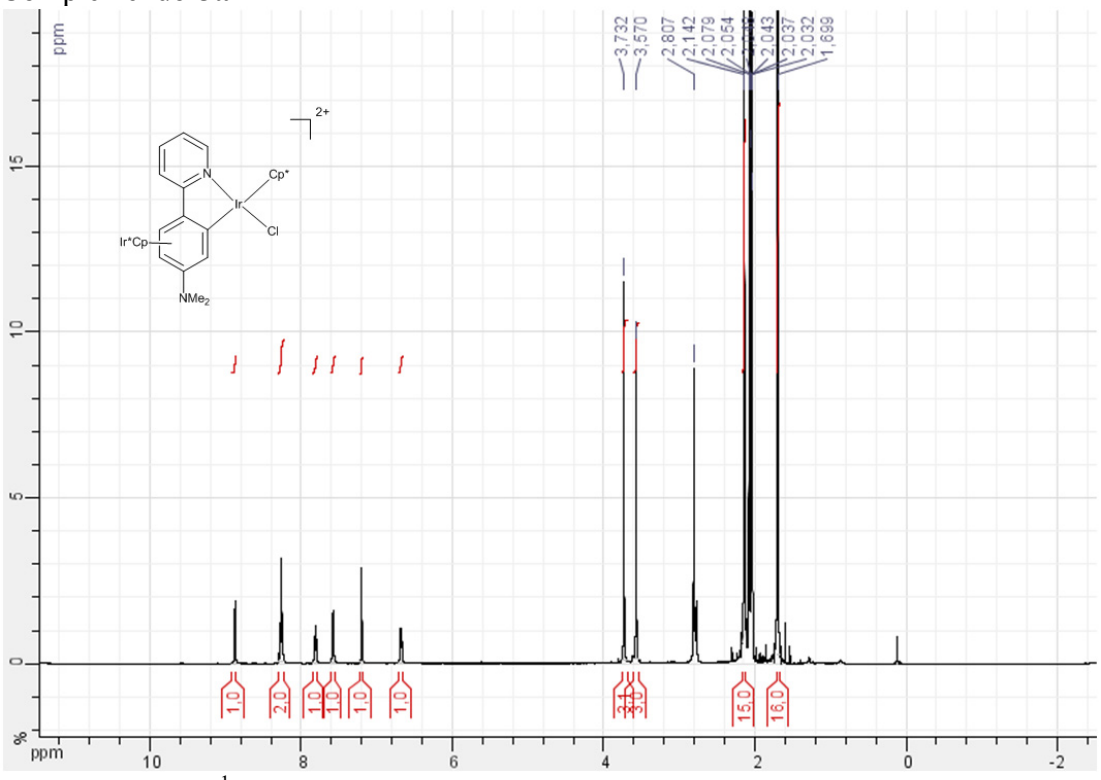


Figure 10 NMR ^{1}H in d_6.acetone

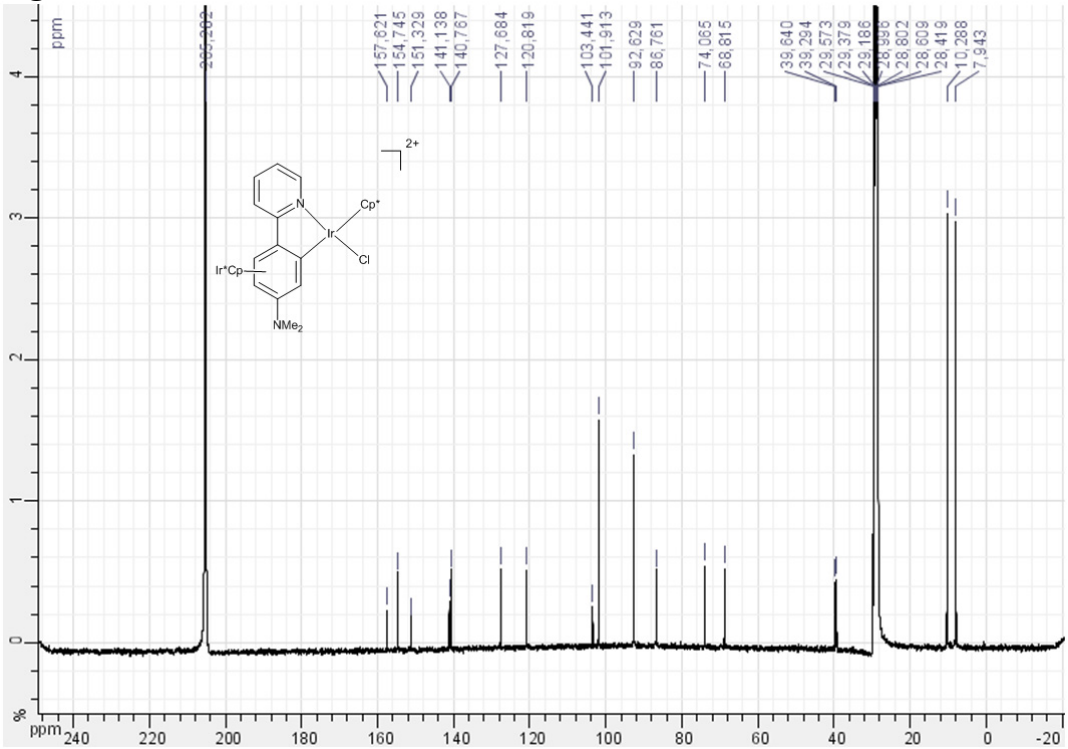


Figure 11 NMR ^{13}C in d_6.acetone

A solution of compound **2a** (230 mg, 0.41 mmol) in acetone (8 mL) was added to a freshly prepared solution of $[Cp^*Ir(CH_3COCH_3)_3](PF_6)_2$ [generated in situ by reaction of $[Cp^*IrCl_2]_2$ (200 mg, 0.25

mmol) and $AgPF_6$ (253 mg, 1 mmol) in acetone (8 mL) at room temperature 30 minutes] and the resulting solution was left to stir for 24 h at room temperature. Upon filtration of the reaction mixture, the filtrate was concentrated and the resulting precipitate was washed with pentane (15 mL). The compound was recrystallized and subsequently isolated as an orange solid with a yield of 78% (370 mg). Anal. Calcd for $C_{33}H_{43}ClF_{12}Ir_2N_2P_2$: C, 33.66 ; H, 3.69; N, 2.38. Found: C, 33.82; H, 4.104; N, 2.108. ^{1}H NMR (d_6.acetone): δ 1.7 (s,15 H, C_5Me_5), 2.14 (s,15 H, C_5Me_5), 3.57 (s, 3 H, NMe), 3.73 (s, 3 H, NMe), 6.68 (dd, 1 H, ^4J = 2.4, 3J =7.1 Hz), 7.2 (d, 1 H, ^4J = 2.3 Hz), 7.58 (d, 1 H, ^3J = 7.0 Hz), 7.81 (ddd, 1 H, ^4J = 2.3, ^3J =5.7, ^3J = 6.6 Hz), 8.27 (m, 2 H, ^3J = 1.7, ^3J =5.4, ^3J =7.0 Hz), 8.88 (d, 1 H, ^3J = 5.5 Hz).^{13}C NMR (d_6.acetone): δ 157.6, 154.7, 151.3, 141.1, 140.7, 127.7, 120.8, 103.4, 101.9, 92.6, 86.7, 74.0, 68.8, 39.6, 39.3, 10.3, 7.9.

Complex **5a**

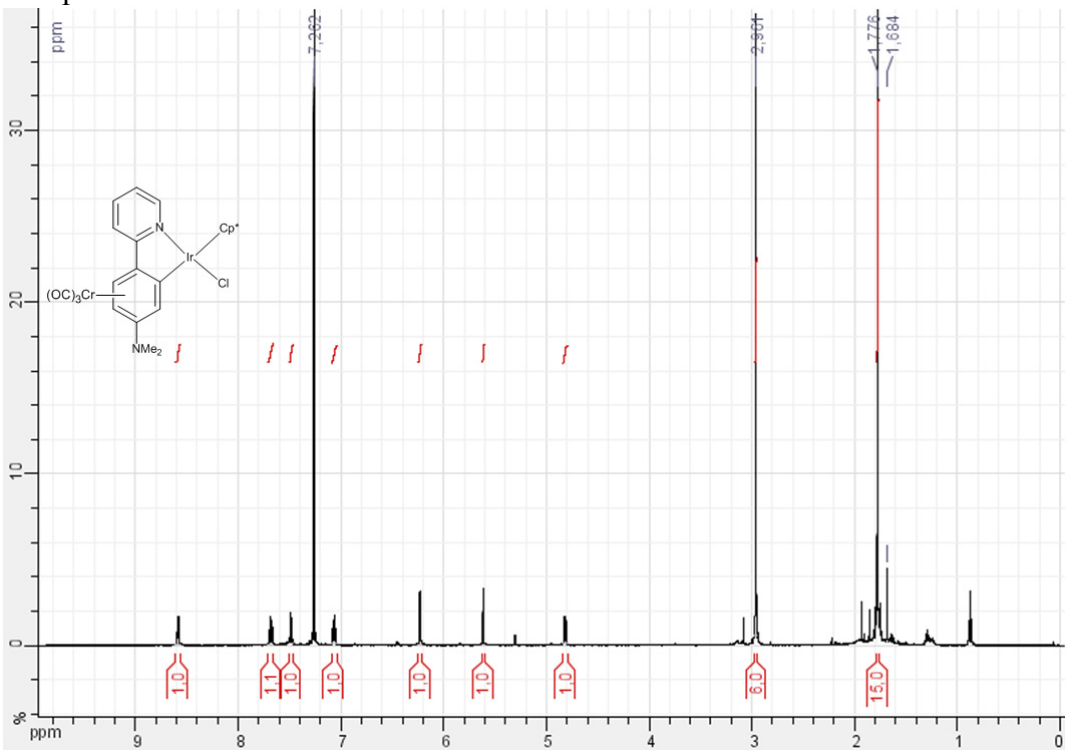


Figure 12 NMR ^{1}H in $CDCl_3$

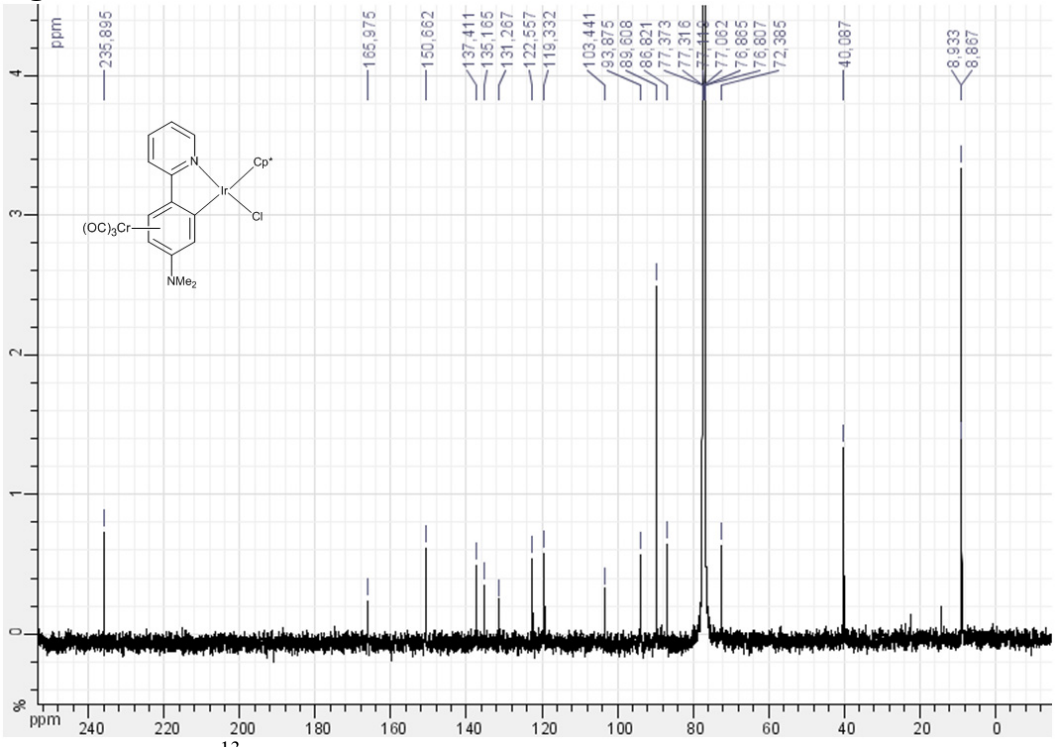


Figure 13 NMR ^{13}C in $CDCl_3$

$[Cp^*IrCl_2]_2$ (0.498 mmol), **1c** (336 mg, 1.006 mmol) and $NaOAc{\cdot}3H_2O$ (324 mg, 3.95mmol) were dissolved in dichloromethane (20 mL), and the resulting mixture was stirred at room temperature for 24 h under argon. The resulting red solution was filtered through Celite, the filtrate was evaporated to

dryness under reduced pressure to afford an orange solid, which was recrystallized from a mixture of pentane (15 mL) and dichloromethane (5 mL) and dried under reduced pressure overnight. Compound **5a** was recovered as an orange powder with a yield of 75% (520 mg). Anal. Calcd for $C_{26}H_{28}ClCrIrN_2O_3$ $0.3CH_2Cl_2$: C, 43.77; H, 3.99; N, 3.88. Found: C, 43.76; H, 4.16; N, 3.55. (IR) υ= 1917, 1829 (C=O). ^{1}H NMR ($CDCl_3$): δ 1.77 (s, 15 H, C_5Me_5), 2.96 (s, 6 H, NMe_2), 4.82 (dd, 1 H, ^4J = 2.4, ^3J =7.1 Hz), 5.61 (d, 1 H, ^4J = 2.4 Hz), 6.23 (d, 1 H, ^3J = 7.1 Hz), 7.07 (ddd, 1 H, ^4J = 1.4, ^3J =5.8, ^3J =7.5 Hz), 7.49 (d, 1 H, ^3J = 8.2 Hz), 7.68 (dt, 1 H, ^2J = 1.5, ^3J =7.8 Hz), 8.59 (d, 1 H, ^3J = 5.8 Hz). ^{13}C NMR ($CDCl_3$): δ 235.9, 165.9, 150.6, 137.4, 135.1, 131.2, 122.5, 119.3, 103.4, 93.9, 89.6, 86.8,72.4, 40.1, 8.9.

Synthesis of 5a by an alternative method

2a (159 mg, 0.282 mmol) and tricarbonyl(η^6-naphthalene)chromium (108 mg, 0.408 mmol) were dissolved in dry and degassed tetrahydrofuran (15 mL). The resulting mixture was stirred at room temperature for 24 h under argon. The resulting solution was filtered through Celite, the filtrate was concentrated to ca. 5 mL, and silica gel was added. The solvent was evaporated under reduced pressure, and the coated silica gel was loaded on the top of a silica gel column packed in mixture pentane and dichloromethane (50/50) at 5 °C. The product was eluted with a 75:25 mixture of dichloromethane and pentane (195 mg, 100%).

Complex **5b**

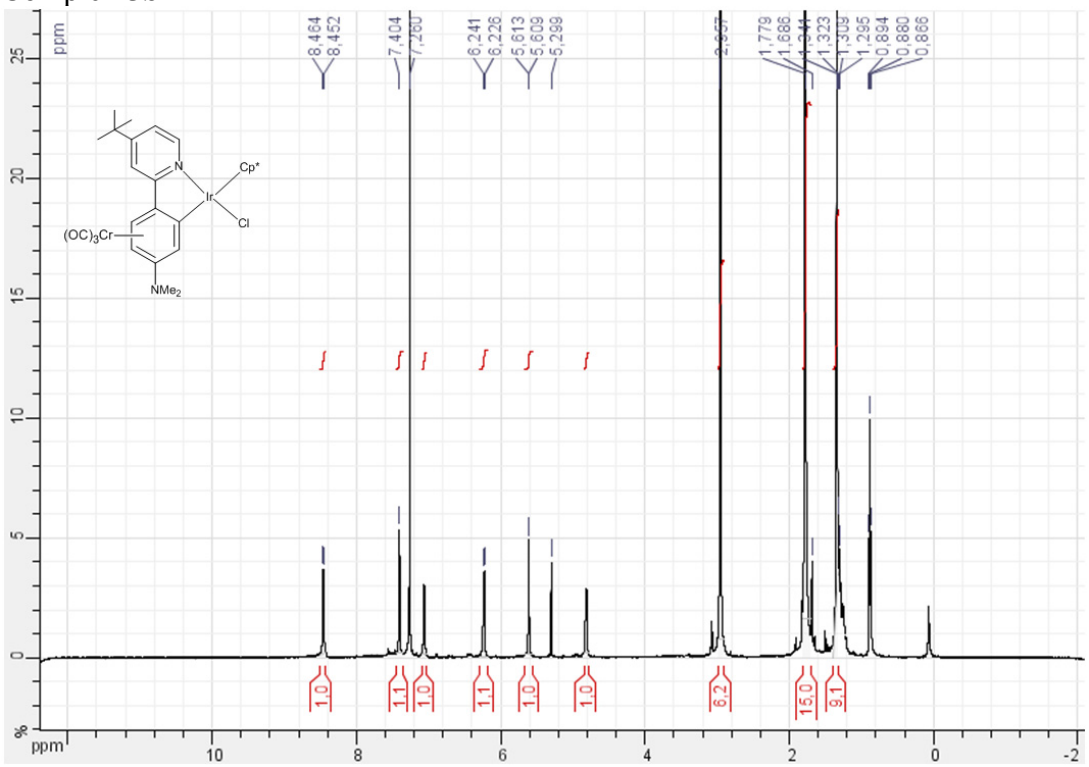


Figure 14 NMR ^{1}H in $CDCl_3$

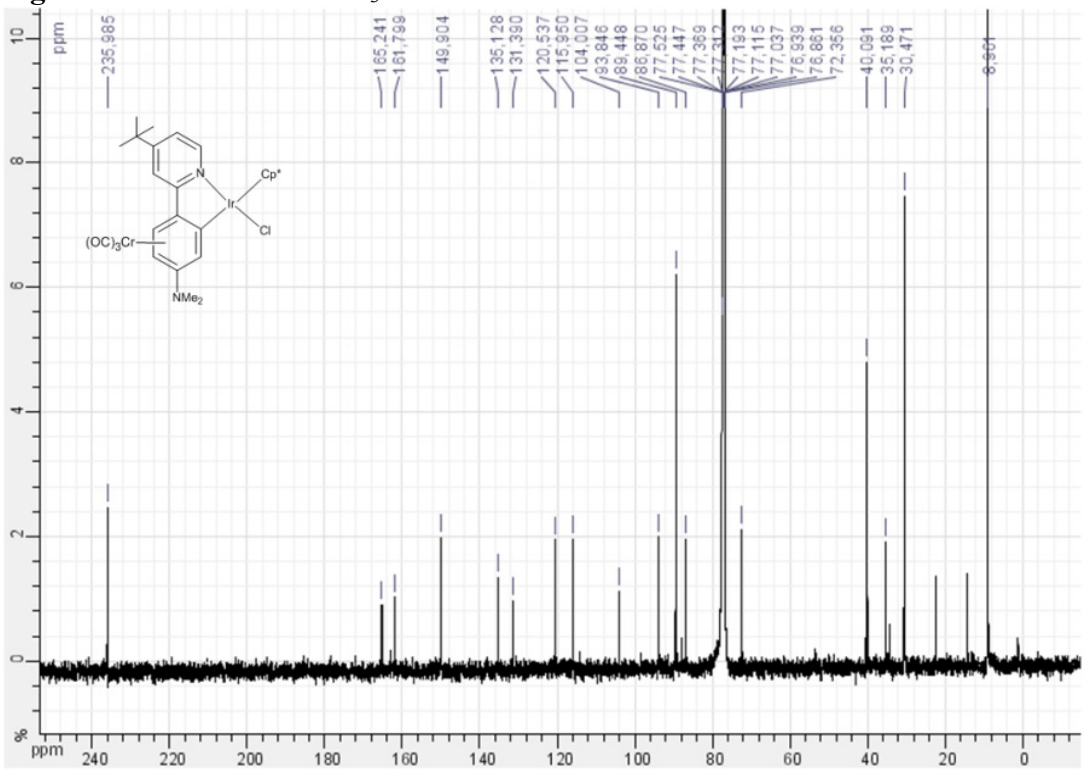


Figure 15 NMR ^{13}C in $CDCl_3$

A similar procedure was applied for the synthesis of complex **2b: 1d** (250 mg, 0.639 mmol), $[Cp^*IrCl_2]_2$ (254 mg, 0.319 mmol) and $NaOAc^{\bullet}3H_2O$ (209.59 mg, 2.55 mmol) in dichloromethane (15

mL). The yield was 70% (336 mg). Anal. Calcd for $C_{30}H_{36}ClCrIrN_2O_3$ $0.6CH_2Cl_2$: C, 45.88; H, 4.888; N, 3.093. Found: C, 45.76; H, 4.67; N, 3.49. (IR) υ= 1917, 1829 (C=O). ^{1}H NMR ($CDCl_3$): δ 1.34 (s, 9 H, *t*Bu), 1.78 (s,15 H, C_5Me_5), 2.96 (s, 6 H, NMe_2), 4.82 (d, 1 H, ^3J = 7.1 Hz), 5.61 (d, 1 H, ^4J = 1.7 Hz), 6.23 (d, 1 H, ^3J = 7.2 Hz), 7.06 (d, 1 H, ^3J = 5.7 Hz), 7.4 (s, 1 H), 8.46 (d, 1 H, ^3J = 6.3 Hz). ^{13}C NMR ($CDCl_3$): δ 235.9, 165.2, 161.8, 149.9, 135.1, 131.4, 120.5, 115.9, 104.0, 93.8, 89.4, 86.8, 72.3, 40.1, 35.2, 30.5, 8.9.

Complex **4a**

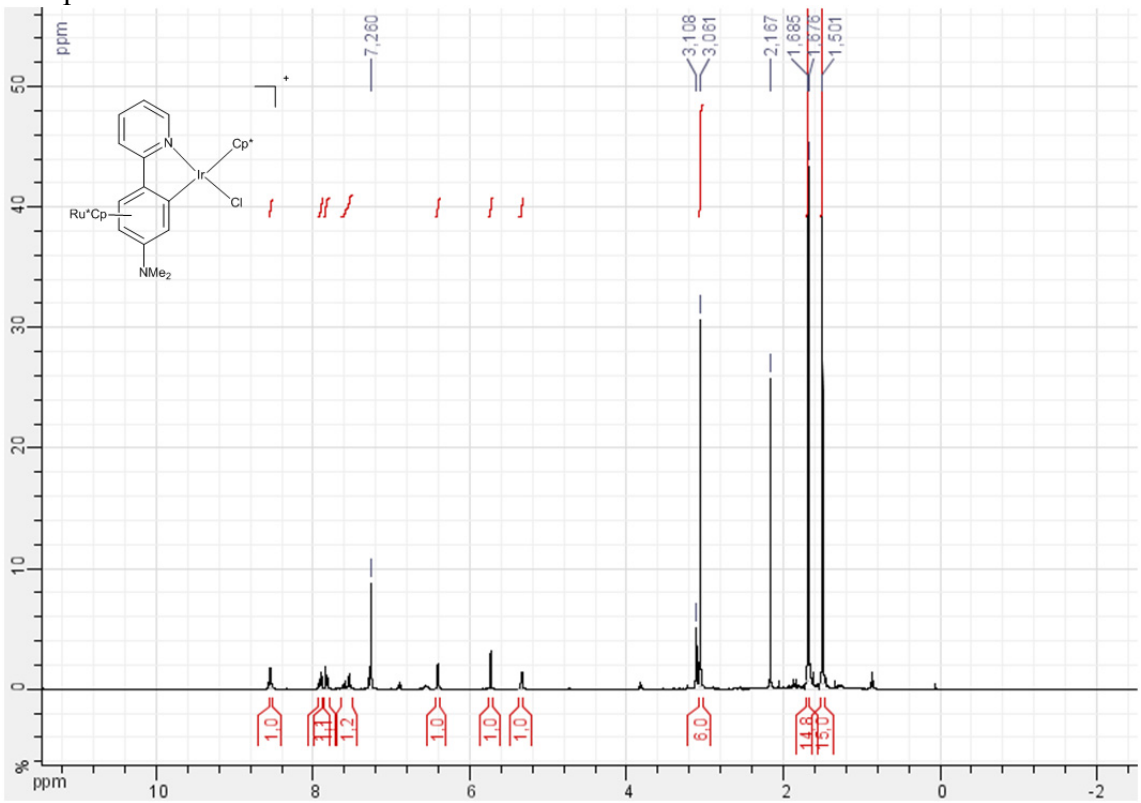


Figure 16 NMR ^{1}H in $CDCl_3$

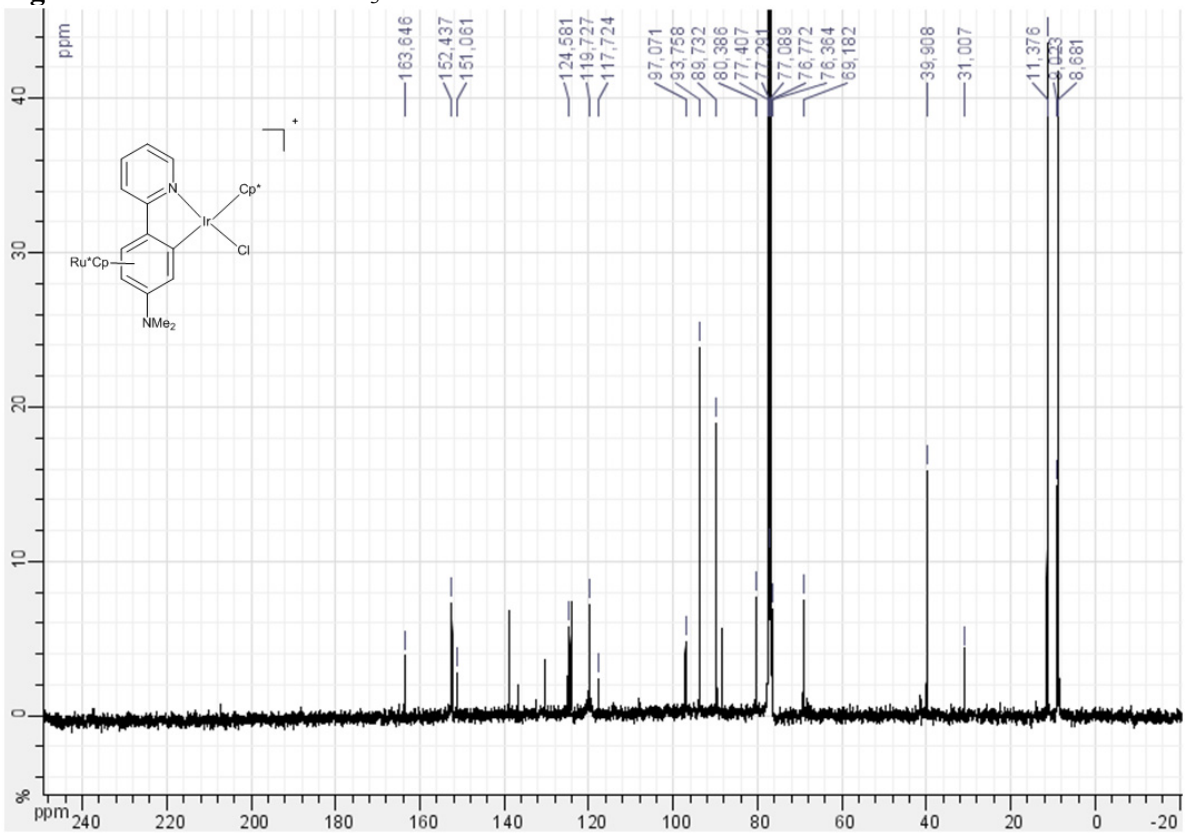


Figure 17 NMR ^{13}C in $CDCl_3$

A mixture compound **2a** (100 mg, 0.178 mmol) and $[Cp^*Ru(NCCH_3)_3]PF_6$ (90 mg, 0.178 mmol) in THF (10 mL) was stirred at room temperature for 24 h under argon. After a flash filtration of the solution through celite, the filtrate was concentrated and the resulting precipitate recrystallized with pentane. The precipitate was washed 3 times with pentane and finally evaporated to dryness under reduced pressure. The compound **4a** was isolated as a yellow-orange solid with a yield of 75% (127 mg). Anal. Calcd for $C_{33}H_{43}ClF_6IrN_2PRu.\ 2CH_2Cl_2.\ H_2O$: C, 37.29; H, 4.51; N, 2.92. Found: C, 37.22; H, 4.37; N, 2.48. ^{1}H NMR ($CDCl_3$): δ1.501 (s, 15 H, C_5Me_5), 1.685 (s, 15 H, C_5Me_5), 3.06 (s, 6 H, NMe_2), 5.34 (dd, 1 H, ^4J = 1.99, ^3J =6.38 Hz), 5.73 (d, 1 H, ^4J = 1.9 Hz), 6.41 (d, 1 H, ^3J = 6.5 Hz), 7.26 (m, 1 H, ^4J= 1.4, ^3J =4.2 Hz), 7.83 (d, 1 H, ^3J = 7.9 Hz), 7.9 (dt, 1 H, ^4J = 1.6, ^3J =7.7 Hz), 8.54 (d, 1 H, ^3J = 5.5 Hz). ^{13}C NMR ($CDCl_3$): δ 163.6, 152.4, 151.0, 124.6, 119.3, 117.7, 97.1, 93.7, 88.7, 80.4, 69.2, 39.9, 31.0, 11.4, 8.7.

Ligand **1b**

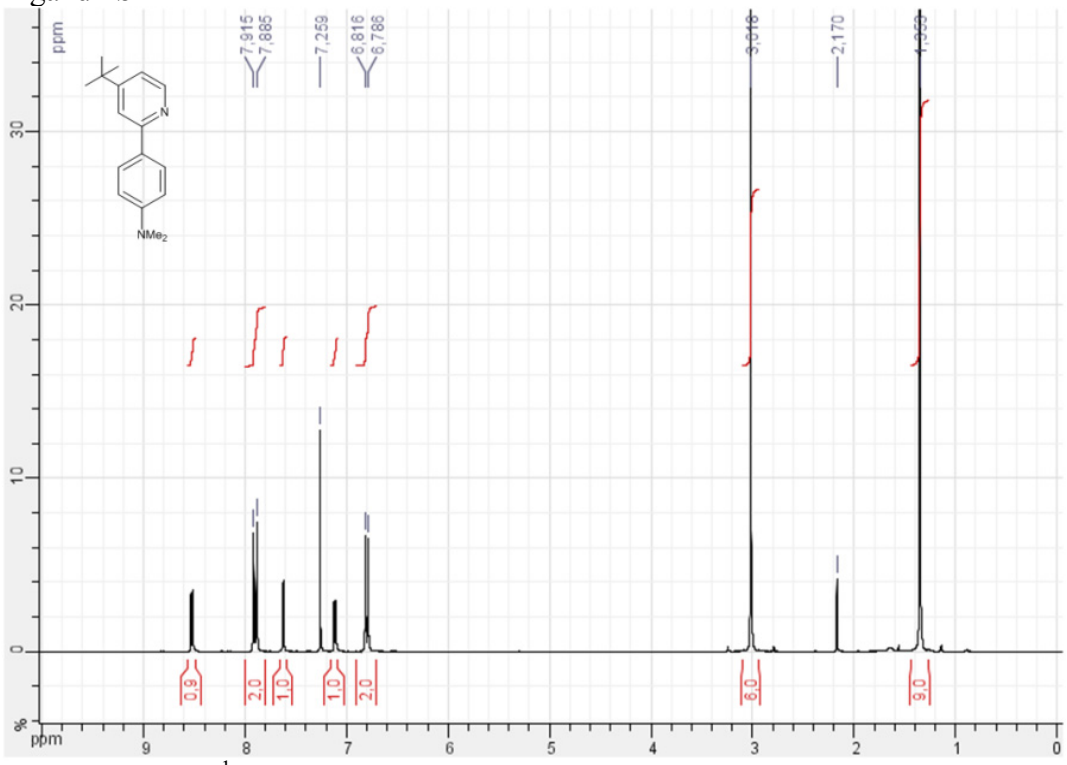


Figure 18 NMR ^{1}H in $CDCl_3$

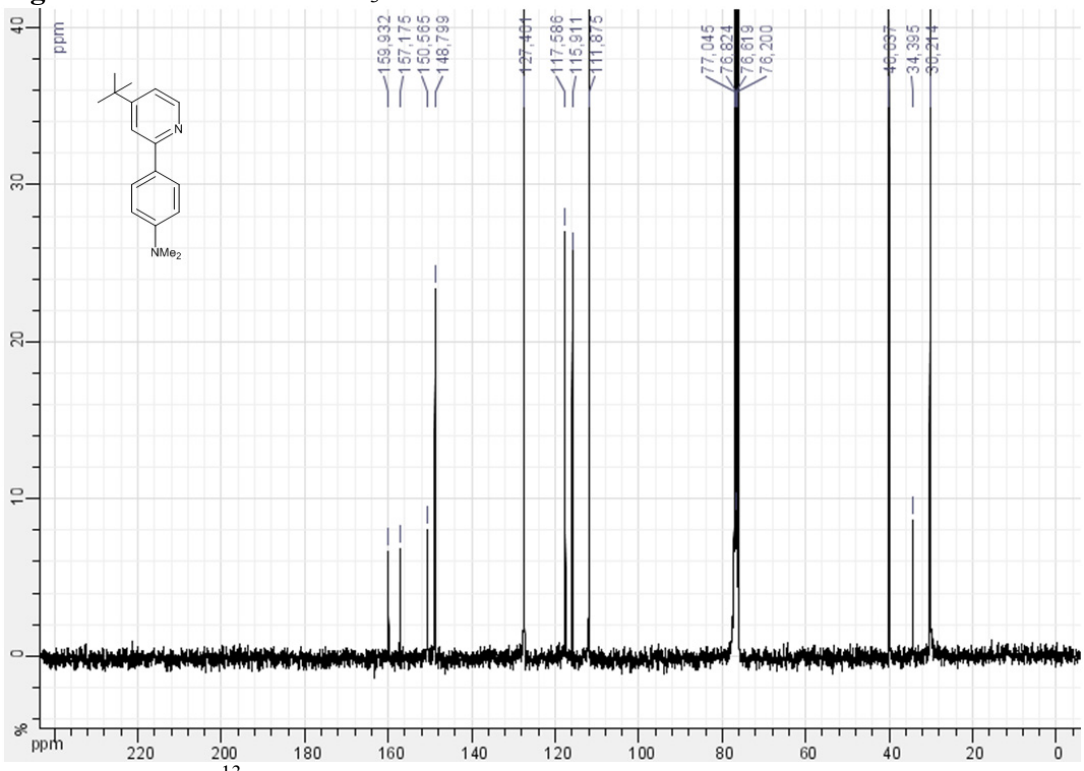


Figure 19 NMR ^{13}C in $CDCl_3$

A solution of 4-lithio,N,N-dimethylaniline (57.5 mmol, prepared by reaction of 4-bromo,N,N-dimethylaniline with excess Li metal) in diethyl ether (125 mL) was added to pure and dry 4-

tbutylpyridine (7.75 g, 57.5 mmol) at room temperature and the resulting solution was left to stir for ca. 7 h. The resulting solution evaporated to dryness and the residue suspended in dry cyclohexane (70 mL) and boiled overnight. The resulting suspension was hydrolized with water and the mixture extracted dichloromethane following convention workup procedure. The organic phase was dried over $MgSO_4$, filtered through Celite and the filtrate was stripped of solvents. The residue was purified by chromatography through SiO_2 and eluted with a 30:70 mixture of CH_2Cl_2 and *n*-pentane. Pure compound **1b** was recovered as off-white crystals upon concentration of the eluate and crystallization (8.7 g, 60 %).

Anal. Calcd for $C_{17}H_{22}N_2$: C, 80.27; H, 8.72; N, 11.02. Found: C, 80.08; H, 8.42; N, 11.00. ^{1}H NMR ($CDCl_3$): δ1.35 (s, 9 H, *t*Bu), 3.02 (s, 6 H, NMe_2), 6.80 (d, 2 H, ^3J = 8.9 Hz), 7.11 (dd, 1 H, ^4J = 1.9, ^3J =5.3 Hz), 7.62 (d, 1 H, ^4J = 2.1 Hz), 7.90 (d, 2 H, ^3J = 8.9 Hz), 8.52 (d, 1 H, ^3J = 5.3 Hz). ^{13}C NMR ($CDCl_3$): δ159.9, 157.2, 150.5, 148.8, 127.4, 117.6, 115.9, 111.8, 40.0, 34.4, 30.2.

Dependence of the ^{1}H NMR spectrum of endo-3a on the nature of the counter anion.

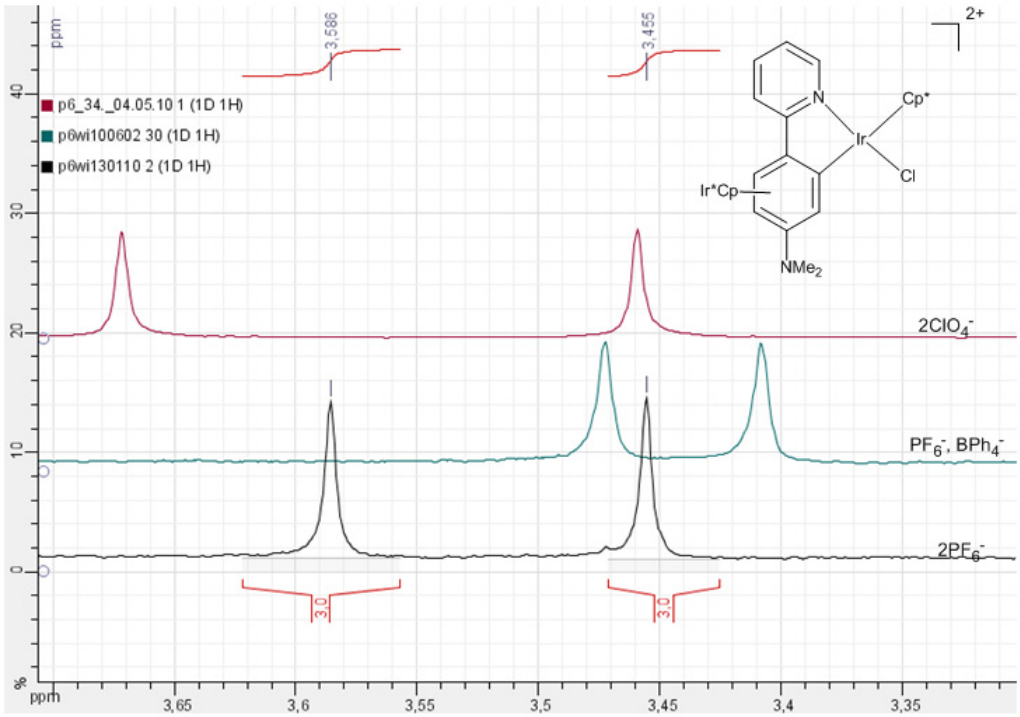


Figure 20: ^{1}H signals of the NMe_2 group in the presence of different anions

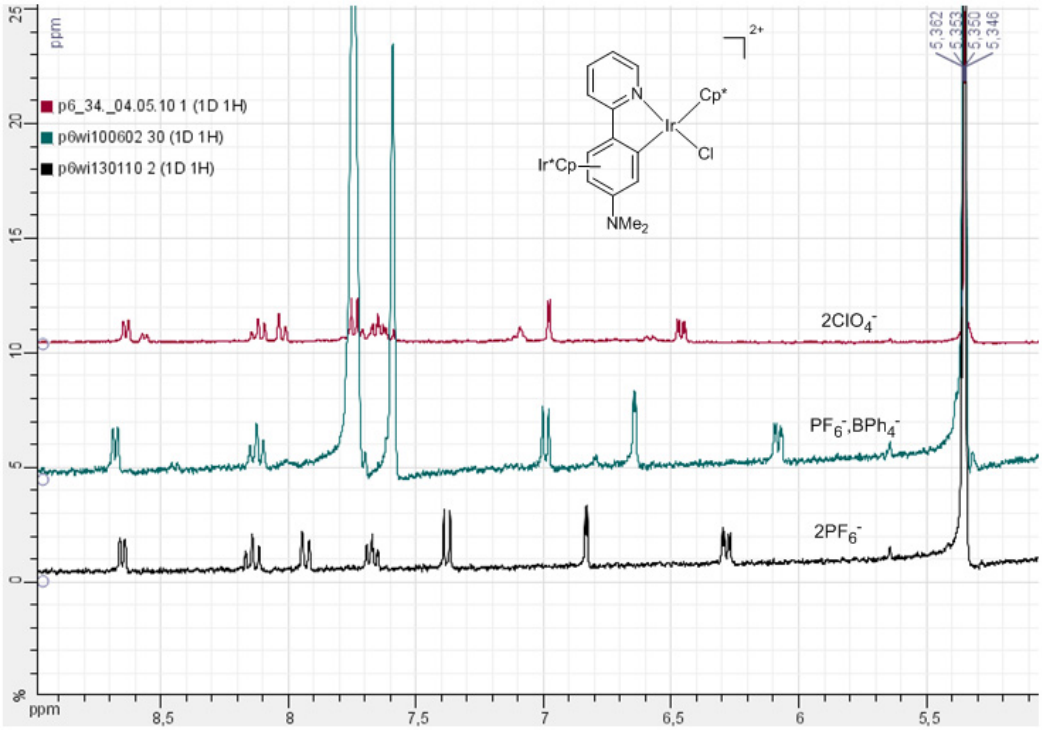


Figure 2: ^{1}H NMR signals in the aromatic region in the presence of different anions

Variable Temperature ^{1}H NMR experiments

Line shape analysis of the rotation of the –NMe_2 group in compound [*endo*-**3a**][PF_6]$_2$ in deuterated acetone[1, 2]

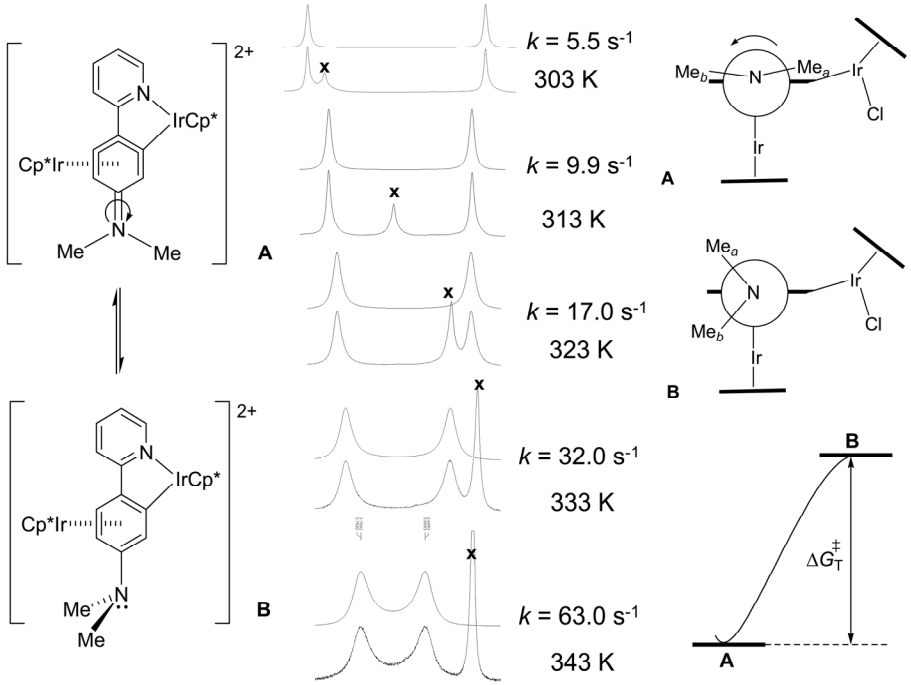


Figure 21 Experimental and simulated portions of the ^{1}H NMR spectrum of a 15 mM solution of [*endo*-**3a**][PF_6]$_2$.

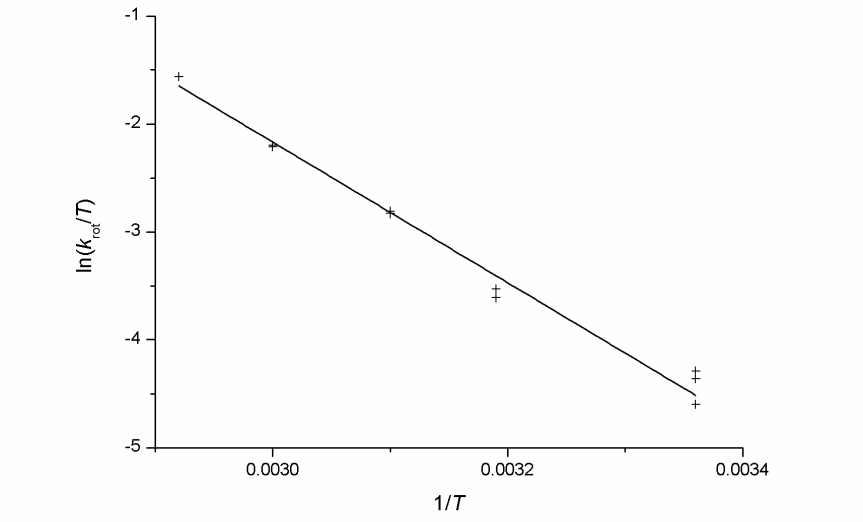


Figure 22 Eyring plot of $\ln(k_{rot}/T) = f(1/T)$. The data of three independent VT experiments carried out with solutions of different ionic strength have been merged here since no major difference in k_{rot} for each temperature was noticed. Variable-temperature (VT) ^{1}H NMR experiments were carried out with 9.3 mM solutions of [*endo*-**3a**][PF_6]$_2$ in d_6-acetone.

	Intercept Value	Intercept Error	Slope Value	Slope Error	Statistics Adj. R^2
I	17.38001	0.62043	-6516.16576	198.99825	0.9871

$$\ln(k_{rot}/T) - \ln[\kappa(k_B / h)] = \Delta S_{rot}/R - \Delta H_{rot}/RT, \textit{ with } \kappa = 1$$

Crystallographic data

2a
3a
4a
5b

2a

Crystal data

$C_{23}H_{28}ClIrN_2$	
M_r = 560.12	D_x = 1.833 Mg m^{-3}
Monoclinic, $P2_1/c$	
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 16.5371 (6) Å	Cell parameters from 9910 reflections
b = 7.5131 (3) Å	θ = 3.0–32.1°
c = 20.9885 (6) Å	μ = 6.72 mm^{-1}
β = 128.903 (2)°	T = 173 K
V = 2029.35 (12) Å^3	Block, yellow
Z = 4	0.38 × 0.30 × 0.20 mm
F(000) = 1096	

Data collection

Bruker APEX-II CCD diffractometer	7014 independent reflections
Radiation source: fine-focus sealed tube	6324 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.017
Detector resolution: ? pixels mm^{-1}	θ_{max} = 32.1°, θ_{min} = 3.0°
φ and ω scans	h = −24 20
Absorption correction: multi-scan sadabs	k = −10 11
T_{min} = 0.184, T_{max} = 0.347	l = −30 31
20707 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier

	map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.023	H-atom parameters constrained
$wR(F^2)$ = 0.052	$w = 1/[\sigma^2(F_o^2) + (0.0166P)^2 + 4.1026P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.14	$(\Delta/\sigma)_{max}$ = 0.003
7014 reflections	$\Delta\rho_{max}$ = 2.90 e Å^{-3}
251 parameters	$\Delta\rho_{min}$ = −1.45 e Å^{-3}
0 restraints	Extinction correction: none
? constraints	Extinction coefficient: ?
Primary atom site location: structure-invariant direct methods	

Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ir1	−0.267470 (6)	−0.258435 (10)	−0.998843 (5)	0.01386 (3)
Cl1	−0.32964 (5)	−0.54194 (8)	−1.06777 (4)	0.02188 (11)
N1	−0.29354 (16)	−0.3639 (3)	−0.92061 (13)	0.0166 (4)
N2	0.13504 (18)	−0.4641 (4)	−0.84389 (16)	0.0290 (5)
C1	−0.12850 (18)	−0.3758 (3)	−0.91031 (14)	0.0150 (4)
C2	−0.04238 (19)	−0.3782 (3)	−0.90755 (15)	0.0181 (4)
H2	−0.0467	−0.3205	−0.9499	0.022*
C3	0.05145 (19)	−0.4634 (3)	−0.84412 (15)	0.0198 (4)
C4	0.0559 (2)	−0.5514 (3)	−0.78263 (16)	0.0227 (5)
H4	0.1179	−0.6103	−0.7394	0.027*
C5	−0.0293 (2)	−0.5524 (3)	−0.78481 (15)	0.0207 (5)

H5	−0.0257	−0.6139	−0.7435	0.025*
C6	−0.12093 (18)	−0.4639 (3)	−0.84718 (14)	0.0158 (4)
C7	−0.21354 (19)	−0.4569 (3)	−0.85414 (14)	0.0170 (4)
C8	−0.2266 (2)	−0.5366 (3)	−0.80067 (16)	0.0229 (5)
H8	−0.1706	−0.5990	−0.7537	0.027*
C9	−0.3209 (2)	−0.5245 (4)	−0.81630 (17)	0.0270 (5)
H9	−0.3301	−0.5788	−0.7804	0.032*
C10	−0.4024 (2)	−0.4322 (4)	−0.88505 (18)	0.0268 (5)
H10	−0.4680	−0.4227	−0.8971	0.032*
C11	−0.3852 (2)	−0.3550 (4)	−0.93532 (17)	0.0228 (5)
H11	−0.4408	−0.2926	−0.9825	0.027*
C12	0.2370 (2)	−0.5113 (5)	−0.76996 (19)	0.0338 (7)
H12A	0.2564	−0.4307	−0.7256	0.051*
H12B	0.2878	−0.5011	−0.7794	0.051*
H12C	0.2359	−0.6340	−0.7547	0.051*
C13	0.1321 (2)	−0.3572 (5)	−0.9026 (2)	0.0342 (7)
H13A	0.0746	−0.3968	−0.9581	0.051*
H13B	0.1978	−0.3702	−0.8932	0.051*
H13C	0.1219	−0.2319	−0.8962	0.051*
C14	−0.2426 (2)	−0.0894 (3)	−1.06843 (14)	0.0182 (4)
C15	−0.20860 (19)	0.0023 (3)	−0.99487 (14)	0.0165 (4)
C16	−0.2977 (2)	0.0214 (3)	−0.99808 (15)	0.0177 (4)
C17	−0.3885 (2)	−0.0456 (3)	−1.07653 (16)	0.0209 (5)
C18	−0.3538 (2)	−0.1134 (3)	−1.11821 (15)	0.0202 (4)
C19	−0.1779 (2)	−0.1286 (4)	−1.09422 (18)	0.0267 (5)
H19A	−0.2017	−0.0550	−1.1417	0.040*
H19B	−0.1848	−0.2547	−1.1089	0.040*
H19C	−0.1049	−0.1017	−1.0490	0.040*

C20	−0.1043 (2)	0.0796 (4)	−0.93120 (16)	0.0246 (5)
H20A	−0.1026	0.2028	−0.9456	0.037*
H20B	−0.0516	0.0096	−0.9277	0.037*
H20C	−0.0897	0.0773	−0.8782	0.037*
C21	−0.3000 (2)	0.1134 (4)	−0.93623 (18)	0.0258 (5)
H21A	−0.2293	0.1211	−0.8841	0.039*
H21B	−0.3438	0.0460	−0.9283	0.039*
H21C	−0.3284	0.2336	−0.9556	0.039*
C22	−0.4982 (2)	−0.0315 (4)	−1.1086 (2)	0.0337 (7)
H22A	−0.5303	0.0749	−1.1430	0.050*
H22B	−0.4995	−0.0228	−1.0627	0.050*
H22C	−0.5369	−0.1373	−1.1412	0.050*
C23	−0.4212 (3)	−0.1961 (4)	−1.20203 (17)	0.0325 (6)
H23A	−0.4681	−0.2830	−1.2055	0.049*
H23B	−0.3774	−0.2560	−1.2119	0.049*
H23C	−0.4623	−0.1031	−1.2433	0.049*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01495 (4)	0.01173 (4)	0.01424 (4)	0.00102 (3)	0.00886 (3)	0.00074 (3)
Cl1	0.0270 (3)	0.0162 (2)	0.0246 (3)	−0.0030 (2)	0.0172 (2)	−0.0042 (2)
N1	0.0184 (9)	0.0156 (8)	0.0198 (9)	−0.0009 (7)	0.0139 (8)	−0.0007 (7)
N2	0.0181 (10)	0.0367 (13)	0.0314 (12)	0.0064 (9)	0.0151 (10)	0.0041 (10)
C1	0.0172 (10)	0.0113 (9)	0.0160 (9)	−0.0001 (7)	0.0102 (8)	0.0005 (7)
C2	0.0193 (10)	0.0168 (10)	0.0199 (10)	0.0033 (8)	0.0132 (9)	0.0032 (8)
C3	0.0161 (10)	0.0182 (10)	0.0214 (11)	0.0015 (8)	0.0100 (9)	−0.0012 (8)
C4	0.0195 (11)	0.0208 (11)	0.0189 (11)	0.0047 (9)	0.0078 (9)	0.0032 (9)
C5	0.0238 (11)	0.0183 (10)	0.0163 (10)	0.0007 (9)	0.0107 (9)	0.0025 (8)

C6	0.0184 (10)	0.0129 (9)	0.0151 (9)	−0.0008 (7)	0.0101 (8)	−0.0005 (7)
C7	0.0224 (11)	0.0133 (9)	0.0176 (10)	−0.0033 (8)	0.0136 (9)	−0.0030 (7)
C8	0.0306 (13)	0.0215 (11)	0.0203 (11)	−0.0041 (10)	0.0178 (10)	−0.0013 (9)
C9	0.0374 (15)	0.0276 (13)	0.0275 (13)	−0.0106 (11)	0.0260 (12)	−0.0069 (10)
C10	0.0294 (13)	0.0284 (13)	0.0344 (14)	−0.0068 (10)	0.0257 (12)	−0.0079 (11)
C11	0.0229 (12)	0.0233 (11)	0.0281 (12)	−0.0018 (9)	0.0189 (11)	−0.0031 (9)
C12	0.0184 (12)	0.0434 (17)	0.0301 (14)	0.0049 (12)	0.0106 (11)	−0.0067 (13)
C13	0.0284 (14)	0.0371 (16)	0.0467 (18)	0.0003 (12)	0.0282 (14)	0.0014 (13)
C14	0.0259 (11)	0.0154 (10)	0.0172 (10)	0.0019 (8)	0.0154 (9)	0.0037 (8)
C15	0.0221 (11)	0.0117 (9)	0.0161 (9)	−0.0006 (8)	0.0122 (9)	0.0005 (7)
C16	0.0238 (11)	0.0112 (9)	0.0201 (10)	0.0037 (8)	0.0148 (9)	0.0024 (8)
C17	0.0199 (11)	0.0165 (10)	0.0216 (11)	0.0043 (8)	0.0107 (9)	0.0028 (8)
C18	0.0234 (11)	0.0168 (10)	0.0164 (10)	0.0038 (8)	0.0105 (9)	0.0038 (8)
C19	0.0363 (15)	0.0265 (13)	0.0291 (13)	0.0021 (11)	0.0262 (12)	0.0021 (10)
C20	0.0276 (13)	0.0208 (11)	0.0225 (11)	−0.0064 (10)	0.0144 (10)	−0.0025 (9)
C21	0.0367 (15)	0.0201 (11)	0.0306 (13)	0.0032 (10)	0.0259 (12)	−0.0013 (10)
C22	0.0211 (13)	0.0325 (15)	0.0390 (16)	0.0088 (11)	0.0148 (12)	0.0057 (12)
C23	0.0354 (15)	0.0303 (14)	0.0168 (11)	0.0020 (12)	0.0091 (11)	−0.0014 (10)

Geometric parameters (Å, °)

Ir1—C1	2.037 (2)	C12—H12A	0.9800
Ir1—N1	2.097 (2)	C12—H12B	0.9800
Ir1—C14	2.161 (2)	C12—H12C	0.9800
Ir1—C16	2.163 (2)	C13—H13A	0.9800
Ir1—C15	2.166 (2)	C13—H13B	0.9800
Ir1—C18	2.238 (2)	C13—H13C	0.9800
Ir1—C17	2.263 (2)	C14—C15	1.443 (3)
Ir1—Cl1	2.4122 (6)	C14—C18	1.446 (4)

N1—C11	1.346 (3)	C14—C19	1.501 (4)
N1—C7	1.366 (3)	C15—C16	1.440 (3)
N2—C3	1.379 (3)	C15—C20	1.484 (4)
N2—C13	1.446 (4)	C16—C17	1.454 (4)
N2—C12	1.446 (4)	C16—C21	1.492 (3)
C1—C2	1.389 (3)	C17—C18	1.409 (4)
C1—C6	1.415 (3)	C17—C22	1.491 (4)
C2—C3	1.413 (3)	C18—C23	1.503 (4)
C2—H2	0.9500	C19—H19A	0.9800
C3—C4	1.410 (4)	C19—H19B	0.9800
C4—C5	1.380 (4)	C19—H19C	0.9800
C4—H4	0.9500	C20—H20A	0.9800
C5—C6	1.400 (3)	C20—H20B	0.9800
C5—H5	0.9500	C20—H20C	0.9800
C6—C7	1.445 (3)	C21—H21A	0.9800
C7—C8	1.404 (3)	C21—H21B	0.9800
C8—C9	1.379 (4)	C21—H21C	0.9800
C8—H8	0.9500	C22—H22A	0.9800
C9—C10	1.392 (4)	C22—H22B	0.9800
C9—H9	0.9500	C22—H22C	0.9800
C10—C11	1.380 (4)	C23—H23A	0.9800
C10—H10	0.9500	C23—H23B	0.9800
C11—H11	0.9500	C23—H23C	0.9800
C1—Ir1—N1	77.94 (9)	N2—C12—H12C	109.5
C1—Ir1—C14	106.65 (9)	H12A—C12—H12C	109.5
N1—Ir1—C14	166.19 (9)	H12B—C12—H12C	109.5
C1—Ir1—C16	123.20 (9)	N2—C13—H13A	109.5
N1—Ir1—C16	101.49 (9)	N2—C13—H13B	109.5
C14—Ir1—C16	64.96 (9)	H13A—C13—H13B	109.5

C1—Ir1—C15	97.70 (9)	N2—C13—H13C	109.5
N1—Ir1—C15	128.32 (8)	H13A—C13—H13C	109.5
C14—Ir1—C15	38.97 (9)	H13B—C13—H13C	109.5
C16—Ir1—C15	38.85 (9)	C15—C14—C18	107.3 (2)
C1—Ir1—C18	142.46 (9)	C15—C14—C19	126.3 (2)
N1—Ir1—C18	139.48 (9)	C18—C14—C19	125.8 (2)
C14—Ir1—C18	38.33 (9)	C15—C14—Ir1	70.70 (13)
C16—Ir1—C18	63.09 (9)	C18—C14—Ir1	73.73 (14)
C15—Ir1—C18	63.77 (9)	C19—C14—Ir1	127.56 (18)
C1—Ir1—C17	160.69 (10)	C16—C15—C14	107.3 (2)
N1—Ir1—C17	107.92 (9)	C16—C15—C20	125.5 (2)
C14—Ir1—C17	63.57 (10)	C14—C15—C20	127.0 (2)
C16—Ir1—C17	38.26 (9)	C16—C15—Ir1	70.48 (13)
C15—Ir1—C17	63.98 (9)	C14—C15—Ir1	70.33 (13)
C18—Ir1—C17	36.47 (9)	C20—C15—Ir1	128.94 (17)
C1—Ir1—Cl1	88.67 (7)	C15—C16—C17	108.5 (2)
N1—Ir1—Cl1	85.19 (6)	C15—C16—C21	126.1 (2)
C14—Ir1—Cl1	107.70 (7)	C17—C16—C21	125.0 (2)
C16—Ir1—Cl1	148.11 (7)	C15—C16—Ir1	70.67 (13)
C15—Ir1—Cl1	146.49 (6)	C17—C16—Ir1	74.58 (13)
C18—Ir1—Cl1	91.51 (7)	C21—C16—Ir1	126.10 (17)
C17—Ir1—Cl1	109.92 (7)	C18—C17—C16	107.2 (2)
C11—N1—C7	119.2 (2)	C18—C17—C22	126.9 (3)
C11—N1—Ir1	123.89 (18)	C16—C17—C22	125.8 (2)
C7—N1—Ir1	116.71 (16)	C18—C17—Ir1	70.82 (14)
C3—N2—C13	119.8 (2)	C16—C17—Ir1	67.16 (13)
C3—N2—C12	119.7 (3)	C22—C17—Ir1	130.6 (2)
C13—N2—C12	116.3 (3)	C17—C18—C14	109.5 (2)
C2—C1—C6	118.0 (2)	C17—C18—C23	125.7 (3)

C2—C1—Ir1	125.72 (17)	C14—C18—C23	124.7 (2)
C6—C1—Ir1	116.28 (17)	C17—C18—Ir1	72.71 (14)
C1—C2—C3	122.4 (2)	C14—C18—Ir1	67.94 (13)
C1—C2—H2	118.8	C23—C18—Ir1	126.29 (19)
C3—C2—H2	118.8	C14—C19—H19A	109.5
N2—C3—C4	121.3 (2)	C14—C19—H19B	109.5
N2—C3—C2	120.7 (2)	H19A—C19—H19B	109.5
C4—C3—C2	118.0 (2)	C14—C19—H19C	109.5
C5—C4—C3	120.5 (2)	H19A—C19—H19C	109.5
C5—C4—H4	119.8	H19B—C19—H19C	109.5
C3—C4—H4	119.8	C15—C20—H20A	109.5
C4—C5—C6	120.7 (2)	C15—C20—H20B	109.5
C4—C5—H5	119.6	H20A—C20—H20B	109.5
C6—C5—H5	119.6	C15—C20—H20C	109.5
C5—C6—C1	120.3 (2)	H20A—C20—H20C	109.5
C5—C6—C7	124.6 (2)	H20B—C20—H20C	109.5
C1—C6—C7	115.0 (2)	C16—C21—H21A	109.5
N1—C7—C8	119.9 (2)	C16—C21—H21B	109.5
N1—C7—C6	114.0 (2)	H21A—C21—H21B	109.5
C8—C7—C6	126.1 (2)	C16—C21—H21C	109.5
C9—C8—C7	120.0 (3)	H21A—C21—H21C	109.5
C9—C8—H8	120.0	H21B—C21—H21C	109.5
C7—C8—H8	120.0	C17—C22—H22A	109.5
C8—C9—C10	119.6 (2)	C17—C22—H22B	109.5
C8—C9—H9	120.2	H22A—C22—H22B	109.5
C10—C9—H9	120.2	C17—C22—H22C	109.5
C11—C10—C9	118.1 (3)	H22A—C22—H22C	109.5
C11—C10—H10	120.9	H22B—C22—H22C	109.5
C9—C10—H10	120.9	C18—C23—H23A	109.5

N1—C11—C10	123.1 (3)	C18—C23—H23B	109.5
N1—C11—H11	118.4	H23A—C23—H23B	109.5
C10—C11—H11	118.4	C18—C23—H23C	109.5
N2—C12—H12A	109.5	H23A—C23—H23C	109.5
N2—C12—H12B	109.5	H23B—C23—H23C	109.5
H12A—C12—H12B	109.5		
C1—Ir1—N1—C11	−176.8 (2)	Cl1—Ir1—C15—C14	7.7 (2)
C14—Ir1—N1—C11	72.2 (4)	C1—Ir1—C15—C20	−15.2 (2)
C16—Ir1—N1—C11	61.3 (2)	N1—Ir1—C15—C20	65.5 (3)
C15—Ir1—N1—C11	92.9 (2)	C14—Ir1—C15—C20	−122.2 (3)
C18—Ir1—N1—C11	−0.4 (3)	C16—Ir1—C15—C20	120.3 (3)
C17—Ir1—N1—C11	22.3 (2)	C18—Ir1—C15—C20	−160.8 (3)
Cl1—Ir1—N1—C11	−87.14 (19)	C17—Ir1—C15—C20	158.4 (3)
C1—Ir1—N1—C7	−1.37 (17)	Cl1—Ir1—C15—C20	−114.5 (2)
C14—Ir1—N1—C7	−112.4 (4)	C14—C15—C16—C17	−4.5 (3)
C16—Ir1—N1—C7	−123.23 (17)	C20—C15—C16—C17	170.0 (2)
C15—Ir1—N1—C7	−91.70 (19)	Ir1—C15—C16—C17	−65.53 (16)
C18—Ir1—N1—C7	174.99 (16)	C14—C15—C16—C21	−177.9 (2)
C17—Ir1—N1—C7	−162.30 (16)	C20—C15—C16—C21	−3.4 (4)
Cl1—Ir1—N1—C7	88.30 (16)	Ir1—C15—C16—C21	121.1 (2)
N1—Ir1—C1—C2	−179.9 (2)	C14—C15—C16—Ir1	61.02 (15)
C14—Ir1—C1—C2	−13.4 (2)	C20—C15—C16—Ir1	−124.5 (2)
C16—Ir1—C1—C2	−84.0 (2)	C1—Ir1—C16—C15	56.14 (17)
C15—Ir1—C1—C2	−52.3 (2)	N1—Ir1—C16—C15	139.15 (13)
C18—Ir1—C1—C2	4.0 (3)	C14—Ir1—C16—C15	−38.01 (13)
C17—Ir1—C1—C2	−69.9 (4)	C18—Ir1—C16—C15	−80.80 (15)
Cl1—Ir1—C1—C2	94.7 (2)	C17—Ir1—C16—C15	−116.4 (2)
N1—Ir1—C1—C6	0.98 (16)	Cl1—Ir1—C16—C15	−121.37 (14)

C14—Ir1—C1—C6	167.52 (17)	C1—Ir1—C16—C17	172.56 (14)
C16—Ir1—C1—C6	96.93 (18)	N1—Ir1—C16—C17	−104.43 (15)
C15—Ir1—C1—C6	128.64 (17)	C14—Ir1—C16—C17	78.41 (16)
C18—Ir1—C1—C6	−175.14 (16)	C15—Ir1—C16—C17	116.4 (2)
C17—Ir1—C1—C6	111.0 (3)	C18—Ir1—C16—C17	35.63 (15)
Cl1—Ir1—C1—C6	−84.39 (17)	Cl1—Ir1—C16—C17	−5.0 (2)
C6—C1—C2—C3	−0.6 (3)	C1—Ir1—C16—C21	−65.0 (3)
Ir1—C1—C2—C3	−179.67 (18)	N1—Ir1—C16—C21	18.0 (2)
C13—N2—C3—C4	−173.4 (3)	C14—Ir1—C16—C21	−159.2 (3)
C12—N2—C3—C4	−17.1 (4)	C15—Ir1—C16—C21	−121.2 (3)
C13—N2—C3—C2	8.4 (4)	C18—Ir1—C16—C21	158.0 (3)
C12—N2—C3—C2	164.6 (3)	C17—Ir1—C16—C21	122.4 (3)
C1—C2—C3—N2	179.5 (2)	Cl1—Ir1—C16—C21	117.5 (2)
C1—C2—C3—C4	1.2 (4)	C15—C16—C17—C18	3.2 (3)
N2—C3—C4—C5	−178.6 (2)	C21—C16—C17—C18	176.7 (2)
C2—C3—C4—C5	−0.3 (4)	Ir1—C16—C17—C18	−59.77 (17)
C3—C4—C5—C6	−1.1 (4)	C15—C16—C17—C22	−172.5 (2)
C4—C5—C6—C1	1.7 (4)	C21—C16—C17—C22	0.9 (4)
C4—C5—C6—C7	−179.6 (2)	Ir1—C16—C17—C22	124.5 (3)
C2—C1—C6—C5	−0.8 (3)	C15—C16—C17—Ir1	62.99 (15)
Ir1—C1—C6—C5	178.32 (18)	C21—C16—C17—Ir1	−123.6 (2)
C2—C1—C6—C7	−179.7 (2)	C1—Ir1—C17—C18	100.0 (3)
Ir1—C1—C6—C7	−0.5 (3)	N1—Ir1—C17—C18	−155.04 (15)
C11—N1—C7—C8	−2.1 (3)	C14—Ir1—C17—C18	36.74 (15)
Ir1—N1—C7—C8	−177.76 (18)	C16—Ir1—C17—C18	119.1 (2)
C11—N1—C7—C6	177.1 (2)	C15—Ir1—C17—C18	80.40 (16)
Ir1—N1—C7—C6	1.5 (3)	Cl1—Ir1—C17—C18	−63.69 (16)
C5—C6—C7—N1	−179.4 (2)	C1—Ir1—C17—C16	−19.1 (4)

C1—C6—C7—N1	−0.6 (3)	N1—Ir1—C17—C16	85.88 (15)
C5—C6—C7—C8	−0.2 (4)	C14—Ir1—C17—C16	−82.35 (16)
C1—C6—C7—C8	178.6 (2)	C15—Ir1—C17—C16	−38.69 (14)
N1—C7—C8—C9	1.5 (4)	C18—Ir1—C17—C16	−119.1 (2)
C6—C7—C8—C9	−177.7 (2)	Cl1—Ir1—C17—C16	177.22 (13)
C7—C8—C9—C10	−0.3 (4)	C1—Ir1—C17—C22	−137.5 (3)
C8—C9—C10—C11	−0.2 (4)	N1—Ir1—C17—C22	−32.5 (3)
C7—N1—C11—C10	1.6 (4)	C14—Ir1—C17—C22	159.3 (3)
Ir1—N1—C11—C10	177.0 (2)	C16—Ir1—C17—C22	−118.3 (3)
C9—C10—C11—N1	−0.4 (4)	C15—Ir1—C17—C22	−157.0 (3)
C1—Ir1—C14—C15	−81.53 (15)	C18—Ir1—C17—C22	122.6 (3)
N1—Ir1—C14—C15	26.1 (4)	Cl1—Ir1—C17—C22	58.9 (3)
C16—Ir1—C14—C15	37.88 (14)	C16—C17—C18—C14	−0.7 (3)
C18—Ir1—C14—C15	115.5 (2)	C22—C17—C18—C14	175.0 (3)
C17—Ir1—C14—C15	80.52 (15)	Ir1—C17—C18—C14	−58.14 (17)
Cl1—Ir1—C14—C15	−175.54 (12)	C16—C17—C18—C23	−179.9 (2)
C1—Ir1—C14—C18	162.97 (14)	C22—C17—C18—C23	−4.2 (4)
N1—Ir1—C14—C18	−89.4 (4)	Ir1—C17—C18—C23	122.7 (3)
C16—Ir1—C14—C18	−77.62 (15)	C16—C17—C18—Ir1	57.47 (16)
C15—Ir1—C14—C18	−115.5 (2)	C22—C17—C18—Ir1	−126.8 (3)
C17—Ir1—C14—C18	−34.98 (14)	C15—C14—C18—C17	−2.1 (3)
Cl1—Ir1—C14—C18	68.96 (14)	C19—C14—C18—C17	−174.0 (2)
C1—Ir1—C14—C19	39.9 (3)	Ir1—C14—C18—C17	61.05 (18)
N1—Ir1—C14—C19	147.6 (3)	C15—C14—C18—C23	177.1 (2)
C16—Ir1—C14—C19	159.4 (3)	C19—C14—C18—C23	5.2 (4)
C15—Ir1—C14—C19	121.5 (3)	Ir1—C14—C18—C23	−119.7 (3)
C18—Ir1—C14—C19	−123.0 (3)	C15—C14—C18—Ir1	−63.16 (15)
C17—Ir1—C14—C19	−158.0 (3)	C19—C14—C18—Ir1	124.9 (2)

Cl1—Ir1—C14—C19	−54.1 (2)	C1—Ir1—C18—C17	−147.69 (16)
C18—C14—C15—C16	4.0 (3)	N1—Ir1—C18—C17	38.2 (2)
C19—C14—C15—C16	175.9 (2)	C14—Ir1—C18—C17	−120.3 (2)
Ir1—C14—C15—C16	−61.12 (15)	C16—Ir1—C18—C17	−37.36 (15)
C18—C14—C15—C20	−170.3 (2)	C15—Ir1—C18—C17	−81.01 (16)
C19—C14—C15—C20	1.5 (4)	Cl1—Ir1—C18—C17	122.53 (14)
Ir1—C14—C15—C20	124.5 (2)	C1—Ir1—C18—C14	−27.4 (2)
C18—C14—C15—Ir1	65.17 (16)	N1—Ir1—C18—C14	158.44 (14)
C19—C14—C15—Ir1	−123.0 (2)	C16—Ir1—C18—C14	82.91 (15)
C1—Ir1—C15—C16	−135.48 (14)	C15—Ir1—C18—C14	39.26 (14)
N1—Ir1—C15—C16	−54.79 (17)	C17—Ir1—C18—C14	120.3 (2)
C14—Ir1—C15—C16	117.5 (2)	Cl1—Ir1—C18—C14	−117.20 (13)
C18—Ir1—C15—C16	78.90 (15)	C1—Ir1—C18—C23	90.3 (3)
C17—Ir1—C15—C16	38.11 (14)	N1—Ir1—C18—C23	−83.8 (3)
Cl1—Ir1—C15—C16	125.22 (13)	C14—Ir1—C18—C23	117.7 (3)
C1—Ir1—C15—C14	107.02 (15)	C16—Ir1—C18—C23	−159.4 (3)
N1—Ir1—C15—C14	−172.30 (13)	C15—Ir1—C18—C23	157.0 (3)
C16—Ir1—C15—C14	−117.5 (2)	C17—Ir1—C18—C23	−122.0 (3)
C18—Ir1—C15—C14	−38.61 (14)	Cl1—Ir1—C18—C23	0.5 (2)
C17—Ir1—C15—C14	−79.40 (15)		

All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Computing details

Data collection: Bruker *APEX2*; cell refinement: Bruker *SAINT*; data reduction: Bruker *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: Bruker *SHELXTL*; software used to prepare material for publication: Bruker *SHELXTL*.

3a

Table 1. Crystal data for 3a

Compound	3a
Molecular formula	$C_{33}H_{43}ClIr_2N_2,C_3H_6O,_2(F_6P)$
Molecular weight	1235.56
Crystal habit	Orange Needle
Crystal dimensions(mm)	0.28x0.12x0.10
Crystal system	monoclinic
Space group	$P2_1/c$
a(Å)	13.019(1)
b(Å)	20.090(1)
c(Å)	17.132(1)
α(°)	90.00
β(°)	108.824(1)
γ(°)	90.00
V(Å^3)	4241.2(5)
Z	4
d(g-cm^{-3})	1.935
F(000)	2384
μ(cm^{-1})	6.492
Absorption corrections	multi-scan ; 0.2637 min, 0.5629 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	-15 18 ; -24 28 ; -24 22
Reflections measured	30593
Unique data	12327
Rint	0.0464
Reflections used	8865
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	519
Reflections / parameter	17
wR2	0.1312
R1	0.0440
Weights a, b	0.0768 ; 0.0000
GoF	0.990
difference peak / hole (e Å^{-3})	2.681(0.354) / -2.894(0.354)

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

atom	x	y	z	U(eq)
Ir(1)	-2412(1)	2201(1)	-1750(1)	23(1)
Ir(2)	-5215(1)	3280(1)	-2826(1)	25(1)
Cl(1)	-5559(2)	2616(1)	-1792(1)	52(1)
N(1)	-5395(4)	2388(2)	-3482(3)	32(1)
N(2)	-771(4)	3580(2)	-1753(3)	32(1)
C(1)	-3652(5)	2998(3)	-2579(4)	24(1)
C(2)	-2694(5)	3295(3)	-2032(4)	24(1)
C(3)	-1626(5)	3206(3)	-2129(4)	27(1)
C(4)	-1512(5)	2600(3)	-2560(4)	28(1)
C(5)	-2429(5)	2242(3)	-3029(4)	29(1)
C(6)	-3498(5)	2431(3)	-3045(4)	26(1)
C(7)	-4495(5)	2082(3)	-3528(4)	28(1)
C(8)	-4534(6)	1489(3)	-3949(4)	36(1)
C(9)	-5539(7)	1209(3)	-4349(5)	49(2)
C(10)	-6471(6)	1514(4)	-4287(5)	56(2)
C(11)	-6374(6)	2100(3)	-3855(6)	50(2)
C(12)	-853(6)	4158(3)	-1256(5)	44(2)
C(13)	299(6)	3437(4)	-1805(6)	49(2)
C(14)	-1540(6)	2048(3)	-453(4)	34(1)
C(15)	-1200(5)	1552(3)	-919(4)	36(1)
C(16)	-2143(6)	1156(3)	-1350(4)	33(1)
C(17)	-3045(5)	1407(3)	-1129(4)	30(1)
C(18)	-2680(5)	1956(3)	-583(4)	30(1)
C(19)	-806(7)	2547(4)	127(4)	54(2)
C(20)	-93(6)	1432(4)	-941(6)	56(2)
C(21)	-2126(7)	559(3)	-1854(5)	52(2)
C(22)	-4137(6)	1093(3)	-1385(5)	43(2)
C(23)	-3316(7)	2316(3)	-118(4)	43(2)
C(24)	-6551(6)	3871(3)	-3692(4)	40(2)
C(25)	-6629(6)	3951(3)	-2900(5)	39(2)
C(26)	-5613(6)	4226(3)	-2378(4)	40(2)
C(27)	-4934(6)	4351(3)	-2871(5)	40(2)
C(28)	-5495(6)	4093(3)	-3681(5)	41(2)
C(29)	-7430(10)	3623(4)	-4445(6)	84(3)
C(30)	-7557(7)	3782(4)	-2616(7)	68(3)
C(31)	-5380(10)	4405(4)	-1481(6)	76(3)
C(32)	-3891(6)	4707(4)	-2589(8)	74(3)
C(33)	-5110(10)	4162(5)	-4423(6)	84(4)
P(1)	-2267(2)	328(1)	-4591(1)	36(1)
F(1)	-3530(4)	261(2)	-4697(3)	51(1)
F(2)	-2054(5)	-365(3)	-4127(4)	85(2)
F(3)	-1018(4)	386(2)	-4489(3)	64(1)
F(4)	-2496(4)	1013(2)	-5077(4)	69(2)
F(5)	-2473(4)	-45(2)	-5453(3)	65(1)
F(6)	-2097(5)	711(3)	-3758(3)	88(2)
P(2)	-1370(2)	4520(1)	-3936(1)	45(1)
F(7)	-1090(10)	3775(3)	-3868(5)	163(4)
F(8)	-1816(7)	4470(4)	-3211(4)	115(3)
F(9)	-1550(10)	5262(3)	-3986(5)	174(5)
F(10)	-850(10)	4551(5)	-4631(6)	171(4)
F(11)	-231(6)	4665(5)	-3253(6)	162(4)
F(12)	-2436(6)	4375(4)	-4605(5)	148(4)
O(1)	-9219(7)	2052(4)	-2762(6)	110(3)
C(34)	-8625(8)	1586(4)	-2621(7)	64(2)
C(35)	-7710(10)	1556(8)	-1860(10)	142(7)
C(36)	-8740(20)	1052(6)	-3210(10)	136(6)

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

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

Ir(1)-C(14)	2.166(6)	Ir(1)-C(15)	2.184(6)
Ir(1)-C(5)	2.186(6)	Ir(1)-C(18)	2.193(6)
Ir(1)-C(16)	2.202(6)	Ir(1)-C(17)	2.218(5)
Ir(1)-C(4)	2.234(5)	Ir(1)-C(2)	2.254(5)
Ir(1)-C(6)	2.261(6)	Ir(1)-C(1)	2.390(6)
Ir(1)-C(3)	2.444(5)	Ir(2)-C(1)	2.021(6)
Ir(2)-N(1)	2.087(5)	Ir(2)-C(28)	2.145(6)
Ir(2)-C(26)	2.175(6)	Ir(2)-C(27)	2.188(6)
Ir(2)-C(24)	2.230(6)	Ir(2)-C(25)	2.251(6)
Ir(2)-Cl(1)	2.373(2)	N(1)-C(7)	1.349(8)
N(1)-C(11)	1.36(1)	N(2)-C(3)	1.326(7)
N(2)-C(13)	1.453(8)	N(2)-C(12)	1.464(8)
C(1)-C(2)	1.426(8)	C(1)-C(6)	1.443(8)
C(2)-C(3)	1.463(8)	C(2)-H(2)	0.9500
C(3)-C(4)	1.456(8)	C(4)-C(5)	1.40(1)
C(4)-H(4)	0.9500	C(5)-C(6)	1.434(8)
C(5)-H(5)	0.9500	C(6)-C(7)	1.472(8)
C(7)-C(8)	1.385(8)	C(8)-C(9)	1.38(1)
C(8)-H(8)	0.9500	C(9)-C(10)	1.39(1)
C(9)-H(9)	0.9500	C(10)-C(11)	1.37(1)
C(10)-H(10)	0.9500	C(11)-H(11)	0.9500
C(12)-H(12A)	0.9800	C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800	C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800	C(13)-H(13C)	0.9800
C(14)-C(15)	1.43(1)	C(14)-C(18)	1.44(1)
C(14)-C(19)	1.51(1)	C(15)-C(16)	1.45(1)
C(15)-C(20)	1.47(1)	C(16)-C(17)	1.44(1)
C(16)-C(21)	1.48(1)	C(17)-C(18)	1.425(8)
C(17)-C(22)	1.49(1)	C(18)-C(23)	1.506(8)
C(19)-H(19A)	0.9800	C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800	C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800	C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800	C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800	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)	1.40(1)
C(24)-C(28)	1.44(1)	C(24)-C(29)	1.50(1)
C(25)-C(26)	1.45(1)	C(25)-C(30)	1.48(1)
C(26)-C(27)	1.43(1)	C(26)-C(31)	1.51(1)
C(27)-C(28)	1.44(1)	C(27)-C(32)	1.47(1)
C(28)-C(33)	1.52(1)	C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800	C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800	C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800	C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800	C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800	C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800	C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800	C(33)-H(33C)	0.9800
P(1)-F(6)	1.573(5)	P(1)-F(3)	1.582(5)
P(1)-F(2)	1.584(5)	P(1)-F(4)	1.586(5)
P(1)-F(5)	1.598(5)	P(1)-F(1)	1.601(5)
P(2)-F(9)	1.507(6)	P(2)-F(12)	1.516(7)
P(2)-F(8)	1.534(6)	P(2)-F(7)	1.538(7)
P(2)-F(10)	1.551(7)	P(2)-F(11)	1.592(8)
O(1)-C(34)	1.19(1)	C(34)-C(36)	1.44(1)
C(34)-C(35)	1.46(2)	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(14)-Ir(1)-C(15)	38.5(2)	C(14)-Ir(1)-C(5)	150.0(3)
C(15)-Ir(1)-C(5)	116.6(2)	C(14)-Ir(1)-C(18)	38.6(2)

C(15)-Ir(1)-C(18)	64.3(2)	C(5)-Ir(1)-C(18)	165.7(2)
C(14)-Ir(1)-C(16)	64.4(2)	C(15)-Ir(1)-C(16)	38.6(2)
C(5)-Ir(1)-C(16)	107.2(2)	C(18)-Ir(1)-C(16)	63.8(2)
C(14)-Ir(1)-C(17)	63.8(2)	C(15)-Ir(1)-C(17)	63.9(2)
C(5)-Ir(1)-C(17)	128.5(2)	C(18)-Ir(1)-C(17)	37.7(2)
C(16)-Ir(1)-C(17)	37.9(2)	C(14)-Ir(1)-C(4)	118.8(2)
C(15)-Ir(1)-C(4)	101.9(2)	C(5)-Ir(1)-C(4)	37.0(2)
C(18)-Ir(1)-C(4)	156.4(2)	C(16)-Ir(1)-C(4)	118.2(2)
C(17)-Ir(1)-C(4)	155.0(2)	C(14)-Ir(1)-C(2)	110.8(2)
C(15)-Ir(1)-C(2)	139.1(2)	C(5)-Ir(1)-C(2)	78.5(2)
C(18)-Ir(1)-C(2)	110.6(2)	C(16)-Ir(1)-C(2)	174.3(2)
C(17)-Ir(1)-C(2)	138.1(2)	C(4)-Ir(1)-C(2)	66.3(2)
C(14)-Ir(1)-C(6)	172.1(2)	C(15)-Ir(1)-C(6)	148.5(2)
C(5)-Ir(1)-C(6)	37.6(2)	C(18)-Ir(1)-C(6)	135.0(2)
C(16)-Ir(1)-C(6)	119.1(2)	C(17)-Ir(1)-C(6)	113.9(2)
C(4)-Ir(1)-C(6)	66.7(2)	C(2)-Ir(1)-C(6)	65.4(2)
C(14)-Ir(1)-C(1)	137.4(2)	C(15)-Ir(1)-C(1)	174.6(2)
C(5)-Ir(1)-C(1)	65.9(2)	C(18)-Ir(1)-C(1)	114.6(2)
C(16)-Ir(1)-C(1)	146.4(2)	C(17)-Ir(1)-C(1)	118.9(2)
C(4)-Ir(1)-C(1)	77.2(2)	C(2)-Ir(1)-C(1)	35.6(2)
C(6)-Ir(1)-C(1)	36.0(2)	C(14)-Ir(1)-C(3)	105.4(2)
C(15)-Ir(1)-C(3)	113.0(2)	C(5)-Ir(1)-C(3)	64.7(2)
C(18)-Ir(1)-C(3)	129.2(2)	C(16)-Ir(1)-C(3)	146.3(2)
C(17)-Ir(1)-C(3)	166.8(2)	C(4)-Ir(1)-C(3)	35.9(2)
C(2)-Ir(1)-C(3)	36.0(2)	C(6)-Ir(1)-C(3)	75.7(2)
C(1)-Ir(1)-C(3)	63.2(2)	C(1)-Ir(2)-N(1)	78.7(2)
C(1)-Ir(2)-C(28)	107.1(2)	N(1)-Ir(2)-C(28)	108.8(2)
C(1)-Ir(2)-C(26)	120.6(3)	N(1)-Ir(2)-C(26)	160.4(2)
C(28)-Ir(2)-C(26)	64.4(3)	C(1)-Ir(2)-C(27)	96.5(2)
N(1)-Ir(2)-C(27)	144.7(3)	C(28)-Ir(2)-C(27)	38.8(3)
C(26)-Ir(2)-C(27)	38.2(3)	C(1)-Ir(2)-C(24)	143.6(3)
N(1)-Ir(2)-C(24)	99.8(2)	C(28)-Ir(2)-C(24)	38.4(3)
C(26)-Ir(2)-C(24)	63.0(3)	C(27)-Ir(2)-C(24)	63.7(3)
C(1)-Ir(2)-C(25)	158.2(2)	N(1)-Ir(2)-C(25)	122.4(2)
C(28)-Ir(2)-C(25)	63.2(2)	C(26)-Ir(2)-C(25)	38.1(3)
C(27)-Ir(2)-C(25)	63.4(2)	C(24)-Ir(2)-C(25)	36.5(3)
C(1)-Ir(2)-Cl(1)	96.1(2)	N(1)-Ir(2)-Cl(1)	84.5(2)
C(28)-Ir(2)-Cl(1)	155.0(2)	C(26)-Ir(2)-Cl(1)	95.9(2)
C(27)-Ir(2)-Cl(1)	130.8(2)	C(24)-Ir(2)-Cl(1)	120.1(2)
C(25)-Ir(2)-Cl(1)	91.7(2)	C(7)-N(1)-C(11)	118.7(5)
C(7)-N(1)-Ir(2)	118.3(4)	C(11)-N(1)-Ir(2)	123.0(4)
C(3)-N(2)-C(13)	122.0(5)	C(3)-N(2)-C(12)	121.6(5)
C(13)-N(2)-C(12)	116.4(5)	C(2)-C(1)-C(6)	116.5(5)
C(2)-C(1)-Ir(2)	129.0(4)	C(6)-C(1)-Ir(2)	114.5(4)
C(2)-C(1)-Ir(1)	67.0(3)	C(6)-C(1)-Ir(1)	67.1(3)
Ir(2)-C(1)-Ir(1)	138.9(3)	C(1)-C(2)-C(3)	122.4(5)
C(1)-C(2)-Ir(1)	77.4(3)	C(3)-C(2)-Ir(1)	79.1(3)
C(1)-C(2)-H(2)	118.8	C(3)-C(2)-H(2)	118.8
Ir(1)-C(2)-H(2)	115.0	N(2)-C(3)-C(4)	120.9(5)
N(2)-C(3)-C(2)	123.8(5)	C(4)-C(3)-C(2)	114.6(5)
N(2)-C(3)-Ir(1)	134.2(4)	C(4)-C(3)-Ir(1)	64.2(3)
C(2)-C(3)-Ir(1)	64.9(3)	C(5)-C(4)-C(3)	120.8(5)
C(5)-C(4)-Ir(1)	69.6(3)	C(3)-C(4)-Ir(1)	79.9(3)
C(5)-C(4)-H(4)	119.6	C(3)-C(4)-H(4)	119.6
Ir(1)-C(4)-H(4)	121.9	C(4)-C(5)-C(6)	121.1(5)
C(4)-C(5)-Ir(1)	73.4(3)	C(6)-C(5)-Ir(1)	74.1(3)
C(4)-C(5)-H(5)	119.4	C(6)-C(5)-H(5)	119.4
Ir(1)-C(5)-H(5)	124.8	C(5)-C(6)-C(1)	120.3(5)
C(5)-C(6)-C(7)	124.0(5)	C(1)-C(6)-C(7)	115.6(5)
C(5)-C(6)-Ir(1)	68.3(3)	C(1)-C(6)-Ir(1)	76.8(3)
C(7)-C(6)-Ir(1)	127.9(4)	N(1)-C(7)-C(8)	122.4(6)
N(1)-C(7)-C(6)	112.1(5)	C(8)-C(7)-C(6)	125.4(6)
C(9)-C(8)-C(7)	118.5(6)	C(9)-C(8)-H(8)	120.8
C(7)-C(8)-H(8)	120.8	C(8)-C(9)-C(10)	119.4(6)
C(8)-C(9)-H(9)	120.3	C(10)-C(9)-H(9)	120.3
C(11)-C(10)-C(9)	119.1(7)	C(11)-C(10)-H(10)	120.4
C(9)-C(10)-H(10)	120.4	N(1)-C(11)-C(10)	121.8(7)

N(1)-C(11)-H(11)	119.1	C(10)-C(11)-H(11)	119.1
N(2)-C(12)-H(12A)	109.5	N(2)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	N(2)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-H(13A)	109.5	N(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	N(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(18)	108.3(5)	C(15)-C(14)-C(19)	125.7(7)
C(18)-C(14)-C(19)	125.9(6)	C(15)-C(14)-Ir(1)	71.4(4)
C(18)-C(14)-Ir(1)	71.7(3)	C(19)-C(14)-Ir(1)	126.1(4)
C(14)-C(15)-C(16)	107.6(6)	C(14)-C(15)-C(20)	127.4(7)
C(16)-C(15)-C(20)	124.9(7)	C(14)-C(15)-Ir(1)	70.1(4)
C(16)-C(15)-Ir(1)	71.4(4)	C(20)-C(15)-Ir(1)	126.0(5)
C(17)-C(16)-C(15)	107.5(5)	C(17)-C(16)-C(21)	127.3(6)
C(15)-C(16)-C(21)	124.9(6)	C(17)-C(16)-Ir(1)	71.6(3)
C(15)-C(16)-Ir(1)	70.0(3)	C(21)-C(16)-Ir(1)	128.4(5)
C(18)-C(17)-C(16)	108.6(5)	C(18)-C(17)-C(22)	127.3(6)
C(16)-C(17)-C(22)	123.9(6)	C(18)-C(17)-Ir(1)	70.2(3)
C(16)-C(17)-Ir(1)	70.4(3)	C(22)-C(17)-Ir(1)	129.2(5)
C(17)-C(18)-C(14)	108.0(5)	C(17)-C(18)-C(23)	126.5(6)
C(14)-C(18)-C(23)	124.9(6)	C(17)-C(18)-Ir(1)	72.1(3)
C(14)-C(18)-Ir(1)	69.7(3)	C(23)-C(18)-Ir(1)	130.6(4)
C(14)-C(19)-H(19A)	109.5	C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5	C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5	H(19B)-C(19)-H(19C)	109.5
C(15)-C(20)-H(20A)	109.5	C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5	C(15)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5	H(20B)-C(20)-H(20C)	109.5
C(16)-C(21)-H(21A)	109.5	C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5	C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5	H(21B)-C(21)-H(21C)	109.5
C(17)-C(22)-H(22A)	109.5	C(17)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5	C(17)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(22B)-C(22)-H(22C)	109.5
C(18)-C(23)-H(23A)	109.5	C(18)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5	C(18)-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(28)	108.5(6)	C(25)-C(24)-C(29)	126.6(8)
C(28)-C(24)-C(29)	124.8(8)	C(25)-C(24)-Ir(2)	72.6(4)
C(28)-C(24)-Ir(2)	67.6(4)	C(29)-C(24)-Ir(2)	127.4(5)
C(24)-C(25)-C(26)	107.8(6)	C(24)-C(25)-C(30)	127.8(8)
C(26)-C(25)-C(30)	124.4(8)	C(24)-C(25)-Ir(2)	70.9(4)
C(26)-C(25)-Ir(2)	68.1(3)	C(30)-C(25)-Ir(2)	125.7(4)
C(27)-C(26)-C(25)	108.5(6)	C(27)-C(26)-C(31)	127.0(8)
C(25)-C(26)-C(31)	124.2(7)	C(27)-C(26)-Ir(2)	71.4(3)
C(25)-C(26)-Ir(2)	73.8(3)	C(31)-C(26)-Ir(2)	125.2(5)
C(26)-C(27)-C(28)	106.8(6)	C(26)-C(27)-C(32)	124.9(8)
C(28)-C(27)-C(32)	128.3(8)	C(26)-C(27)-Ir(2)	70.4(3)
C(28)-C(27)-Ir(2)	69.0(3)	C(32)-C(27)-Ir(2)	127.8(5)
C(27)-C(28)-C(24)	108.1(6)	C(27)-C(28)-C(33)	124.9(8)
C(24)-C(28)-C(33)	126.2(8)	C(27)-C(28)-Ir(2)	72.2(4)
C(24)-C(28)-Ir(2)	74.0(4)	C(33)-C(28)-Ir(2)	127.7(5)
C(24)-C(29)-H(29A)	109.5	C(24)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5	C(24)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5	H(29B)-C(29)-H(29C)	109.5
C(25)-C(30)-H(30A)	109.5	C(25)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5	C(25)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(30B)-C(30)-H(30C)	109.5
C(26)-C(31)-H(31A)	109.5	C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5	C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(27)-C(32)-H(32A)	109.5	C(27)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5	C(27)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(32B)-C(32)-H(32C)	109.5
C(28)-C(33)-H(33A)	109.5	C(28)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5	C(28)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5	H(33B)-C(33)-H(33C)	109.5

F(6)-P(1)-F(3)	91.4(3)	F(6)-P(1)-F(2)	91.4(3)
F(3)-P(1)-F(2)	90.1(3)	F(6)-P(1)-F(4)	90.0(3)
F(3)-P(1)-F(4)	90.4(3)	F(2)-P(1)-F(4)	178.6(4)
F(6)-P(1)-F(5)	178.1(3)	F(3)-P(1)-F(5)	89.9(3)
F(2)-P(1)-F(5)	90.0(3)	F(4)-P(1)-F(5)	88.6(3)
F(6)-P(1)-F(1)	89.0(3)	F(3)-P(1)-F(1)	179.4(3)
F(2)-P(1)-F(1)	89.4(3)	F(4)-P(1)-F(1)	90.1(2)
F(5)-P(1)-F(1)	89.7(3)	F(9)-P(2)-F(12)	93.6(5)
F(9)-P(2)-F(8)	91.2(5)	F(12)-P(2)-F(8)	96.1(5)
F(9)-P(2)-F(7)	175.0(6)	F(12)-P(2)-F(7)	90.5(5)
F(8)-P(2)-F(7)	91.1(5)	F(9)-P(2)-F(10)	90.8(5)
F(12)-P(2)-F(10)	87.1(6)	F(8)-P(2)-F(10)	176.2(6)
F(7)-P(2)-F(10)	86.6(5)	F(9)-P(2)-F(11)	87.1(5)
F(12)-P(2)-F(11)	178.2(5)	F(8)-P(2)-F(11)	85.6(5)
F(7)-P(2)-F(11)	88.7(5)	F(10)-P(2)-F(11)	91.3(6)
O(1)-C(34)-C(36)	122(1)	O(1)-C(34)-C(35)	120(1)
C(36)-C(34)-C(35)	118(1)	C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5	H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5	H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5	C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5	H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5	H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5		

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

atom	x	y	z	U(eq)
H(2)	-2751	3559	-1588.9999	29
H(4)	-807.9999	2445	-2523	34
H(5)	-2340	1868	-3340	35
H(8)	-3887	1278	-3963	43
H(9)	-5593	813	-4662	58
H(10)	-7164.0005	1320	-4539	67
H(11)	-7011	2309	-3816	60
H(12A)	-1581	4351	-1477	65
H(12B)	-312	4491	-1275	65
H(12C)	-722	4018	-684	65
H(13A)	633	3075	-1423	73
H(13B)	754	3836	-1657	73
H(13C)	233	3303	-2369	73
H(19A)	-452	2336	662	81
H(19B)	-1238	2927	200	81
H(19C)	-253	2702	-107.0000	81
H(20A)	340	1838	-776	84
H(20B)	-126	1309	-1502	84
H(20C)	242	1071	-560	84
H(21A)	-1883	173	-1492.0001	77
H(21B)	-1626	634	-2168	77
H(21C)	-2857	476	-2236	77
H(22A)	-4108	680	-1074	65
H(22B)	-4364	993	-1976.0001	65
H(22C)	-4658	1400	-1273	65
H(23A)	-4093.9998	2243	-393.0000	64
H(23B)	-3159	2794	-107.0000	64
H(23C)	-3111	2146	447	64
H(29A)	-7595.0005	3158	-4362	127
H(29B)	-7176	3653	-4925	127
H(29C)	-8080.0005	3896	-4539	127
H(30A)	-7932	4191	-2552	101
H(30B)	-7292	3551	-2085	101
H(30C)	-8062.0005	3492	-3022	101
H(31A)	-4604	4493	-1227	114
H(31B)	-5596	4035	-1195	114
H(31C)	-5795	4804	-1441	114
H(32A)	-3423	4549	-2898	111
H(32B)	-3537	4623	-1999	111
H(32C)	-4019	5184	-2681	111
H(33A)	-5518	4516	-4784	126
H(33B)	-5220	3741	-4727	126
H(33C)	-4333	4275	-4237	126
H(35A)	-7039	1491	-1988	214
H(35B)	-7815	1184	-1521	214
H(35C)	-7669	1974	-1553.0001	214
H(36A)	-9295	1169	-3726	204
H(36B)	-8948	643	-2985	204
H(36C)	-8043	982	-3303	204

4a

Table 1. Crystal data for **4a**

Compound	**4a**
Molecular formula	$C_{33}H_{43}ClIrN_2Ru,F_6P$
Molecular weight	941.38
Crystal habit	Orange Plate

Crystal dimensions(mm)	0.24x0.18x0.12
Crystal system	monoclinic
Space group	$P2_1/c$
a(Å)	8.671(1)
b(Å)	13.989(1)
c(Å)	28.862(1)
α(°)	90.00
β(°)	105.194(2)
γ(°)	90.00
V(Å^3)	3378.5(5)
Z	4
d(g-cm^{-3})	1.851
F(000)	1848
μ(cm^{-1})	4.568
Absorption corrections	multi-scan ; 0.4069 min, 0.6102 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	-12 12 ; -19 18 ; -31 40
Reflections measured	29565
Unique data	9531
Rint	0.0298
Reflections used	7714
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	454
Reflections / parameter	16
wR2	0.0704
R1	0.0314
Weights a, b	0.0378 ; 0.0000
GoF	1.023
difference peak / hole (e Å^{-3})	1.624(0.118) / -1.549(0.118)

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

atom	x	y	z	U(eq)
Ir(1)	8450(1)	-1379(1)	-1163(1)	26(1)
Ru(1)	7935(1)	-4272(1)	-1522(1)	25(1)
Cl(1)	8766(1)	-1371(1)	-1960(1)	35(1)
N(1)	6036(3)	-1695(2)	-1467(1)	30(1)
N(2)	10850(3)	-4923(2)	-515(1)	33(1)
C(1)	4964(4)	-1058(2)	-1718(1)	36(1)
C(2)	3354(4)	-1248(3)	-1854(2)	43(1)
C(3)	2809(4)	-2104(3)	-1728(2)	46(1)
C(4)	3891(4)	-2781(2)	-1488(2)	40(1)
C(5)	5519(3)	-2565(2)	-1366(1)	30(1)
C(6)	6830(3)	-3208(2)	-1130(1)	26(1)
C(7)	8396(3)	-2840(2)	-1085(1)	24(1)
C(8)	9692(3)	-3471(2)	-933(1)	26(1)
C(9)	9532(4)	-4388(2)	-739(1)	28(1)
C(10)	7955(3)	-4738(2)	-789(1)	29(1)
C(11)	6610(3)	-4151(2)	-977(1)	31(1)
C(12)	10654(4)	-5932(2)	-425(1)	39(1)
C(13)	12437(4)	-4594(2)	-510(2)	45(1)
C(14)	8544(4)	-4284(2)	-2217(1)	32(1)
C(15)	6853(4)	-4150(2)	-2297(1)	36(1)
C(16)	6241(4)	-4977(2)	-2107(1)	35(1)
C(17)	7553(4)	-5606(2)	-1920(1)	38(1)
C(18)	8974(4)	-5176(2)	-1979(1)	34(1)
C(19)	9645(5)	-3665(2)	-2405(2)	51(1)
C(20)	5910(5)	-3321(3)	-2558(2)	52(1)
C(21)	4519(4)	-5171(3)	-2123(2)	54(1)
C(22)	7412(5)	-6596(2)	-1717(2)	52(1)
C(23)	10609(4)	-5627(3)	-1852(2)	52(1)
C(24A)	9421(6)	-1134(3)	-408(2)	33(1)
C(25A)	10632(4)	-927(3)	-645(2)	31(1)
C(26A)	10079(7)	-118(4)	-943(3)	41(1)
C(27A)	8514(7)	135(5)	-915(3)	38(1)
C(28A)	8107(5)	-500(4)	-579(2)	38(1)
C(29A)	9560(10)	-1858(3)	-11(2)	62(2)
C(30A)	12272(5)	-1374(4)	-537(3)	67(2)
C(31A)	11000(10)	382(5)	-1251(3)	76(2)
C(32A)	7530(10)	961(4)	-1174(3)	79(3)
C(33A)	6572(6)	-530(5)	-424(3)	71(2)
C(24B)	8740(20)	-1000(10)	-421(6)	33(1)
C(25B)	10270(20)	-1030(10)	-521(7)	31(1)
C(26B)	10290(30)	-370(20)	-900(10)	41(1)
C(27B)	8830(30)	160(20)	-1010(10)	38(1)
C(28B)	7860(20)	-290(20)	-735(6)	38(1)
C(29B)	8430(30)	-1590(10)	-17(6)	62(2)
C(30B)	11680(20)	-1630(10)	-263(8)	67(2)
C(31B)	11640(30)	-20(20)	-1090(10)	76(2)
C(32B)	8410(30)	1020(10)	-1330(10)	79(3)
C(33B)	6270(20)	30(20)	-670(10)	71(2)
P(1)	4595(1)	-7215(1)	-717(1)	41(1)
F(1)	4660(3)	-7630(2)	-1226(1)	67(1)
F(2)	4481(4)	-6165(2)	-932(1)	84(1)
F(3)	4529(3)	-6791(2)	-209(1)	66(1)
F(4)	4714(3)	-8265(2)	-506(1)	76(1)
F(5)	2705(2)	-7296(2)	-874(1)	68(1)
F(6)	6497(3)	-7119(2)	-565(1)	71(1)

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

Table 3. Bond lengths (A) and angles (deg) for 4a

Ir(1)-C(7)	2.058(3)	Ir(1)-N(1)	2.094(2)
Ir(1)-C(28B)	2.11(2)	Ir(1)-C(26B)	2.12(3)
Ir(1)-C(24A)	2.149(5)	Ir(1)-C(25B)	2.15(2)
Ir(1)-C(24B)	2.16(2)	Ir(1)-C(28A)	2.170(6)
Ir(1)-C(25A)	2.176(5)	Ir(1)-C(27B)	2.20(3)
Ir(1)-C(27A)	2.232(8)	Ir(1)-C(26A)	2.246(7)
Ru(1)-C(16)	2.165(3)	Ru(1)-C(17)	2.172(3)
Ru(1)-C(11)	2.183(3)	Ru(1)-C(18)	2.186(3)
Ru(1)-C(15)	2.195(4)	Ru(1)-C(14)	2.204(3)
Ru(1)-C(10)	2.210(3)	Ru(1)-C(6)	2.232(3)
Ru(1)-C(8)	2.259(3)	Ru(1)-C(9)	2.325(3)
Ru(1)-C(7)	2.344(3)	N(1)-C(1)	1.353(4)
N(1)-C(5)	1.354(4)	N(2)-C(9)	1.378(4)
N(2)-C(13)	1.448(4)	N(2)-C(12)	1.453(4)
C(1)-C(2)	1.373(5)	C(2)-C(3)	1.371(5)
C(3)-C(4)	1.385(5)	C(4)-C(5)	1.395(4)
C(5)-C(6)	1.470(4)	C(6)-C(11)	1.420(4)
C(6)-C(7)	1.427(4)	C(7)-C(8)	1.405(4)
C(8)-C(9)	1.422(4)	C(9)-C(10)	1.423(4)
C(10)-C(11)	1.414(4)	C(14)-C(18)	1.426(5)
C(14)-C(15)	1.435(4)	C(14)-C(19)	1.494(4)
C(15)-C(16)	1.439(5)	C(15)-C(20)	1.503(5)
C(16)-C(17)	1.428(5)	C(16)-C(21)	1.507(4)
C(17)-C(18)	1.421(4)	C(17)-C(22)	1.521(5)
C(18)-C(23)	1.506(4)	C(24A)-C(28A)	1.425(2)
C(24A)-C(25A)	1.426(2)	C(24A)-C(29A)	1.510(2)
C(25A)-C(26A)	1.426(2)	C(25A)-C(30A)	1.510(2)
C(26A)-C(27A)	1.426(2)	C(26A)-C(31A)	1.510(2)
C(27A)-C(28A)	1.427(2)	C(27A)-C(32A)	1.511(2)
C(28A)-C(33A)	1.511(2)	C(24B)-C(25B)	1.425(2)
C(24B)-C(28B)	1.425(2)	C(24B)-C(29B)	1.510(2)
C(25B)-C(26B)	1.425(2)	C(25B)-C(30B)	1.510(2)
C(26B)-C(27B)	1.425(2)	C(26B)-C(31B)	1.510(2)
C(27B)-C(28B)	1.425(2)	C(27B)-C(32B)	1.510(2)
C(28B)-C(33B)	1.510(2)	P(1)-F(4)	1.583(2)
P(1)-F(5)	1.586(2)	P(1)-F(2)	1.588(3)
P(1)-F(1)	1.594(3)	P(1)-F(3)	1.595(3)
P(1)-F(6)	1.597(2)		

C(7)-Ir(1)-N(1)	77.7(1)	C(7)-Ir(1)-C(28B)	129.8(5)
N(1)-Ir(1)-C(28B)	91.8(5)	C(7)-Ir(1)-C(26B)	131.1(5)
N(1)-Ir(1)-C(26B)	150.3(5)	C(28B)-Ir(1)-C(26B)	64.9(8)
C(7)-Ir(1)-C(24A)	93.5(1)	N(1)-Ir(1)-C(24A)	122.8(1)
C(28B)-Ir(1)-C(24A)	51.7(4)	C(26B)-Ir(1)-C(24A)	57.7(6)
C(7)-Ir(1)-C(25B)	99.3(4)	N(1)-Ir(1)-C(25B)	146.6(4)
C(28B)-Ir(1)-C(25B)	64.3(6)	C(26B)-Ir(1)-C(25B)	39.0(3)
C(24A)-Ir(1)-C(25B)	23.9(4)	C(7)-Ir(1)-C(24B)	97.9(4)
N(1)-Ir(1)-C(24B)	108.3(4)	C(28B)-Ir(1)-C(24B)	39.0(2)
C(26B)-Ir(1)-C(24B)	65.8(7)	C(24A)-Ir(1)-C(24B)	16.2(3)
C(25B)-Ir(1)-C(24B)	38.6(2)	C(7)-Ir(1)-C(28A)	117.8(2)
N(1)-Ir(1)-C(28A)	96.9(1)	C(28B)-Ir(1)-C(28A)	14.3(4)
C(26B)-Ir(1)-C(28A)	65.3(7)	C(24A)-Ir(1)-C(28A)	38.54(8)
C(25B)-Ir(1)-C(28A)	54.6(4)	C(24B)-Ir(1)-C(28A)	24.8(4)
C(7)-Ir(1)-C(25A)	104.7(1)	N(1)-Ir(1)-C(25A)	160.6(1)
C(28B)-Ir(1)-C(25A)	71.7(5)	C(26B)-Ir(1)-C(25A)	28.2(5)
C(24A)-Ir(1)-C(25A)	38.51(8)	C(25B)-Ir(1)-C(25A)	14.8(4)
C(24B)-Ir(1)-C(25A)	52.4(4)	C(28A)-Ir(1)-C(25A)	64.7(2)
C(7)-Ir(1)-C(27B)	162.2(7)	N(1)-Ir(1)-C(27B)	111.9(6)
C(28B)-Ir(1)-C(27B)	38.5(4)	C(26B)-Ir(1)-C(27B)	38.5(4)
C(24A)-Ir(1)-C(27B)	68.6(7)	C(25B)-Ir(1)-C(27B)	64.2(8)
C(24B)-Ir(1)-C(27B)	65.2(8)	C(28A)-Ir(1)-C(27B)	47.9(6)
C(25A)-Ir(1)-C(27B)	61.2(7)	C(7)-Ir(1)-C(27A)	155.0(2)
N(1)-Ir(1)-C(27A)	105.9(2)	C(28B)-Ir(1)-C(27A)	27.6(6)

C(26B)-Ir(1)-C(27A)	45.4(6)	C(24A)-Ir(1)-C(27A)	63.4(2)
C(25B)-Ir(1)-C(27A)	63.8(5)	C(24B)-Ir(1)-C(27A)	57.3(4)
C(28A)-Ir(1)-C(27A)	37.8(1)	C(25A)-Ir(1)-C(27A)	63.9(2)
C(27B)-Ir(1)-C(27A)	11.0(5)	C(7)-Ir(1)-C(26A)	141.2(1)
N(1)-Ir(1)-C(26A)	140.4(1)	C(28B)-Ir(1)-C(26A)	59.7(6)
C(26B)-Ir(1)-C(26A)	10.1(5)	C(24A)-Ir(1)-C(26A)	62.5(2)
C(25B)-Ir(1)-C(26A)	46.7(5)	C(24B)-Ir(1)-C(26A)	67.8(4)
C(28A)-Ir(1)-C(26A)	62.6(2)	C(25A)-Ir(1)-C(26A)	37.6(1)
C(27B)-Ir(1)-C(26A)	29.1(6)	C(27A)-Ir(1)-C(26A)	37.1(1)
C(16)-Ru(1)-C(17)	38.4(1)	C(16)-Ru(1)-C(11)	102.7(1)
C(17)-Ru(1)-C(11)	114.3(1)	C(16)-Ru(1)-C(18)	64.3(1)
C(17)-Ru(1)-C(18)	38.1(1)	C(11)-Ru(1)-C(18)	149.0(1)
C(16)-Ru(1)-C(15)	38.5(1)	C(17)-Ru(1)-C(15)	64.0(1)
C(11)-Ru(1)-C(15)	124.3(1)	C(18)-Ru(1)-C(15)	64.1(1)
C(16)-Ru(1)-C(14)	64.0(1)	C(17)-Ru(1)-C(14)	63.3(1)
C(11)-Ru(1)-C(14)	162.3(1)	C(18)-Ru(1)-C(14)	37.9(1)
C(15)-Ru(1)-C(14)	38.1(1)	C(16)-Ru(1)-C(10)	116.5(1)
C(17)-Ru(1)-C(10)	102.4(1)	C(11)-Ru(1)-C(10)	37.5(1)
C(18)-Ru(1)-C(10)	120.4(1)	C(15)-Ru(1)-C(10)	153.3(1)
C(14)-Ru(1)-C(10)	157.7(1)	C(16)-Ru(1)-C(6)	114.0(1)
C(17)-Ru(1)-C(6)	144.6(1)	C(11)-Ru(1)-C(6)	37.5(1)
C(18)-Ru(1)-C(6)	172.6(1)	C(15)-Ru(1)-C(6)	109.8(1)
C(14)-Ru(1)-C(6)	134.7(1)	C(10)-Ru(1)-C(6)	67.0(1)
C(16)-Ru(1)-C(8)	177.2(1)	C(17)-Ru(1)-C(8)	143.5(1)
C(11)-Ru(1)-C(8)	78.4(1)	C(18)-Ru(1)-C(8)	115.9(1)
C(15)-Ru(1)-C(8)	138.7(1)	C(14)-Ru(1)-C(8)	114.4(1)
C(10)-Ru(1)-C(8)	65.9(1)	C(6)-Ru(1)-C(8)	65.3(1)
C(16)-Ru(1)-C(9)	146.7(1)	C(17)-Ru(1)-C(9)	115.1(1)
C(11)-Ru(1)-C(9)	66.3(1)	C(18)-Ru(1)-C(9)	108.2(1)
C(15)-Ru(1)-C(9)	169.3(1)	C(14)-Ru(1)-C(9)	131.3(1)
C(10)-Ru(1)-C(9)	36.5(1)	C(6)-Ru(1)-C(9)	77.3(1)
C(8)-Ru(1)-C(9)	36.1(1)	C(16)-Ru(1)-C(7)	142.6(1)
C(17)-Ru(1)-C(7)	178.9(1)	C(11)-Ru(1)-C(7)	66.1(1)
C(18)-Ru(1)-C(7)	141.2(1)	C(15)-Ru(1)-C(7)	116.7(1)
C(14)-Ru(1)-C(7)	116.6(1)	C(10)-Ru(1)-C(7)	77.3(1)
C(6)-Ru(1)-C(7)	36.2(1)	C(8)-Ru(1)-C(7)	35.5(1)
C(9)-Ru(1)-C(7)	64.1(1)	C(1)-N(1)-C(5)	119.2(3)
C(1)-N(1)-Ir(1)	123.8(2)	C(5)-N(1)-Ir(1)	116.8(2)
C(9)-N(2)-C(13)	120.1(3)	C(9)-N(2)-C(12)	119.3(3)
C(13)-N(2)-C(12)	117.5(2)	N(1)-C(1)-C(2)	122.0(3)
C(3)-C(2)-C(1)	119.3(3)	C(2)-C(3)-C(4)	119.6(3)
C(3)-C(4)-C(5)	119.1(3)	N(1)-C(5)-C(4)	120.7(3)
N(1)-C(5)-C(6)	113.0(2)	C(4)-C(5)-C(6)	126.3(3)
C(11)-C(6)-C(7)	120.6(3)	C(11)-C(6)-C(5)	124.2(3)
C(7)-C(6)-C(5)	115.0(3)	C(11)-C(6)-Ru(1)	69.4(2)
C(7)-C(6)-Ru(1)	76.2(2)	C(5)-C(6)-Ru(1)	123.8(2)
C(8)-C(7)-C(6)	117.7(3)	C(8)-C(7)-Ir(1)	128.2(2)
C(6)-C(7)-Ir(1)	113.4(2)	C(8)-C(7)-Ru(1)	68.9(2)
C(6)-C(7)-Ru(1)	67.6(2)	Ir(1)-C(7)-Ru(1)	142.7(2)
C(7)-C(8)-C(9)	122.5(3)	C(7)-C(8)-Ru(1)	75.6(2)
C(9)-C(8)-Ru(1)	74.5(2)	N(2)-C(9)-C(8)	121.4(3)
N(2)-C(9)-C(10)	121.2(3)	C(8)-C(9)-C(10)	117.5(3)
N(2)-C(9)-Ru(1)	134.7(2)	C(8)-C(9)-Ru(1)	69.4(2)
C(10)-C(9)-Ru(1)	67.3(2)	C(11)-C(10)-C(9)	120.8(3)
C(11)-C(10)-Ru(1)	70.2(2)	C(9)-C(10)-Ru(1)	76.2(2)
C(10)-C(11)-C(6)	119.7(3)	C(10)-C(11)-Ru(1)	72.3(2)
C(6)-C(11)-Ru(1)	73.1(2)	C(18)-C(14)-C(15)	108.7(3)
C(18)-C(14)-C(19)	124.8(3)	C(15)-C(14)-C(19)	126.0(3)
C(18)-C(14)-Ru(1)	70.4(2)	C(15)-C(14)-Ru(1)	70.6(2)
C(19)-C(14)-Ru(1)	131.0(2)	C(14)-C(15)-C(16)	107.2(3)
C(14)-C(15)-C(20)	125.5(3)	C(16)-C(15)-C(20)	127.2(3)
C(14)-C(15)-Ru(1)	71.3(2)	C(16)-C(15)-Ru(1)	69.6(2)
C(20)-C(15)-Ru(1)	127.1(3)	C(17)-C(16)-C(15)	107.7(3)
C(17)-C(16)-C(21)	125.8(3)	C(15)-C(16)-C(21)	126.5(3)
C(17)-C(16)-Ru(1)	71.0(2)	C(15)-C(16)-Ru(1)	71.8(2)
C(21)-C(16)-Ru(1)	124.7(3)	C(18)-C(17)-C(16)	108.9(3)
C(18)-C(17)-C(22)	126.2(3)	C(16)-C(17)-C(22)	124.8(3)

C(18)-C(17)-Ru(1)	71.5(2)	C(16)-C(17)-Ru(1)	70.6(2)
C(22)-C(17)-Ru(1)	126.6(3)	C(17)-C(18)-C(14)	107.6(3)
C(17)-C(18)-C(23)	125.7(3)	C(14)-C(18)-C(23)	126.5(3)
C(17)-C(18)-Ru(1)	70.4(2)	C(14)-C(18)-Ru(1)	71.7(2)
C(23)-C(18)-Ru(1)	127.3(3)	C(28A)-C(24A)-C(25A)	109.3(3)
C(28A)-C(24A)-C(29A)	125.2(4)	C(25A)-C(24A)-C(29A)	125.4(4)
C(28A)-C(24A)-Ir(1)	71.5(3)	C(25A)-C(24A)-Ir(1)	71.8(3)
C(29A)-C(24A)-Ir(1)	126.5(3)	C(24A)-C(25A)-C(26A)	106.1(3)
C(24A)-C(25A)-C(30A)	126.0(4)	C(26A)-C(25A)-C(30A)	127.1(4)
C(24A)-C(25A)-Ir(1)	69.7(2)	C(26A)-C(25A)-Ir(1)	73.9(3)
C(30A)-C(25A)-Ir(1)	128.6(4)	C(27A)-C(26A)-C(25A)	109.7(3)
C(27A)-C(26A)-C(31A)	125.1(4)	C(25A)-C(26A)-C(31A)	125.2(4)
C(27A)-C(26A)-Ir(1)	70.9(4)	C(25A)-C(26A)-Ir(1)	68.5(3)
C(31A)-C(26A)-Ir(1)	125.9(6)	C(26A)-C(27A)-C(28A)	107.1(3)
C(26A)-C(27A)-C(32A)	125.6(5)	C(28A)-C(27A)-C(32A)	127.2(5)
C(26A)-C(27A)-Ir(1)	72.0(4)	C(28A)-C(27A)-Ir(1)	68.8(4)
C(32A)-C(27A)-Ir(1)	127.1(6)	C(24A)-C(28A)-C(27A)	107.7(3)
C(24A)-C(28A)-C(33A)	124.5(4)	C(27A)-C(28A)-C(33A)	127.8(4)
C(24A)-C(28A)-Ir(1)	69.9(3)	C(27A)-C(28A)-Ir(1)	73.4(4)
C(33A)-C(28A)-Ir(1)	121.6(4)	C(25B)-C(24B)-C(28B)	105(1)
C(25B)-C(24B)-C(29B)	120(2)	C(28B)-C(24B)-C(29B)	134(2)
C(25B)-C(24B)-Ir(1)	71(1)	C(28B)-C(24B)-Ir(1)	69(1)
C(29B)-C(24B)-Ir(1)	129(1)	C(24B)-C(25B)-C(26B)	109(1)
C(24B)-C(25B)-C(30B)	127(2)	C(26B)-C(25B)-C(30B)	124(2)
C(24B)-C(25B)-Ir(1)	71(1)	C(26B)-C(25B)-Ir(1)	69(1)
C(30B)-C(25B)-Ir(1)	128(1)	C(27B)-C(26B)-C(25B)	109(1)
C(27B)-C(26B)-C(31B)	119(2)	C(25B)-C(26B)-C(31B)	131(2)
C(27B)-C(26B)-Ir(1)	74(2)	C(25B)-C(26B)-Ir(1)	72(1)
C(31B)-C(26B)-Ir(1)	131(2)	C(26B)-C(27B)-C(28B)	106(1)
C(26B)-C(27B)-C(32B)	127(2)	C(28B)-C(27B)-C(32B)	127(2)
C(26B)-C(27B)-Ir(1)	68(2)	C(28B)-C(27B)-Ir(1)	67(1)
C(32B)-C(27B)-Ir(1)	131(2)	C(24B)-C(28B)-C(27B)	111(1)
C(24B)-C(28B)-C(33B)	118(2)	C(27B)-C(28B)-C(33B)	129(2)
C(24B)-C(28B)-Ir(1)	72(1)	C(27B)-C(28B)-Ir(1)	74(2)
C(33B)-C(28B)-Ir(1)	131(2)	F(4)-P(1)-F(5)	90.1(2)
F(4)-P(1)-F(2)	179.5(2)	F(5)-P(1)-F(2)	90.0(2)
F(4)-P(1)-F(1)	90.1(2)	F(5)-P(1)-F(1)	89.6(1)
F(2)-P(1)-F(1)	89.4(2)	F(4)-P(1)-F(3)	90.3(2)
F(5)-P(1)-F(3)	90.3(1)	F(2)-P(1)-F(3)	90.1(2)
F(1)-P(1)-F(3)	179.6(2)	F(4)-P(1)-F(6)	90.8(1)
F(5)-P(1)-F(6)	179.0(2)	F(2)-P(1)-F(6)	89.1(2)
F(1)-P(1)-F(6)	90.0(1)	F(3)-P(1)-F(6)	90.0(1)

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

atom	U11	U22	U33	U23	U13	U12
Ir(1)	27(1)	25(1)	23(1)	0(1)	3(1)	3(1)
Ru(1)	24(1)	27(1)	25(1)	-4(1)	6(1)	-2(1)
Cl(1)	30(1)	49(1)	25(1)	2(1)	5(1)	5(1)
N(1)	25(1)	38(1)	24(2)	-5(1)	1(1)	8(1)
N(2)	35(1)	29(1)	33(2)	4(1)	4(1)	8(1)
C(1)	37(2)	43(2)	27(2)	3(2)	7(1)	14(1)
C(2)	32(2)	56(2)	38(2)	-3(2)	1(2)	18(2)
C(3)	26(2)	63(2)	46(3)	-14(2)	1(2)	10(2)
C(4)	27(2)	43(2)	47(3)	-11(2)	5(2)	1(1)
C(5)	25(1)	35(2)	29(2)	-8(1)	6(1)	3(1)
C(6)	23(1)	30(1)	26(2)	-7(1)	6(1)	2(1)
C(7)	24(1)	25(2)	22(2)	-3(1)	3(1)	2(1)
C(8)	26(1)	26(1)	25(2)	-6(1)	7(1)	0(1)
C(9)	41(2)	26(2)	20(2)	-4(1)	10(1)	-1(1)
C(10)	34(2)	27(2)	29(2)	-1(1)	13(1)	-1(1)
C(11)	27(1)	36(2)	31(2)	-5(1)	11(1)	-2(1)
C(12)	52(2)	31(2)	33(2)	1(2)	9(2)	10(1)
C(13)	30(2)	40(2)	59(3)	7(2)	4(2)	12(1)
C(14)	32(2)	40(2)	26(2)	-10(1)	10(1)	-7(1)
C(15)	35(2)	42(2)	25(2)	-6(2)	-2(1)	-2(1)
C(16)	33(2)	42(2)	30(2)	-15(2)	7(1)	-11(1)
C(17)	48(2)	36(2)	34(2)	-12(2)	14(2)	-8(1)
C(18)	38(2)	40(2)	27(2)	-12(1)	11(1)	-2(1)
C(19)	63(2)	54(2)	44(3)	-17(2)	30(2)	-25(2)
C(20)	53(2)	57(2)	37(3)	0(2)	-7(2)	7(2)
C(21)	38(2)	77(3)	49(3)	-25(2)	14(2)	-22(2)
C(22)	80(3)	33(2)	45(3)	-7(2)	20(2)	-12(2)
C(23)	45(2)	67(2)	47(3)	-14(2)	16(2)	17(2)
C(24A)	40(3)	27(2)	29(2)	-6(2)	2(3)	-3(2)
C(25A)	27(2)	31(2)	32(3)	-7(2)	4(2)	-6(2)
C(26A)	53(3)	26(4)	45(3)	-15(3)	18(3)	-16(2)
C(27A)	57(4)	21(2)	30(4)	-5(2)	3(2)	7(2)
C(28A)	45(3)	43(4)	24(4)	-18(3)	7(3)	-2(2)
C(29A)	116(6)	39(3)	26(3)	-2(2)	7(4)	-12(3)
C(30A)	31(3)	84(4)	74(5)	-46(4)	-9(2)	9(2)
C(31A)	116(6)	68(5)	53(6)	-10(3)	38(5)	-48(4)
C(32A)	110(6)	39(3)	63(6)	-10(3)	-21(4)	34(4)
C(33A)	56(3)	88(5)	78(6)	-48(4)	34(4)	-10(3)
C(24B)	40(3)	27(2)	29(2)	-6(2)	2(3)	-3(2)
C(25B)	27(2)	31(2)	32(3)	-7(2)	4(2)	-6(2)
C(26B)	53(3)	26(4)	45(3)	-15(3)	18(3)	-16(2)
C(27B)	57(4)	21(2)	30(4)	-5(2)	3(2)	7(2)
C(28B)	45(3)	43(4)	24(4)	-18(3)	7(3)	-2(2)
C(29B)	116(6)	39(3)	26(3)	-2(2)	7(4)	-12(3)
C(30B)	31(3)	84(4)	74(5)	-46(4)	-9(2)	9(2)
C(31B)	116(6)	68(5)	53(6)	-10(3)	38(5)	-48(4)
C(32B)	110(6)	39(3)	63(6)	-10(3)	-21(4)	34(4)
C(33B)	56(3)	88(5)	78(6)	-48(4)	34(4)	-10(3)
P(1)	41(1)	39(1)	45(1)	1(1)	13(1)	7(1)
F(1)	69(2)	80(2)	58(2)	-18(1)	27(1)	5(1)
F(2)	119(2)	46(1)	87(3)	14(2)	26(2)	5(1)
F(3)	60(1)	88(2)	48(2)	-18(1)	11(1)	8(1)
F(4)	90(2)	50(1)	85(3)	21(1)	15(2)	7(1)
F(5)	39(1)	96(2)	65(2)	-18(2)	7(1)	14(1)
F(6)	42(1)	85(2)	87(2)	-18(2)	16(1)	-1(1)

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 4a

atom	x	y	z	U(eq)
H(1)	5335	-461.0000	-1802	43
H(2)	2627	-792	-2033	52
H(3)	1694	-2232	-1806	56
H(4)	3529	-3384	-1408	48
H(8)	10712	-3274.9998	-961.9999	31
H(10)	7803	-5375	-695	35
H(11)	5564	-4386	-1001.0001	37
H(12A)	9884	-6007	-233	59
H(12B)	11686	-6203	-251	59
H(12C)	10261	-6266.0005	-732	59
H(13A)	12571	-4616	-837	67
H(13B)	13235	-5007	-300	67
H(13C)	12580	-3935.9998	-390	67
H(19A)	10742	-3747	-2207	76
H(19B)	9326	-2994	-2396	76
H(19C)	9590	-3847	-2737	76
H(20A)	6581	-2746.9998	-2507	79
H(20B)	4972	-3212.0002	-2436	79
H(20C)	5564	-3465	-2902	79
H(21A)	4004	-5511	-2420	81
H(21B)	3965	-4564	-2113	81
H(21C)	4467	-5563	-1846	81
H(22A)	7259	-7070.9995	-1975	78
H(22B)	6496	-6612	-1578	78
H(22C)	8391	-6743.9995	-1468	78
H(23A)	10756	-5990	-2127	78
H(23B)	10710	-6057.9995	-1578	78
H(23C)	11425	-5126	-1767	78
H(29A)	9898	-1536.0001	301	94
H(29B)	10346	-2345	-34	94
H(29C)	8517	-2162	-43	94
H(30A)	13036	-970	-310	100
H(30B)	12607	-1435	-835	100
H(30C)	12239	-2009	-396	100
H(31A)	10266	554	-1560	114
H(31B)	11829	-46	-1305	114
H(31C)	11495	961	-1088	114
H(32A)	7914	1559	-1005.9999	118
H(32B)	6408	864	-1181	118
H(32C)	7639	996	-1503	118
H(33A)	6296	-1196	-378	106
H(33B)	5712	-236.0000	-673	106
H(33C)	6714	-179	-122	106
H(29D)	8881	-2230	-25	94
H(29E)	7280	-1636	-56.0000	94
H(29F)	8941	-1284	291	94
H(30D)	11355	-2076	-46	100
H(30E)	12529	-1210	-78	100
H(30F)	12088	-1987	-499	100
H(31D)	11217	143	-1432	114
H(31E)	12444	-523	-1059	114
H(31F)	12120	549	-914	114
H(32D)	9262	1499	-1232	118
H(32E)	7402	1292	-1297	118
H(32F)	8304	829	-1661	118
H(33D)	5758	-512	-552	106
H(33E)	5590	256	-973	106
H(33F)	6442	547	-430	106

5b

Table 1. Crystal data for 5b

Compound	5b
Molecular formula	$C_{30}H_{36}ClCrIrN_2O_3,C_3H_6O$
Molecular weight	810.34
Crystal habit	Orange Needle
Crystal dimensions(mm)	0.34x0.04x0.02
Crystal system	monoclinic
Space group	$P2_1/c$
a(Å)	10.649(1)
b(Å)	15.812(1)
c(Å)	21.131(1)
α(°)	90.00
β(°)	107.397(3)
γ(°)	90.00
V(Å^3)	3395.3(4)
Z	4
d(g-cm^{-3})	1.585
F(000)	1616
μ(cm^{-1})	4.351
Absorption corrections	multi-scan ; 0.3193 min, 0.9180 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	29.95
HKL ranges	-12 14 ; -22 20 ; -24 29
Reflections measured	26792
Unique data	9667
Rint	0.0494
Reflections used	6935
Criterion	I > 2σI)
Refinement type	Fsqd
Hydrogen atoms	constr
Parameters refined	391
Reflections / parameter	17
wR2	0.0624
R1	0.0495
Weights a, b	0.0095 ; 4.6460
GoF	1.127
difference peak / hole (e Å^{-3})	0.943(0.193) / -0.940(0.193)

Table 2. Atomic Coordinates (A x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5b

atom	x	y	z	U(eq)
Ir(1)	3505(1)	-5334(1)	-3025(1)	16(1)
Cr(1)	244(1)	-3865(1)	-3482(1)	19(1)
Cl(1)	3559(1)	-6041(1)	-4023(1)	27(1)
O(1)	-539(4)	-2067(3)	-3803(2)	49(1)
O(2)	2106(3)	-3075(3)	-2282(2)	43(1)
O(3)	-1654(3)	-4033(3)	-2695(2)	35(1)
N(1)	3947(4)	-4257(3)	-3500(2)	18(1)
N(2)	-1877(4)	-5513(3)	-4069(2)	25(1)
C(1)	1674(4)	-4935(3)	-3570(2)	18(1)
C(2)	471(4)	-5305(4)	-3577(2)	20(1)
C(3)	-754(4)	-5087(3)	-4056(2)	21(1)
C(4)	-737(4)	-4417(3)	-4496(2)	21(1)
C(5)	447(4)	-4012(3)	-4482(2)	20(1)
C(6)	1650(4)	-4260(3)	-4021(2)	19(1)
C(7)	2921(4)	-3872(3)	-3964(2)	18(1)
C(8)	3139(4)	-3206(3)	-4340(2)	20(1)
C(9)	4402(4)	-2900(3)	-4266(2)	18(1)
C(10)	5428(4)	-3308(3)	-3793(2)	23(1)
C(11)	5158(4)	-3970(3)	-3430(2)	23(1)
C(12)	-1866(5)	-6086(4)	-3526(2)	31(1)
C(13)	-3143(4)	-5159(4)	-4449(2)	29(1)
C(14)	4631(5)	-2171(3)	-4694(2)	24(1)
C(15)	3890(6)	-1384(4)	-4559(2)	35(1)
C(16)	4078(5)	-2415(4)	-5428(2)	31(1)
C(17)	6088(5)	-1951(4)	-4546(3)	43(2)
C(18)	4428(5)	-5110(3)	-1974(2)	24(1)
C(19)	5286(5)	-5688(4)	-2176(2)	26(1)
C(20)	4559(5)	-6421(4)	-2421(2)	29(1)
C(21)	3240(5)	-6318(4)	-2375(2)	26(1)
C(22)	3187(5)	-5520(3)	-2067(2)	24(1)
C(23)	4865(6)	-4293(4)	-1632(2)	48(2)
C(24)	6728(5)	-5573(5)	-2080(3)	54(2)
C(25)	5046(7)	-7194(4)	-2686(3)	54(2)
C(26)	2192(6)	-6993(4)	-2532(3)	52(2)
C(27)	2081(6)	-5215(4)	-1825(2)	46(2)
C(28)	-251(5)	-2773(4)	-3688(2)	30(1)
C(29)	1416(5)	-3415(4)	-2746(2)	26(1)
C(30)	-924(4)	-3963(3)	-3012(2)	22(1)
O(4)	505(5)	-2609(4)	-548(3)	89(2)
C(31)	-252(7)	-3183(6)	-698(3)	58(2)
C(32)	-1581(7)	-3141(6)	-630(4)	91(3)
C(33)	140(10)	-3961(8)	-979(5)	149(5)

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

Table 3. Bond lengths (A) and angles (deg) for 5b

Ir(1)-C(1)	2.046(4)	Ir(1)-N(1)	2.101(4)
Ir(1)-C(21)	2.150(5)	Ir(1)-C(22)	2.170(4)
Ir(1)-C(18)	2.171(4)	Ir(1)-C(20)	2.233(5)
Ir(1)-C(19)	2.257(4)	Ir(1)-Cl(1)	2.402(1)
Cr(1)-C(30)	1.815(5)	Cr(1)-C(28)	1.820(6)
Cr(1)-C(29)	1.823(5)	Cr(1)-C(5)	2.201(4)
Cr(1)-C(6)	2.224(4)	Cr(1)-C(4)	2.260(4)
Cr(1)-C(2)	2.305(5)	Cr(1)-C(1)	2.321(5)
Cr(1)-C(3)	2.359(5)	O(1)-C(28)	1.163(6)
O(2)-C(29)	1.165(5)	O(3)-C(30)	1.173(5)
N(1)-C(11)	1.333(5)	N(1)-C(7)	1.373(5)
N(2)-C(3)	1.366(6)	N(2)-C(13)	1.460(6)
N(2)-C(12)	1.460(6)	C(1)-C(2)	1.404(6)
C(1)-C(6)	1.427(6)	C(2)-C(3)	1.434(6)
C(2)-H(2)	0.9500	C(3)-C(4)	1.411(6)
C(4)-C(5)	1.407(6)	C(4)-H(4)	0.9500
C(5)-C(6)	1.413(6)	C(5)-H(5)	0.9500
C(6)-C(7)	1.457(6)	C(7)-C(8)	1.380(6)
C(8)-C(9)	1.393(6)	C(8)-H(8)	0.9500
C(9)-C(10)	1.400(6)	C(9)-C(14)	1.529(6)
C(10)-C(11)	1.377(7)	C(10)-H(10)	0.9500
C(11)-H(11)	0.9500	C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800	C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800	C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800	C(14)-C(17)	1.528(7)
C(14)-C(16)	1.535(6)	C(14)-C(15)	1.545(7)
C(15)-H(15A)	0.9800	C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800	C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800	C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800	C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800	C(18)-C(22)	1.433(7)
C(18)-C(19)	1.444(7)	C(18)-C(23)	1.485(7)
C(19)-C(20)	1.404(7)	C(19)-C(24)	1.498(6)
C(20)-C(21)	1.446(7)	C(20)-C(25)	1.500(7)
C(21)-C(22)	1.428(7)	C(21)-C(26)	1.507(7)
C(22)-C(27)	1.498(6)	C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800	C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800	C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800	C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800	C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800	C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800	C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800	C(27)-H(27C)	0.9800
O(4)-C(31)	1.19(1)	C(31)-C(32)	1.47(1)
C(31)-C(33)	1.48(1)	C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800	C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800	C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800		

C(1)-Ir(1)-N(1)	78.1(2)	C(1)-Ir(1)-C(21)	107.3(2)
N(1)-Ir(1)-C(21)	169.5(2)	C(1)-Ir(1)-C(22)	100.3(2)
N(1)-Ir(1)-C(22)	132.5(2)	C(21)-Ir(1)-C(22)	38.6(2)
C(1)-Ir(1)-C(18)	126.1(2)	N(1)-Ir(1)-C(18)	105.0(2)
C(21)-Ir(1)-C(18)	64.6(2)	C(22)-Ir(1)-C(18)	38.5(2)
C(1)-Ir(1)-C(20)	142.2(2)	N(1)-Ir(1)-C(20)	138.7(2)
C(21)-Ir(1)-C(20)	38.5(2)	C(22)-Ir(1)-C(20)	63.5(2)
C(18)-Ir(1)-C(20)	62.9(2)	C(1)-Ir(1)-C(19)	163.2(2)
N(1)-Ir(1)-C(19)	109.0(2)	C(21)-Ir(1)-C(19)	63.4(2)
C(22)-Ir(1)-C(19)	63.5(2)	C(18)-Ir(1)-C(19)	38.0(2)
C(20)-Ir(1)-C(19)	36.4(2)	C(1)-Ir(1)-Cl(1)	85.3(1)
N(1)-Ir(1)-Cl(1)	83.7(1)	C(21)-Ir(1)-Cl(1)	105.4(2)
C(22)-Ir(1)-Cl(1)	143.8(2)	C(18)-Ir(1)-Cl(1)	148.3(1)
C(20)-Ir(1)-Cl(1)	90.2(1)	C(19)-Ir(1)-Cl(1)	110.3(1)

C(30)-Cr(1)-C(28)	90.9(2)	C(30)-Cr(1)-C(29)	88.5(2)
C(28)-Cr(1)-C(29)	84.8(2)	C(30)-Cr(1)-C(5)	142.8(2)
C(28)-Cr(1)-C(5)	88.6(2)	C(29)-Cr(1)-C(5)	128.5(2)
C(30)-Cr(1)-C(6)	158.8(2)	C(28)-Cr(1)-C(6)	109.6(2)
C(29)-Cr(1)-C(6)	98.8(2)	C(5)-Cr(1)-C(6)	37.2(2)
C(30)-Cr(1)-C(4)	106.7(2)	C(28)-Cr(1)-C(4)	97.0(2)
C(29)-Cr(1)-C(4)	164.7(2)	C(5)-Cr(1)-C(4)	36.8(2)
C(6)-Cr(1)-C(4)	66.2(2)	C(30)-Cr(1)-C(2)	94.0(2)
C(28)-Cr(1)-C(2)	161.2(2)	C(29)-Cr(1)-C(2)	113.4(2)
C(5)-Cr(1)-C(2)	76.6(2)	C(6)-Cr(1)-C(2)	64.8(2)
C(4)-Cr(1)-C(2)	64.3(2)	C(30)-Cr(1)-C(1)	123.7(2)
C(28)-Cr(1)-C(1)	145.4(2)	C(29)-Cr(1)-C(1)	93.2(2)
C(5)-Cr(1)-C(1)	65.8(2)	C(6)-Cr(1)-C(1)	36.5(2)
C(4)-Cr(1)-C(1)	76.7(2)	C(2)-Cr(1)-C(1)	35.3(2)
C(30)-Cr(1)-C(3)	86.2(2)	C(28)-Cr(1)-C(3)	126.9(2)
C(29)-Cr(1)-C(3)	147.9(2)	C(5)-Cr(1)-C(3)	65.0(2)
C(6)-Cr(1)-C(3)	77.0(2)	C(4)-Cr(1)-C(3)	35.5(2)
C(2)-Cr(1)-C(3)	35.8(2)	C(1)-Cr(1)-C(3)	64.3(2)
C(11)-N(1)-C(7)	117.8(4)	C(11)-N(1)-Ir(1)	124.8(3)
C(7)-N(1)-Ir(1)	117.1(3)	C(3)-N(2)-C(13)	118.7(4)
C(3)-N(2)-C(12)	119.4(4)	C(13)-N(2)-C(12)	117.4(4)
C(2)-C(1)-C(6)	118.1(4)	C(2)-C(1)-Ir(1)	126.2(4)
C(6)-C(1)-Ir(1)	115.5(3)	C(2)-C(1)-Cr(1)	71.7(3)
C(6)-C(1)-Cr(1)	68.1(3)	Ir(1)-C(1)-Cr(1)	135.8(2)
C(1)-C(2)-C(3)	122.8(4)	C(1)-C(2)-Cr(1)	72.9(3)
C(3)-C(2)-Cr(1)	74.1(3)	C(1)-C(2)-H(2)	118.6
C(3)-C(2)-H(2)	118.6	Cr(1)-C(2)-H(2)	126.3
N(2)-C(3)-C(4)	122.7(4)	N(2)-C(3)-C(2)	120.1(4)
C(4)-C(3)-C(2)	117.2(4)	N(2)-C(3)-Cr(1)	132.2(3)
C(4)-C(3)-Cr(1)	68.4(3)	C(2)-C(3)-Cr(1)	70.1(3)
C(5)-C(4)-C(3)	121.0(4)	C(5)-C(4)-Cr(1)	69.3(2)
C(3)-C(4)-Cr(1)	76.1(3)	C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5	Cr(1)-C(4)-H(4)	127.1
C(4)-C(5)-C(6)	120.7(4)	C(4)-C(5)-Cr(1)	73.9(2)
C(6)-C(5)-Cr(1)	72.3(2)	C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7	Cr(1)-C(5)-H(5)	126.0
C(5)-C(6)-C(1)	120.0(4)	C(5)-C(6)-C(7)	124.6(4)
C(1)-C(6)-C(7)	115.4(4)	C(5)-C(6)-Cr(1)	70.5(2)
C(1)-C(6)-Cr(1)	75.4(2)	C(7)-C(6)-Cr(1)	126.2(3)
N(1)-C(7)-C(8)	120.9(4)	N(1)-C(7)-C(6)	113.2(4)
C(8)-C(7)-C(6)	125.9(4)	C(7)-C(8)-C(9)	121.6(4)
C(7)-C(8)-H(8)	119.2	C(9)-C(8)-H(8)	119.2
C(8)-C(9)-C(10)	116.1(4)	C(8)-C(9)-C(14)	121.0(4)
C(10)-C(9)-C(14)	122.8(4)	C(11)-C(10)-C(9)	120.0(4)
C(11)-C(10)-H(10)	120.0	C(9)-C(10)-H(10)	120.0
N(1)-C(11)-C(10)	123.6(4)	N(1)-C(11)-H(11)	118.2
C(10)-C(11)-H(11)	118.2	N(2)-C(12)-H(12A)	109.5
N(2)-C(12)-H(12B)	109.5	H(12A)-C(12)-H(12B)	109.5
N(2)-C(12)-H(12C)	109.5	H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5	N(2)-C(13)-H(13A)	109.5
N(2)-C(13)-H(13B)	109.5	H(13A)-C(13)-H(13B)	109.5
N(2)-C(13)-H(13C)	109.5	H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5	C(17)-C(14)-C(9)	112.4(4)
C(17)-C(14)-C(16)	108.9(4)	C(9)-C(14)-C(16)	109.1(4)
C(17)-C(14)-C(15)	108.8(5)	C(9)-C(14)-C(15)	108.5(4)
C(16)-C(14)-C(15)	109.1(4)	C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5	H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5	H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5	C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5	H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5	H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5	C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5	H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5	H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5	C(22)-C(18)-C(19)	108.2(5)
C(22)-C(18)-C(23)	127.0(5)	C(19)-C(18)-C(23)	124.1(5)
C(22)-C(18)-Ir(1)	70.7(2)	C(19)-C(18)-Ir(1)	74.2(3)

C(23)-C(18)-Ir(1)	128.3(4)	C(20)-C(19)-C(18)	107.7(4)
C(20)-C(19)-C(24)	125.4(5)	C(18)-C(19)-C(24)	126.6(6)
C(20)-C(19)-Ir(1)	70.9(3)	C(18)-C(19)-Ir(1)	67.8(2)
C(24)-C(19)-Ir(1)	131.4(3)	C(19)-C(20)-C(21)	108.8(5)
C(19)-C(20)-C(25)	126.6(5)	C(21)-C(20)-C(25)	124.6(6)
C(19)-C(20)-Ir(1)	72.7(3)	C(21)-C(20)-Ir(1)	67.6(3)
C(25)-C(20)-Ir(1)	125.7(3)	C(22)-C(21)-C(20)	107.6(4)
C(22)-C(21)-C(26)	126.7(5)	C(20)-C(21)-C(26)	125.1(6)
C(22)-C(21)-Ir(1)	71.5(3)	C(20)-C(21)-Ir(1)	73.9(3)
C(26)-C(21)-Ir(1)	126.9(3)	C(21)-C(22)-C(18)	107.6(4)
C(21)-C(22)-C(27)	125.6(5)	C(18)-C(22)-C(27)	126.5(5)
C(21)-C(22)-Ir(1)	69.9(2)	C(18)-C(22)-Ir(1)	70.8(2)
C(27)-C(22)-Ir(1)	129.3(3)	C(18)-C(23)-H(23A)	109.5
C(18)-C(23)-H(23B)	109.5	H(23A)-C(23)-H(23B)	109.5
C(18)-C(23)-H(23C)	109.5	H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5	C(19)-C(24)-H(24A)	109.5
C(19)-C(24)-H(24B)	109.5	H(24A)-C(24)-H(24B)	109.5
C(19)-C(24)-H(24C)	109.5	H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5	C(20)-C(25)-H(25A)	109.5
C(20)-C(25)-H(25B)	109.5	H(25A)-C(25)-H(25B)	109.5
C(20)-C(25)-H(25C)	109.5	H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5	C(21)-C(26)-H(26A)	109.5
C(21)-C(26)-H(26B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(21)-C(26)-H(26C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5	C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5	O(1)-C(28)-Cr(1)	178.0(5)
O(2)-C(29)-Cr(1)	175.0(5)	O(3)-C(30)-Cr(1)	178.3(4)
O(4)-C(31)-C(32)	122.4(8)	O(4)-C(31)-C(33)	119.2(7)
C(32)-C(31)-C(33)	118.4(8)	C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5	H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5	H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5	C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5	H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5	H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5		

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 5b

atom	U11	U22	U33	U23	U13	U12
Ir(1)	19(1)	15(1)	18(1)	1(1)	9(1)	1(1)
Cr(1)	16(1)	19(1)	23(1)	-1(1)	8(1)	0(1)
Cl(1)	33(1)	27(1)	24(1)	-4(1)	12(1)	5(1)
O(1)	62(3)	24(3)	64(3)	7(2)	23(2)	12(2)
O(2)	32(2)	47(3)	44(2)	-14(2)	0(2)	-6(2)
O(3)	32(2)	35(3)	48(2)	1(2)	28(2)	-1(2)
N(1)	18(2)	19(3)	20(2)	2(2)	9(2)	-1(2)
N(2)	23(2)	27(3)	26(2)	-2(2)	10(2)	-8(2)
C(1)	22(2)	16(3)	17(2)	-4(2)	10(2)	1(2)
C(2)	23(2)	16(3)	24(2)	-5(2)	12(2)	-2(2)
C(3)	24(2)	23(3)	18(2)	-6(2)	12(2)	-2(2)
C(4)	18(2)	24(3)	21(2)	-2(2)	7(2)	-2(2)
C(5)	20(2)	22(3)	20(2)	-2(2)	9(2)	0(2)
C(6)	19(2)	18(3)	22(2)	-2(2)	10(2)	-3(2)
C(7)	21(2)	20(3)	17(2)	0(2)	12(2)	3(2)
C(8)	16(2)	27(3)	19(2)	1(2)	7(2)	0(2)
C(9)	22(2)	19(3)	15(2)	-2(2)	9(2)	-2(2)
C(10)	18(2)	28(3)	25(2)	-2(2)	9(2)	-7(2)
C(11)	20(2)	26(3)	24(2)	2(2)	7(2)	-1(2)
C(12)	33(3)	31(4)	31(3)	-6(2)	12(2)	-16(3)
C(13)	23(3)	29(4)	38(3)	-5(2)	11(2)	-5(2)
C(14)	28(3)	23(3)	21(2)	-1(2)	8(2)	-4(2)
C(15)	57(4)	22(4)	28(3)	1(2)	16(2)	-9(3)
C(16)	41(3)	28(4)	25(3)	1(2)	15(2)	-5(3)
C(17)	40(3)	45(5)	43(3)	12(3)	10(3)	-15(3)
C(18)	34(3)	25(3)	13(2)	3(2)	6(2)	2(2)
C(19)	21(3)	37(4)	21(2)	13(2)	8(2)	3(2)
C(20)	45(3)	24(3)	20(2)	7(2)	15(2)	17(3)
C(21)	34(3)	26(3)	17(2)	7(2)	5(2)	-5(2)
C(22)	32(3)	23(4)	23(2)	6(2)	17(2)	9(2)
C(23)	73(5)	33(4)	25(3)	-2(2)	-7(3)	-5(3)
C(24)	31(3)	91(7)	39(3)	35(3)	8(2)	-1(3)
C(25)	85(5)	37(5)	49(4)	7(3)	35(3)	33(4)
C(26)	58(4)	31(4)	55(4)	16(3)	-2(3)	-21(3)
C(27)	53(4)	60(5)	38(3)	17(3)	33(3)	23(4)
C(28)	35(3)	23(4)	33(3)	3(2)	13(2)	5(3)
C(29)	22(3)	25(3)	33(3)	0(2)	11(2)	-1(2)
C(30)	19(2)	20(3)	26(2)	-4(2)	4(2)	-3(2)
O(4)	54(3)	117(6)	100(4)	-53(4)	27(3)	-25(4)
C(31)	42(4)	89(7)	41(4)	-30(4)	7(3)	-3(4)
C(32)	54(5)	120(10)	104(6)	-20(6)	37(4)	-7(5)
C(33)	96(8)	160(10)	190(10)	-120(10)	29(7)	10(8)

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 5b

atom	x	y	z	U(eq)
H(2)	469	-5718	-3251	24
H(4)	-1538	-4238	-4805	25
H(5)	438	-3568	-4786	24
H(8)	2411	-2949	-4655	24
H(10)	6311	-3129	-3721	28
H(11)	5874	-4236	-3113	28
H(12A)	-1259	-6555	-3517	47
H(12B)	-2754.0002	-6310	-3591.0002	47
H(12C)	-1579	-5779	-3104	47
H(13A)	-3215	-4577	-4304	44
H(13B)	-3856	-5501.0005	-4377	44
H(13C)	-3210	-5161	-4922	44
H(15A)	4246	-1221	-4092.0002	53
H(15B)	2952	-1516	-4658	53
H(15C)	4003	-916	-4841	53
H(16A)	4201	-1944	-5705	46
H(16B)	3138	-2542	-5531	46
H(16C)	4543	-2915	-5517	46
H(17A)	6450	-1797	-4077	65
H(17B)	6184	-1474.0001	-4823	65
H(17C)	6563	-2442	-4641	65
H(23A)	4099	-3930	-1675	72
H(23B)	5472	-4013.0002	-1834	72
H(23C)	5314	-4399	-1162	72
H(24A)	7230	-5797	-1646	82
H(24B)	6922	-4970	-2103	82
H(24C)	6975	-5878.0005	-2429	82
H(25A)	5703	-7028	-2903	81
H(25B)	4306	-7474	-3009.0002	81
H(25C)	5445	-7583	-2321	81
H(26A)	1401	-6777	-2442	79
H(26B)	2515	-7492	-2256	79
H(26C)	1980	-7149	-3001	79
H(27A)	2105	-5511	-1414	69
H(27B)	1240	-5329	-2162	69
H(27C)	2173	-4605	-1740	69
H(32A)	-1593	-3425	-220	136
H(32B)	-2201	-3422	-1010.0001	136
H(32C)	-1838	-2548	-616	136
H(33A)	-464	-4063	-1421.9999	223
H(33B)	121	-4443	-691	223
H(33C)	1039	-3892	-1009	223

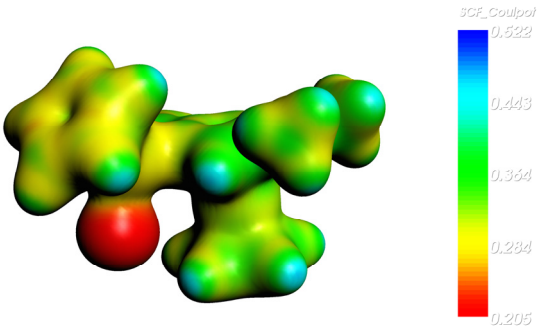
Computational details

Theoretical and Computational details.

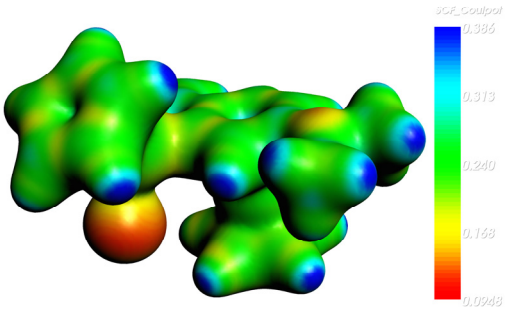
Geometry optimization and ground singlet state electronic structure determination were performed by using the methods of the Density Functional Theory (DFT). The *Becke*[3]-*Perdew*[4, 5] (BP86) and the *Perdew-Burke-Ernzerhof*[6] (PBE) GGA functionals as well as the *Tao-Perdew-Staroverov-Scuseria* (TPSS) metaGGA functional[7] implemented in the *Amsterdam Density Functional* package[8, 9] (abbr. *ADF, version 2009.01*) were used. Opposed to a similar functional that is typically termed BP86, the implementation in ADF employs the *Vosko-Wilk-Nusair* parametrization for the LDA correlation energy part.[10] The PBE functional in ADF200 employs the PW92 parametrization of the LDA correlation energy part. In calculations carried out with the ADF package, scalar relativistic effects were treated within the *Zeroth Order Regular Approximation* (ZORA).[11, 12] As a consequence, in all cases *ad hoc* all-electron TZP (ZORA for Ir, Ru, Cr) and DZP (ZORA for remaining main group elements) basis sets were used. [13] Geometry optimizations by energy gradient minimization were carried out in all cases without symmetry constraint. Integration grid accuracy spanned 5 to 6, energy gradient convergence criterion was set to 10^{-3} au and tight SCF convergence criteria (10^{-7} au) was used. Wiberg bond indices for ADF-optimized geometries (using all electron TZP basis sets) were computed with the GENNBO 5.0 extension of ADF[14]. Representations of molecular structures and orbitals were drawn using *ADFview* v09. Solvation by acetone was accounted for using the COSMO[15-17] procedure with Klamt's values of van der Waals radii for atoms. Thermodynamic data were computed from the statistical data, namely internal energy and entropy, generated by vibrational frequency calculations. The latter were computed by analytical integration and by two point numerical differentiation for geometries optimized respectively in the gas phase and in acetonitrile (COSMO).[8]

Coulomb potential maps for the following models drawn over the SCF electron density isosurface

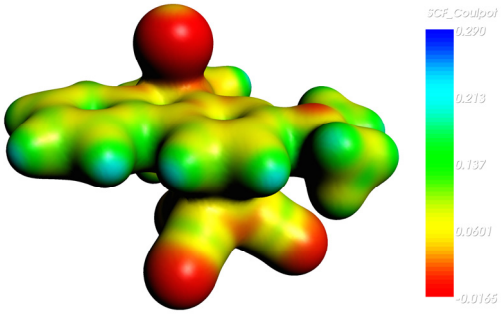
III, charge 2+ (0.035 e/bohr^3)



IV, charge 1+ (0.025 e/bohr^3)



V, neutral (0.025 e/bohr^3)



Dimethylaniline at TPSS/TZP

Geometry CYCLE 2
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Energy gradients wrt nuclear displacements
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Atom	Cartesian (a.u./angstrom) X	Y	Z
1 C	0.000061	0.000034	0.000063
2 C	0.000017	0.000234	-0.000011
3 C	-0.000031	0.000230	0.000129
4 C	-0.000024	0.000117	0.000512
5 C	0.000003	-0.000273	0.000358
6 C	0.000020	-0.000265	-0.000526
7 H	0.000052	-0.000123	0.000025
8 H	-0.000012	-0.000059	0.000085
9 H	-0.000008	-0.000016	0.000047
10 H	0.000028	0.000052	-0.000045
11 H	-0.000002	-0.000081	0.000323
12 N	-0.000071	-0.000011	-0.000357
13 C	-0.000025	0.000157	-0.000022
14 H	0.000030	-0.000057	0.000036
15 H	0.000014	0.000143	-0.000263
16 H	0.000013	0.000048	0.000066
17 C	-0.000027	-0.000164	-0.000568
18 H	-0.000019	-0.000129	0.000084
19 H	-0.000062	0.000101	0.000062
20 H	0.000043	0.000060	0.000000

Geometry Convergence after Step 2
---

current energy	-4.46173895 Hartree		
abs of energy change	0.00085923	0.00100000	T
constrained gradient max	0.00056789	0.00100000	T
constrained gradient rms	0.00017157	0.00066667	T
gradient max	0.00056789		
gradient rms	0.00017157		
cart. step max	0.00472343	0.01000000	T
cart. step rms	0.00134636	0.00666667	T

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

Electrostatic Energy:	-3.343971421350849	-90.9941	-2098.37	-8779.60
Kinetic Energy:	4.089879086778282	111.2913	2566.44	10737.98
Coulomb (Steric+OrbInt) Energy:	-1.120168257182293	-30.4813	-702.92	-2941.00
XC Energy:	-4.087476743146226	-111.2259	-2564.93	-10731.67
Total Bonding Energy:	-4.461737334901086	-121.4101	-2799.78	-11714.29

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
71.170682	0.539450	0.009623
125.433169	235.608254	7.407659
165.169300	87.304780	3.614477
177.130409	0.153834	0.006830
274.913468	106.568606	7.343505
277.732443	4.035233	0.280914
393.924809	8.698585	0.858895
411.713420	0.745933	0.076979
458.950062	39.306253	4.521735
503.808753	89.526283	11.305619
535.707394	10.818507	1.452690
618.989182	0.103309	0.016029
687.767916	115.121357	19.846132
737.366324	60.964055	11.267698
744.243867	193.015856	36.006949
802.264469	0.005660	0.001138
855.365551	10.091364	2.163614
938.509513	59.796860	14.066794
950.819163	0.144739	0.034496
968.782400	0.479368	0.116405
990.732566	56.346127	13.992605
1037.348063	36.613590	9.520174
1057.231174	67.975064	18.013481
1093.751290	3.861965	1.058778
1111.696424	5.826501	1.623574
1130.507282	207.862014	58.901529
1165.323242	3.871461	1.130835
1171.656701	50.926673	14.956286
1197.210463	33.624254	10.090234
1230.244559	94.364842	29.099112
1335.536258	436.179224	146.015422
1337.923208	1.164839	0.390639

1352.025998	16.752875	5.677439
1431.132647	3.597788	1.290606
1466.317808	8.661951	3.183625
1467.160875	30.004734	11.034320
1486.238686	10.958496	4.082419
1490.447034	53.964032	20.160394
1509.028106	10.878394	4.114719
1516.411329	58.134711	22.096862
1526.395986	199.038277	76.152101
1581.298098	19.560849	7.753174
1615.888314	289.047110	117.073349
2924.345177	91.001587	66.704583
2932.536364	145.792591	107.165977
3029.810080	32.768020	24.885346
3031.880659	41.643051	31.647013
3076.779073	4.167205	3.213803
3084.360893	46.170352	35.694922
3112.744244	4.422184	3.450312
3120.059620	13.423257	10.497814
3143.571790	28.845712	22.729125
3156.985146	11.884645	9.404524
3161.321618	0.235452	0.186573

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	40.288	28.798	21.756	90.842
	Internal Energy (Kcal/mole):	0.889	0.889	110.624	112.401
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	27.451	33.412

TS-dimethylaniline at TPSS

Geometry CYCLE 11
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000007	0.000306	0.000050
2	C	-0.000181	0.000050	-0.000075
3	C	0.000023	0.000061	0.000065
4	C	-0.000179	0.000062	-0.000008
5	C	0.000575	-0.000008	-0.000201
6	C	-0.000332	-0.000463	0.000360
7	H	-0.000143	0.000032	-0.000097
8	H	0.000129	-0.000012	0.000054
9	H	-0.000085	-0.000003	-0.000128
10	H	0.000015	-0.000058	0.000108
11	H	-0.000040	0.000201	-0.000126
12	N	0.000627	0.000548	0.000381
13	C	-0.000213	-0.000632	-0.000346
14	H	0.000071	-0.000079	0.000132
15	H	-0.000183	0.000257	-0.000242
16	H	0.000013	-0.000048	0.000061
17	C	-0.000224	-0.000562	-0.000323
18	H	-0.000026	-0.000022	0.000431
19	H	0.000265	0.000049	0.000114
20	H	-0.000104	0.000320	-0.000210

Geometry Convergence after Step 11
---

current energy	-4.45630430 Hartree		
abs of energy change	0.00001941	0.00100000	T
constrained gradient max	0.00063171	0.00100000	T
constrained gradient rms	0.00024662	0.00066667	T
gradient max	0.00063171		
gradient rms	0.00024662		
cart. step max	0.00665736	0.01000000	T
cart. step rms	0.00206888	0.00666667	T

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

Electrostatic Energy:	-3.295092313594319	-89.6640	-2067.70	-8651.26
Kinetic Energy:	4.083285281999387	111.1118	2562.30	10720.66
Coulomb (Steric+OrbInt) Energy:	-1.185039709411491	-32.2466	-743.62	-3111.32
XC Energy:	-4.059456109426393	-110.4634	-2547.35	-10658.10
Total Bonding Energy:	-4.456302850432816	-121.2622	-2796.37	-11700.02

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-56.847230	19.848424	-0.282822
129.137959	17.627052	0.570574
189.630191	24.107891	1.145895
243.455355	2.659260	0.162277
250.756399	10.145588	0.637687
317.820701	1.532537	0.122088
322.456958	1.992864	0.161075
409.041648	0.277914	0.028494
440.992967	18.592868	2.055210
523.195355	35.266588	4.624932
548.198649	108.765862	14.945438
616.826631	0.040219	0.006218
697.700282	176.261291	30.825059
740.575061	23.665585	4.393032
773.163438	70.395533	13.642516
838.102630	0.680510	0.142958
915.781551	0.220049	0.050511
926.249029	120.706259	28.024355
969.075050	0.195831	0.047568
985.547135	0.083201	0.020553
1004.063245	1.062102	0.267304
1027.797666	29.005467	7.472494
1032.999534	54.234623	14.042836
1074.374606	23.360891	6.291051
1092.566906	31.018321	8.494629
1136.614487	103.779111	29.566587
1159.617156	29.061148	8.447058
1163.711871	16.172791	4.717463
1175.042152	11.918078	3.510247
1181.937251	57.344775	16.988942
1284.675368	55.169013	17.765060

1305.305117	1.062117	0.347506
1331.017374	0.448348	0.149581
1423.636501	6.889056	2.458311
1450.214615	4.684715	1.702917
1456.810713	0.347466	0.126880
1480.083701	21.955603	8.145349
1492.778540	31.362244	11.734932
1494.161107	10.017287	3.751679
1498.893609	45.655833	17.153200
1511.429594	30.593570	11.590339
1589.896428	5.364372	2.137794
1604.130974	59.669807	23.992336
2883.999060	54.322057	39.268959
2892.051929	161.840677	117.319943
3015.697809	37.907073	28.654058
3018.305049	74.113564	56.071077
3076.455112	16.345395	12.604455
3078.378111	27.264551	21.037706
3107.703139	4.988822	3.886115
3117.362477	2.022152	1.580081
3126.402039	15.471591	12.124333
3137.443035	18.142348	14.267484
3148.416680	13.657833	10.778345

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	40.288	28.780	16.911	85.979
	Internal Energy (Kcal/mole):	0.889	0.889	109.535	111.312
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	25.377	31.339

dimethylaniline BP86/TZP,DZP

Geometry CYCLE 7
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000080	0.000220	-0.000044
2	C	-0.000066	-0.000179	-0.000005
3	C	0.000039	0.000201	-0.000035
4	C	-0.000059	-0.000345	-0.000015
5	C	-0.000001	0.000079	0.000060
6	C	0.000046	-0.000043	0.000131
7	H	-0.000051	0.000004	-0.000002
8	H	0.000057	0.000048	0.000079
9	H	-0.000039	0.000241	-0.000015
10	H	0.000018	0.000040	-0.000036
11	H	0.000017	-0.000041	-0.000129
12	N	0.000065	0.000299	-0.000118
13	C	-0.000229	-0.000189	0.000502
14	H	-0.000028	0.000076	-0.000092
15	H	0.000164	0.000023	0.000086
16	H	-0.000020	-0.000190	-0.000097
17	C	-0.000024	-0.000182	-0.000225
18	H	-0.000061	-0.000140	0.000066
19	H	0.000288	0.000015	-0.000137
20	H	-0.000036	0.000063	0.000026

Geometry Convergence after Step 7

---

current energy -4.35612063 Hartree

abs of energy change	0.00000111	0.00100000	T
constrained gradient max	0.00050201	0.00100000	T
constrained gradient rms	0.00013843	0.00066667	T
gradient max	0.00050201		
gradient rms	0.00013843		
cart. step max	0.00472666	0.01000000	T
cart. step rms	0.00160111	0.00666667	T

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

Electrostatic Energy:	-3.317534128118646	-90.2747	-2081.78	-8710.18
Kinetic Energy:	4.050633218134081	110.2233	2541.81	10634.94
Coulomb (Steric+OrbInt) Energy:	-1.140504850833189	-31.0347	-715.68	-2994.40
XC Energy:	-3.948704248737393	-107.4497	-2477.85	-10367.32
Total Bonding Energy:	-4.356110009555146	-118.5358	-2733.50	-11436.97

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
87.094894	0.174279	0.003805
120.869054	318.720191	9.656123
158.131655	32.720133	1.296916
177.599785	0.456986	0.020343
268.936120	66.595159	4.489209
279.319801	2.815455	0.197119
394.570973	2.904976	0.287307
411.852010	0.704667	0.072745
461.867804	45.140397	5.225900
503.431775	105.229403	13.278707
538.610365	6.725428	0.907973
615.993964	0.475445	0.073410
682.679284	169.171058	28.948153
733.111289	235.282054	43.235131
737.092458	14.208048	2.625031
786.428020	0.038240	0.007538
839.740634	14.097131	2.967249
930.150241	0.074848	0.017451
937.743187	47.518360	11.169235
948.212221	1.573823	0.374058
977.883062	52.818336	12.946421
1025.062092	48.331429	12.418178
1046.389982	64.051693	16.799728
1081.354891	5.668834	1.536526
1093.510823	3.318895	0.909692
1108.213408	145.139136	40.316795
1150.955948	3.816765	1.101114
1153.425949	35.567773	10.283109
1181.933495	37.553849	11.125654
1227.689729	95.120654	29.271267
1322.683295	10.343764	3.429356

1326.799488	399.397713	132.827788
1337.606012	13.497116	4.525299
1399.294943	1.146820	0.402238
1435.571611	18.917577	6.807199
1440.874196	0.061111	0.022071
1444.569392	26.212891	9.491424
1449.009454	48.829556	17.735036
1470.606336	4.520426	1.666303
1484.782711	32.320239	12.028613
1496.011667	324.009985	121.498648
1559.860462	20.785592	8.126924
1598.044763	320.275199	128.289266
2881.417910	107.938675	77.958129
2889.445156	161.727454	117.132193
2986.744032	40.406310	30.249992
2988.164520	40.848403	30.595507
3043.489264	3.198451	2.439998
3049.959565	42.800822	32.720826
3087.124676	5.014602	3.880330
3092.686446	14.426387	11.183341
3114.657938	27.178309	21.218313
3124.018269	17.727860	13.881870
3128.616835	0.584468	0.458344

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	40.288	28.810	21.642	90.740
	Internal Energy (Kcal/mole):	0.889	0.889	109.267	111.045
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	27.807	33.769

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TS-dimethylaniline BP86/TZP,DZP

Geometry CYCLE 11
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	0.000228	-0.000128	-0.000340
2	C	-0.000084	0.000193	-0.000126
3	C	0.000070	-0.000039	-0.000062
4	C	0.000026	-0.000082	0.000052
5	C	-0.000074	-0.000035	-0.000065
6	C	0.000031	0.000088	0.000124
7	H	-0.000023	-0.000115	0.000103
8	H	-0.000067	0.000038	0.000062
9	H	0.000021	-0.000056	0.000060
10	H	0.000006	0.000047	-0.000081
11	H	0.000090	-0.000123	0.000031
12	N	-0.000678	-0.000640	0.000850
13	C	0.000134	0.000863	-0.000856
14	H	-0.000153	-0.000184	0.000132
15	H	0.000029	-0.000150	0.000188
16	H	0.000154	-0.000083	0.000118
17	C	0.000646	0.000658	0.000116
18	H	-0.000137	-0.000049	-0.000131
19	H	-0.000178	-0.000203	-0.000192
20	H	-0.000041	0.000002	0.000015

Geometry Convergence after Step 11
---

current energy	-4.34788809 Hartree		
abs of energy change	0.00000149	0.00100000	T
constrained gradient max	0.00086327	0.00100000	T
constrained gradient rms	0.00027850	0.00066667	T
gradient max	0.00086327		
gradient rms	0.00027850		
cart. step max	0.00978050	0.01000000	T
cart. step rms	0.00342448	0.00666667	T

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

Electrostatic Energy:	-3.273078161609319	-89.0650	-2053.89	-8593.47
Kinetic Energy:	4.031535746909071	109.7037	2529.83	10584.80
Coulomb (Steric+OrbInt) Energy:	-1.184225312222722	-32.2244	-743.11	-3109.18
XC Energy:	-3.922120351292322	-106.7263	-2461.17	-10297.53
Total Bonding Energy:	-4.347888078215292	-118.3121	-2728.34	-11415.38

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-59.540700	15.658033	-0.233684
134.535484	22.923724	0.773037
194.529064	29.582437	1.442436
247.961176	4.833085	0.300390
257.344050	11.237694	0.724885
322.712000	0.351087	0.028399
327.045579	3.134272	0.256935
406.560843	0.135373	0.013795
445.040918	21.943660	2.447863
525.912476	30.898197	4.073096
546.532873	118.223504	16.195643
613.907926	0.649524	0.099949
691.709388	222.209883	38.526993
740.080961	24.861957	4.612035
765.460154	73.634166	14.127979
821.055070	0.816000	0.167935
899.419873	0.866041	0.195245
925.790337	120.406288	27.940867
949.237843	0.237061	0.056404
965.909311	0.024564	0.005947
992.013081	0.301578	0.074989
1014.430498	36.358934	9.245098
1023.637576	45.166128	11.588765
1060.861742	31.362417	8.339622
1073.601502	24.933400	6.709694
1121.877687	90.324739	25.399800
1137.875537	38.534780	10.990709
1147.906521	2.179276	0.627042
1157.854696	11.442186	3.320788
1174.519919	64.576272	19.011283
1267.709171	51.380774	16.326698
1282.354092	1.776842	0.571130

1321.992089	0.813804	0.269666
1389.035260	1.623266	0.565173
1413.771309	0.464063	0.164450
1433.926301	1.289539	0.463489
1436.229796	23.711258	8.536043
1447.864248	42.896206	15.567712
1450.766270	21.150001	7.691055
1464.967412	4.868596	1.787762
1480.637399	83.651330	31.045570
1570.930655	5.464874	2.151866
1586.590635	58.181268	23.138017
2841.402482	68.126959	48.521009
2849.215047	180.726256	129.069775
2979.175412	58.599238	43.758872
2980.469965	47.402298	35.412959
3036.317424	14.840895	11.294976
3038.123532	30.044249	22.879412
3079.077069	6.418546	4.953764
3088.123807	0.289969	0.224452
3095.661456	16.813728	13.046546
3104.923596	23.574034	18.346909
3115.937347	14.878208	11.620302

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	40.288	28.787	16.772	85.848
	Internal Energy (Kcal/mole):	0.889	0.889	108.146	109.923
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	25.693	31.654

****

V

G E O M E T R Y U P D A T E *** 19 ***

*** Using NEW gradient routines ***

Energy gradients wrt nuclear displacements

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 C	0.000045	0.000005	-0.000011
2 H	-0.000026	0.000024	-0.000050
3 C	0.000019	0.000053	0.000016
4 H	0.000055	0.000029	-0.000039
5 C	0.000035	0.000028	-0.000010
6 H	0.000079	0.000038	0.000028
7 C	0.000064	0.000037	0.000026
8 H	0.000052	0.000006	0.000006
9 C	0.000040	-0.000011	-0.000002
10 C	0.000145	-0.000041	0.000179
11 C	-0.000048	0.000025	-0.000143
12 C	-0.000061	-0.000078	0.000028
13 H	-0.000015	0.000007	-0.000006
14 C	-0.000001	0.000016	-0.000009
15 N	0.000039	-0.000024	0.000025
16 C	-0.000054	0.000018	-0.000016
17 H	0.000011	-0.000042	-0.000013
18 C	-0.000110	-0.000041	-0.000084
19 H	0.000024	-0.000035	-0.000035
20 C	-0.000304	0.000410	0.000087
21 C	-0.000151	0.000161	0.000117
22 C	0.000069	-0.000718	0.000238
23 C	-0.000014	-0.000003	-0.000096
24 C	0.000026	0.000192	-0.000072
25 C	-0.000231	0.000179	-0.000029
26 C	-0.000126	-0.000028	-0.000109
27 C	-0.000045	0.000096	-0.000037
28 H	0.000039	0.000024	-0.000009
29 H	0.000010	0.000008	0.000065
30 H	0.000010	0.000058	0.000041
31 H	-0.000081	0.000082	0.000000
32 H	-0.000071	-0.000006	-0.000048
33 N	-0.000105	0.000186	-0.000135
34 Ir	0.000107	-0.000603	0.000355
35 O	0.000237	-0.000448	-0.000098
36 O	-0.000151	0.000090	-0.000069
37 O	-0.000199	0.000301	0.000013
38 Cr	0.000637	0.000222	-0.000333
39 Cl	-0.000182	-0.000045	-0.000140
40 C	0.000026	-0.000016	0.000053
41 H	0.000091	-0.000010	0.000047
42 H	0.000018	-0.000057	0.000073
43 H	0.000065	-0.000027	0.000056
44 C	-0.000011	-0.000031	0.000031
45 H	0.000039	-0.000022	0.000020
46 H	0.000029	-0.000018	0.000063
47 H	-0.000025	0.000007	0.000023

Geometry Convergence Tests

Energy old : -11.18096267
        new : -11.18096759

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	-0.00000493	0.00100000	YES	0.06240439
gradient max	0.00069375	0.00100000	YES	0.65663607
gradient rms	0.00014202	0.00066667	YES	0.91490827
cart. step max	0.00275662	0.01000000	YES	1.00738279
cart. step rms	0.00085481	0.00666667	YES	1.01977222

prediction dE : -0.00000327

****
Geometry CONVERGED
****

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

Electrostatic Energy:	-10.250530134594040	-278.9311	-6432.31	-26912.76
Kinetic Energy:	12.347216971911195	335.9849	7748.00	32417.61
Coulomb (Steric+OrbInt) Energy:	-2.989579188181153	-81.3506	-1875.99	-7849.14
XC Energy:	-10.288078926245573	-279.9529	-6455.87	-27011.35

Total Bonding Energy: -11.180971277109572 -304.2497 -7016.17 -29355.64

List of All Frequencies:

Intensities
==========

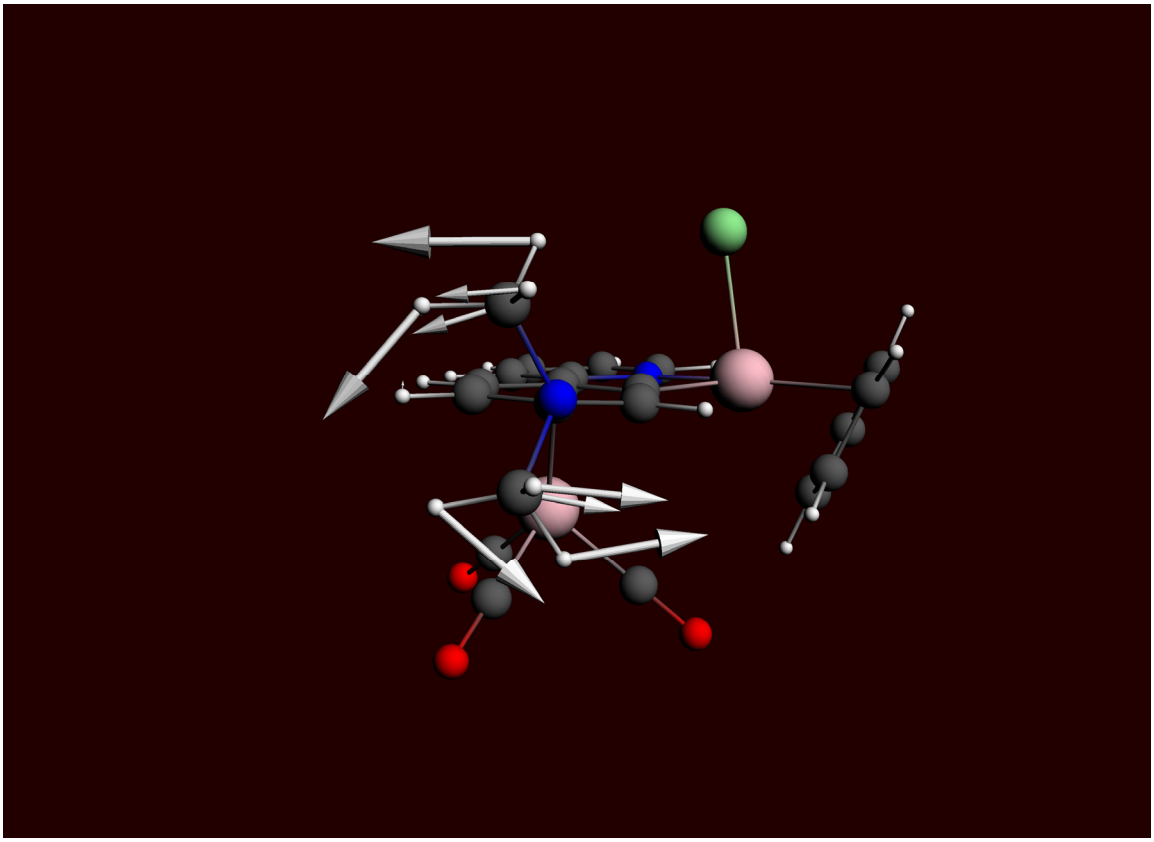
Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
22.526084	303.763406	1.715139
39.528106	174.181636	1.725784
52.358456	145.668845	1.911752
54.342642	135.153582	1.840969
61.863210	253.620925	3.932743
66.906939	220.473893	3.697485
72.709035	69.660475	1.269559
82.764916	44.197087	0.916892
86.699470	26.324279	0.572072
94.417596	0.272045	0.006438
106.337348	85.373837	2.275562
112.855868	29.483046	0.834016
121.159940	81.674703	2.480417
124.743722	21.287056	0.665599
136.824807	135.208923	4.637119
156.578599	73.448296	2.882652
165.205991	46.419930	1.922243
166.940887	0.585776	0.024512
194.941824	55.569256	2.715299
226.493565	50.359470	2.859006
237.332548	14.094216	0.838448
246.449589	42.208430	2.607386
253.298016	54.851728	3.482573
283.154094	29.891649	2.121538
296.622938	14.478900	1.076511
303.252901	223.471633	16.986560
314.869556	114.805281	9.060885
329.816307	39.084198	3.231107
338.811971	20.366545	1.729634
370.843598	33.047794	3.071930
379.257729	56.004762	5.323993
421.290635	3.927828	0.414775
433.516459	40.840891	4.437914
435.860110	56.887405	6.215003
458.775861	5.929847	0.681902
471.365207	13.362321	1.578765
483.292772	101.919828	12.346591
489.955099	8.549682	1.049988
499.040700	40.124481	5.019072
511.340865	123.164083	15.786020
531.156144	3.667965	0.488344
538.153771	233.783845	31.535444
544.638108	101.066948	13.797336
553.020628	34.125251	4.730372
565.347504	43.010912	6.094979
574.048213	39.585765	5.695941
587.919293	2.779045	0.409535
634.896000	226.900567	36.109065
647.001983	86.919231	14.096119
647.448978	383.577081	62.249558
656.015058	78.974918	12.986169
669.789327	50.811330	8.530546
696.196018	437.544766	76.354054
718.865910	160.815461	28.977023
720.671134	98.320686	17.760701
745.475266	181.875837	33.984925
774.203560	75.954242	14.739585
781.151379	203.983813	39.940085
796.059899	69.536572	13.875131
799.003052	36.623008	7.334669
799.526567	5.108666	1.023808
818.562143	17.477049	3.585897
821.884530	38.950477	8.024198
830.592490	8.524073	1.774652
834.461550	158.594484	33.172063
873.103442	4.083842	0.893743
882.057806	10.985766	2.428877
894.236151	24.069828	5.395147
909.229004	0.758777	0.172928
937.322177	0.276386	0.064936
940.117682	92.616593	21.824741
968.111326	32.932711	7.991547
990.126818	19.656076	4.878269
998.937470	71.564985	17.919132
1013.060106	112.314837	28.520059
1039.386732	44.480091	11.588331
1041.347516	12.560037	3.278421
1046.306618	6.260333	1.641854
1050.835671	34.004021	8.956599
1053.554026	58.542877	15.459981
1093.312761	1.283536	0.351747
1093.853822	41.771623	11.452985
1106.806658	4.443809	1.232836
1110.247068	116.195602	32.336082
1127.278609	3.598291	1.016730
1156.697901	32.552453	9.438038
1165.078171	51.592414	15.066729

1222.094437	86.982564	26.644958
1225.097677	54.464568	16.724874
1233.378598	0.365030	0.112850
1272.701032	2.828845	0.902430
1293.352598	15.871253	5.145247
1313.741695	65.312977	21.507381
1331.770161	19.070264	6.365962
1336.235317	218.408020	73.152572
1338.236246	6.235579	2.091643
1359.292418	13.653350	4.651898
1378.258596	15.933227	5.504432
1387.335546	18.650013	6.485429
1400.625343	41.656615	14.624601
1404.211517	104.713955	36.856591
1419.883617	17.488925	6.224349
1430.076042	68.812707	24.666404
1442.187367	2.598289	0.939263
1448.093230	10.944263	3.972474
1454.947974	168.779368	61.552386
1459.311695	129.648880	47.423642
1467.663931	11.109377	4.086904
1486.418929	113.429365	42.261489
1501.543125	141.560796	53.279345
1535.576102	1172.138459	451.157655
1548.924916	34.362118	13.340999
1595.279167	149.302028	59.700844
1870.936583	1658.800796	777.913614
1874.858944	1642.850363	772.048667
1932.908678	2382.712683	1154.412665
2936.737413	53.632937	39.479784
2942.171525	62.387723	46.009254
3021.909875	20.894663	15.826867
3025.069263	15.603563	11.831428
3072.519815	1.373849	1.058063
3079.917185	23.647505	18.255866
3127.603810	3.386989	2.655239
3130.305103	2.520855	1.977938
3145.131329	0.503413	0.396864
3152.321144	1.651332	1.304797
3168.322369	0.119193	0.094659
3172.318928	3.772359	2.999632
3172.601560	0.833094	0.662503
3174.711849	0.884845	0.704125
3175.493834	2.438783	1.941166
3183.477070	0.872749	0.696417
3188.419800	1.441654	1.152165
3198.424258	3.420506	2.742234

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.185	36.144	105.431	186.760
	Internal Energy (Kcal/mole):	0.889	0.889	226.847	228.625
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	101.271	107.233

****

TS1-V



Geometry CYCLE 65
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	0.000093	0.000006	0.000096
2	H	-0.000014	-0.000005	-0.000005
3	C	-0.000004	0.000011	-0.000008
4	H	0.000006	0.000007	0.000013
5	C	-0.000029	-0.000005	0.000002
6	H	0.000000	-0.000009	0.000005
7	C	-0.000009	-0.000006	0.000030
8	H	0.000013	0.000007	0.000005
9	C	-0.000015	0.000002	-0.000043
10	C	-0.000195	-0.000069	0.000042
11	C	0.000049	-0.000083	0.000172
12	C	0.000038	0.000166	0.000166
13	H	-0.000001	0.000018	-0.000013
14	C	0.000202	0.000010	0.000050
15	N	-0.000151	0.000017	0.000087
16	C	0.000059	-0.000005	0.000047
17	H	-0.000007	0.000011	-0.000001
18	C	0.000049	0.000036	0.000047
19	H	-0.000033	0.000012	-0.000032
20	C	-0.000045	0.000119	0.000045
21	C	-0.000078	-0.000041	-0.000038
22	C	0.000117	-0.000356	0.000366
23	C	-0.000110	0.000032	0.000051
24	C	0.000028	0.000020	0.000047
25	C	-0.000018	-0.000013	-0.000002
26	C	0.000187	0.000038	-0.000056
27	C	0.000046	-0.000048	-0.000091
28	H	0.000000	-0.000012	0.000007
29	H	0.000004	0.000004	-0.000018
30	H	-0.000003	-0.000013	-0.000002
31	H	0.000026	0.000026	0.000041
32	H	0.000016	0.000020	-0.000012
33	N	-0.000201	0.000091	-0.000145
34	Ir	0.000117	-0.000056	0.000123
35	O	0.000045	-0.000037	-0.000077
36	O	-0.000074	0.000026	-0.000166
37	O	-0.000149	0.000022	-0.000007
38	Cr	-0.000031	-0.000100	-0.000564
39	Cl	0.000000	0.000027	-0.000077

```
    40 C     0.000005 -0.000009 -0.000037
    41 H    -0.000004  0.000025 -0.000003
    42 H     0.000016 -0.000006 -0.000006
    43 H    -0.000024 -0.000021 -0.000014
    44 C     0.000084  0.000212 -0.000081
    45 H     0.000055 -0.000007 -0.000011
    46 H    -0.000019 -0.000056  0.000040
    47 H    -0.000041 -0.000011  0.000027
 ----------------------------------------

---------------------------------------
Geometry Convergence after Step  65
---------------------------------------
current energy                          -11.27434073 Hartree
abs of energy change               0.00000454     0.00100000    T
constrained gradient max           0.00056447     0.00100000    T
constrained gradient rms           0.00009250     0.00066667    T
gradient max                       0.00056447
gradient rms                       0.00009250
cart. step max                     0.00620827     0.01000000    T
cart. step rms                     0.00175878     0.00666667    T


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

  Electrostatic Energy:           -10.192832711128343       -277.3611         -6396.10        -26761.28
  Kinetic Energy:                  10.085509623764992        274.4407          6328.75         26479.50
  Coulomb (Steric+OrbInt) Energy:  -0.864038087507424        -23.5117          -542.19         -2268.53
  XC Energy:                      -10.302979557120729       -280.3583         -6465.22        -27050.47
                                  -------------------     -----------       ----------      -----------
  Total Bonding Energy:           -11.274340731991504       -306.7904         -7074.76        -29600.78


 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2             km/mole
             ----------          ----------            ----------
             -69.127986           15.086930            -0.261416
              26.642271           67.476662             0.450612
              35.805556          225.241979             2.021519
              54.173049          125.847114             1.708853
              60.485451          215.159099             3.262036
              75.587212          110.745318             2.098224
              80.466325           40.754436             0.821991
              84.018844            3.679193             0.077483
              94.970553            5.319345             0.126627
             105.846663            6.333968             0.168047
             109.213439           10.101774             0.276536
             115.387150          104.835129             3.032092
             116.708743            5.469756             0.160011
             123.331412            4.827077             0.149223
             139.075219           13.749406             0.479305
             157.522483           72.629154             2.867686
             188.201590           31.959520             1.507654
             201.381009            8.566296             0.432404
             224.969374           65.303303             3.682448
             228.127539            3.687570             0.210861
             235.374780           18.304025             1.079903
             239.364701           34.626555             2.077531
             260.174510           86.916027             5.668168
             272.490694           24.551263             1.676886
             280.407513           18.167054             1.276886
             285.220699          170.381374            12.180952
             301.633206          105.936194             8.009430
             312.352789           13.289769             1.040497
             333.242745           90.127231             7.528263
             352.601903           67.794219             5.991773
             384.858334           33.707042             3.251619
             403.576368           11.819752             1.195672
             407.478733            5.367573             0.548228
             425.542210           32.366491             3.452362
             436.536301           44.213334             4.837842
             446.845653            1.368958             0.153330
             474.793466           53.836512             6.407074
             481.802270            2.975957             0.359396
             497.834974            9.450408             1.179272
             500.970752           32.516225             4.083105
             508.821702          140.733419            17.949028
             533.470263          100.479137            13.435820
             546.439636          218.912684            29.984112
             556.273298           11.779659             1.642476
             566.163241           46.421922             6.587837
             567.456036           51.784191             7.365589
             589.546497           46.123611             6.815841
             630.456821          518.915660            82.003086
             641.169838          202.867768            32.603499
             649.862558           13.578857             2.211886
             668.199142           55.393625             9.277774
             679.418046          156.032957            26.572443
             691.406235          255.294641            44.243865
             712.570358           28.186909             5.034464
             716.553028          149.528159            26.856499
             738.600510          339.638302            62.878813
```

744.211183	217.621285	40.595289
756.030636	254.561551	48.240330
776.122360	31.723266	6.171435
799.303531	51.726068	10.363329
803.856405	26.328398	5.304946
810.743447	8.104650	1.647008
812.560582	51.501158	10.489404
835.761240	5.612030	1.175656
842.717493	0.683815	0.144444
847.014160	1.236667	0.262556
865.987531	12.754888	2.768639
884.128454	4.295072	0.951840
917.717633	0.240354	0.055289
933.290660	246.049207	57.559493
943.100287	0.333488	0.078834
962.860201	37.138581	8.963273
994.369318	34.115474	8.503098
1002.914758	41.033516	10.315275
1014.027069	55.551750	14.119696
1031.014879	30.569530	7.900085
1034.282674	26.203717	6.793291
1035.385681	16.146078	4.190321
1044.230670	5.525302	1.446207
1050.577959	15.745308	4.146269
1078.927874	10.853990	2.935350
1093.147053	34.736095	9.517824
1100.006457	23.405272	6.453376
1112.606254	6.260973	1.746069
1122.560512	178.255024	50.156776
1139.446115	13.527525	3.863583
1156.580082	12.437264	3.605609
1180.303405	41.011285	12.133193
1195.224449	32.906810	9.858556
1228.614623	0.063724	0.019624
1259.296643	27.512454	8.684313
1274.417821	39.119177	12.496247
1293.028728	23.583308	7.643477
1306.216115	31.023140	10.157313
1323.478479	34.367347	11.400948
1331.248372	2.661683	0.888165
1339.912524	10.023253	3.366380
1365.323047	8.906170	3.047926
1385.967300	18.704434	6.497939
1398.442913	10.208133	3.578237
1400.250341	90.254120	31.677492
1423.317696	10.233959	3.651099
1425.609258	8.672362	3.098960
1433.755089	79.157679	28.447630
1440.833792	36.913306	13.331373
1443.966210	17.230548	6.236403
1449.217180	24.449483	8.881396
1456.648310	162.010022	59.152712
1467.447821	96.683061	35.562406
1474.938600	19.702795	7.284166
1500.971340	428.104924	161.064821
1555.591785	20.368444	7.942031
1591.765081	136.803216	54.582491
1886.773509	1531.713491	724.394889
1895.052135	1403.484073	666.663566
1946.647834	2455.252787	1198.013394
2866.472915	102.914432	73.943873
2883.840156	84.273118	60.916974
2996.881200	35.661073	26.788105
3006.588548	37.997581	28.635714
3052.971881	12.823352	9.813015
3075.268644	12.346326	9.516974
3124.630719	2.863258	2.242525
3128.917464	1.084989	0.850937
3138.219871	2.671113	2.101133
3139.498409	2.077071	1.634518
3145.123339	0.383374	0.302230
3155.282477	1.717284	1.358183
3160.137886	0.463128	0.366847
3170.021417	1.770592	1.406886
3171.108699	0.842133	0.669375
3182.556403	2.443881	1.949550
3184.081492	0.212235	0.169387
3200.251131	2.271526	1.822132

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.185	36.168	99.981	181.333
	Internal Energy (Kcal/mole):	0.889	0.889	225.008	226.785
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	100.097	106.059

****

TS2-V

```
 Geometry CYCLE 41
 ==============

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

     Atom      Cartesian (a.u./angstrom)
               X         Y         Z
 ----------------------------------------
     1 C    -0.000151  0.000284  0.000147
     2 H    -0.000003  0.000042 -0.000035
     3 C     0.000196 -0.000115 -0.000142
     4 H    -0.000173  0.000081  0.000109
     5 C    -0.000326  0.000052  0.000196
     6 H    -0.000043 -0.000207  0.000063
     7 C     0.000564 -0.000250  0.000276
     8 H    -0.000050 -0.000120  0.000150
     9 C    -0.000542  0.000077 -0.000854
    10 C    -0.000183 -0.000163 -0.000375
    11 C     0.000532 -0.000118 -0.000818
    12 C    -0.000244  0.000105 -0.000237
    13 H     0.000063 -0.000003  0.000157
    14 C    -0.000366  0.000332 -0.000080
    15 N    -0.000102 -0.000398 -0.000037
    16 C     0.000109 -0.000212  0.000004
    17 H     0.000023 -0.000002  0.000050
    18 C     0.000155  0.000241 -0.000087
    19 H     0.000014  0.000025 -0.000006
    20 C    -0.000098  0.000117  0.000338
    21 C     0.000599 -0.000346  0.000370
    22 C     0.000174 -0.000042  0.000990
    23 C     0.000151  0.000116  0.000048
    24 C    -0.000234 -0.000082 -0.000209
    25 C    -0.000105 -0.000223  0.000253
    26 C     0.000135 -0.000303  0.000423
    27 C     0.000106 -0.000148 -0.000195
    28 H     0.000040  0.000064  0.000011
    29 H     0.000021  0.000055  0.000009
    30 H     0.000046  0.000138 -0.000099
    31 H    -0.000023  0.000037 -0.000116
    32 H     0.000072  0.000086 -0.000108
    33 N    -0.000219 -0.000045 -0.000489
    34 Ir    0.000017  0.000851  0.000901
    35 O     0.000115 -0.000855 -0.000471
    36 O     0.000016  0.000365 -0.000533
    37 O    -0.000352  0.000099 -0.000482
    38 Cr   -0.000078  0.000144  0.000591
    39 Cl   -0.000038 -0.000017  0.000163
    40 C     0.000046  0.000108 -0.000147
    41 H     0.000050 -0.000008  0.000008
    42 H    -0.000077 -0.000119  0.000102
    43 H     0.000018  0.000040  0.000026
    44 C     0.000258  0.000174  0.000116
    45 H    -0.000042  0.000108 -0.000023
    46 H    -0.000007  0.000026  0.000031
    47 H    -0.000067  0.000007  0.000015
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Geometry Convergence after Step  41
--------------------------------------
current energy                          -11.16485526 Hartree
energy change                -0.00000776     0.00100000    T
constrained gradient max      0.00099011     0.00100000    T
constrained gradient rms      0.00027313     0.00066667    T
gradient max                  0.00099011
gradient rms                  0.00027313
cart. step max                0.00563994     0.01000000    T
cart. step rms                0.00175992     0.00666667    T


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

  Electrostatic Energy:            -10.214278627581541       -277.9447         -6409.56        -26817.58
  Kinetic Energy:                   12.292409724899045        334.4935          7713.60         32273.72
  Coulomb (Steric+OrbInt) Energy:   -2.981608285363222        -81.1337         -1870.99         -7828.21
  XC Energy:                       -10.261378066994137       -279.2263         -6439.11        -26941.24
                                   --------------------     -----------       ----------      -----------
  Total Bonding Energy:            -11.164855255039855       -303.8112         -7006.05        -29313.32


 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2              km/mole
             ----------          ----------            ----------
            -62.737230           21.288613            -0.334773
             21.269003           64.445652             0.343573
             37.675295          248.141748             2.343336
```

52.769643	127.739142	1.689609
64.528903	231.930998	3.751381
67.593743	14.876354	0.252047
81.571263	32.081638	0.655952
84.940319	7.629489	0.162438
92.661573	3.921289	0.091077
108.011739	9.080097	0.245833
115.196162	17.272143	0.498726
116.116898	41.982779	1.221925
121.523200	84.035053	2.559751
127.797913	7.447778	0.238577
146.381310	24.706888	0.906529
159.775000	64.658844	2.589494
195.640513	12.134992	0.595081
206.119828	18.900759	0.976511
228.232129	73.131823	4.183707
229.678573	21.229560	1.222192
236.592635	15.489151	0.918559
247.486846	20.109251	1.247458
257.890265	80.635910	5.212445
282.149142	6.231179	0.440684
284.682220	21.000844	1.498564
303.198155	221.801457	16.856563
320.437776	32.437063	2.605333
330.964092	69.885379	5.797560
335.886238	25.625677	2.157474
374.805447	66.372816	6.235542
381.976673	31.136187	2.981126
403.120123	10.074766	1.017999
412.918610	8.239304	0.852772
433.601954	25.390080	2.759519
443.668327	32.937535	3.662921
457.808860	2.789071	0.320053
482.180627	51.992595	6.283901
486.518651	5.006964	0.610593
504.409324	13.051694	1.650168
512.869791	84.073772	10.808010
519.294195	49.097293	6.390710
538.581378	94.445250	12.749981
551.234040	100.565655	13.895167
552.536761	102.328736	14.172186
566.761047	57.444554	8.160691
567.413188	48.491397	6.896714
600.094324	46.861680	7.048804
634.491854	463.447266	73.706272
645.554495	173.365434	28.052624
650.988535	19.381991	3.162640
670.245473	67.412039	11.325292
681.324507	114.100351	19.485837
695.218125	309.223764	53.885513
713.987729	24.574276	4.397943
720.490830	220.187103	39.764764
749.267890	147.810134	27.759996
789.349079	271.975865	53.811803
799.092982	68.777916	13.776040
803.350876	24.026221	4.838033
805.195371	3.926097	0.792392
815.845382	21.599085	4.416938
820.349646	10.597639	2.179145
831.664995	136.666494	28.489744
834.247067	51.778896	10.827434
869.958558	10.135920	2.210242
881.075814	3.318503	0.732881
883.874166	5.000979	1.107959
904.753435	27.300444	6.191245
910.701441	0.594886	0.135796
933.761915	262.919067	61.536998
939.101483	0.415975	0.097917
965.929872	34.597818	8.376689
992.869842	29.803827	7.417242
1003.676069	38.400536	9.660707
1011.716052	65.025945	16.490103
1030.853187	29.345043	7.582451
1034.060286	45.623023	11.825186
1041.067042	10.997202	2.869716
1045.009482	7.066255	1.850920
1051.439391	19.457327	5.127970
1078.643583	12.536704	3.389529
1095.598141	34.744490	9.541470
1101.478875	11.637956	3.213150
1115.849615	3.242410	0.906884
1122.551516	187.087432	52.641586
1139.396762	12.429832	3.549918
1157.820368	11.005571	3.193977
1179.292828	39.883139	11.789328
1197.178448	52.633404	15.794228
1232.921629	0.061829	0.019108
1263.845680	26.931693	8.531704
1274.502971	40.283083	12.868906
1289.355674	17.962404	5.805174
1303.590218	29.903856	9.771165
1329.810866	32.776497	10.925227
1333.971058	2.407764	0.805079
1341.568487	4.113193	1.383152
1356.450048	7.235267	2.460008
1386.870779	17.599593	6.118102
1398.268781	10.288722	3.606037
1399.821986	101.609789	35.652208
1424.194302	10.804602	3.857057

1426.423252	8.238860	2.945734
1435.321958	76.354391	27.470174
1440.610215	37.563568	13.564113
1445.020459	29.286076	10.607505
1450.007592	24.507094	8.907179
1456.174351	161.668350	59.008755
1468.627257	106.480746	39.197714
1475.749019	25.448260	9.413447
1503.596414	435.196416	164.019189
1550.522033	21.008594	8.164940
1594.968518	105.994278	42.375282
1881.137155	1532.864385	722.773574
1892.237974	1442.022931	683.952578
1944.354446	2441.959422	1190.123280
2867.307713	104.787125	75.311326
2885.096266	81.020078	58.591017
2996.795620	36.913821	27.728361
3005.061680	37.818779	28.486492
3052.645805	12.696468	9.714880
3074.241405	13.443974	10.359617
3125.336404	2.375118	1.860630
3130.714881	1.122503	0.880865
3138.862562	3.084055	2.426456
3140.666792	1.509727	1.188498
3145.217407	0.384140	0.302844
3156.360719	1.374695	1.087605
3167.417787	0.466484	0.370357
3173.674395	1.540882	1.225773
3178.773058	0.833771	0.664331
3187.079414	1.421342	1.135454
3191.128828	2.477626	1.981793
3202.423240	2.503636	2.009685

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.185	36.162	98.884	180.232
	Internal Energy (Kcal/mole):	0.889	0.889	225.601	227.379
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	99.181	105.143

****

II

Geometry CYCLE 9
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000009	0.000111	0.000016
2	H	0.000020	-0.000044	-0.000040
3	C	0.000011	-0.000084	0.000052
4	H	0.000071	0.000022	0.000000
5	C	-0.000050	-0.000024	-0.000081
6	H	0.000058	0.000072	0.000021
7	C	-0.000064	-0.000043	0.000025
8	H	0.000027	0.000058	0.000028
9	C	-0.000052	0.000100	0.000011
10	C	0.000035	0.000120	0.000086
11	C	0.000324	-0.000339	-0.000290
12	C	-0.000159	0.000135	-0.000044
13	H	-0.000015	-0.000102	-0.000078
14	C	-0.000030	-0.000039	0.000098
15	N	0.000167	-0.000159	0.000530
16	C	0.000017	-0.000129	-0.000014
17	H	-0.000015	0.000140	0.000012
18	C	0.000011	-0.000017	-0.000068
19	H	-0.000022	0.000080	0.000039
20	Cl	0.000050	0.000035	-0.000247
21	C	-0.000063	-0.000053	-0.000177
22	C	-0.000163	-0.000281	-0.000053
23	C	-0.000247	0.000178	-0.000052
24	C	0.000249	0.000134	-0.000253
25	C	0.000197	-0.000149	0.000121
26	H	-0.000028	-0.000009	-0.000026
27	H	-0.000047	0.000020	-0.000008
28	H	-0.000006	-0.000051	0.000047
29	H	0.000020	-0.000004	0.000059
30	H	0.000053	0.000034	-0.000026
31	N	-0.000196	-0.000216	-0.000088
32	Ir	-0.000080	0.000312	0.000925
33	C	-0.000010	0.000309	-0.000094
34	H	-0.000074	0.000010	-0.000102
35	H	0.000074	0.000026	-0.000049
36	H	-0.000088	-0.000065	0.000053
37	C	0.000085	-0.000149	-0.000277
38	H	-0.000003	0.000027	-0.000070
39	H	0.000037	0.000024	-0.000032
40	H	-0.000084	0.000012	0.000043

Geometry Convergence after Step 9
---

current energy	-9.12330744 Hartree		
energy change	-0.00000207	0.00100000	T
constrained gradient max	0.00092536	0.00100000	T
constrained gradient rms	0.00015069	0.00066667	T
gradient max	0.00092536		
gradient rms	0.00015069		
cart. step max	0.00951725	0.01000000	T
cart. step rms	0.00221713	0.00666667	T

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

Electrostatic Energy:	-8.117518802494171	-220.8889	-5093.82	-21312.54
Kinetic Energy:	10.300182031559117	280.2822	6463.46	27043.12
Coulomb (Steric+OrbInt) Energy:	-2.676159899475039	-72.8220	-1679.32	-7026.26
XC Energy:	-8.629809850124204	-234.8291	-5415.29	-22657.56
Total Bonding Energy:	-9.123306520534296	-248.2578	-5724.96	-23953.24

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
30.679474	38.698702	0.297593
46.733893	105.326892	1.233813
54.995554	215.603390	2.972085
61.871945	53.447284	0.828891
92.763343	2.435172	0.056622
105.815217	11.981492	0.317788
116.279662	17.672813	0.515095
132.238733	44.765637	1.483821

142.628480	10.229847	0.365724
178.505675	5.225450	0.233805
189.534483	3.358233	0.159543
214.179669	34.341269	1.843625
229.593639	12.985461	0.747301
248.071862	60.523254	3.763378
250.270129	6.713160	0.421128
289.051102	31.967761	2.316141
306.101223	224.090913	17.193622
317.321679	20.179971	1.605086
323.547081	25.480517	2.066445
335.343907	2.863283	0.240676
373.094682	58.375847	5.459217
424.778521	15.013639	1.598551
433.338916	44.239866	4.805290
449.623914	10.538583	1.187708
469.064398	4.903631	0.576538
514.493891	40.139116	5.176379
535.482765	28.059306	3.766175
549.798828	34.063897	4.694358
567.732091	51.951184	7.392936
572.811614	31.780706	4.563031
591.913038	31.990509	4.746321
653.164769	5.765202	0.943877
674.365837	24.887223	4.206783
698.858702	82.289570	14.414920
715.492029	149.576754	26.825447
722.260477	4.070925	0.736996
737.336692	362.178214	66.936999
762.760640	89.938018	17.195296
767.066805	139.976832	26.913329
788.000018	101.267929	20.002129
799.242705	81.879174	16.403261
804.583635	25.057941	5.053528
806.687226	1.285736	0.259977
818.332919	9.284290	1.904394
824.049636	6.870648	1.419153
825.529633	154.772579	32.026152
872.483070	6.429177	1.406017
876.526851	22.513156	4.946291
888.643280	3.948684	0.879545
905.139769	0.932363	0.211533
931.924551	0.131885	0.030807
951.137217	127.001696	30.278250
966.068522	40.958019	9.918019
988.644646	20.518207	5.084611
997.711617	51.189072	12.801485
1014.540986	201.514471	51.245284
1039.994318	4.511039	1.175941
1040.502941	33.649705	8.776122
1044.749741	6.086175	1.593803
1052.398018	40.105056	10.579307
1056.532267	104.144938	27.580301
1092.806563	56.246676	15.407005
1101.568520	43.616748	12.043227
1105.195667	1.519021	0.420805
1106.737918	3.461857	0.960355
1150.129745	0.232968	0.067162
1153.495259	121.350298	35.086070
1165.156566	67.635376	19.753146
1232.722840	236.725756	73.145738
1233.259950	0.034102	0.010542
1242.635636	24.694478	7.691689
1275.062076	14.186578	4.534058
1295.324245	62.491991	20.289947
1328.408790	126.631306	42.164883
1330.523759	42.736712	14.252853
1334.926976	202.187344	67.653388
1337.308693	15.924738	5.338043
1352.117347	551.834743	187.025789
1386.165006	18.501595	6.428389
1397.069704	10.111076	3.540736
1411.663131	29.148475	10.313949
1417.846679	205.753124	73.122963
1423.777648	29.349245	10.474111
1435.173538	103.735263	37.317187
1438.017413	19.057886	6.869371
1447.658050	58.571899	21.253642
1460.373379	503.609102	184.346777
1463.878424	34.463720	12.645769
1472.526480	158.294788	58.426221
1494.603706	315.615949	118.239631
1534.861294	127.773624	49.157345
1540.767894	247.853748	95.721783
1585.916201	1648.506841	655.313417
1594.943144	73.506408	29.386541
2916.716045	96.424350	70.495101
2925.200718	181.772250	133.278877
2982.175855	35.049469	26.199486
2988.425476	27.311946	20.458470
3068.675716	1.951175	1.500809
3078.213984	32.092759	24.761898
3110.253274	12.521918	9.762132
3122.722436	2.636619	2.063758
3142.139094	2.188810	1.723898
3147.756889	2.560874	2.020540
3152.076444	8.967066	7.084761
3159.220160	9.711628	7.690419
3165.428030	0.858815	0.681413

3167.405972	0.313921	0.249231
3168.035837	2.124218	1.686814
3179.316852	0.290840	0.231775
3185.141006	0.085358	0.068148
3195.396009	4.714462	3.776025

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	44.456	34.845	67.969	147.270
	Internal Energy (Kcal/mole):	0.889	0.889	204.183	205.960
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	72.175	78.136

****

TS2-II

Geometry CYCLE 40
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000009	-0.000002	-0.000009
2	H	-0.000004	0.000002	-0.000001
3	C	-0.000005	-0.000002	-0.000014
4	H	0.000001	-0.000001	-0.000005
5	C	0.000002	-0.000001	0.000005
6	H	0.000000	0.000004	0.000004
7	C	0.000004	-0.000002	-0.000004
8	H	-0.000003	-0.000002	0.000000
9	C	0.000059	0.000009	-0.000020
10	C	0.000033	-0.000052	-0.000022
11	C	-0.000067	0.000128	0.000030
12	C	-0.000034	-0.000031	-0.000034
13	H	0.000007	0.000006	0.000008
14	C	0.000030	0.000018	0.000052
15	N	-0.000019	-0.000011	-0.000036
16	C	0.000003	0.000002	-0.000006
17	H	-0.000008	0.000003	-0.000004
18	C	0.000007	0.000000	-0.000008
19	H	0.000000	-0.000002	0.000004
20	H	-0.000003	0.000009	-0.000003
21	H	-0.000004	0.000003	-0.000002
22	C	0.000003	0.000010	0.000005
23	C	-0.000089	-0.000250	0.000244
24	C	-0.000056	0.000039	-0.000027
25	C	-0.000091	0.000083	-0.000034
26	C	0.000115	0.000003	-0.000012
27	C	-0.000216	-0.000240	0.000342
28	H	-0.000007	0.000002	-0.000009
29	H	0.000020	0.000020	0.000016
30	H	-0.000001	0.000021	0.000025
31	H	-0.000022	0.000000	0.000024
32	H	-0.000004	-0.000012	-0.000011
33	N	0.000017	-0.000011	0.000105
34	Ir	0.000316	0.000276	-0.000697
35	H	-0.000002	-0.000004	0.000008
36	H	-0.000001	0.000004	-0.000004
37	H	-0.000002	0.000002	-0.000003
38	H	0.000005	-0.000007	-0.000002
39	Cl	0.000013	0.000001	0.000080
40	C	0.000011	-0.000017	0.000017

Geometry Convergence after Step 40
---

current energy	-9.11308579 Hartree		
energy change	-0.00000113	0.00100000	T
constrained gradient max	0.00069708	0.00100000	T
constrained gradient rms	0.00009621	0.00066667	T
gradient max	0.00069708		
gradient rms	0.00009621		
cart. step max	0.00229228	0.01000000	T
cart. step rms	0.00074277	0.00666667	T

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

Electrostatic Energy:	-8.068113034761669	-219.5445	-5062.82	-21182.83
Kinetic Energy:	10.268185605258807	279.4115	6443.38	26959.12
Coulomb (Steric+OrbInt) Energy:	-2.714187387019308	-73.8568	-1703.18	-7126.10
XC Energy:	-8.598971123668818	-233.9899	-5395.94	-22576.60
Total Bonding Energy:	-9.113085940190988	-247.9797	-5718.55	-23926.40

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-70.383936	26.145372	-0.461261
36.799091	56.230527	0.518665
49.480215	231.685371	2.873481
54.620204	142.816135	1.955279
88.484277	3.122836	0.069262
106.736005	19.389686	0.518752
117.493021	22.775080	0.670734
124.665830	20.203235	0.631315
133.832418	27.049260	0.907392
174.469193	7.861537	0.343799
204.853312	14.079753	0.722963

226.419949	4.830232	0.274133
233.909249	61.725172	3.618993
236.827898	4.850692	0.287948
261.220481	7.668013	0.502074
264.608364	9.852469	0.653472
279.782167	32.413560	2.273133
304.629559	191.598164	14.629903
311.450453	80.660626	6.296927
333.833802	1.068688	0.089425
366.814269	38.428546	3.533282
371.056210	48.322548	4.494357
399.012405	3.510747	0.351127
427.244254	7.807801	0.836148
435.917910	24.268986	2.651761
443.407899	35.451969	3.940233
516.434382	21.824870	2.825172
521.963485	22.055857	2.885640
550.380203	32.896239	4.538237
565.098836	31.120123	4.408022
568.514531	45.658938	6.506470
623.487365	49.216967	7.691669
652.509954	12.263358	2.005740
672.333010	13.285189	2.238877
712.511853	129.436593	23.116775
720.768434	147.766064	26.696144
722.007696	158.662924	28.714109
757.130825	160.448017	30.449723
763.747142	166.880191	31.947175
791.978438	110.719388	21.979363
799.375296	42.205469	8.456634
810.701063	40.838384	8.298648
813.124312	47.668641	9.715559
819.543762	21.757346	4.469471
826.551080	147.590044	30.577701
834.021968	11.372711	2.377495
857.997603	31.424269	6.758173
875.830930	4.664112	1.023923
878.850055	25.601896	5.639817
908.303504	0.560118	0.127523
910.530219	0.445807	0.101746
936.014746	162.612422	38.151751
936.869956	0.813340	0.190998
966.558586	41.436779	10.039041
989.805528	28.666718	7.112232
1005.435264	69.394102	17.488588
1020.370460	27.592340	7.057071
1030.297388	40.300500	10.407612
1039.446497	11.440314	2.980699
1042.613193	24.044365	6.283688
1046.061289	14.187853	3.720077
1052.595450	54.326276	14.333409
1076.569120	19.105538	5.155601
1092.756584	51.897127	14.214933
1104.792762	5.469941	1.514752
1117.314160	16.336760	4.575297
1133.591929	148.638471	42.234372
1141.091644	23.004313	6.579727
1155.169557	11.239661	3.254446
1175.677721	42.491087	12.521726
1224.057741	41.675521	12.786775
1233.836970	0.054684	0.016912
1259.926790	14.482447	4.573675
1276.312084	87.116374	27.869857
1289.941417	21.620294	6.990523
1308.533971	85.106673	27.914296
1319.653370	33.609572	11.117341
1330.748046	8.433358	2.813030
1337.129992	1.585934	0.531541
1372.238188	35.853147	12.332038
1385.998133	17.582720	6.108390
1394.434374	1.048392	0.366437
1415.020972	93.869145	33.293834
1421.443820	2.201868	0.784511
1423.592442	3.386172	1.208294
1435.556960	30.328953	10.913296
1442.254268	52.364119	18.930135
1448.777481	62.875405	22.832873
1450.072857	137.989640	50.155016
1461.982826	283.843092	104.015646
1470.272006	10.771107	3.969503
1537.283556	104.036863	40.088453
1548.182768	96.004406	37.255592
1571.749043	394.657912	155.482705
1593.062409	99.057549	39.554731
2847.170151	89.208693	63.664696
2864.352668	101.685480	73.006832
2986.999439	93.636838	70.106769
2989.116224	20.048154	15.020876
3045.910913	19.340606	14.766085
3052.392380	19.306164	14.771154
3109.294533	16.492430	12.853594
3111.145135	1.649451	1.286287
3124.691964	1.365439	1.069443
3136.064903	5.215937	4.100110
3142.733535	1.297503	1.022102
3148.774772	2.123816	1.676241
3165.629912	0.506928	0.402239
3168.121509	0.517752	0.411152
3170.038500	1.573488	1.250277

```
        3178.883953           0.466909           0.372036
        3185.790819           0.012266           0.009795
        3195.876316           3.886203           3.113103
```

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	44.456	34.799	64.837	144.092
	Internal Energy (Kcal/mole):	0.889	0.889	203.566	205.344
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	71.904	77.866

****

TS1-II

Geometry CYCLE 30
==========

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

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 C	0.000014	0.000011	-0.000087
2 H	0.000019	0.000004	0.000020
3 C	0.000030	0.000028	0.000038
4 H	-0.000010	-0.000014	-0.000011
5 C	0.000028	0.000028	0.000050
6 H	-0.000010	-0.000004	-0.000032
7 C	-0.000008	-0.000047	-0.000010
8 H	0.000005	0.000010	-0.000004
9 C	-0.000075	0.000107	-0.000068
10 C	0.000086	-0.000070	-0.000136
11 C	-0.000140	-0.000089	0.000016
12 C	-0.000002	-0.000030	0.000047
13 H	0.000005	0.000002	0.000019
14 C	0.000094	0.000005	0.000016
15 N	-0.000029	0.000017	-0.000001
16 C	-0.000044	-0.000019	-0.000099
17 H	0.000013	0.000002	0.000013
18 C	0.000010	0.000016	0.000085
19 H	-0.000012	0.000004	-0.000020
20 H	0.000012	-0.000002	-0.000009
21 H	-0.000003	-0.000005	0.000009
22 C	-0.000025	0.000028	-0.000006
23 C	0.000120	-0.000288	0.000151
24 C	-0.000750	-0.000314	0.000144
25 C	0.000297	0.000120	0.000088
26 C	0.000037	-0.000048	-0.000079
27 C	-0.000090	-0.000085	0.000021
28 H	0.000014	-0.000028	0.000001
29 H	-0.000009	0.000006	-0.000038
30 H	-0.000011	0.000044	0.000018
31 H	-0.000034	0.000035	-0.000019
32 H	-0.000003	-0.000022	0.000037
33 N	-0.000243	-0.000365	0.000373
34 Ir	0.000620	0.000975	-0.000555
35 H	0.000012	-0.000022	-0.000002
36 H	-0.000005	0.000009	-0.000011
37 H	0.000004	0.000006	0.000006
38 H	-0.000007	0.000001	0.000014
39 Cl	0.000098	-0.000013	-0.000012
40 C	-0.000008	0.000010	0.000035

Geometry Convergence after Step 30
---

current energy	-9.11314048 Hartree		
energy change	-0.00000955	0.00100000	T
constrained gradient max	0.00097515	0.00100000	T
constrained gradient rms	0.00015998	0.00066667	T
gradient max	0.00097515		
gradient rms	0.00015998		
cart. step max	0.00580950	0.01000000	T
cart. step rms	0.00190657	0.00666667	T

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

Electrostatic Energy:	-8.068336467598352	-219.5506	-5062.96	-21183.41
Kinetic Energy:	10.257201732876013	279.1127	6436.49	26930.28
Coulomb (Steric+OrbInt) Energy:	-2.703885129227857	-73.5765	-1696.71	-7099.05
XC Energy:	-8.598120732408098	-233.9668	-5395.40	-22574.36
Total Bonding Energy:	-9.113140596358294	-247.9812	-5718.58	-23926.55

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-62.999543	4.480100	-0.070746
34.145302	35.820576	0.306578
50.607078	270.796335	3.435043
55.099454	126.027074	1.740561
91.742596	3.581405	0.082357
105.059095	22.965363	0.604763
117.447590	21.669508	0.637927
127.315322	34.498459	1.100927
142.295889	13.343215	0.475917
192.745410	6.426426	0.310479
202.186790	22.420447	1.136253
207.632993	0.999646	0.052026

231.780643	16.425740	0.954290
235.026594	42.469749	2.501928
251.969034	8.507139	0.537290
259.554737	12.123888	0.788767
279.617590	54.228854	3.800782
302.714802	103.437318	7.848542
307.386367	130.972386	10.091191
335.467524	3.507916	0.294970
366.908185	31.586336	2.904924
371.719045	49.948954	4.653924
398.044399	7.597329	0.758002
431.381714	4.039022	0.436733
441.153024	45.684781	5.051715
449.315545	14.999633	1.689313
518.584871	22.409763	2.912964
523.283390	12.900517	1.692085
550.196911	27.085727	3.735397
566.579087	46.109593	6.548320
568.830906	35.144336	5.010910
622.804261	53.197172	8.304590
653.079506	9.315876	1.524993
676.080051	29.297557	4.964867
711.999217	136.293377	24.323851
717.193440	21.685033	3.898293
720.815420	277.424683	50.124175
755.883220	130.463000	24.718387
766.918603	196.429920	37.760261
789.903504	42.474082	8.409615
794.151286	82.801390	16.482343
809.070976	23.371658	4.739737
810.696306	5.765179	1.171518
819.617693	11.724782	2.408763
826.383155	137.939817	28.572561
833.411793	11.173901	2.334224
872.654623	37.892933	8.288552
875.668486	7.209235	1.582366
881.690579	14.863531	3.284856
902.559317	0.975858	0.220770
909.164611	0.673499	0.153482
936.154585	0.442400	0.103810
938.013499	364.694734	85.746549
965.797373	39.296365	9.512977
990.640539	27.872167	6.920937
1004.846604	61.018720	15.368834
1020.085445	24.554443	6.278338
1030.039007	40.596899	10.481528
1039.116694	17.973349	4.681353
1042.038123	15.761517	4.116799
1046.103808	14.476776	3.795987
1051.528161	52.533550	13.846363
1077.619433	18.705766	5.052647
1093.048970	50.001131	13.699273
1104.938074	3.881915	1.075133
1127.520498	184.176858	52.052019
1130.362758	3.802310	1.077317
1143.119136	25.732622	7.373159
1155.173361	12.203157	3.533438
1174.653248	42.740495	12.584249
1215.232890	46.842633	14.268519
1233.915194	0.054013	0.016706
1258.544396	20.013717	6.313561
1275.923865	27.365833	8.752084
1289.993435	29.822986	9.643101
1311.389079	88.107274	28.961523
1321.428268	27.596191	9.140518
1331.050470	8.739583	2.915838
1337.599484	0.863964	0.289667
1372.541803	29.171955	10.036197
1385.748320	17.791791	6.179909
1394.523864	1.842967	0.644201
1415.477049	71.988708	25.541434
1423.239980	11.541114	4.117219
1426.587132	5.367983	1.919497
1435.761689	23.709445	8.532608
1444.829864	106.709065	38.645247
1448.964484	25.115560	9.121761
1450.563784	76.004314	27.634597
1463.338976	298.409947	109.455177
1470.507095	34.195475	12.604158
1528.216063	59.885286	22.939448
1547.570226	83.372509	32.340841
1577.375743	490.779790	194.043857
1593.010499	116.646411	46.576633
2851.815088	70.534398	50.419716
2857.066680	180.763141	129.451869
2986.730212	80.421780	60.207106
2988.709799	16.498048	12.359315
3046.443135	20.799034	15.882334
3051.957978	20.564482	15.731654
3104.244187	10.220686	7.952689
3123.883531	8.498438	6.654448
3124.510510	0.167594	0.131256
3125.837973	8.691036	6.809513
3142.536979	1.060082	0.835022
3148.743389	2.298149	1.813817
3166.091750	0.612447	0.486038
3168.084786	0.612297	0.486224
3169.986235	1.774543	1.410009
3179.478104	0.387455	0.308785

```
        3185.515228            0.141381            0.112888
        3195.878720            3.774547            3.023662
```

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	44.456	34.874	64.816	144.146
	Internal Energy (Kcal/mole):	0.889	0.889	203.576	205.353
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	71.894	77.856

IV

```
 Geometry CYCLE 7
 ==============

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

     Atom      Cartesian (a.u./angstrom)
               X          Y          Z
 ----------------------------------------
     1 C    -0.000007  0.000077 -0.000070
     2 H    -0.000043 -0.000024 -0.000055
     3 C     0.000004  0.000035  0.000094
     4 H     0.000052  0.000005  0.000047
     5 C    -0.000050 -0.000068 -0.000098
     6 H    -0.000040  0.000010 -0.000067
     7 C     0.000121 -0.000006  0.000083
     8 H     0.000020  0.000010  0.000053
     9 C    -0.000196  0.000121  0.000036
    10 C     0.000040  0.000002 -0.000111
    11 C    -0.000149 -0.000274  0.000348
    12 C     0.000178 -0.000094 -0.000071
    13 H    -0.000047 -0.000017  0.000012
    14 C    -0.000364  0.000153 -0.000117
    15 N     0.000132 -0.000033  0.000021
    16 C     0.000009  0.000041 -0.000001
    17 H     0.000000 -0.000010 -0.000028
    18 C    -0.000068  0.000080  0.000021
    19 H     0.000021  0.000012  0.000021
    20 Cl    0.000188  0.000051  0.000050
    21 C    -0.000125 -0.000005  0.000052
    22 C     0.000097  0.000148 -0.000207
    23 C     0.000056  0.000000 -0.000008
    24 C     0.000199  0.000118  0.000091
    25 C    -0.000126  0.000043  0.000054
    26 H     0.000015 -0.000002  0.000022
    27 H    -0.000015 -0.000016  0.000011
    28 H     0.000010  0.000030 -0.000055
    29 H    -0.000005  0.000037 -0.000008
    30 H    -0.000008 -0.000009  0.000020
    31 N     0.000045 -0.000098  0.000107
    32 Ir   -0.000245 -0.000370 -0.000166
    33 C    -0.000026 -0.000048  0.000022
    34 H     0.000007  0.000029 -0.000036
    35 H    -0.000009  0.000037 -0.000030
    36 H     0.000004 -0.000023  0.000009
    37 C     0.000080  0.000049 -0.000022
    38 H    -0.000044 -0.000032 -0.000020
    39 H    -0.000043 -0.000042 -0.000015
    40 H     0.000016 -0.000006  0.000012
    41 Ru    0.000134  0.000099 -0.000080
    42 C     0.000042  0.000093  0.000032
    43 C     0.000077 -0.000065 -0.000112
    44 C     0.000152 -0.000091 -0.000039
    45 C    -0.000102 -0.000079  0.000115
    46 C     0.000062  0.000116  0.000088
    47 H     0.000007  0.000023 -0.000012
    48 H     0.000010  0.000001 -0.000009
    49 H    -0.000026  0.000005  0.000019
    50 H     0.000000 -0.000011  0.000010
    51 H    -0.000041 -0.000001 -0.000015
 ----------------------------------------

---------------------------------------
Geometry Convergence after Step   7
---------------------------------------
current energy                          -11.48437019 Hartree
abs of energy change              0.00000311     0.00100000    T
constrained gradient max          0.00036978     0.00100000    T
constrained gradient rms          0.00009132     0.00066667    T
gradient max                      0.00036978
gradient rms                      0.00009132
cart. step max                    0.00895224     0.01000000    T
cart. step rms                    0.00229212     0.00666667    T


 Number of elements of the density matrix on this node (used, total):     35923    264628


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

  Electrostatic Energy:           -10.731117243576886       -292.0086         -6733.88        -28174.54
  Kinetic Energy:                  12.646203372343393        344.1207          7935.61         33202.60
  Coulomb (Steric+OrbInt) Energy:  -2.692056743742128        -73.2546         -1689.29         -7067.99
  XC Energy:                      -10.707400426287801       -291.3632         -6719.00        -28112.28
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -11.484371041263422       -312.5056         -7206.55        -30152.21



 List of All Frequencies:


 Intensities
```

==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
34.981966	177.324048	1.554855
49.865766	188.461418	2.355608
54.624282	171.918297	2.353889
59.404928	117.416684	1.748358
70.351648	0.389687	0.006872
80.511578	54.221399	1.094226
94.479077	27.489441	0.650998
108.844115	49.600766	1.353229
122.515121	34.655042	1.064227
125.656998	35.506807	1.118346
135.045121	88.259722	2.987580
144.921108	89.784541	3.261454
156.325331	48.758296	1.910539
169.294353	197.384622	8.375946
192.841355	84.416333	4.080419
224.415003	34.191226	1.923289
239.224284	35.348297	2.119590
248.660374	115.292120	7.185951
263.724583	156.575057	10.350260
282.523509	3.199119	0.226549
298.455763	12.788078	0.956673
306.451631	170.144458	13.069465
324.829455	4.260283	0.346874
331.658652	46.689902	3.881435
343.713829	17.077794	1.471319
359.956010	43.516281	3.926262
373.253831	143.903656	13.463382
377.288753	230.471193	21.795587
381.172644	32.175305	3.074132
391.258833	115.371275	11.314619
437.693415	21.623920	2.372370
441.982385	9.848739	1.091098
468.544525	113.110652	13.284109
486.872378	51.951272	6.340002
513.231690	68.468161	8.808059
528.735617	54.289362	7.195010
552.304382	44.442893	6.152603
563.842931	38.649510	5.462359
566.628283	13.252201	1.882194
568.719638	8.867961	1.264154
572.453777	16.475765	2.364090
581.486176	177.880624	25.926632
639.244864	95.566523	15.312676
650.376959	41.957061	6.839877
666.247391	17.615817	2.941822
717.022652	22.851878	4.107077
729.718766	147.056370	26.897841
755.416314	247.112322	46.790623
791.891595	81.666062	16.210090
795.444691	186.059342	37.097064
804.488508	11.328595	2.284410
811.144287	121.164246	24.634892
816.771332	154.226337	31.574545
820.021624	29.265360	6.015299
820.991617	23.259246	4.786438
822.313270	98.715520	20.347020
826.773677	83.225819	17.247366
832.372145	22.406661	4.674905
839.439447	116.891892	24.595284
840.918245	29.847665	6.291326
847.263335	3.471213	0.737187
867.543991	4.619105	1.004448
878.763390	4.852401	1.068825
890.508229	6.008052	1.341065
892.726913	12.778975	2.859517
895.128650	15.274220	3.427067
898.524534	5.431317	1.223244
920.986227	1.589424	0.366920
935.470216	94.926108	22.258388
950.409811	0.060646	0.014447
971.349481	37.292425	9.079757
989.881148	60.104308	14.913059
990.635279	47.335297	11.753764
991.514068	7.576858	1.883068
992.898096	61.873614	15.398848
1012.278407	36.207255	9.186998
1038.447535	33.358796	8.683064
1044.002735	1.600468	0.418819
1046.648866	29.779959	7.812737
1047.979904	34.615276	9.092825
1049.105095	6.370427	1.675196
1050.361984	11.038184	2.906128
1053.750831	26.233058	6.928910
1090.577887	2.686029	0.734252
1096.168660	31.259263	8.588833
1104.496083	27.924794	7.730939
1105.001064	11.646397	3.225762
1111.839244	128.646127	35.852281
1120.033465	2.765465	0.776385
1161.139498	45.274106	13.176873
1163.141613	11.057151	3.223695
1211.046231	91.937265	27.908107
1218.057226	41.751058	12.747154
1235.448751	0.108841	0.033705

1236.177856	0.078548	0.024339
1272.161456	6.107847	1.947639
1286.348472	3.529783	1.138111
1300.821580	34.658192	11.300605
1332.762185	182.892832	61.098059
1334.712076	9.399784	3.144731
1342.209001	3.092484	1.040413
1351.101187	3.776348	1.278904
1355.330866	6.421706	2.181594
1358.661938	7.268622	2.475378
1368.645335	2.834498	0.972401
1390.537899	23.971981	8.355353
1397.768583	144.243594	50.537049
1405.202779	4.837361	1.703827
1406.177371	37.509237	13.220760
1407.464221	15.088408	5.323029
1423.393494	10.389940	3.706945
1432.734342	112.999802	40.580877
1441.928900	6.435939	2.326129
1448.505109	11.118070	4.036710
1451.834069	100.985423	36.749695
1461.244621	125.377256	45.921890
1463.925071	7.812389	2.866690
1481.788370	132.056183	49.048191
1491.551347	58.379175	21.826004
1538.603816	1067.186536	411.571423
1554.611682	6.188206	2.411375
1596.096299	54.362307	21.748787
2936.631495	55.548820	40.888611
2941.973076	54.920979	40.500001
3033.033271	15.826685	12.032205
3035.681360	9.846145	7.492047
3082.192185	1.080216	0.834542
3088.989776	7.857376	6.083760
3125.873221	2.215598	1.735963
3133.493870	1.293574	1.016011
3147.230046	2.010971	1.586399
3147.519274	1.680839	1.326089
3152.601104	0.883606	0.698242
3153.783494	4.627109	3.657797
3158.833117	0.179279	0.141950
3165.123192	0.074570	0.059160
3167.893481	0.659812	0.523925
3172.437642	0.760943	0.605094
3174.720739	1.135115	0.903282
3174.802739	0.245262	0.195175
3176.665449	0.682764	0.543651
3182.617265	4.056830	3.236304
3188.678531	1.906924	1.524130
3188.803828	2.103330	1.681176
3198.505604	1.712191	1.372706

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.330	36.105	88.929	170.364
	Internal Energy (Kcal/mole):	0.889	0.889	261.060	262.837
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	95.890	101.852

****

TS1-IV

```
 Geometry CYCLE 25
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 C    -0.000106 -0.000075  0.000036
     2 H     0.000004 -0.000003  0.000000
     3 C     0.000055  0.000035  0.000014
     4 H     0.000006  0.000040 -0.000001
     5 C    -0.000039 -0.000028 -0.000019
     6 H    -0.000029 -0.000046  0.000019
     7 C     0.000000  0.000023 -0.000005
     8 H     0.000025  0.000030 -0.000004
     9 C     0.000025 -0.000008 -0.000007
    10 C    -0.000023  0.000059 -0.000010
    11 C    -0.000128 -0.000109 -0.000145
    12 C    -0.000105  0.000027  0.000133
    13 H     0.000026 -0.000037  0.000000
    14 C     0.000229 -0.000163 -0.000007
    15 N    -0.000159  0.000142 -0.000069
    16 C    -0.000253  0.000008  0.000157
    17 H     0.000013  0.000012 -0.000038
    18 C     0.000342  0.000156  0.000094
    19 H     0.000002  0.000013  0.000023
    20 Cl   -0.000020 -0.000033  0.000074
    21 C     0.000047 -0.000017  0.000046
    22 C    -0.000064  0.000016 -0.000007
    23 C    -0.000052 -0.000043  0.000021
    24 C     0.000035  0.000062  0.000053
    25 C     0.000034  0.000065  0.000069
    26 H    -0.000009 -0.000010 -0.000008
    27 H    -0.000016  0.000003 -0.000009
    28 H     0.000007  0.000013  0.000006
    29 H     0.000009  0.000020 -0.000005
    30 H     0.000000  0.000008  0.000008
    31 N     0.000211  0.000018  0.000001
    32 Ir   -0.000080  0.000041 -0.000259
    33 C    -0.000027 -0.000051 -0.000009
    34 H    -0.000005  0.000019  0.000009
    35 H     0.000000 -0.000014  0.000023
    36 H    -0.000013 -0.000010 -0.000010
    37 C     0.000076 -0.000061  0.000002
    38 H     0.000011  0.000005  0.000001
    39 H     0.000007  0.000064 -0.000040
    40 H     0.000011 -0.000006  0.000008
    41 Ru   -0.000406 -0.000415 -0.000239
    42 C     0.000097 -0.000022  0.000017
    43 C     0.000047 -0.000021  0.000021
    44 C     0.000033  0.000052 -0.000065
    45 C     0.000155  0.000163 -0.000026
    46 C     0.000020  0.000089  0.000114
    47 H     0.000012 -0.000019 -0.000013
    48 H     0.000035 -0.000008 -0.000008
    49 H    -0.000010 -0.000015  0.000018
    50 H    -0.000023  0.000018  0.000038
    51 H    -0.000004  0.000014 -0.000004
 ----------------------------------------

---------------------------------------
Geometry Convergence after Step  25
---------------------------------------
current energy                          -11.46684707 Hartree
abs of energy change              0.00001437     0.00100000    T
constrained gradient max          0.00041533     0.00100000    T
constrained gradient rms          0.00008718     0.00066667    T
gradient max                      0.00041533
gradient rms                      0.00008718
cart. step max                    0.00744534     0.01000000    T
cart. step rms                    0.00252766     0.00666667    T

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

  Electrostatic Energy:           -10.701576987020477       -291.2047         -6715.34        -28096.99
  Kinetic Energy:                  12.618572850690242        343.3688          7918.27         33130.06
  Coulomb (Steric+OrbInt) Energy:  -2.698666559238063        -73.4345         -1693.44         -7085.35
  XC Energy:                      -10.685174533770104       -290.7584         -6705.05        -28053.92
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -11.466845229338402       -312.0287         -7195.55        -30106.20

 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2          km/mole
             ----------          ----------          ----------
             -97.337607           38.865142           -0.948242
              34.896247           57.589986            0.503737
```

55.658226	198.572798	2.770302
68.499140	11.711029	0.201075
75.258608	113.444689	2.140023
94.553572	44.111224	1.045454
101.909500	15.118749	0.386197
111.454191	30.699791	0.857650
123.919014	60.749421	1.886940
129.047636	42.934940	1.388798
153.070050	37.348652	1.432990
175.344711	90.238968	3.966111
191.163440	15.073124	0.722248
199.854200	26.198441	1.312402
215.480764	6.112313	0.330135
228.775274	12.144436	0.696409
231.865969	4.124228	0.239694
243.765764	186.543259	11.398044
253.449864	50.757062	3.224531
274.266475	62.501541	4.296764
284.221146	35.123778	2.502279
305.690905	165.116737	12.651782
322.530941	16.693512	1.349575
331.685234	27.575930	2.292632
344.019763	4.528203	0.390470
367.842288	45.848334	4.227302
373.015794	76.447432	7.147731
378.390995	233.286184	22.126253
384.980501	33.247982	3.208353
393.890761	49.130394	4.850697
407.947200	89.749329	9.177264
441.907918	15.393308	1.705068
448.417027	63.136214	7.096410
470.610600	188.881269	22.280692
516.009735	46.376106	5.998329
522.242816	67.249214	8.803143
552.341336	41.807784	5.788190
559.734101	53.112104	7.451665
564.122217	33.538574	4.742375
568.419564	4.874709	0.694538
572.662058	5.148983	0.739091
610.814783	26.353404	4.034822
647.237017	24.311649	3.944172
666.422002	23.817744	3.978579
685.377108	20.714719	3.558662
713.351458	22.440457	4.012484
730.580318	156.787170	28.711545
757.408000	204.611671	38.845289
793.261034	54.332040	10.803145
796.580933	187.115154	37.360866
806.963432	7.018414	1.419616
819.774602	3.127301	0.642602
820.439659	5.389114	1.108261
821.602424	23.547291	4.849319
825.531865	438.419395	90.719714
828.441090	76.347222	15.853784
830.214427	2.529063	0.526293
842.771681	103.736871	21.913974
845.544835	19.254072	4.080725
845.921346	6.920782	1.467450
854.866500	23.740345	5.087019
895.269804	3.685721	0.827093
896.495464	7.693339	1.728785
897.828044	25.913002	5.831617
902.217935	5.924440	1.339790
904.314955	30.635824	6.944282
907.915851	1.182990	0.269218
921.268807	1.942851	0.448646
931.450408	238.824813	55.759292
951.614717	0.066920	0.015962
971.845523	35.900003	8.745201
991.574970	32.283236	8.023811
991.981743	20.748354	5.158998
993.447021	23.358882	5.816676
996.289073	73.003160	18.230773
1008.897846	34.048445	8.610385
1027.619985	36.093889	9.297031
1032.637850	42.249628	10.935761
1045.095762	1.684690	0.441321
1047.042977	0.655439	0.172018
1049.670638	4.396628	1.156780
1051.017856	20.658899	5.442461
1053.018946	10.212704	2.695597
1078.635187	9.359487	2.530491
1095.521564	8.691686	2.386728
1097.080833	29.444468	8.096930
1106.975915	27.610262	7.661023
1111.012699	0.749888	0.208830
1120.722852	201.272505	56.540644
1138.941129	8.928426	2.548909
1163.334010	5.909606	1.723221
1177.789498	38.099730	11.247802
1195.535073	42.452612	12.721690
1235.383105	0.529025	0.163816
1236.802298	0.041122	0.012748
1262.454673	22.762658	7.203057
1271.419757	46.114786	14.696273
1281.262506	5.173970	1.661652
1298.555973	35.554872	11.572784
1320.881229	14.895420	4.931677
1336.581333	4.884929	1.636559

1342.320264	3.056336	1.028337
1346.235469	5.679166	1.916389
1360.714079	14.394814	4.909655
1364.010301	1.498758	0.512421
1383.031699	138.598943	48.047426
1391.163934	26.378942	9.198431
1399.419472	9.967778	3.496426
1406.277276	16.581714	5.844918
1407.700096	27.851800	9.827464
1423.755719	12.406948	4.427703
1426.668784	11.620211	4.155423
1434.359362	73.470116	26.414766
1440.840592	24.840762	8.971373
1447.012844	39.657060	14.383712
1451.432872	56.454966	20.538900
1457.576322	127.531968	46.593833
1466.403950	26.718930	9.820888
1476.964854	28.870622	10.688195
1494.131922	345.794191	129.504455
1555.067946	6.075022	2.367965
1596.263407	33.188901	13.279310
2881.264695	55.585936	40.144509
2887.096420	105.084757	76.046474
3013.311839	17.551399	13.256653
3020.011556	20.563854	15.566507
3063.433677	7.288020	5.596237
3087.471132	12.587290	9.741217
3115.390324	1.274415	0.995180
3126.355458	0.521816	0.408916
3127.781127	1.466229	1.149519
3134.481407	1.466633	1.152299
3147.384183	2.251421	1.776170
3154.260097	4.114219	3.252842
3160.564265	0.048641	0.038534
3166.744096	0.139451	0.110691
3168.724411	0.612679	0.486626
3172.358212	0.811492	0.645274
3176.002867	0.497781	0.396276
3176.246190	0.560523	0.446258
3177.170957	3.094330	2.464253
3182.428971	4.834662	3.856585
3189.378386	4.067111	3.251398
3189.467719	1.724812	1.378917
3198.859035	1.415275	1.134786

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.330	36.113	81.871	163.314
	Internal Energy (Kcal/mole):	0.889	0.889	259.886	261.663
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	93.756	99.717

****

TS2-IV

```
 Geometry CYCLE 62
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 C     0.000055  0.000014  0.000002
     2 H    -0.000004 -0.000089  0.000021
     3 C    -0.000022 -0.000088  0.000020
     4 H     0.000017 -0.000014  0.000006
     5 C     0.000053  0.000045 -0.000015
     6 H     0.000012  0.000035 -0.000011
     7 C    -0.000085 -0.000136  0.000042
     8 H     0.000039  0.000078  0.000019
     9 C     0.000179  0.000267 -0.000086
    10 C    -0.000183 -0.000733  0.000286
    11 C     0.000303  0.000206  0.000123
    12 C    -0.000087 -0.000127  0.000043
    13 H     0.000062  0.000060 -0.000010
    14 C    -0.000300 -0.000094  0.000206
    15 N    -0.000113  0.000083 -0.000410
    16 C     0.000002  0.000169  0.000009
    17 H     0.000005 -0.000077  0.000039
    18 C     0.000161  0.000607 -0.000199
    19 H    -0.000056 -0.000111 -0.000005
    20 Cl    0.000109 -0.000079 -0.000149
    21 C     0.000052  0.000099  0.000016
    22 C     0.000103  0.000031 -0.000053
    23 C     0.000091  0.000007 -0.000027
    24 C     0.000071  0.000010 -0.000063
    25 C     0.000050  0.000030 -0.000027
    26 H    -0.000013  0.000005  0.000005
    27 H     0.000057  0.000061  0.000035
    28 H     0.000008  0.000030  0.000004
    29 H    -0.000092 -0.000045 -0.000017
    30 H    -0.000110 -0.000051 -0.000034
    31 N     0.000195  0.000087 -0.000072
    32 Ir   -0.000844 -0.000119  0.000453
    33 C    -0.000404 -0.000448  0.000573
    34 H    -0.000097  0.000207 -0.000315
    35 H     0.000146  0.000101 -0.000033
    36 H     0.000282 -0.000067 -0.000179
    37 C     0.000170 -0.000138  0.000052
    38 H     0.000181  0.000089  0.000255
    39 H     0.000006  0.000222 -0.000195
    40 H     0.000056 -0.000113 -0.000027
    41 Ru    0.000270 -0.000261 -0.000876
    42 C    -0.000086 -0.000128  0.000043
    43 C     0.000092  0.000150  0.000088
    44 C     0.000070  0.000173  0.000133
    45 C     0.000011  0.000133  0.000119
    46 C    -0.000190 -0.000017  0.000099
    47 H    -0.000028 -0.000002  0.000032
    48 H    -0.000079 -0.000007  0.000025
    49 H    -0.000068 -0.000029 -0.000011
    50 H    -0.000022 -0.000048  0.000016
    51 H    -0.000028  0.000023  0.000045
 ----------------------------------------

---------------------------------------
Geometry Convergence after Step  62
---------------------------------------
current energy                          -11.46704846 Hartree
energy change                -0.00001040     0.00100000    T
constrained gradient max      0.00087621     0.00100000    T
constrained gradient rms      0.00018627     0.00066667    T
gradient max                  0.00087621
gradient rms                  0.00018627
cart. step max                0.00523537     0.01000000    T
cart. step rms                0.00135406     0.00666667    T


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

  Electrostatic Energy:            -10.701620493014072       -291.2059         -6715.37        -28097.10
  Kinetic Energy:                   12.627798232256140        343.6199          7924.06         33154.28
  Coulomb (Steric+OrbInt) Energy:   -2.708304865198770        -73.6967         -1699.49         -7110.65
  XC Energy:                       -10.684921618175501       -290.7515         -6704.89        -28053.26
                                   --------------------     -----------       ----------      -----------
  Total Bonding Energy:            -11.467048744132203       -312.0343         -7195.68        -30106.73


 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2          km/mole
```

-81.170651	25.404491	-0.516877
36.042691	69.106876	0.624333
55.616574	190.251726	2.652228
69.909425	1.841412	0.032267
76.692639	87.223881	1.676746
91.939283	69.434914	1.600137
102.864961	11.938167	0.307810
111.345710	27.717726	0.773587
124.333012	76.316859	2.378401
128.182403	43.461519	1.396405
153.094233	19.065838	0.731632
172.843324	48.722179	2.110850
179.294358	88.626317	3.982973
224.211412	18.478197	1.038473
228.978324	3.422594	0.196439
236.488565	5.320879	0.315407
243.147559	23.629290	1.440120
245.340410	160.638515	9.878633
260.191082	84.828018	5.532352
266.962597	6.185289	0.413893
298.123955	109.919383	8.213896
307.192788	132.896340	10.232980
322.620301	12.623637	1.020832
330.695020	15.758393	1.306224
343.547242	5.352024	0.460874
368.531678	45.164174	4.172026
371.319900	75.325391	7.010802
378.411652	190.250702	18.045497
385.162970	57.084427	5.511125
395.800947	65.133465	6.461883
415.219396	95.968225	9.988107
442.513443	12.824351	1.422460
451.990811	180.518171	20.451662
455.827934	34.186361	3.905997
512.817664	24.398436	3.136195
521.831795	110.451203	14.447046
552.205292	40.173494	5.560556
561.632473	80.531112	11.336891
563.201527	31.338176	4.424005
568.913063	9.573449	1.365188
571.616404	3.670279	0.525874
613.213602	22.258700	3.421288
645.176030	24.659733	3.987904
664.204307	11.319442	1.884537
686.877886	24.491024	4.216621
715.972704	35.856279	6.434870
730.830672	157.476279	28.847619
757.708388	205.861191	39.098009
794.138906	71.037235	14.140364
796.617168	229.140123	45.753980
806.432076	10.556511	2.133862
820.285652	1.568525	0.322504
820.961344	3.509611	0.722204
821.753069	60.714180	12.505744
825.029109	408.271683	84.429963
828.049993	78.530104	16.299369
831.522453	9.371571	1.953280
842.382611	109.294928	23.077431
845.200710	6.857241	1.452738
846.325088	15.327318	3.251483
855.922395	21.908288	4.700249
893.063856	8.249827	1.846739
895.590067	5.267058	1.182376
896.676011	6.032579	1.355866
897.833869	17.099975	3.848305
903.059575	11.341513	2.567234
913.991304	4.283795	0.981406
921.916502	3.474605	0.802925
929.063312	120.302394	28.015453
951.843438	0.069699	0.016629
972.001337	37.327389	9.094368
991.992149	29.193089	7.258825
993.115907	21.301086	5.302489
994.468283	13.331079	3.323030
995.664866	79.879662	19.935516
1009.126355	32.593851	8.244405
1028.387987	36.957001	9.526465
1033.620496	38.752963	10.040240
1045.072846	1.768198	0.463186
1048.299973	0.993102	0.260950
1049.976612	5.502762	1.448233
1052.766958	21.436976	5.656839
1053.107364	11.092030	2.927937
1079.362356	2.392129	0.647187
1087.510556	13.290197	3.622788
1096.969789	28.460673	7.825605
1106.571121	26.453373	7.337337
1109.134177	4.047809	1.125336
1123.301226	199.956601	56.300215
1138.686447	16.774279	4.787691
1163.119782	5.941936	1.732330
1182.432767	40.401894	11.974469
1200.889313	46.588714	14.023673
1236.842256	0.065450	0.020291
1237.756686	0.415804	0.129004
1261.296986	18.009937	5.693871
1271.806363	57.945635	18.472250
1280.103555	4.369578	1.402047

1298.612219	29.740777	9.680769
1317.156222	11.484172	3.791535
1335.959970	5.701926	1.909383
1341.675632	2.658943	0.894200
1343.874617	1.861381	0.627007
1360.592949	11.747072	4.006230
1363.556077	3.225752	1.102509
1380.079917	134.579095	46.554312
1391.199012	25.094753	8.750850
1398.798106	8.634132	3.027274
1407.083289	17.890409	6.309837
1408.173432	23.367353	8.247907
1423.560885	12.741259	4.546388
1425.292011	19.674865	7.029002
1435.172196	46.028687	16.558106
1443.335329	44.215184	15.996197
1448.590052	96.406277	35.004903
1451.286586	34.394485	12.511808
1459.445997	104.318378	38.161631
1470.822265	52.111144	19.211836
1478.211805	50.560250	18.733717
1491.759465	287.261991	107.412553
1554.835686	6.058860	2.361312
1595.944405	34.302770	13.722240
2880.758810	50.912799	36.763084
2885.915556	80.171361	57.993717
3011.281905	22.389830	16.899750
3016.072697	20.991669	15.869631
3059.810646	8.092760	6.206822
3074.105752	13.461000	10.372280
3114.065947	1.083267	0.845554
3121.313685	2.156983	1.687572
3133.569399	1.381876	1.085392
3135.683746	0.307690	0.241838
3147.224382	2.117140	1.670149
3153.804674	4.358028	3.445108
3160.017002	0.087541	0.069339
3166.683963	0.225449	0.178949
3168.516112	0.692479	0.549972
3172.050906	0.884746	0.703456
3175.885241	0.683323	0.543963
3176.353978	2.107079	1.677598
3176.748016	2.096000	1.668984
3182.173397	4.794639	3.824351
3189.135738	3.492440	2.791773
3189.387547	1.247282	0.997126
3198.643657	1.456190	1.167514

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.330	36.081	81.370	162.780
	Internal Energy (Kcal/mole):	0.889	0.889	259.883	261.661
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	93.665	99.626

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III

```
 Geometry CYCLE 20
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 C     0.000082  0.000216  0.000020
     2 H    -0.000039  0.000031 -0.000030
     3 C     0.000104 -0.000091 -0.000083
     4 H     0.000002 -0.000036  0.000008
     5 C     0.000014  0.000019  0.000008
     6 H     0.000013 -0.000063  0.000009
     7 C    -0.000087 -0.000134 -0.000075
     8 H     0.000005 -0.000037 -0.000003
     9 C     0.000021 -0.000011  0.000084
    10 C    -0.000383  0.000027 -0.000843
    11 C     0.000214 -0.000191 -0.000008
    12 C     0.000482 -0.000153  0.000122
    13 H    -0.000030  0.000030  0.000011
    14 C    -0.000430 -0.000077 -0.000109
    15 N    -0.000067  0.000085  0.000030
    16 C     0.000210  0.000250  0.000036
    17 H     0.000036 -0.000032 -0.000022
    18 C     0.000399  0.000482  0.000191
    19 H    -0.000016 -0.000028 -0.000023
    20 Cl    0.000086 -0.000074  0.000293
    21 C     0.000146  0.000075 -0.000063
    22 C    -0.000117 -0.000032 -0.000136
    23 C    -0.000104 -0.000037  0.000032
    24 C     0.000036 -0.000063 -0.000064
    25 C     0.000121  0.000002 -0.000024
    26 H     0.000012 -0.000020  0.000093
    27 H     0.000008 -0.000065  0.000036
    28 H    -0.000018 -0.000004  0.000009
    29 H    -0.000064 -0.000028 -0.000008
    30 H     0.000023 -0.000059  0.000008
    31 N     0.000010 -0.000273  0.000097
    32 Ir   -0.000430  0.000390 -0.000099
    33 C    -0.000005 -0.000088 -0.000006
    34 H    -0.000007  0.000003  0.000013
    35 H     0.000001 -0.000016  0.000015
    36 H    -0.000062  0.000035  0.000005
    37 C    -0.000043 -0.000090  0.000008
    38 H     0.000010  0.000033  0.000006
    39 H     0.000043  0.000041 -0.000018
    40 H     0.000009  0.000026  0.000000
    41 Ir   -0.000651  0.000111  0.000672
    42 C     0.000292 -0.000224  0.000113
    43 C     0.000031  0.000042  0.000058
    44 C     0.000031  0.000018 -0.000186
    45 C    -0.000039  0.000032 -0.000021
    46 C     0.000232  0.000144 -0.000017
    47 H    -0.000016 -0.000045 -0.000042
    48 H     0.000008 -0.000056 -0.000061
    49 H    -0.000021 -0.000015 -0.000027
    50 H    -0.000038 -0.000024 -0.000012
    51 H    -0.000014 -0.000023  0.000007
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Geometry Convergence after Step  20
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current energy                          -11.11602195 Hartree
abs of energy change               0.00000291     0.00100000    T
constrained gradient max           0.00084345     0.00100000    T
constrained gradient rms           0.00016076     0.00066667    T
gradient max                       0.00084345
gradient rms                       0.00016076
cart. step max                     0.00542116     0.01000000    T
cart. step rms                     0.00152811     0.00666667    T

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

  Electrostatic Energy:           -10.881796876753072       -296.1088         -6828.43        -28570.15
  Kinetic Energy:                  13.398480784897288        364.5912          8407.67         35177.71
  Coulomb (Steric+OrbInt) Energy:  -3.123682559614579        -84.9997         -1960.14         -8201.23
  XC Energy:                      -10.509025772584714       -285.9651         -6594.51        -27591.44
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -11.116024424055077       -302.4824         -6975.41        -29185.12
 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2             km/mole
             ----------          ----------           ----------
              12.849866            0.000000             0.000000
              26.246493          247.893084             1.630849
              38.844212           75.337488             0.733526
```

48.885114	156.264263	1.914760
58.063166	148.613343	2.162901
63.949464	45.051146	0.722139
66.244464	39.794994	0.660779
80.770905	47.542758	0.962537
98.829152	50.198384	1.243520
105.803894	50.283808	1.333546
118.734299	140.620986	4.185086
120.520544	31.801380	0.960694
126.887491	53.464002	1.700428
141.494846	365.144099	12.950394
155.394324	113.851138	4.434561
202.255264	120.430374	6.105397
219.074869	203.283912	11.162813
249.802828	46.286628	2.898217
254.177560	149.555724	9.528363
263.499362	231.777203	15.308349
275.919979	8.406106	0.581375
287.107092	10.847694	0.780655
311.693842	141.612619	11.063900
327.422338	188.771660	15.492559
333.143277	31.613648	2.639877
337.561081	76.718082	6.491248
342.402190	75.815955	6.506916
351.006639	47.843779	4.209387
367.701800	21.933431	2.021531
369.761687	44.216366	4.098105
380.447106	111.642280	10.646358
433.373713	35.293532	3.833856
440.906455	32.773217	3.621960
465.391108	42.350045	4.940262
483.928454	59.124735	7.171804
508.293285	172.436884	21.969623
528.378527	42.052943	5.569544
545.443062	5.839300	0.798341
550.038007	3.798567	0.523710
552.457815	41.693633	5.773603
557.682163	33.289957	4.653482
560.154956	43.424160	6.097021
597.118920	131.904067	19.742270
628.416518	156.172383	24.599705
649.499131	110.858874	18.047918
660.438791	13.054337	2.161053
715.242603	20.248007	3.630059
728.878331	115.650446	21.129072
759.404457	246.086802	46.842443
787.412853	19.043620	3.758634
809.564991	72.571261	14.726328
815.893391	11.313753	2.313759
817.924623	4.464094	0.915218
818.582068	25.459080	5.223757
830.508169	109.584031	22.812309
838.676655	181.205234	38.092841
840.301452	67.899405	14.301420
846.710272	273.909967	58.132732
852.783654	40.055929	8.562168
855.272329	15.126973	3.242907
857.367557	34.187217	7.346980
867.751969	32.500192	7.069026
894.852401	34.531062	7.745321
902.466662	10.212893	2.310245
906.952832	3.758688	0.854474
908.464275	8.051886	1.833511
914.317884	8.459200	1.938673
919.628792	5.918040	1.364170
928.513104	45.632900	10.620481
929.778560	6.384273	1.487884
959.757904	0.157086	0.037790
976.337203	31.550300	7.721140
989.522239	21.237453	5.267518
992.327428	6.130832	1.524939
994.129093	120.982616	30.146981
997.346341	47.800089	11.949584
1010.301119	27.986744	7.087307
1034.983330	49.513637	12.845063
1037.089162	95.261291	24.763420
1048.728736	1.007818	0.264925
1053.391845	10.661173	2.814965
1054.321376	2.507285	0.662605
1054.970433	18.677667	4.939022
1055.140900	7.905276	2.090767
1075.373523	2.169117	0.584683
1098.817472	5.251970	1.446525
1100.125783	13.085817	3.608455
1100.856712	5.966216	1.646296
1116.607314	31.553095	8.831216
1120.264968	66.471369	18.665234
1162.630460	58.164791	16.950400
1170.793695	2.219330	0.651299
1191.236785	17.629802	5.264094
1198.626579	123.767950	37.185204
1238.716056	0.160942	0.049971
1239.372692	0.158336	0.049188
1270.869621	25.800834	8.218883
1280.644866	34.185097	10.973460
1303.316034	13.495638	4.408808
1315.327615	1.754405	0.578418
1333.967007	5.877504	1.965242
1338.946163	55.793280	18.725054

1342.233126	3.528365	1.187079
1345.204963	3.660286	1.234189
1346.731949	6.361466	2.147417
1351.379766	4.563532	1.545812
1391.689979	47.509249	16.572909
1394.365918	38.770450	13.550511
1401.232364	41.982817	14.745510
1403.645241	61.016299	21.467491
1407.557211	26.998912	9.525557
1426.773668	20.265322	7.247474
1428.562680	155.404595	55.646932
1440.249185	18.378921	6.634920
1448.928677	28.211532	10.245939
1451.080909	15.812903	5.751502
1456.117600	29.998689	10.949059
1469.434072	108.426535	39.935926
1473.115308	38.521553	14.223897
1484.952039	31.973056	11.900758
1557.064538	0.678224	0.264703
1586.963543	1134.900752	451.442980
1593.205465	19.605415	7.829354
2976.589683	10.173026	7.590095
2979.108503	6.775914	5.059788
3069.352445	0.731887	0.563078
3075.940829	0.774747	0.597332
3106.165634	1.465239	1.140804
3111.539969	1.917138	1.495226
3136.648669	1.807080	1.420762
3140.834129	1.352308	1.064630
3147.255615	5.096571	4.020575
3150.234343	0.819480	0.647082
3154.984864	22.326078	17.655816
3158.849467	6.440375	5.099389
3170.126853	0.914685	0.726819
3171.044902	2.503555	1.989929
3172.660345	2.842930	2.260830
3178.534021	2.378520	1.895011
3179.870849	3.168224	2.525244
3183.742790	14.236644	11.361186
3185.898106	23.802131	19.007534
3187.698851	20.393914	16.295059
3188.904349	11.840237	9.464114
3198.653739	4.857750	3.894758
3198.778408	4.549096	3.647433

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.716	36.321	92.745	174.783
	Internal Energy (Kcal/mole):	0.889	0.889	261.602	263.379
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	95.914	101.876

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TS1-III

```
 Geometry CYCLE 41
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 C     0.000067  0.000015  0.000134
     2 H     0.000026 -0.000060 -0.000011
     3 C     0.000007  0.000055  0.000009
     4 H    -0.000009 -0.000042  0.000042
     5 C     0.000095 -0.000013  0.000076
     6 H     0.000031  0.000028  0.000038
     7 C     0.000088  0.000037  0.000084
     8 H     0.000001  0.000001  0.000040
     9 C    -0.000200 -0.000071 -0.000037
    10 C     0.000296 -0.000049 -0.000295
    11 C    -0.000190 -0.000089  0.000234
    12 C     0.000143 -0.000168  0.000315
    13 H     0.000041  0.000064  0.000030
    14 C     0.000150 -0.000209  0.000189
    15 N     0.000071  0.000153 -0.000080
    16 C    -0.000037  0.000216  0.000035
    17 H     0.000039 -0.000018  0.000037
    18 C    -0.000006 -0.000232 -0.000162
    19 H    -0.000036  0.000015 -0.000009
    20 Cl    0.000070  0.000024  0.000204
    21 C     0.000098 -0.000026 -0.000070
    22 C    -0.000003 -0.000139  0.000039
    23 C     0.000106  0.000053  0.000146
    24 C     0.000036 -0.000019  0.000066
    25 C    -0.000068  0.000130  0.000060
    26 H    -0.000015  0.000019 -0.000008
    27 H    -0.000009 -0.000003  0.000046
    28 H    -0.000011 -0.000014  0.000033
    29 H    -0.000013  0.000004 -0.000013
    30 H    -0.000002  0.000015  0.000014
    31 N    -0.000067  0.000039 -0.000007
    32 Ir   -0.000242 -0.000066 -0.000398
    33 C     0.000023 -0.000043 -0.000094
    34 H     0.000050  0.000030  0.000049
    35 H    -0.000049  0.000076  0.000060
    36 H    -0.000016 -0.000016  0.000053
    37 C    -0.000023  0.000011  0.000132
    38 H    -0.000001  0.000000  0.000007
    39 H    -0.000039 -0.000021  0.000028
    40 H     0.000021 -0.000008 -0.000039
    41 Ir   -0.000763  0.000383 -0.000914
    42 C     0.000028 -0.000109  0.000142
    43 C     0.000072  0.000050 -0.000117
    44 C    -0.000061 -0.000117 -0.000116
    45 C     0.000185 -0.000076 -0.000110
    46 C     0.000073  0.000107  0.000070
    47 H    -0.000001  0.000031  0.000046
    48 H     0.000028 -0.000008  0.000028
    49 H     0.000045  0.000022  0.000001
    50 H    -0.000024  0.000022  0.000007
    51 H    -0.000005  0.000015 -0.000013
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Geometry Convergence after Step  41
---------------------------------------
current energy                          -11.08199539 Hartree
abs of energy change              0.00000445     0.00100000    T
constrained gradient max          0.00091388     0.00100000    T
constrained gradient rms          0.00013971     0.00066667    T
gradient max                      0.00091388
gradient rms                      0.00013971
cart. step max                    0.00904993     0.01000000    T
cart. step rms                    0.00321292     0.00666667    T


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

  Electrostatic Energy:           -10.847965368341191       -295.1882         -6807.20        -28481.33
  Kinetic Energy:                  13.394723884680545        364.4890          8405.32         35167.84
  Coulomb (Steric+OrbInt) Energy:  -3.143309433586680        -85.5338         -1972.46         -8252.76
  XC Energy:                      -10.485447688567479       -285.3235         -6579.72        -27529.54
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -11.081998605814805       -301.5565         -6954.06        -29095.78

 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
           -109.536423           61.646998           -1.692577
```

20.121521	72.556664	0.365945
35.030705	48.236008	0.423544
56.078954	246.731056	3.468181
62.607251	15.233583	0.239059
74.109541	132.749037	2.465946
92.103890	19.886623	0.459110
95.478823	19.473713	0.466051
108.225872	51.742141	1.403633
117.699161	170.069377	5.017386
124.099894	36.467691	1.134378
141.116988	166.640689	5.894384
152.927797	189.665818	7.270321
186.169283	8.895949	0.415124
195.811957	47.455249	2.329172
201.530023	12.882978	0.650780
216.647831	60.421472	3.281132
220.872234	104.634417	5.792870
231.358668	133.539934	7.744172
257.356307	61.772174	3.984793
270.055125	120.167452	8.134247
281.860289	20.448056	1.444654
310.364120	163.923136	12.752338
317.985938	85.699191	6.830661
327.196677	54.954582	4.507034
339.571840	61.821907	5.262016
343.567584	58.673907	5.052837
348.638979	175.644710	15.349318
361.968320	45.564916	4.134083
365.424740	175.546829	16.079369
383.576660	46.674478	4.487554
397.846356	54.860865	5.470866
435.213645	56.966551	6.214418
438.043502	27.722898	3.043925
456.586733	129.841701	14.859889
508.222242	101.786359	12.966457
518.411563	96.720864	12.568195
542.195274	0.227135	0.030869
546.159606	7.410413	1.014472
551.420912	30.755442	4.250923
556.681953	65.366091	9.120901
559.947842	21.877533	3.070605
609.217184	63.227241	9.655048
642.694973	12.256939	1.974536
660.764617	6.086911	1.008142
681.110961	42.841636	7.314118
715.823765	27.102468	4.862874
729.081319	120.308380	21.986187
761.566275	218.326458	41.676587
792.043759	17.213514	3.417408
811.268930	49.575533	10.081155
816.863733	7.059015	1.445346
817.494606	6.226218	1.275814
819.783871	19.248324	3.955217
833.468845	174.210969	36.395102
846.307712	106.374612	22.565469
851.817555	102.863303	21.962669
854.989846	193.272545	41.419914
857.976010	99.314580	21.358278
860.965966	44.899904	9.689681
874.069526	38.746488	8.488997
878.921698	30.719192	6.767652
909.261018	97.940127	22.321702
913.010173	104.707427	23.962447
916.844389	16.438128	3.777688
917.538321	9.080317	2.088350
920.309300	28.482451	6.570361
928.624616	7.758913	1.806006
933.235609	0.261639	0.061203
934.574410	54.549510	12.778586
961.026939	0.168400	0.040565
974.943008	28.990272	7.084506
989.326741	20.589573	5.105816
993.066872	7.488119	1.863929
994.433430	75.831713	18.901865
998.941299	37.609112	9.416968
1006.050796	40.875663	10.307724
1020.717332	56.091374	14.350916
1029.528209	71.172951	18.366707
1049.951085	1.463159	0.385069
1052.889663	1.299011	0.342826
1053.275940	2.126932	0.561531
1054.079384	2.940612	0.776943
1056.053999	29.209352	7.731898
1071.251761	7.990542	2.145586
1095.093860	20.521915	5.633098
1099.367426	3.412609	0.940389
1100.771635	6.056669	1.671126
1112.946573	25.278622	7.051894
1116.321219	284.435771	79.588710
1133.520496	19.664650	5.587193
1160.731657	28.668273	8.340872
1171.731629	1.689028	0.496070
1192.471431	68.475548	20.467348
1238.823308	0.433247	0.134531
1239.312958	0.097036	0.030143
1258.715593	43.560413	13.743510
1267.363949	69.668656	22.131806
1277.028869	16.598687	5.313155
1303.644934	27.045697	8.837625

1307.137409	23.753891	7.782768
1312.843468	36.106757	11.881725
1342.623808	12.042024	4.052583
1346.188486	2.580708	0.870809
1346.974218	41.369561	13.967487
1349.707460	4.200323	1.421021
1366.535257	152.186597	52.128511
1393.943007	38.042111	13.291919
1399.405824	39.262588	13.772116
1401.699637	21.689597	7.620518
1405.466768	67.253098	23.692503
1424.920235	49.066802	17.524933
1430.257600	35.850528	12.852508
1437.288543	133.299809	48.023251
1440.157193	14.022657	5.061955
1445.988154	46.426845	16.827205
1450.911235	50.519796	18.373018
1457.162216	188.516788	68.855083
1461.099127	6.153880	2.253755
1474.866947	78.594555	29.055167
1484.287308	173.049772	64.382387
1556.590050	8.265270	3.224849
1590.504684	27.861589	11.107566
2902.412061	44.361287	32.273144
2918.047663	40.150652	29.367235
3031.207910	5.513543	4.189137
3038.647603	7.487187	5.702655
3074.832238	0.696576	0.536869
3085.079564	9.146450	7.072892
3129.652405	1.692001	1.327318
3136.681773	6.749017	5.306266
3137.646914	2.468230	1.941188
3141.469017	1.626270	1.280571
3146.508992	9.317294	7.348469
3154.255406	24.903184	19.689278
3170.393532	0.643652	0.511496
3171.610669	2.471059	1.964450
3172.024151	2.564924	2.039337
3176.232026	3.170508	2.524173
3179.095730	3.699922	2.948318
3183.068443	17.634476	14.069757
3184.348827	34.304469	27.381007
3185.483817	19.298573	15.409150
3187.892114	17.070107	13.640112
3196.805901	4.930718	3.950977
3197.752004	7.562543	6.061648

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.716	36.317	90.560	172.594
	Internal Energy (Kcal/mole):	0.889	0.889	260.721	262.498
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	95.990	101.952

****

TS2-III

```
 Geometry CYCLE 16
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ------------------------------------------
     1 C     0.000039 -0.000012  0.000001
     2 H    -0.000018 -0.000006 -0.000033
     3 C     0.000084  0.000051  0.000126
     4 H    -0.000027 -0.000003 -0.000036
     5 C    -0.000093 -0.000046 -0.000116
     6 H     0.000007  0.000018  0.000011
     7 C     0.000063  0.000004  0.000050
     8 H    -0.000008  0.000016  0.000012
     9 C    -0.000020 -0.000041 -0.000050
    10 C     0.000026 -0.000098  0.000034
    11 C    -0.000090  0.000256 -0.000381
    12 C     0.000669 -0.000094 -0.000003
    13 H    -0.000095 -0.000003  0.000030
    14 C     0.000167 -0.000595  0.000317
    15 N    -0.000041  0.000124  0.000131
    16 C    -0.000344  0.000286  0.000030
    17 H     0.000073 -0.000107 -0.000006
    18 C     0.000246  0.000295 -0.000059
    19 H    -0.000040 -0.000021  0.000035
    20 Cl   -0.000059 -0.000028  0.000000
    21 C     0.000026  0.000026 -0.000022
    22 C    -0.000043 -0.000014 -0.000008
    23 C    -0.000044  0.000010 -0.000046
    24 C     0.000008  0.000004 -0.000017
    25 C    -0.000007 -0.000004 -0.000048
    26 H    -0.000003  0.000004 -0.000008
    27 H    -0.000005 -0.000001 -0.000005
    28 H     0.000011  0.000011  0.000012
    29 H    -0.000008 -0.000009 -0.000010
    30 H     0.000003 -0.000004 -0.000005
    31 N    -0.000105 -0.000056  0.000016
    32 Ir    0.000239  0.000048  0.000159
    33 C     0.000014 -0.000078 -0.000078
    34 H    -0.000001  0.000029  0.000014
    35 H     0.000009 -0.000011 -0.000013
    36 H     0.000000  0.000009 -0.000018
    37 C    -0.000015  0.000069 -0.000030
    38 H     0.000006  0.000009  0.000001
    39 H     0.000026 -0.000025  0.000037
    40 H     0.000010 -0.000027  0.000019
    41 Ir   -0.000916 -0.000181 -0.000401
    42 C     0.000152 -0.000036  0.000073
    43 C     0.000045  0.000025  0.000122
    44 C     0.000040  0.000140  0.000078
    45 C     0.000060  0.000103 -0.000026
    46 C    -0.000011 -0.000012  0.000052
    47 H    -0.000002 -0.000006 -0.000006
    48 H     0.000021 -0.000005  0.000004
    49 H    -0.000005 -0.000035  0.000030
    50 H    -0.000036  0.000035  0.000019
    51 H    -0.000006 -0.000017  0.000011
 ------------------------------------------

---------------------------------------
Geometry Convergence after Step  16
---------------------------------------
current energy                          -11.08201986 Hartree
energy change                 -0.00000262     0.00100000    T
constrained gradient max       0.00091559     0.00100000    T
constrained gradient rms       0.00013819     0.00066667    T
gradient max                   0.00091559
gradient rms                   0.00013819
cart. step max                 0.00276863     0.01000000    T
cart. step rms                 0.00050927     0.00666667    T

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

  Electrostatic Energy:           -10.852099643989787       -295.3007         -6809.80        -28492.18
  Kinetic Energy:                  13.381819517948202        364.1378          8397.22         35133.96
  Coulomb (Steric+OrbInt) Energy:  -3.127108870052638        -85.0930         -1962.29         -8210.22
  XC Energy:                      -10.484631057469914       -285.3013         -6579.21        -27527.39
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -11.082020053564136       -301.5571         -6954.07        -29095.84

 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2          km/mole
             ----------          ----------          ----------
           -100.783642           27.367006           -0.691346
             26.563634           91.278530            0.607763
```

38.239149	41.220668	0.395095
57.245967	210.923394	3.026549
62.449388	24.122456	0.377596
73.265571	74.532358	1.368746
88.202539	70.572577	1.560253
96.329107	16.315071	0.393935
107.886003	48.411914	1.309168
117.337783	199.583793	5.870042
124.855384	56.130345	1.756641
143.026676	148.890687	5.337804
150.474844	155.495245	5.864879
174.024040	76.668737	3.344303
209.857266	34.935567	1.837680
219.516405	20.323830	1.118280
220.909632	23.966595	1.327086
233.290646	192.065044	11.231137
237.230739	26.367492	1.567898
258.479819	64.947718	4.207931
265.012323	74.730008	4.964085
295.032512	79.946748	5.912195
310.256370	133.265034	10.363704
323.398894	99.118503	8.034731
324.840645	29.991526	2.442008
340.073238	61.752515	5.263870
343.666489	54.999169	4.737742
351.762459	177.880868	15.683999
361.965714	20.709374	1.878938
365.012179	167.696930	15.343009
385.242963	54.693754	5.281418
404.996175	72.260901	7.335545
435.946489	58.811371	6.426471
437.692953	158.082054	17.343238
443.837958	2.788329	0.310203
506.972903	37.864434	4.811653
516.246560	178.363129	23.080240
543.343409	2.872967	0.391276
546.093562	5.707425	0.781241
551.341955	28.209717	3.898503
556.875679	73.666982	10.282748
560.696264	29.420522	4.134815
610.183744	68.654035	10.500374
640.218802	6.905763	1.108200
659.524780	2.068950	0.342026
682.897312	55.990664	9.584050
718.276162	32.585936	5.866779
729.483919	120.554876	22.043400
762.078282	218.635127	41.763568
794.850291	54.058997	10.770389
810.601855	66.820424	13.576721
817.038660	13.414667	2.747265
818.285831	7.714473	1.582302
820.282126	15.751156	3.238574
833.215492	184.017036	38.432040
844.631668	106.272883	22.499242
851.704191	224.639832	47.957178
855.126078	55.010834	11.791158
857.324247	95.298723	20.479071
861.005044	62.090822	13.400197
873.659517	26.091841	5.713800
879.633829	26.310214	5.801020
907.797951	48.773086	11.098071
912.202820	48.878940	11.176125
915.634278	8.075516	1.853405
916.356745	14.436801	3.315993
920.904528	3.766199	0.869352
925.058918	55.785852	12.935152
931.857757	0.824672	0.192623
938.467388	0.215841	0.050773
961.799008	0.083570	0.020147
974.976380	29.976442	7.325753
990.806300	21.440857	5.324870
994.166699	48.981388	12.205860
995.332716	28.875779	7.204105
999.284171	35.703426	8.942871
1006.171439	38.478119	9.704293
1024.888527	54.080394	13.892952
1030.768772	61.839738	15.977431
1050.253342	1.728434	0.455014
1053.623758	4.767970	1.259207
1054.129876	4.024501	1.063370
1055.111544	1.277876	0.337960
1057.660513	29.933544	7.935650
1074.182395	1.014509	0.273157
1086.560231	17.930213	4.883344
1099.195057	3.745826	1.032049
1100.983623	6.513931	1.797637
1111.530411	16.413437	4.572976
1120.710816	297.116358	83.463808
1134.012583	32.186738	9.148985
1168.259800	36.523773	10.695304
1172.097980	1.344362	0.394965
1195.836515	74.393891	22.299091
1239.814151	0.146764	0.045609
1241.682910	0.401635	0.125003
1257.132071	27.311774	8.606149
1271.608349	76.442565	24.365016
1275.596227	6.217180	1.987855
1301.371283	83.130162	27.116767
1304.884041	5.930661	1.939783

1308.793282	7.942491	2.605589
1342.555940	9.888361	3.327628
1346.408656	2.971577	1.002864
1347.501980	41.263900	13.937271
1349.859572	3.033588	1.026416
1365.589972	158.577092	54.279875
1393.872324	37.576348	13.128516
1400.954538	38.583853	13.549014
1402.780386	19.009679	6.684094
1405.963978	60.874271	21.452901
1425.563314	50.007667	17.869038
1430.910607	32.813704	11.769170
1438.385105	94.246688	33.979685
1443.260069	24.761390	8.957724
1448.320313	69.455290	25.214364
1451.082583	39.412840	14.335338
1458.556172	218.375993	79.837352
1466.016226	10.128333	3.721815
1476.977021	75.732885	28.037308
1482.502384	168.020300	62.436022
1556.597980	7.418084	2.894318
1590.756864	27.829565	11.096558
2900.462900	39.576331	28.772719
2908.724014	39.811001	29.025765
3028.025496	5.998427	4.552763
3032.557635	8.110710	6.165183
3072.304507	1.076633	0.829106
3074.901066	5.906060	4.552051
3126.999976	0.972062	0.761903
3133.857237	0.995984	0.782365
3137.519491	6.261118	4.923981
3145.350710	2.471263	1.948346
3148.266992	16.821725	13.274561
3154.139597	25.407351	20.087152
3170.491461	0.692940	0.550681
3170.770032	5.428734	4.314609
3171.493019	2.760139	2.194182
3175.874279	5.035270	4.008336
3179.546220	3.453433	2.752290
3183.013415	17.523368	13.980868
3184.298947	33.257110	26.544614
3186.213324	18.403287	14.697664
3188.058310	16.301822	13.026882
3197.316190	6.027960	4.830967
3197.833771	5.938008	4.759647

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.716	36.295	89.477	171.488
	Internal Energy (Kcal/mole):	0.889	0.889	260.750	262.527
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	95.882	101.844

****

[endo-3a]2+

PBE/TZP,DZP

Geometry CYCLE 63
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	0.000158	0.000183	-0.000085
2	H	-0.000162	0.000010	0.000081
3	C	-0.000190	-0.000202	-0.000128
4	H	-0.000036	0.000000	0.000062
5	C	0.000274	-0.000016	0.000018
6	H	0.000054	0.000023	0.000144
7	C	0.000167	0.000179	0.000044
8	H	-0.000300	-0.000028	-0.000359
9	C	0.000251	-0.000103	0.000201
10	C	0.000104	0.000322	0.000017
11	C	-0.000037	-0.000588	-0.000130
12	C	-0.000483	0.000270	0.000347
13	H	-0.000014	-0.000106	-0.000053
14	C	-0.000506	0.000507	-0.000519
15	N	-0.000141	-0.000011	0.000016
16	C	-0.000189	-0.000758	0.000025
17	H	-0.000018	-0.000111	0.000272
18	C	-0.000231	0.000023	0.000289
19	H	0.000061	-0.000023	-0.000065
20	Cl	-0.000021	0.000122	0.000155
21	C	-0.000151	-0.000697	-0.000345
22	C	-0.000019	-0.000115	-0.000354
23	C	0.000169	-0.000013	-0.000106
24	C	-0.000444	0.000257	0.000347
25	C	0.000076	0.000512	0.000088
26	N	0.000284	-0.000364	-0.000307
27	Ir	0.000276	0.000462	-0.000063
28	C	-0.000041	0.000318	-0.000175
29	H	0.000062	-0.000014	0.000054
30	H	0.000188	0.000230	-0.000070
31	H	0.000236	-0.000022	-0.000037
32	C	0.000191	-0.000150	0.000018
33	H	0.000050	-0.000030	-0.000128
34	H	-0.000113	0.000304	0.000226
35	H	-0.000392	-0.000080	0.000003
36	Ir	0.000875	0.000065	0.000510
37	C	-0.000167	0.000008	0.000006
38	C	-0.000203	-0.000232	-0.000134
39	C	-0.000001	-0.000350	-0.000205
40	C	-0.000067	-0.000245	-0.000079
41	C	0.000061	0.000278	-0.000185
42	C	-0.000432	-0.000045	0.000215
43	H	0.000182	-0.000006	-0.000132
44	H	0.000141	0.000166	0.000016
45	H	0.000193	-0.000171	-0.000120
46	C	-0.000079	0.000115	0.000238
47	H	0.000000	-0.000031	-0.000011
48	H	0.000146	-0.000046	-0.000105
49	H	-0.000059	-0.000124	-0.000015
50	C	0.000193	-0.000069	-0.000061
51	H	-0.000028	0.000064	0.000020
52	H	-0.000059	-0.000139	0.000069
53	H	-0.000007	0.000151	0.000029
54	C	0.000176	-0.000115	-0.000014
55	H	0.000065	-0.000059	-0.000049
56	H	-0.000127	0.000145	-0.000011
57	H	-0.000055	0.000010	0.000135
58	C	-0.000180	-0.000162	0.000004
59	H	0.000141	0.000042	-0.000009
60	H	-0.000002	-0.000014	-0.000053
61	H	-0.000005	0.000055	0.000072
62	C	0.000268	-0.000047	0.000154
63	H	0.000081	0.000071	-0.000089
64	H	-0.000346	0.000163	0.000087
65	H	-0.000040	0.000056	-0.000011
66	C	0.000084	0.000218	0.000138
67	H	-0.000031	-0.000150	-0.000082
68	H	0.000089	-0.000036	-0.000090
69	H	-0.000057	-0.000060	0.000123
70	C	-0.000227	-0.000127	0.000067
71	H	0.000156	0.000281	0.000026
72	H	0.000027	-0.000070	0.000039
73	H	0.000130	-0.000057	-0.000092
74	C	0.000028	0.000207	0.000180
75	H	-0.000152	0.000027	0.000021
76	H	-0.000037	0.000042	-0.000017
77	H	0.000248	-0.000125	-0.000133
78	C	0.000121	-0.000104	0.000154
79	H	-0.000007	-0.000020	0.000045
80	H	-0.000231	0.000059	0.000011
81	H	0.000079	0.000090	-0.000149

Geometry Convergence after Step 63

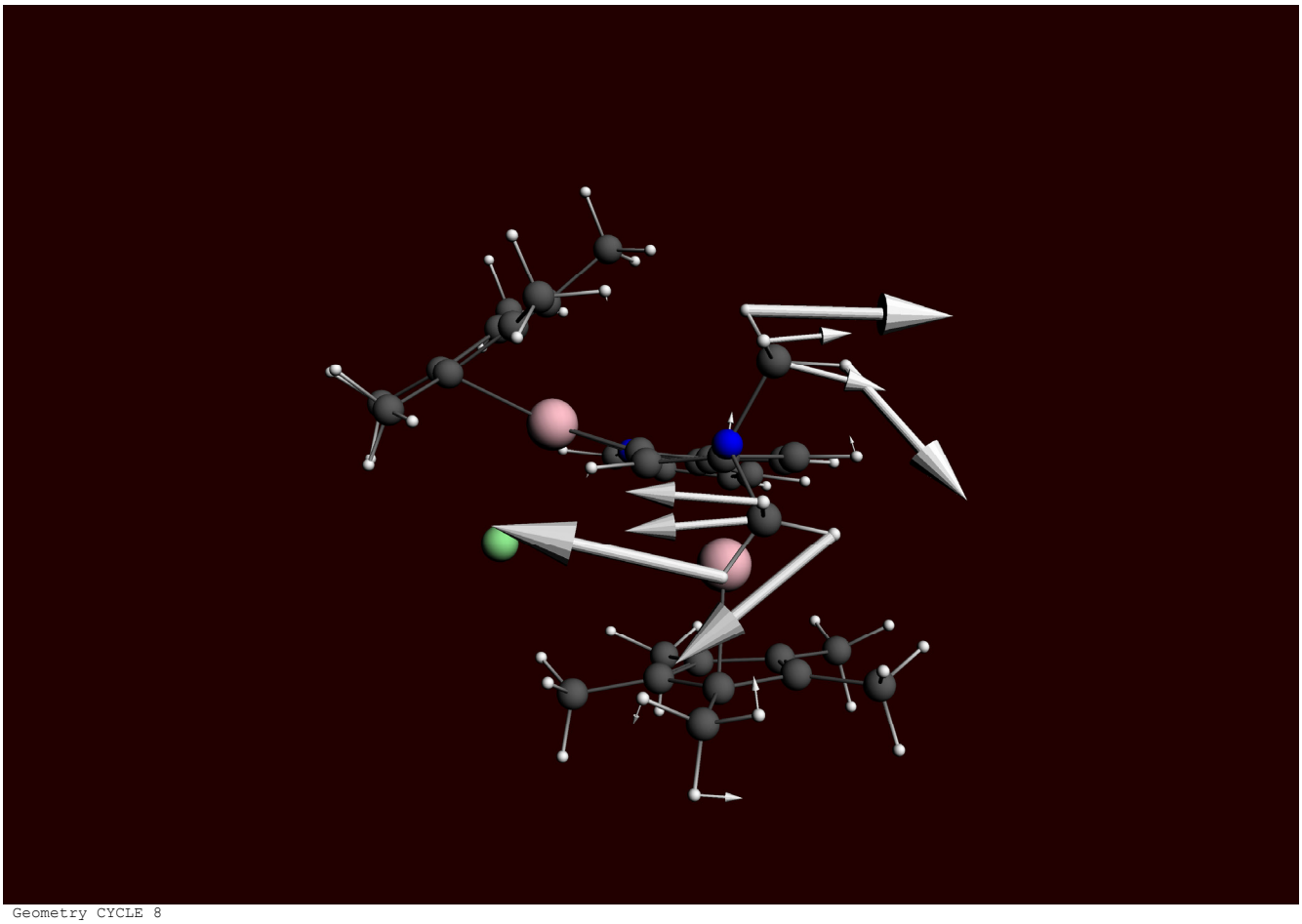
```
---------------------------------------
current energy                          -17.60126000 Hartree
abs of energy change              0.00012899     0.00100000    T
constrained gradient max          0.00087516     0.00100000    T
constrained gradient rms          0.00019665     0.00066667    T
gradient max                      0.00087516
gradient rms                      0.00019665
cart. step max                    0.00652286     0.01000000    T
cart. step rms                    0.00219634     0.00666667    T


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

  Electrostatic Energy:           -14.969080433309829       -407.3294         -9393.24        -39301.32
  Kinetic Energy:                  19.527067825845677        531.3586         12253.42         51268.31
  Coulomb (Steric+OrbInt) Energy:  -5.683039233298416       -154.6434         -3566.16        -14920.82
  XC Energy:                      -16.276795270827705       -442.9141        -10213.84        -42734.72
  Solvation:                       -0.199412991870775         -5.4263          -125.13          -523.56
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -17.601260103461048       -478.9547        -11044.96        -46212.10

 List of All Frequencies:


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

               Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                 cm-1          1e-40 esu2 cm2           km/mole
              ----------          ----------          ----------
                3.749375            0.000000            0.000000
               15.196128            0.000000            0.000000
               38.456905          299.451646            2.886550
               40.768341          380.094494            3.884120
               49.350060          249.030499            3.080479
               61.450333          113.073548            1.741660
               75.825454           68.348424            1.299037
               78.965249           74.375499            1.472123
               83.303635          289.603459            6.047081
               85.140979          203.464507            4.342155
               92.975452          149.575408            3.485833
               94.360766            5.594978            0.132333
              109.439614           33.664612            0.923477
              111.660142          287.902954            8.057909
              117.264140           54.283514            1.595553
              119.309344            7.348312            0.219756
              121.030624           16.918270            0.513250
              122.080109          157.046680            4.805646
              124.413130           24.006355            0.748636
              127.489269           21.590083            0.689932
              130.752562           17.556281            0.575388
              136.656219          115.413221            3.953330
              146.085200           85.251753            3.121674
              147.028088          111.347568            4.103544
              150.180026          310.200055           11.677022
              152.223917           42.318059            1.614681
              153.657284          294.180758           11.330406
              157.057206          147.664275            5.813148
              160.556320          248.421940            9.997592
              162.917314           53.010448            2.164745
              178.608634          387.726679           17.358261
              189.364312          457.321434           21.706898
              196.143037           99.357340            4.884847
              201.578079          796.425922           40.240814
              220.606195          435.195684           24.064695
              242.138795          127.829819            7.758444
              246.561413          566.730965           35.025160
              268.354574           25.916779            1.743284
              269.951197           19.391267            1.312108
              271.231119          114.869702            7.809497
              277.747586          233.145887           16.231405
              279.600591           70.760601            4.959155
              281.803920           44.475495            3.141564
              284.325114           74.863360            5.335346
              293.525197           54.413553            4.003414
              295.591157          158.960847           11.777678
              298.047886           49.308078            3.683682
              300.389491           70.228336            5.287802
              329.496561          224.785281           18.565080
              336.758600           50.369319            4.251702
              362.913947           54.508718            4.958470
              371.650022            7.059606            0.657647
              407.783022          132.418634           13.534939
              410.989165           17.120930            1.763745
              425.095827            0.884567            0.094253
              429.272334           74.488648            8.014955
              430.273026           34.374735            3.707333
              436.492370           82.306767            9.005136
              440.929536           38.507649            4.255928
              465.256484           55.331535            6.452726
              484.441730          134.338298           16.312460
              511.015439          454.563009           58.224556
              521.060777            5.643425            0.737071
              522.702795            3.965694            0.519580
              522.778539           21.905317            2.870419
              524.138725           13.358110            1.754968
              528.389337          144.626765           19.154940
```

538.028069	0.049878	0.006726
538.266477	3.010025	0.406112
559.681163	110.301418	15.473903
579.244993	58.125214	8.439271
581.141101	71.879602	10.470449
587.628014	235.089466	34.626909
593.772078	8.612391	1.281804
594.769314	2.971360	0.442978
597.287176	9.232132	1.382176
599.259150	135.766395	20.393184
624.019958	629.355737	98.440259
645.812790	194.687707	31.515430
658.844208	63.650313	10.511419
713.099017	27.238176	4.868621
729.479868	382.887069	70.010323
755.895448	452.126267	85.664235
781.130718	5.028909	0.984636
785.000291	3.370646	0.663225
785.638775	10.210403	2.010684
786.093286	3.674286	0.723978
788.361659	40.047771	7.913743
842.112966	221.336395	46.719830
858.378788	17.195674	3.699783
891.911086	51.653128	11.547720
908.312869	15.323167	3.488687
928.528976	51.481500	11.981873
930.380382	20.948644	4.885337
931.770557	18.582053	4.339910
932.085612	5.222980	1.220260
932.837366	35.235148	8.238727
937.699245	3.022248	0.710349
957.353923	1.434310	0.344186
985.285339	723.608470	178.707892
994.522645	123.329576	30.743973
995.608848	228.249184	56.960796
996.539710	648.015592	161.866932
997.635784	300.493083	75.142315
999.543294	218.004928	54.619283
1000.124400	148.399718	37.201904
1001.579071	63.949267	16.054577
1005.024118	144.571976	36.419894
1005.498055	38.195048	9.626454
1005.775569	27.072823	6.825158
1009.232601	62.673588	15.854549
1031.648153	63.551594	16.433729
1041.688736	99.371055	25.946330
1050.056601	43.491979	11.447218
1056.540818	73.400679	19.438575
1059.516249	36.384651	9.662820
1063.236445	114.223101	30.441207
1063.610562	105.001989	27.993567
1070.742114	6.473972	1.737536
1082.849564	0.805633	0.218667
1088.209577	0.518287	0.141371
1092.708541	11.968103	3.277991
1104.086299	200.654716	55.530357
1109.248482	3.513910	0.977007
1137.337748	11.500828	3.278662
1141.627888	22.232662	6.362006
1143.641044	4.762124	1.365113
1144.395856	9.962906	2.857856
1147.214665	6.101686	1.754578
1159.120535	110.194191	32.015875
1198.130313	365.707696	109.828797
1201.509339	18.244683	5.494669
1265.104724	42.649497	13.524414
1284.347242	19.004305	6.118043
1304.389715	63.319145	20.702390
1327.245438	6.237806	2.075206
1332.733020	43.142564	14.412097
1336.617853	10.330742	3.461121
1338.530792	177.791871	59.651083
1339.010963	31.704879	10.641144
1341.954917	33.151854	11.151257
1342.983560	2.168962	0.730131
1351.625099	93.309120	31.612469
1353.133945	226.412086	76.792440
1353.822997	24.340787	8.259896
1354.624388	189.573381	64.368638
1355.205787	101.265849	34.399040
1356.537124	42.855273	14.571827
1373.211923	31.450594	10.825413
1375.473188	1.174415	0.404904
1375.955860	4.609283	1.589703
1378.950254	7.620813	2.634074
1387.118396	20.001763	6.954403
1389.575757	145.272323	50.599145
1390.690297	6.975126	2.431423
1392.340316	26.367991	9.202387
1395.600217	112.873289	39.484830
1398.960065	70.904462	24.863196
1405.439505	12.197125	4.296825
1405.984935	230.505970	81.234575
1406.574037	141.327396	49.827262
1410.886423	209.542644	74.104152
1412.028088	41.119537	14.553573
1413.499001	45.477079	16.112619
1414.754199	18.245984	6.470329
1417.322815	7.989660	2.838410

1418.408907	19.578281	6.960719
1423.260883	10.730070	3.827940
1425.008706	30.423244	10.866786
1426.057280	29.339824	10.487514
1427.101466	95.693635	34.230715
1428.549724	117.589859	42.105934
1429.478045	9.099886	3.260555
1430.291505	154.151420	55.264998
1433.590038	36.991840	13.292571
1435.487169	201.506535	72.504760
1437.103791	220.633562	79.476326
1441.982940	37.052489	13.392313
1443.585213	145.033876	52.479531
1445.118517	125.890859	45.601144
1446.192427	174.103190	63.111846
1447.190514	30.694648	11.134390
1455.501508	362.472803	132.241009
1457.529331	72.382116	26.443969
1457.538334	378.662433	138.340798
1459.830431	145.619742	53.284481
1485.988482	265.472719	98.881128
1499.309795	247.002216	92.826141
1553.396169	58.840177	22.910484
1567.005845	2159.448657	848.186917
1592.948343	56.740247	22.655361
2957.906924	5.388201	3.994904
2960.646356	5.494928	4.077807
2961.991591	5.599310	4.157157
2962.154119	12.431440	9.230116
2963.582341	3.622364	2.690836
2964.445344	2.926457	2.174521
2965.792545	6.184198	4.597293
2967.532582	9.131680	6.792415
2967.719952	2.382994	1.772654
2967.793573	1.830308	1.361558
2969.392954	21.802944	16.227846
2973.957211	17.072270	12.726356
3038.887772	5.038276	3.837732
3039.456866	2.020501	1.539335
3041.795603	23.562080	17.964773
3042.426351	7.373274	5.622876
3043.055777	2.784464	2.123878
3043.214456	1.160908	0.885541
3047.116995	24.066274	18.381293
3050.208206	9.807866	7.498633
3051.222026	1.980685	1.514842
3052.802713	9.046002	6.922030
3064.437281	3.434130	2.637822
3066.278581	4.438468	3.411322
3071.336576	1.779116	1.369650
3072.464263	12.816208	9.870166
3072.589308	7.827316	6.028308
3074.116986	6.374611	4.911929
3074.728253	1.272476	0.980696
3077.754111	1.167429	0.900621
3079.365291	21.733792	16.775474
3085.244171	1.307400	1.011058
3087.003870	0.326540	0.252669
3089.250803	0.520582	0.403107
3105.496720	0.352636	0.274495
3111.762038	2.149575	1.676629
3134.051703	0.553879	0.435110
3142.641061	9.161868	7.217003
3146.058426	2.477320	1.953561
3147.590058	2.668783	2.105569
3150.272847	50.420064	39.813434
3161.359704	9.733546	7.712995
3165.347601	52.480103	41.638412

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	46.228	37.575	154.042	237.845
	Internal Energy (Kcal/mole):	0.889	0.889	438.018	439.795
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	152.958	158.919

TS1-[endo-3a]2+



Geometry CYCLE 8
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000105	-0.000110	-0.000192
2	H	-0.000030	0.000098	0.000112
3	C	0.000021	0.000043	0.000072
4	H	0.000010	-0.000017	0.000002
5	C	-0.000119	-0.000058	-0.000011
6	H	-0.000027	0.000001	-0.000027
7	C	0.000025	0.000110	-0.000126
8	H	0.000131	0.000024	-0.000073
9	C	-0.000217	-0.000042	-0.000533
10	C	-0.000160	-0.000011	-0.000139
11	C	-0.000148	-0.000120	0.000183
12	C	0.000166	-0.000191	0.000515
13	H	0.000000	-0.000076	-0.000028
14	C	-0.000089	0.000515	0.000055
15	N	-0.000417	-0.000659	-0.000459
16	C	-0.000015	-0.000182	-0.000205
17	H	-0.000007	0.000029	-0.000030
18	C	0.000123	0.000095	-0.000112
19	H	-0.000100	-0.000022	0.000143
20	Cl	0.000041	-0.000117	-0.000030
21	C	-0.000138	-0.000052	-0.000187
22	C	-0.000060	-0.000121	-0.000050
23	C	-0.000095	0.000005	-0.000269
24	C	-0.000075	-0.000090	0.000110
25	C	-0.000046	-0.000215	0.000188
26	N	0.000768	0.000271	0.000965
27	Ir	0.000112	0.000658	0.000145
28	C	0.000075	-0.000375	0.000282
29	H	-0.000066	0.000069	0.000017
30	H	-0.000040	0.000063	0.000012
31	H	-0.000032	-0.000007	-0.000056
32	C	0.000452	0.000497	-0.000040
33	H	-0.000071	-0.000002	-0.000074
34	H	-0.000089	0.000054	0.000096
35	H	0.000024	0.000035	0.000074
36	Ir	0.000483	-0.000198	-0.000001
37	C	0.000002	0.000025	0.000174

```
    38 C    -0.000138  0.000069  0.000159
    39 C     0.000102  0.000021  0.000024
    40 C    -0.000191  0.000061 -0.000412
    41 C    -0.000088 -0.000081  0.000081
    42 C     0.000138 -0.000008  0.000101
    43 H    -0.000017  0.000005 -0.000117
    44 H     0.000052  0.000166  0.000070
    45 H    -0.000042 -0.000053  0.000090
    46 C     0.000105 -0.000098 -0.000085
    47 H     0.000029 -0.000006 -0.000013
    48 H    -0.000007 -0.000032  0.000061
    49 H    -0.000071  0.000101  0.000000
    50 C    -0.000020 -0.000052 -0.000008
    51 H    -0.000015  0.000025 -0.000034
    52 H     0.000026 -0.000013 -0.000011
    53 H     0.000005  0.000003  0.000026
    54 C     0.000001  0.000060 -0.000028
    55 H    -0.000021 -0.000043  0.000026
    56 H     0.000006  0.000004 -0.000007
    57 H    -0.000049  0.000022 -0.000046
    58 C     0.000002 -0.000023  0.000087
    59 H     0.000005  0.000025 -0.000057
    60 H    -0.000052  0.000047  0.000026
    61 H     0.000024 -0.000035 -0.000012
    62 C    -0.000177  0.000040 -0.000075
    63 H     0.000071 -0.000019 -0.000024
    64 H     0.000027  0.000040 -0.000024
    65 H     0.000119  0.000008  0.000003
    66 C    -0.000052  0.000001 -0.000042
    67 H    -0.000048 -0.000024  0.000008
    68 H     0.000083  0.000046  0.000028
    69 H    -0.000037  0.000062  0.000014
    70 C     0.000225 -0.000005  0.000013
    71 H    -0.000189 -0.000079 -0.000085
    72 H    -0.000028 -0.000037  0.000004
    73 H    -0.000042  0.000064 -0.000188
    74 C     0.000057 -0.000088  0.000055
    75 H     0.000014  0.000046 -0.000078
    76 H     0.000042 -0.000006 -0.000010
    77 H    -0.000001  0.000017 -0.000020
    78 C    -0.000073 -0.000175  0.000039
    79 H     0.000001 -0.000025 -0.000035
    80 H     0.000003  0.000065 -0.000001
    81 H    -0.000065 -0.000020 -0.000007
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----------------------------------------
Geometry Convergence after Step   8
----------------------------------------
current energy                          -17.57104584 Hartree
abs of energy change                0.00017250     0.00100000    T
constrained gradient max            0.00096464     0.00100000    T
constrained gradient rms            0.00016155     0.00066667    T
gradient max                        0.00096464
gradient rms                        0.00016155
cart. step max                      0.00343365     0.01000000    T
cart. step rms                      0.00083448     0.00666667    T


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

  Electrostatic Energy:           -14.925141864459953       -406.1338         -9365.67        -39185.95
  Kinetic Energy:                  19.469055468629847        529.7800         12217.02         51116.00
  Coulomb (Steric+OrbInt) Energy:  -5.667182711332075       -154.2119         -3556.21        -14879.19
  XC Energy:                      -16.250350020275029       -442.1945        -10197.25        -42665.29
  Solvation:                       -0.197427028992267         -5.3723          -123.89          -518.34
                                  --------------------     -----------      ----------       -----------
  Total Bonding Energy:           -17.571046156429475       -478.1325        -11026.00        -46132.78


 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2             km/mole
             ----------          ----------           ----------
            -104.854548          129.281384            -3.397828
              21.386652           99.296652             0.532299
              41.014121          618.386568             6.357283
              42.685782          411.985063             4.408012
              49.282033          252.994535             3.125200
              63.149352          152.085222             2.407321
              75.363397           11.249191             0.212500
              85.243995          191.238393             4.086175
              89.475630           20.231611             0.453747
              98.357483          249.212410             6.144056
             105.492554           64.689250             1.710535
             109.012874           15.997136             0.437117
             113.610937           61.241191             1.743981
             114.664327           61.781980             1.775694
             116.043509          101.010020             2.938078
             119.995430           23.369811             0.702907
             123.719376           53.501554             1.659137
             127.171763          100.851579             3.214782
             135.475451           22.986292             0.780562
```

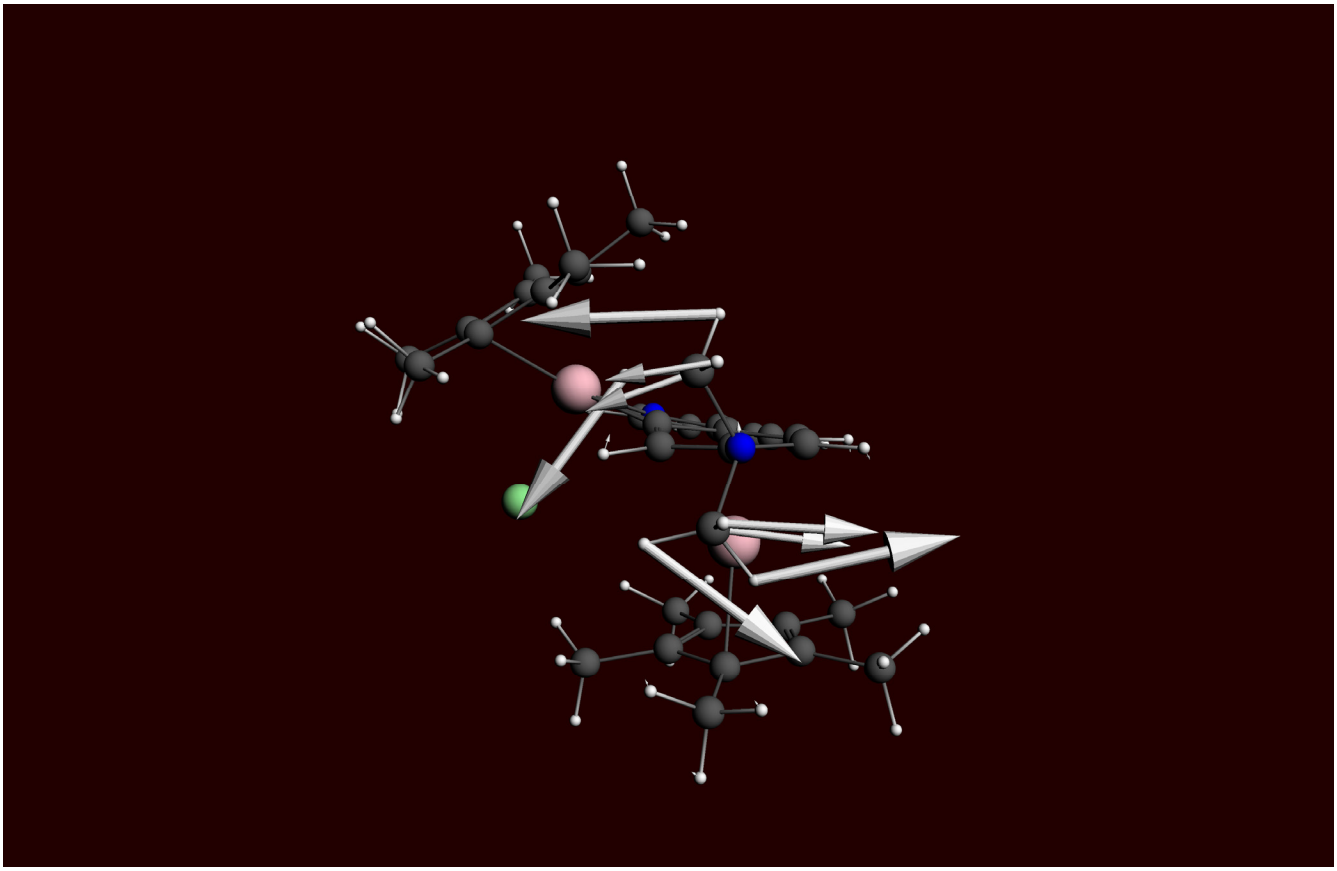
139.017298	39.184782	1.365414
147.303381	321.412114	11.867330
150.498478	376.700548	14.210404
153.471800	8.227122	0.316486
154.572897	169.577611	6.570220
154.897861	38.423784	1.491845
158.176826	80.534149	3.193015
161.701051	208.580302	8.454038
168.749666	105.762112	4.473538
176.748538	421.333385	18.666366
181.197532	122.324712	5.555774
192.145250	104.992142	5.056669
198.623536	194.625448	9.689657
201.859259	444.810392	22.506174
204.968974	230.362779	11.835279
211.035708	199.916364	10.575048
221.057600	505.762835	28.024020
223.405977	56.365543	3.156360
238.543672	180.454513	10.789808
261.148383	18.943752	1.240028
267.954316	103.803803	6.971915
271.667439	146.309148	9.962931
276.452741	205.939826	14.270504
278.308718	107.535866	7.501675
281.016362	4.469517	0.314826
284.863304	29.723219	2.122318
292.472753	89.699050	6.575841
293.820737	65.423838	4.818330
297.384477	50.168218	3.739599
299.920118	68.414284	5.143165
320.398828	264.164881	21.215050
333.486265	158.349456	13.236483
362.103701	57.130413	5.185354
377.781815	13.770728	1.303995
394.889336	69.731719	6.902141
404.730635	58.548327	5.939620
411.900391	19.111221	1.973144
427.012934	45.603273	4.881071
427.775734	137.678981	14.762566
430.120683	81.625063	8.800187
440.213302	17.690353	1.951991
442.016826	80.943031	8.968015
460.203676	324.230637	37.400913
510.628463	272.624993	34.893839
517.433304	197.717171	25.643473
522.416161	11.044337	1.446220
522.813834	7.298494	0.956441
523.075798	12.169953	1.595628
525.182434	91.665839	12.066902
538.539339	0.345694	0.046665
538.794668	1.657119	0.223797
556.971634	142.270384	19.862122
579.796606	51.665439	7.508512
584.060431	60.667856	8.881667
591.417527	15.645088	2.319264
593.722926	12.345435	1.837250
596.128872	5.894867	0.880830
596.641160	23.678227	3.541118
607.426690	221.315577	33.696433
638.422000	48.861727	7.819063
656.847015	49.939112	8.222107
679.156786	126.714329	21.571177
712.090070	54.983104	9.813914
729.379798	387.417411	70.828971
758.066988	357.059592	67.846330
782.907178	6.175691	1.211920
784.642038	1.656681	0.325828
786.452683	0.976674	0.192531
789.212132	24.202811	4.787818
791.036179	48.738131	9.663697
857.370034	62.636115	13.460810
861.741719	138.477033	29.911138
907.696933	233.718009	53.175443
921.709489	2.177338	0.503035
927.884936	232.282645	54.024276
931.015360	1.767421	0.412453
932.100669	9.822096	2.294801
932.261149	58.104736	13.577731
932.939860	21.251702	4.969646
940.643723	11.464071	2.702975
959.337662	1.385755	0.333224
986.591325	824.895367	203.992512
990.347999	248.868138	61.778192
992.764433	162.882535	40.532071
994.557686	753.216451	187.770708
995.576247	347.752698	86.780691
998.090305	106.174527	26.562457
999.432172	129.165031	32.357604
999.567464	105.688040	26.479881
1001.240950	103.177089	25.894048
1004.336434	35.428651	8.918913
1005.476143	6.973049	1.757408
1007.736349	101.365463	25.604424
1019.140715	84.943503	21.699133
1026.160274	62.795914	16.151939
1049.716582	24.007507	6.316801
1057.133345	88.945837	23.568583
1060.068101	28.482281	7.568095
1063.341769	101.922771	27.165779

1065.826066	116.552391	31.137633
1071.172961	37.144739	9.973210
1083.788888	1.239474	0.336713
1088.521928	32.115848	8.762633
1089.566232	1.346107	0.367630
1100.182833	0.766492	0.211374
1111.668288	515.017063	143.507601
1132.848603	32.884448	9.337713
1138.289156	6.762262	1.929402
1142.493852	10.959844	3.138602
1144.389865	15.059234	4.319714
1146.736806	27.232596	7.827640
1149.179839	6.203433	1.786891
1165.045047	93.693496	27.360891
1187.610897	195.115383	58.082293
1255.882364	74.148816	23.341634
1262.263578	117.239287	37.093797
1276.739103	4.919380	1.574311
1305.370243	51.481937	16.844831
1313.908124	33.077548	10.893724
1316.828369	59.412807	19.610439
1331.946863	30.956179	10.335044
1336.808372	10.589156	3.548204
1340.874095	25.643045	8.618579
1342.619973	8.513775	2.865189
1351.820834	7.660063	2.595551
1352.214226	255.404909	86.567089
1352.751073	223.727718	75.860509
1353.817408	95.595137	32.439486
1354.274094	89.146715	30.261468
1354.479824	32.176767	10.924285
1364.310674	429.220430	146.781639
1373.092974	46.029008	15.841986
1375.469427	3.138811	1.082167
1375.483070	23.309679	8.036549
1379.133320	18.451646	6.378513
1384.138108	12.538686	4.350203
1388.952789	13.322124	4.638088
1390.886710	13.710909	4.780090
1391.584232	22.002666	7.674726
1399.492728	79.154382	27.766662
1403.273299	14.573949	5.126224
1407.408951	252.035221	88.911844
1408.412748	224.082063	79.107036
1410.077574	38.180407	13.494650
1411.071299	28.019108	9.910175
1413.003371	7.546181	2.672689
1414.199779	1.946706	0.690064
1416.093938	10.937169	3.882174
1416.697091	30.257180	10.744433
1421.136015	60.480236	21.544042
1423.937458	21.431289	7.649222
1424.186267	56.310515	20.101773
1425.276167	117.454398	41.961053
1426.197731	215.083773	76.889220
1427.715849	29.556813	10.577364
1428.030241	278.331107	99.627039
1432.153632	122.481060	43.967990
1435.240520	178.982146	64.389117
1437.243367	236.035666	85.032709
1440.764252	56.844467	20.528593
1443.034741	20.286654	7.337790
1443.301007	85.037247	30.764097
1445.692608	111.274194	40.322596
1449.058554	78.827536	28.631358
1451.453605	179.668354	65.366137
1454.775067	330.284392	120.437566
1459.269242	477.801845	174.767760
1462.366348	145.803253	53.444309
1464.207725	191.298290	70.208849
1485.145306	378.083743	140.745663
1502.440622	264.275968	99.525200
1554.253178	2.801580	1.091448
1592.490470	38.516707	15.374608
2900.775992	74.431819	54.119141
2910.278793	75.530853	55.098155
2957.012506	6.894451	5.110118
2959.922511	3.025139	2.244418
2961.896167	5.076803	3.769105
2962.498980	6.070499	4.507759
2962.994030	5.160380	3.832574
2964.016523	18.184907	13.510449
2965.138838	2.057086	1.528887
2966.686010	5.128931	3.813964
2967.677358	13.426754	9.987707
2968.554327	7.844065	5.836658
3021.534947	11.771485	8.915320
3034.309590	14.468524	11.004294
3039.254344	41.818408	31.857568
3040.080502	3.427954	2.612150
3040.375746	7.317518	5.576595
3042.210362	5.259651	4.010737
3044.427736	1.857796	1.417691
3044.921828	1.848263	1.410646
3049.351513	27.071256	20.691595
3051.024872	8.249392	6.308785
3052.482054	9.830702	7.521695
3054.051239	12.677724	9.705003
3067.536402	3.068017	2.358987

3072.204971	10.442276	8.041247
3074.202119	0.462993	0.356767
3075.145397	4.666476	3.596936
3076.013099	1.340622	1.033648
3077.639183	0.790517	0.609828
3079.748762	2.001794	1.545300
3084.585190	19.748572	15.268998
3088.938361	0.529308	0.409822
3090.418121	0.923418	0.715309
3100.695897	1.246491	0.968783
3105.794451	5.352643	4.166957
3135.524752	7.101835	5.581602
3136.606825	9.212000	7.242560
3137.656848	16.608174	13.061872
3144.667283	5.339746	4.208946
3148.419777	40.659589	32.087337
3152.732816	52.963313	41.854328
3164.917731	15.797500	12.532244

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	46.228	37.599	159.572	243.399
	Internal Energy (Kcal/mole):	0.889	0.889	438.448	440.226
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	156.824	162.786

TS2-[endo-3a]2+



Geometry CYCLE 89
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	0.000005	0.000029	-0.000013
2	H	0.000007	-0.000001	-0.000001
3	C	0.000015	0.000003	0.000001
4	H	-0.000006	-0.000004	-0.000003
5	C	0.000009	-0.000002	-0.000005
6	H	-0.000016	-0.000004	0.000003
7	C	-0.000029	0.000034	-0.000011
8	H	-0.000054	-0.000188	-0.000037
9	C	0.000006	-0.000020	-0.000069
10	C	-0.000143	0.000024	-0.000030
11	C	0.000239	0.000174	-0.000027
12	C	-0.000280	0.000177	-0.000121
13	H	-0.000016	-0.000007	0.000009
14	C	-0.000008	-0.000060	-0.000077
15	N	0.000025	0.000036	0.000138
16	C	0.000028	-0.000089	0.000060
17	H	-0.000019	0.000024	0.000007
18	C	0.000123	0.000073	-0.000019
19	H	0.000031	0.000164	0.000058
20	Cl	-0.000060	-0.000057	0.000021
21	C	-0.000031	-0.000108	0.000101
22	C	-0.000177	0.000020	-0.000043
23	C	-0.000025	-0.000015	0.000063
24	C	-0.000154	0.000028	-0.000037
25	C	-0.000017	-0.000113	0.000046
26	N	-0.000121	0.000028	-0.000056
27	Ir	0.000534	0.000175	0.000226
28	C	-0.000090	0.000001	-0.000163
29	H	0.000001	-0.000019	0.000027
30	H	0.000049	0.000002	-0.000064
31	H	0.000003	0.000000	0.000020
32	C	0.000045	-0.000069	-0.000023
33	H	-0.000005	-0.000005	0.000015
34	H	-0.000007	-0.000005	0.000016
35	H	-0.000014	-0.000004	-0.000004
36	Ir	0.000203	-0.000672	-0.000291
37	C	-0.000233	0.000201	-0.000084

```
   38 C    -0.000036  0.000009  0.000245
   39 C     0.000003  0.000027  0.000031
   40 C     0.000132  0.000040  0.000068
   41 C     0.000016 -0.000080  0.000009
   42 C     0.000005  0.000010 -0.000008
   43 H    -0.000018  0.000006  0.000009
   44 H     0.000003 -0.000002 -0.000026
   45 H    -0.000003  0.000025 -0.000005
   46 C     0.000023  0.000021  0.000011
   47 H     0.000026  0.000003  0.000006
   48 H     0.000006 -0.000019  0.000001
   49 H    -0.000002 -0.000005  0.000005
   50 C     0.000043  0.000010  0.000017
   51 H     0.000002 -0.000008  0.000019
   52 H    -0.000015  0.000004 -0.000019
   53 H    -0.000005 -0.000010 -0.000023
   54 C    -0.000031  0.000032 -0.000014
   55 H    -0.000001  0.000001 -0.000006
   56 H    -0.000019 -0.000005  0.000007
   57 H     0.000020 -0.000006 -0.000013
   58 C     0.000032  0.000022 -0.000028
   59 H    -0.000020  0.000002  0.000041
   60 H     0.000037 -0.000025 -0.000009
   61 H    -0.000012  0.000002 -0.000007
   62 C     0.000022  0.000046 -0.000047
   63 H    -0.000006  0.000008  0.000003
   64 H     0.000061 -0.000013  0.000029
   65 H     0.000004 -0.000006 -0.000015
   66 C    -0.000017 -0.000007  0.000039
   67 H     0.000006  0.000008  0.000012
   68 H     0.000007 -0.000012  0.000005
   69 H     0.000010  0.000012 -0.000025
   70 C     0.000061  0.000104 -0.000124
   71 H    -0.000048  0.000035  0.000017
   72 H    -0.000046  0.000037  0.000001
   73 H     0.000014 -0.000055  0.000180
   74 C    -0.000042  0.000023 -0.000025
   75 H     0.000004 -0.000002 -0.000022
   76 H     0.000004  0.000002  0.000003
   77 H     0.000001 -0.000012  0.000016
   78 C    -0.000015  0.000021 -0.000008
   79 H    -0.000005  0.000002  0.000020
   80 H    -0.000011  0.000015  0.000001
   81 H    -0.000007 -0.000007 -0.000001
 ----------------------------------------

----------------------------------------
Geometry Convergence after Step  89
----------------------------------------
current energy                            -17.57656931 Hartree
energy change                  -0.00001498     0.00100000    T
constrained gradient max        0.00067249     0.00100000    T
constrained gradient rms        0.00008626     0.00066667    T
gradient max                    0.00067249
gradient rms                    0.00008626
cart. step max                  0.00930994     0.01000000    T
cart. step rms                  0.00271428     0.00666667    T

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

  Electrostatic Energy:           -14.925301598698599       -406.1381         -9365.77        -39186.37
  Kinetic Energy:                  19.469623987421016        529.7954         12217.37         51117.49
  Coulomb (Steric+OrbInt) Energy:  -5.666550189620267       -154.1947         -3555.81        -14877.53
  XC Energy:                      -16.250764923941865       -442.2058        -10197.51        -42666.38
  Solvation:                       -0.203576828887520         -5.5396          -127.75          -534.49
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:           -17.576569553727236       -478.2828        -11029.47        -46147.28


 List of All Frequencies:


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
             -94.887231           79.662055           -1.894686
              18.107168            0.000000            0.000000
              42.177635          769.130279            8.131304
              46.847316           93.423870            1.097035
              50.413818          338.087444            4.272250
              67.781457          193.622175            3.289607
              77.431991           96.098176            1.865149
              84.683141          171.671314            3.643953
              89.617958           16.960326            0.380985
              97.247438          164.223722            4.003060
             106.757087           19.848773            0.531139
             110.027423           46.866844            1.292542
             113.474291          172.673492            4.911354
             116.353011           29.156431            0.850335
             118.069519           60.673982            1.795636
             120.796634           42.452253            1.285386
             122.843380          132.241527            4.071905
             128.583022           37.137555            1.196947
             132.432531           25.977107            0.862310
```

139.853631	72.553432	2.543371
144.642122	267.863655	9.711507
148.628307	134.938783	5.027087
153.506876	156.200664	6.010198
154.467673	225.118316	8.716186
155.483863	41.164103	1.604287
159.474505	65.208860	2.606609
160.333624	108.404430	4.356620
169.928051	237.532077	10.117318
173.896414	455.382411	19.849289
184.279512	348.497976	16.097387
186.677311	211.513847	9.897110
198.090576	303.174718	15.053409
199.386688	85.914387	4.293783
211.960866	263.825079	14.016831
215.330437	224.021225	12.091291
227.662821	512.538905	29.248057
235.846603	38.343253	2.266714
243.144127	34.864801	2.124854
257.236031	15.125066	0.975230
267.815798	78.068078	5.240681
274.019901	63.764562	4.379652
277.439312	370.122678	25.739006
281.673392	18.856242	1.331310
284.553030	44.397481	3.166647
288.373440	87.140743	6.298753
292.762986	64.905294	4.762932
297.098187	72.385691	5.390522
298.301838	64.750235	4.841449
300.264566	66.945566	5.038531
322.104011	242.038932	19.541569
332.311251	87.518765	7.289946
361.882496	68.214110	6.187566
380.254389	21.949721	2.092095
398.915535	72.875352	7.286848
403.044751	48.662618	4.916169
411.278926	19.927572	2.054324
421.455311	267.382272	28.246342
427.592648	91.371141	9.793036
430.301798	44.539876	4.803969
439.091858	12.211242	1.343981
443.713450	102.073568	11.352564
447.775948	167.395737	18.788116
506.588163	60.316459	7.658945
516.686391	438.310410	56.765815
522.017241	11.326743	1.482067
522.980557	1.949577	0.255567
523.243849	19.424983	2.547668
525.966377	132.876768	17.518024
538.196960	0.636176	0.085822
539.593126	2.344779	0.317137
556.024306	184.704394	25.742402
580.275556	50.387947	7.328904
584.540573	56.865731	8.331887
590.717328	14.437781	2.137757
593.234984	6.392602	0.950566
595.345057	6.832895	1.019651
596.210247	26.950434	4.027572
609.591109	239.251025	36.556996
634.758408	42.712572	6.795826
653.413763	21.508307	3.522675
680.567367	159.747246	27.251008
714.634128	61.301533	10.980779
730.229030	381.265661	69.785446
758.534158	372.788882	70.878769
783.181687	6.459071	1.267975
785.771859	1.445795	0.284762
786.498024	1.161263	0.228932
789.602660	14.675780	2.904610
793.151423	194.866831	38.741114
861.198832	21.165899	4.568969
866.571355	180.061464	39.111383
905.509514	38.878927	8.824403
923.546963	163.584896	37.868688
927.145992	28.852708	6.705216
931.796611	2.515466	0.587513
932.278841	6.970559	1.628889
932.567368	27.950806	6.533601
934.355365	16.159390	3.784558
940.195125	11.155475	2.628961
959.103057	2.176151	0.523157
985.387711	790.709219	195.299897
989.044166	285.515135	70.782010
992.318731	204.275408	50.809550
994.058200	682.403963	170.032297
994.918423	376.237000	93.826830
997.547035	150.570838	37.648902
998.910566	24.366182	6.100876
999.537567	178.787612	44.793460
1000.851738	134.506891	33.743673
1004.543809	32.777923	8.253314
1005.229813	5.590430	1.408603
1008.012100	111.810635	28.250552
1022.276213	98.099323	25.136936
1026.747747	48.940182	12.595268
1049.387000	27.663127	7.276374
1057.542279	90.193979	23.908556
1060.416250	29.858113	7.936277
1063.283949	111.300401	29.663614

1065.296271	109.923143	29.351994
1071.787040	6.729982	1.808009
1076.396750	35.876077	9.679555
1084.253112	0.421251	0.114485
1089.385229	0.841447	0.229766
1096.713930	13.205946	3.630287
1113.338788	476.730018	133.038674
1132.007708	35.510855	10.076010
1137.804637	4.198320	1.197351
1142.818927	12.818606	3.671946
1144.686182	13.075571	3.751675
1146.943850	30.158988	8.670357
1149.445260	8.253814	2.378050
1172.883779	117.324513	34.492273
1191.638236	197.915830	59.115726
1252.775326	50.258950	15.782096
1264.995972	138.266924	43.841511
1273.669678	2.652360	0.846774
1306.479390	61.570790	20.163010
1306.887934	51.965992	17.022982
1311.568083	33.757171	11.097750
1331.799787	40.020955	13.359938
1336.750438	10.176164	3.409671
1340.534357	41.376570	13.903063
1342.620422	2.634645	0.886652
1351.320302	42.438264	14.374541
1352.071631	264.781749	89.735816
1352.903595	246.403650	83.558774
1354.099727	39.035928	13.249309
1354.456808	26.256798	8.914254
1354.636098	105.293289	35.752088
1360.935891	398.845472	136.056847
1373.110011	43.239418	14.882067
1374.775781	12.020618	4.142254
1375.845206	7.220485	2.490084
1379.774335	14.388142	4.976120
1384.858454	15.707705	5.452507
1388.351987	18.837371	6.555381
1390.376904	17.923236	6.246360
1391.322579	16.125012	5.623490
1399.896133	77.960514	27.355747
1403.388621	28.205866	9.921914
1406.960130	84.013387	29.628410
1407.947212	130.477592	46.046898
1409.254924	299.271399	105.714083
1411.058100	22.633214	8.005145
1411.887796	4.189418	1.482627
1414.548960	0.421863	0.149578
1415.335532	10.636981	3.773600
1417.008761	28.541287	10.137343
1420.128291	53.992990	19.219542
1424.006084	21.428684	7.648661
1425.027622	61.213317	21.864888
1425.969091	20.661206	7.384887
1426.549566	218.063489	77.973655
1427.653309	120.787501	43.223788
1428.034419	174.440925	62.440321
1433.267919	292.234824	104.987457
1436.060015	216.619909	77.973859
1437.531054	65.444356	23.581287
1441.626293	59.572809	21.526769
1444.030514	110.260388	39.909286
1444.736243	114.777564	41.564603
1446.002696	67.123069	24.328704
1448.012154	190.120128	69.004653
1454.162771	360.232150	131.302671
1456.359928	356.837516	130.261867
1458.517205	228.769366	83.634891
1461.002895	111.009292	40.652614
1470.122471	255.684175	94.218337
1480.951463	281.433619	104.470788
1502.879362	255.510883	96.252406
1554.020542	2.824294	1.100132
1592.015241	38.559442	15.387074
2901.248650	63.748384	46.358801
2909.078566	77.448867	56.474005
2956.118312	7.458931	5.526834
2960.322044	2.825218	2.096375
2961.843975	4.018987	2.983712
2962.010235	8.154235	6.054076
2963.150752	4.200685	3.119981
2964.635649	14.917844	11.085505
2964.647794	5.810149	4.317560
2967.096455	3.764227	2.799533
2967.677107	13.836312	10.292362
2968.793342	9.038016	6.725602
3021.417809	14.106581	10.683428
3032.923701	17.373720	13.207857
3038.165920	42.933066	32.695009
3039.397708	7.464930	5.687106
3040.220573	2.915345	2.221637
3043.292284	0.869267	0.663093
3043.483083	2.175915	1.659934
3044.101963	4.428901	3.379350
3049.490160	31.033370	23.721068
3052.548773	11.607931	8.881688
3054.500991	2.210536	1.692451
3055.204050	15.554040	11.911364
3067.733130	4.360637	3.353093

3071.996585	8.908583	6.859736
3073.211893	0.500837	0.385804
3073.839270	5.251367	4.046053
3075.864468	0.760756	0.586530
3077.894983	1.496085	1.154219
3082.365654	3.955833	3.056330
3084.773630	18.181925	14.058573
3089.119268	0.777980	0.602395
3090.775868	0.808744	0.626551
3095.449588	12.625992	9.796418
3102.573098	0.989542	0.769545
3120.499745	2.690979	2.104808
3135.813540	0.961732	0.755931
3140.819562	15.300341	12.045426
3145.497375	1.470741	1.159588
3150.842988	33.903442	26.776180
3152.345934	88.718257	70.101117
3163.178571	17.421457	13.812944

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	46.228	37.578	152.335	236.141
	Internal Energy (Kcal/mole):	0.889	0.889	437.832	439.610
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	154.797	160.759

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