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Supporting Information

Titanium tetrachloride-mediated synthesis of N-aryl-substituted azacycles from cyclic ethers

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Experimental Section

General Considerations. Starting materials including cyclic ethers, $TiCl_4$ and solvents were dried and distilled prior to use according to standard procedures, amines were used as purchased without further purification. Either pure $TiCl_4$ liquid or its solution in dichloromethane would efficiently facilitate the reaction. All reactions were performed under an atmosphere of argon using standard Schlenck techniques. NMR spectra were recorded on a Bruker 400 spectrometer using $CDCl_3$ as solvent, and the chemical shifts were reported in ppm with respect to the reference (internal $SiMe_4$ for ^1H NMR spectra). The products are known compounds and were identified by comparison with the reported NMR spectra of the compounds in literature.

General procedure and preliminary reaction condition screening: A solution of 1.2 mmol of $TiCl_4$ and 1 mmol of aniline in 4 mL of dry solvent was stirred at room temperature for 30 minutes. To the mixture was added 10 mmol of THF and the temperature was slowly elevated. After refluxing or stirring at certain temperature for 24 h, 10 mL of saturated $NaHCO_3$ solution and 10 mL of dichloromethane were added and stirred for 1h. The mixture was extracted with 3 x 10 mL of dichloromethane and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue was isolated by column chromatography on silica. Results are listed below.

Solvent	Reaction temperature (^oC)	Isolated yield (%)
THF	refluxing	NR
cyclohexane	refluxing	NR
acetonitrile	refluxing	NR
benzene	refluxing	< 5%
dioxane	refluxing	NR

toluene	refluxing	68%
toluene	80	< 5%
octane	refluxing	NR
DMF	refluxing	Complicated mixture

Thus further screening of Lewis acid was carried out by refluxing the reaction mixture in toluene.

Synthesis of N-phenylpyrrolidine (3a): A solution of 0.13 mL (1.2 mmol) of $TiCl_4$ and 0.10 mL (1 mmol) of aniline in 4 mL of dry toluene was stirred at room temperature for 30 minutes. To the mixture was added 1.0 mL (10 mmol) of THF and the temperature was slowly elevated to 110 ^oC. After refluxing for 24 h, 10 mL of saturated $NaHCO_3$ solution and 10 mL of dichloromethane were added and stirred for 1h. The mixture was extracted with 3 x 10 mL of dichloromethane and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue was isolated by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent to give yellow liquid (100 mg, yield 68%). ^1H NMR: (400MHz, $CDCl_3$) δ = 7.28-7.16 (m, 2H), 6.66 (t, J = 7.9 Hz, 1H), 6.57 (d, J = 7.9 Hz, 2H), 3.28 (t, J = 6.5 Hz, 4H), 2.04-1.93 (m, 4H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 129.2, 115.4, 111.7, 47.6, 25.5 ppm.

Synthesis of N-(4-fluorophenyl)pyrrolidine (3b): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 4-fluoroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave brown liquid (137 mg, yield 83%). ^1H NMR: (400MHz, $CDCl_3$) δ = 6.99-6.90 (m, 2H), 6.52-6.45 (m, 2H), 3.25 (t, J = 6.6 Hz, 4H), 2.04-1.99 (m, 4H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.8(d, $^1J_{CF}$ = 232.9 Hz), 144.8, 115.5 (d, $^2J_{CF}$ = 22.2 Hz), 112.1 (d, $^3J_{CF}$ = 7.4 Hz), 48.1, 25.5 ppm.

Synthesis of N-(4-chlorophenyl)pyrrolidine (3c): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 4-chloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave white solid (130 mg, yield 72%). ^1H NMR: (400MHz, $CDCl_3$) δ = 7.14 (d, J = 8.6 Hz, 1H), 6.45 (d, J = 8.6 Hz, 1H), 3.24 (t, J = 6.0 Hz, 2H), 2.00 (t, J = 6.0 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 128.9, 120.1, 112.6, 47.7, 25.5 ppm.

Synthesis of N-(3-chlorophenyl)pyrrolidine (3d): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 3-chloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (137 mg, yield 76%). ^1H NMR: (400MHz, $CDCl_3$) δ = 7.12 (t, J = 7.9 Hz, 1H), 6.62 (d, J = 7.9 Hz, 1H), 6.53 (s, 1H), 6.43 (d, J = 8.3 Hz,

1H), 3.27 (t, J = 5.9 Hz, 5H), 2.02 (d, J = 5.9 Hz, 4H) ppm.^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 134.9, 130.0, 115.1, 111.4, 109.9, 47.6, 25.5 ppm.

Synthesis of N-(2-chlorophenyl)pyrrolidine (3e): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 2-chloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (103 mg, yield 57%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.31 (d, J = 7.8 Hz, 1H), 7.15 (t, J = 7.8 Hz, 1H), 6.90 (d, J = 7.8 Hz, 1H), 6.79 (t, J = 7.8 Hz, 1H), 3.39 (t, J = 5.8 Hz, 4H), 1.97 (d, J = 5.8 Hz, 4H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.2, 131.3, 127.2, 123.4, 120.2, 117.1, 50.9, 25.2 ppm.

Synthesis of N-(2,6-dichlorophenyl)pyrrolidine (3f): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 2,6-dichloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (108 mg, yield 50%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.53-7.50 (m, 2H), 7.24-7.20 (m, 1H), 3.55-3.51 (m, 4H), 2.24-2.18 (m, 4H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 136.6, 128.9, 126.0, 49.9, 26.5 ppm.

Synthesis of N-(3-nitrophenyl)pyrrolidine (3g): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 3-nitroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (113 mg, yield 59%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.46 (d, J = 8.1 Hz, 1H), 7.33 (s, 1H), 7.31 (t, J = 8.1 Hz, 1H), 6.80 (d, J = 8.1 Hz, 1H), 3.34 (t, J = 5.7 Hz, 4H), 2.07 (t, J = 5.7 Hz, 4H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 148.2, 129.5, 117.2, 109.8, 105.6, 47.8, 25.5 ppm.

Synthesis of N-(4-methylphenyl)pyrrolidine (3h): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 4-methylaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave light yellow liquid (97 mg, yield 60%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.10 (d, J = 7.7 Hz, 2H), 6.56 (d, J = 7.7 Hz, 2H), 3.32 (d, J = 5.1 Hz, 3H), 2.32 (s, 3H), 2.05 (d, J = 5.1 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.2, 129.7, 124.5, 111.8, 47.9, 25.5, 20.3 ppm.

Synthesis of N-phenyl-2-methylpyrrolidine (3i): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using 2-methyl tetrahydrofuran instead of tetrahydrofuran. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave light yellow liquid (107 mg, yield 67%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.24-7.17 (m, 2H), 6.63 (td, J = 7.3, 0.9 Hz, 1H), 6.60-6.55 (m, 2H), 3.87 (p, J = 6.2 Hz, 1H), 3.47-3.37 (m, 1H), 3.16 (dt, J = 16.2, 8.0 Hz, 1H), 2.15-1.89 (m, 3H), 1.69 (td, J = 6.4, 2.5 Hz, 1H), 1.17 (d, J = 6.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.2, 129.2, 115.1, 111.8, 53.6, 48.2, 33.1, 23.3, 19.4 ppm.

Synthesis of N-(4-chlorophenyl)-2-methylpyrrolidine (3j): The reaction was carried out as above-mentioned procedure for N-phenyl-2-methylpyrrolidine, using 4-chloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (117 mg, yield 60%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.14 (d, J = 7.5 Hz, 2H), 6.48 (d, J = 7.5 Hz, 2H), 3.83 (p, J = 6.2 Hz, 1H), 3.38 (t, J = 8.1 Hz, 1H), 3.12 (dd, J = 16.2, 7.8 Hz, 1H), 2.14-2.02 (m, 2H), 2.02-1.92 (m, 1H), 1.79-1.63 (m, 1H), 1.15 (d, J = 6.0 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.8, 128.9, 119.9, 112.8, 53.8, 48.3, 33.1, 23.3, 19.1 ppm.

Synthesis of N-(3-chlorophenyl)-2-methylpyrrolidine (3k): The reaction was carried out as above-mentioned procedure for N-phenyl-2-methylpyrrolidine, using 3-chloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave light yellow liquid (148 mg, yield 76%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.11 (t, J = 8.3 Hz, 2H), 6.62-6.58 (m, 1H), 6.54 (t, J = 2.1 Hz, 1H), 6.44 (dd, J = 8.3, 2.1 Hz, 1H), 3.91-3.79 (m, 1H), 3.39 (ddd, J = 9.6, 6.3, 2.1 Hz, 1H), 3.19-3.10 (m, 1H), 2.18-1.90 (m, 3H), 1.71 (ddd, J = 6.3, 4.7, 2.1 Hz, 1H), 1.17 (d, J = 6.3 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.1, 135.0, 130.0, 114.9, 111.5, 110.0, 53.7, 48.1, 33.0, 23.2, 19.1 ppm.

Synthesis of N-phenylpiperidine (3l): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using tetrahydropyran instead of tetrahydrofuran. After refluxing in xylenes for 24 h, aqueous work-up and isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (101 mg, yield 63%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.24 (t, J = 7.3 Hz, 2H), 6.94 (d, J = 8.0 Hz, 2H), 6.82 (t, J = 7.3 Hz, 1H), 3.18-3.10 (m, 4H), 1.71 (dd, J = 10.2, 5.1 Hz, 4H), 1.63 -1.48 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.3, 129.0, 119.2, 116.6, 50.7, 25.9, 24.4 ppm.

Synthesis of N-(4-fluorophenyl)piperidine (3m): The reaction was carried out as above-mentioned procedure for N-phenylpiperidine, using 4-fluoroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (120 mg, yield 67%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.00-6.91 (m, 2H), 6.92-6.84 (m, 2H), 3.11-2.99 (m, 4H), 1.72 (dt, J = 11.3, 5.7 Hz, 4H), 1.64 – 1.49 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0 (d, ^1J = 238.5 Hz), 149.1, 118.4 (d, ^3J = 7.6 Hz), 115.4(d, ^2J = 22.1 Hz), 51.8, 26.0, 24.1 ppm.

Synthesis of N-(2,4-difluorophenyl)piperidine (3n): The reaction was carried out as above-mentioned procedure for N-phenylpiperidine, using 2,4-difluoroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave yellow liquid (158 mg, yield 80%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 6.95-6.86 (m, 1H), 6.78 (tdt, J = 5.8, 4.0, 2.9 Hz, 2H), 3.00-2.89 (m, 4H), 1.78-1.67 (m, 4H), 1.56 (ddd, J = 11.5, 6.9, 4.5 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0 (d, ^1J = 205.3 Hz), 156.6, 119.7 (dd, J = 9.2, 4.3 Hz),

110.6 (dd, J = 21.3, 3.7 Hz), 105.4-103.4 (m), 52.7, 26.3, 24.3 ppm.

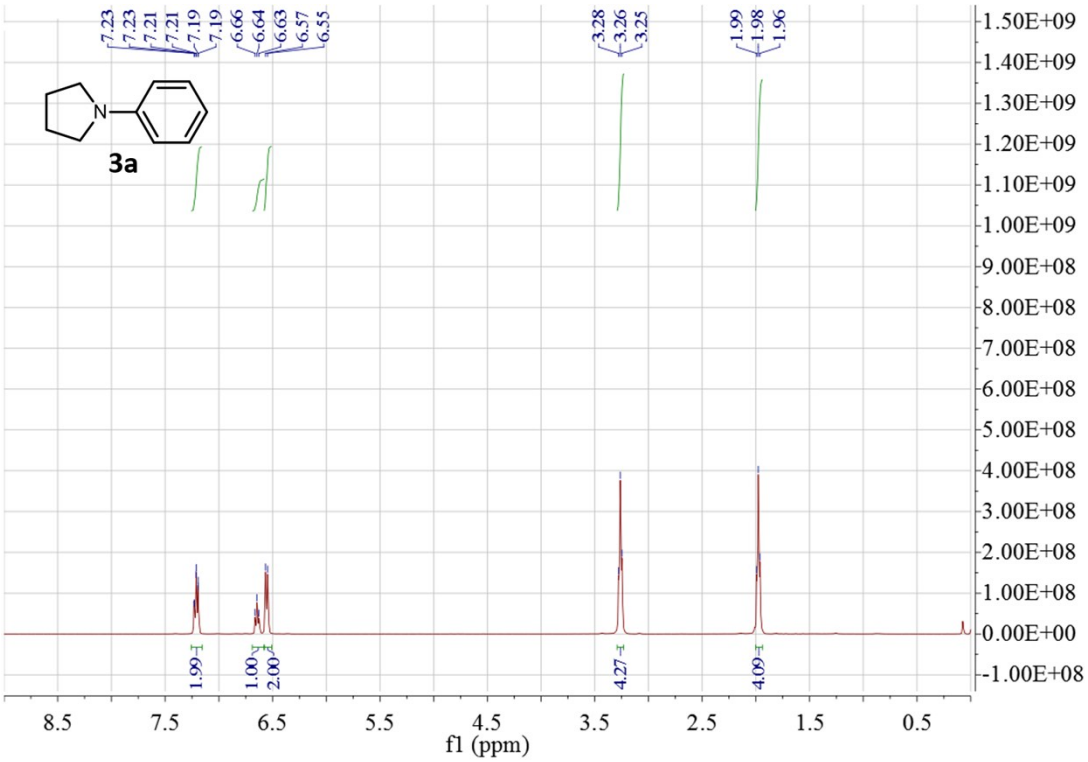
Synthesis of N-(3,5-dichlorophenyl)piperidine (3o): The reaction was carried out as above-mentioned procedure for N-phenylpiperidine, using 3,5-dichloroaniline instead of aniline. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave light yellow liquid (96 mg, yield 42%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 6.72 (d, J = 12.2 Hz, 3H), 3.55 (t, J = 6.6 Hz, 2H), 3.21-3.12 (m, 4H), 1.71-1.63 (m, 4H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.2, 135.3, 117.9, 113.9, 49.6, 31.9, 25.4 ppm.

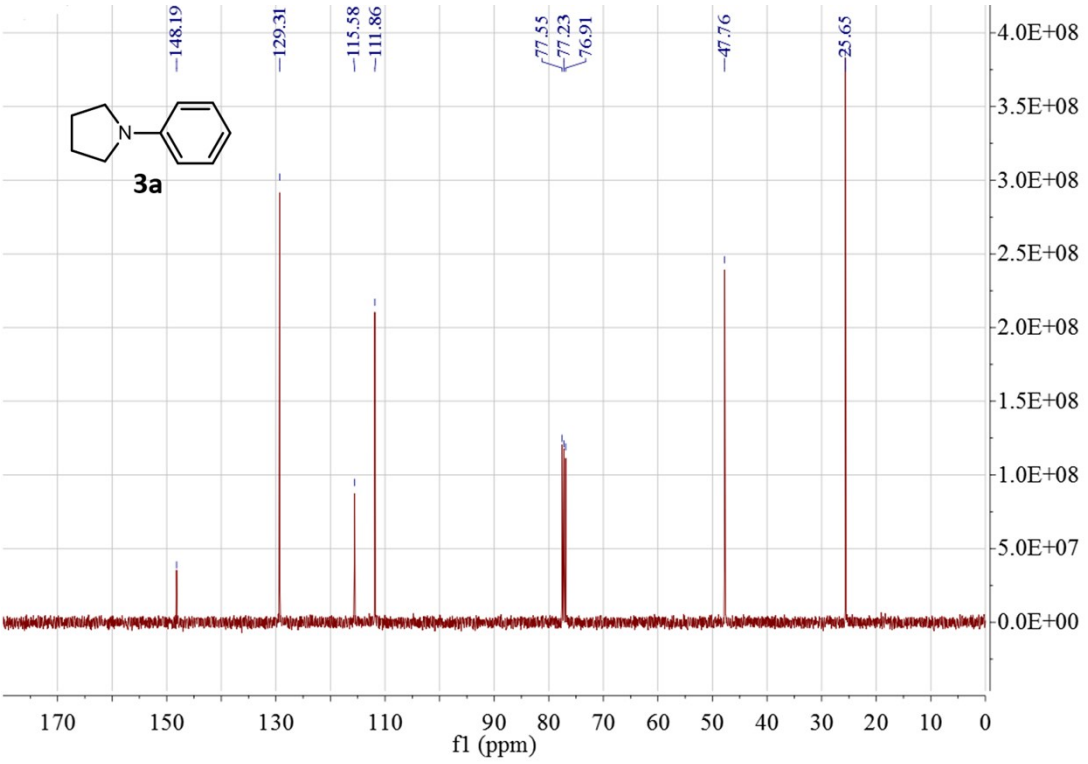
Synthesis of N-phenylisoindoline (3p): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using phthalan instead of tetrahydrofuran. After refluxing in xylenes for 24 h, aqueous work-up and isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave white solid (62 mg, yield 32%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.42-7.27 (m, 1H), 6.75 (t, J = 7.8 Hz, 1H), 6.69 (d, J = 7.8 Hz, 1H), 4.66 (s, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.0, 137.9, 129.4, 127.2, 122.6, 116.3, 111.7, 53.9 ppm.

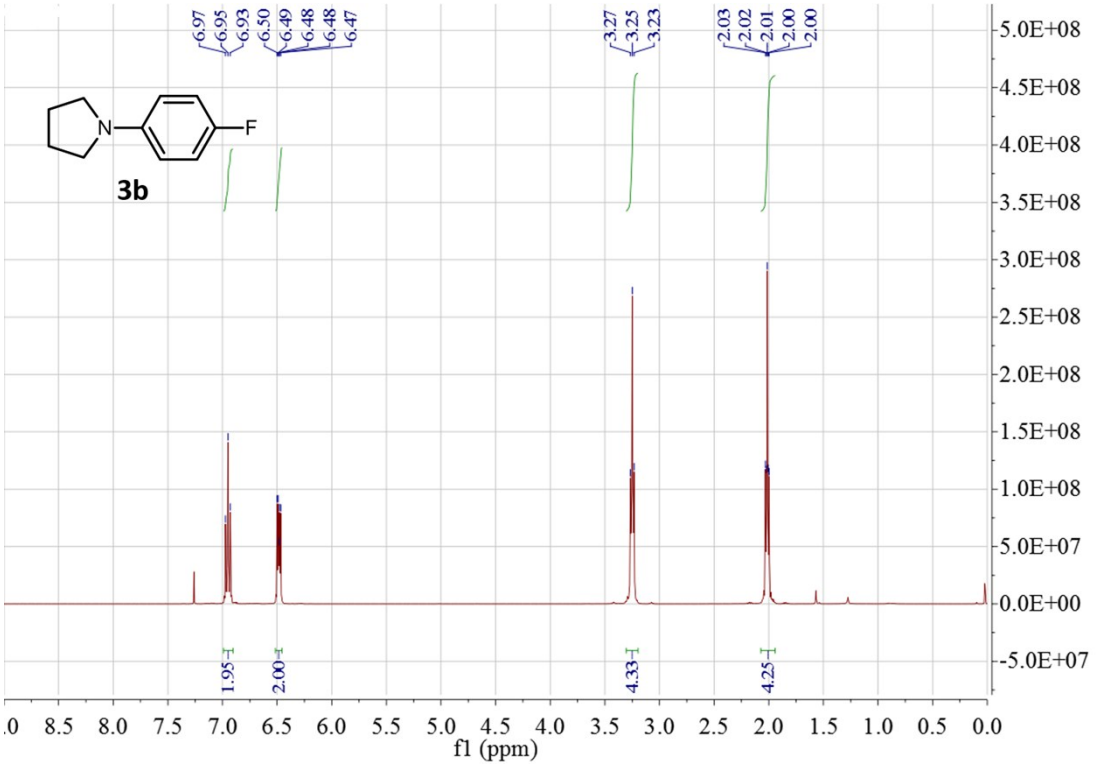
Synthesis of N-(4-fluorophenyl)tetrahydroisoquinoline (3q): The reaction was carried out as above-mentioned procedure for N-phenylpyrrolidine, using isochroman instead of tetrahydrofuran, 4-fluoroaniline instead of aniline. After refluxing in xylenes for 24 h, aqueous work-up and isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave white solid (181 mg, yield 80%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.23-7.13 (m, 4H), 7.11-6.83 (m, 4H), 4.34 (s, 2H), 3.49 (t, J = 5.9 Hz, 2H), 2.99 (t, J = 5.9 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0 (d, $^1J_{CF}$ = 235.6 Hz), 147.3, 134.5, 134.3, 128.6, 126.7 (d, $^3J_{CF}$ = 11.0 Hz), 126.1, 117.4, 117.3, 115.8 (d, $^2J_{CF}$ = 22.2 Hz), 51.9, 47.8, 29.0 ppm.

Synthesis of N-(2-chlorophenyl)tetrahydroisoquinoline (3r): The reaction was carried out as above-mentioned procedure for N-(4-fluorophenyl)tetrahydro isoquinoline, using 2-chloroaniline and isochroman. Isolation by column chromatography on silica using CH_2Cl_2/hexanes (1:4 v/v) as eluent gave white solid (119 mg, yield 49%). ^{1}H NMR: (400MHz, $CDCl_3$) δ = 7.45 (d, J = 7.7 Hz, 1H), 7.33-7.20 (m, 4H), 7.20-7.12 (m, 2H), 7.04 (t, J = 7.7 Hz, 1H), 4.33 (s, 2H), 3.45 (t, J = 5.8 Hz, 2H), 3.08 (t, J = 5.7 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2, 134.7, 134.6, 130.8, 129.0, 128.9, 127.6, 126.4, 126.4, 125.8, 123.7, 120.7, 53.3, 50.0, 29.1ppm.

NMR spectra of the Products



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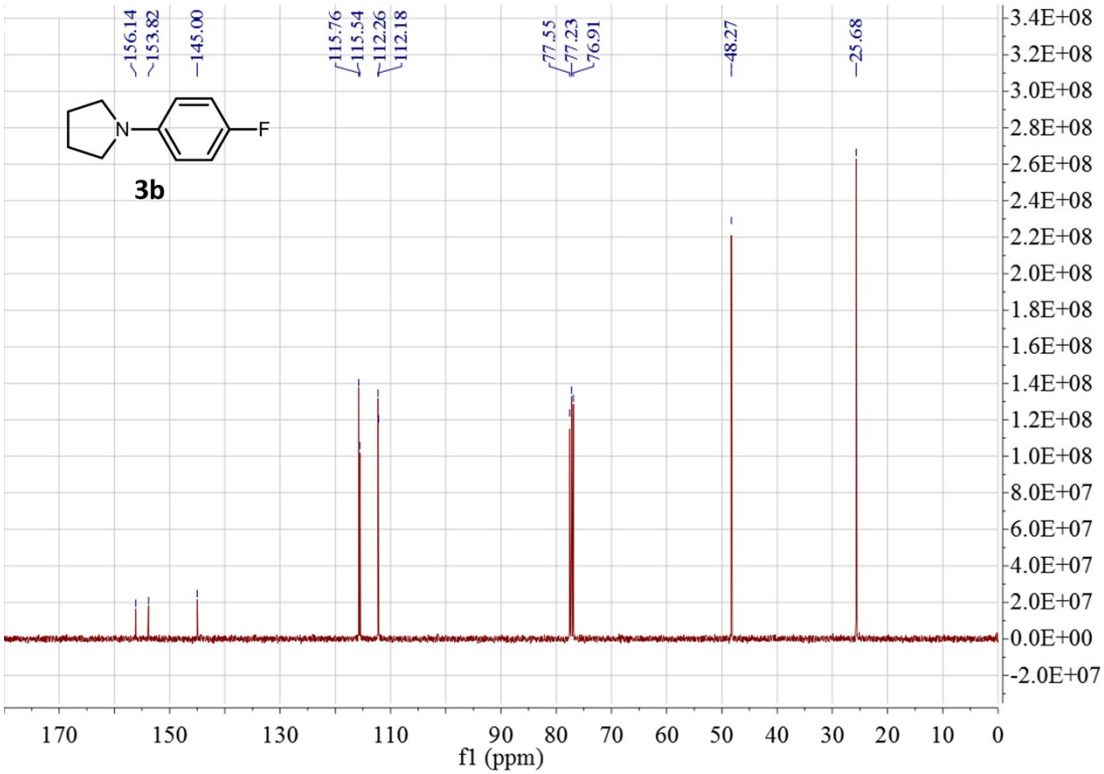
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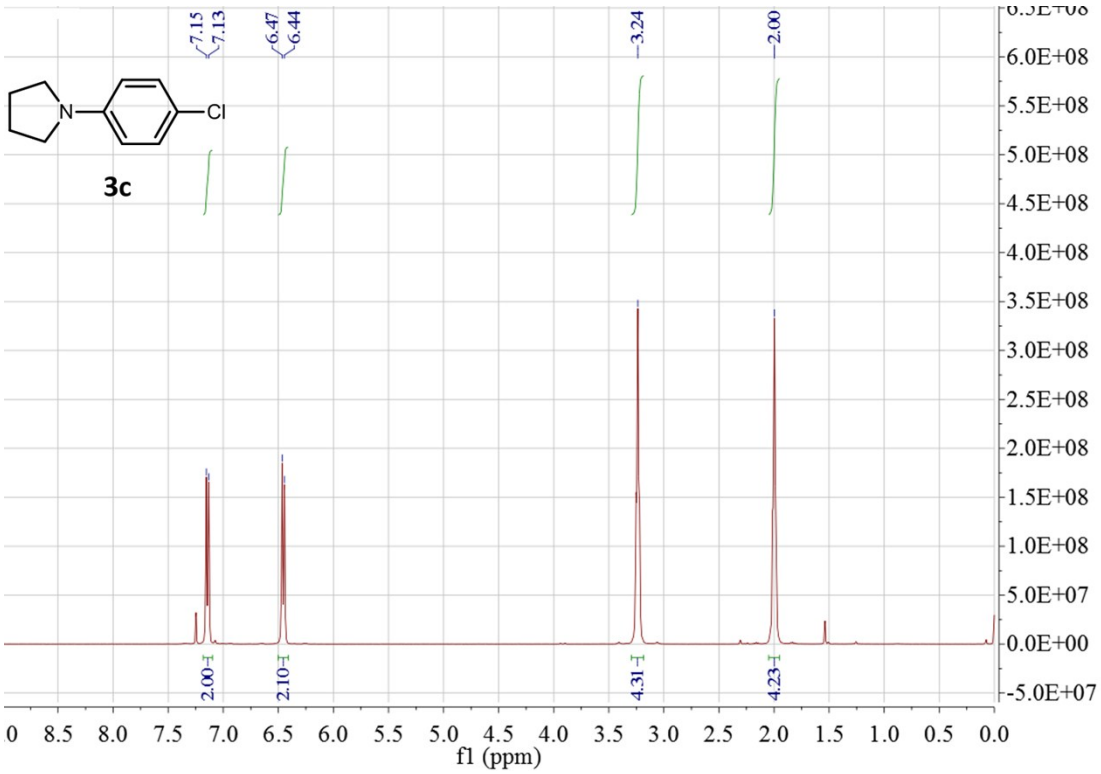
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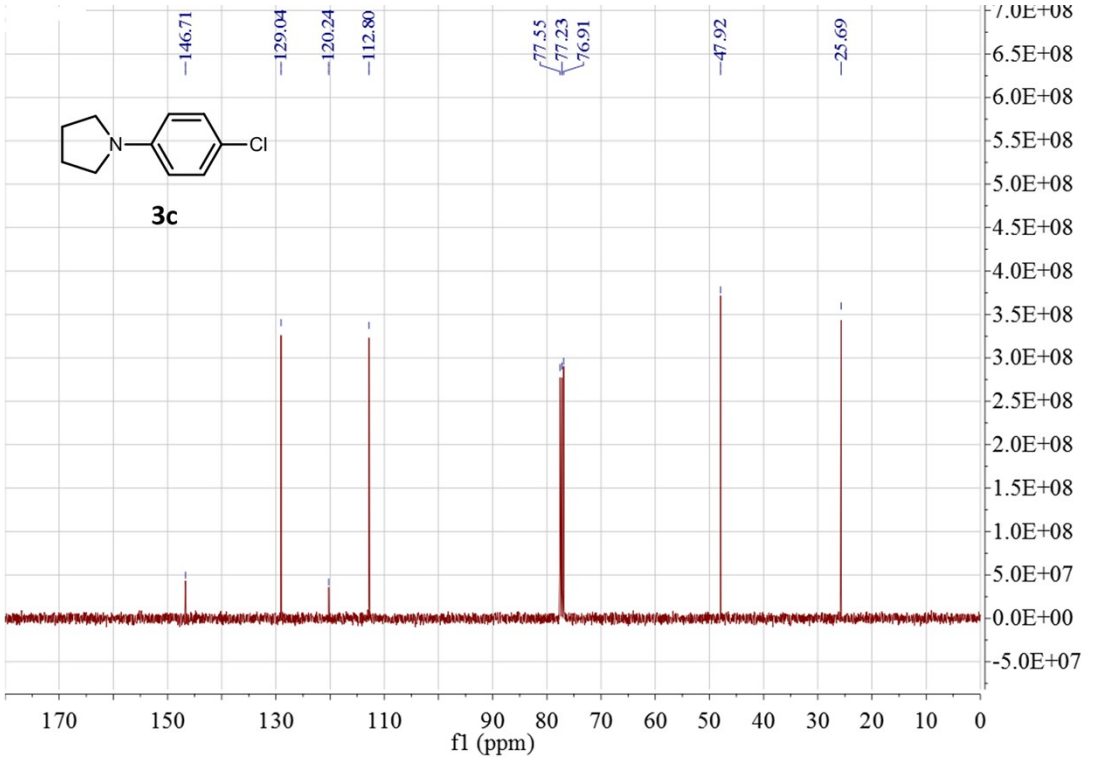
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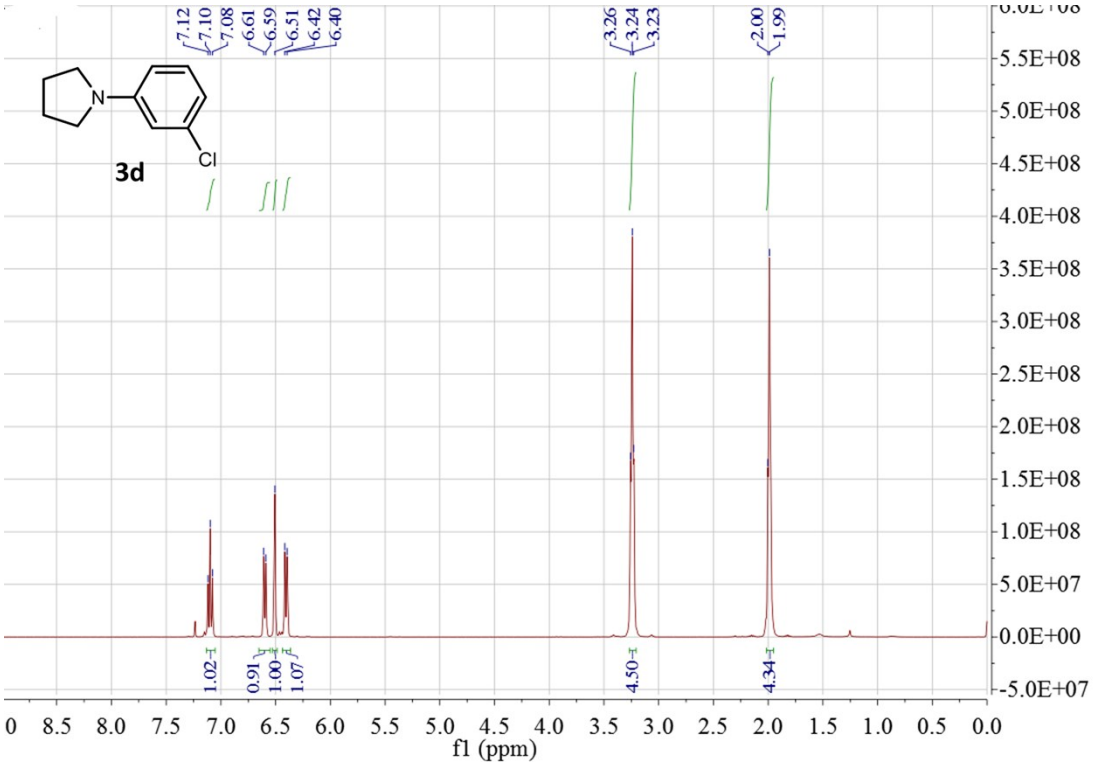
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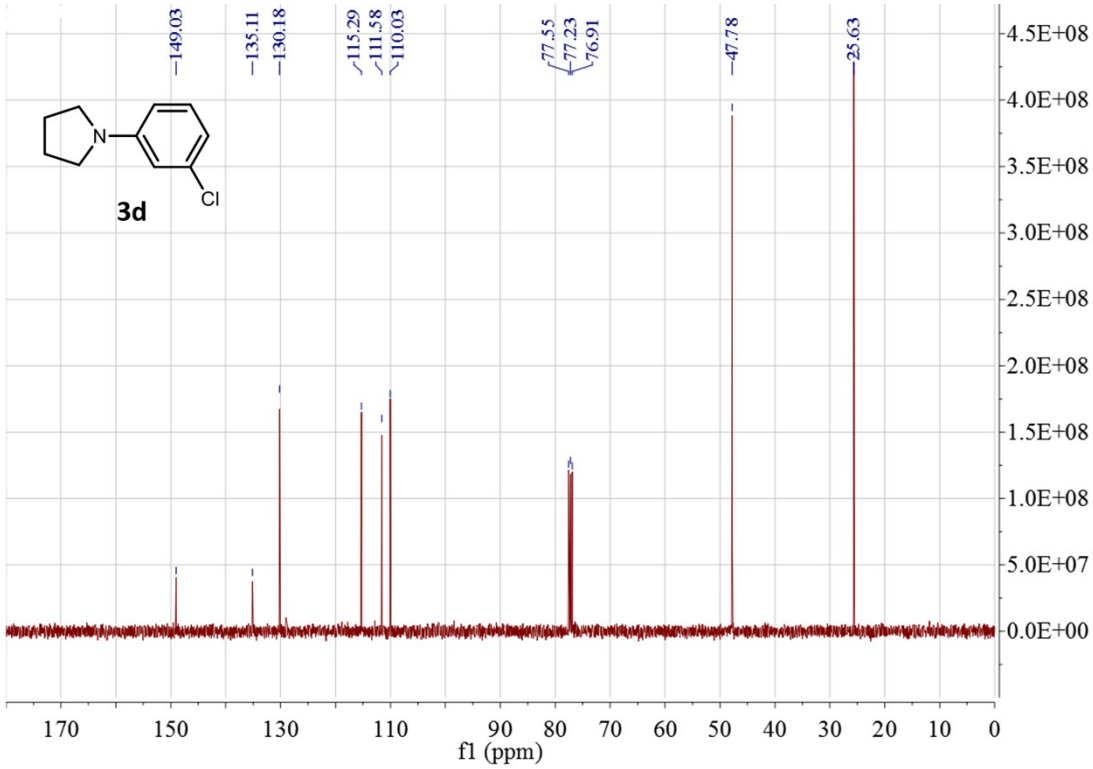
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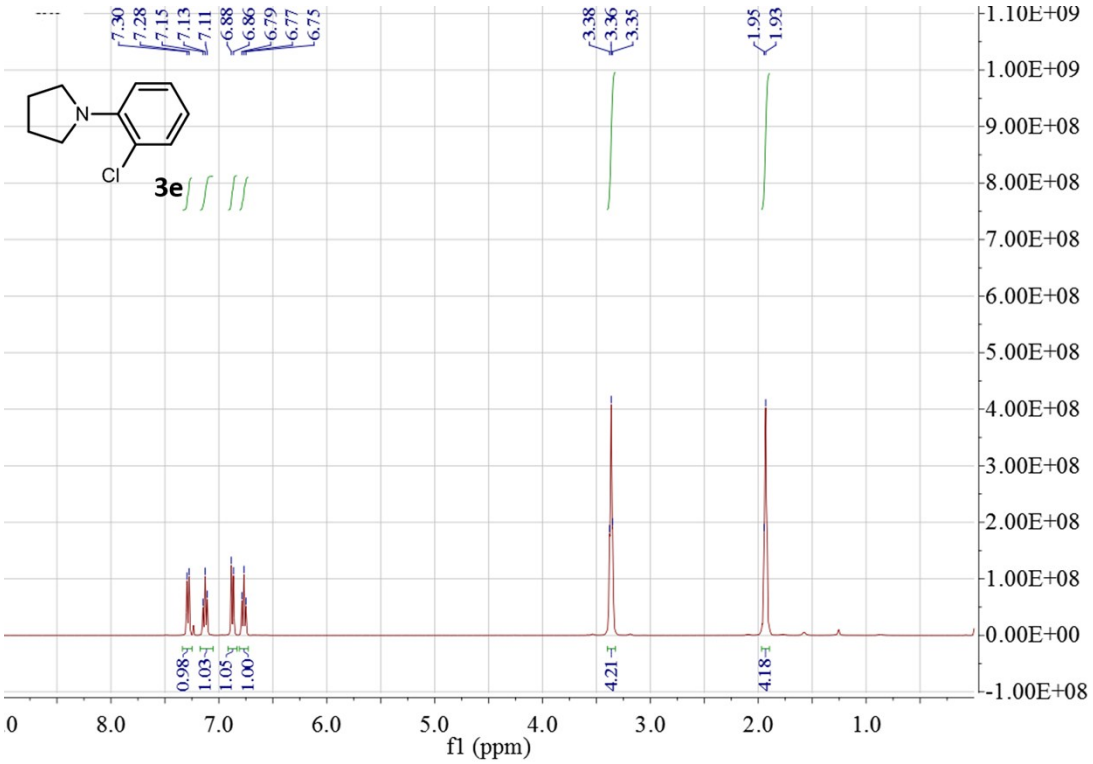
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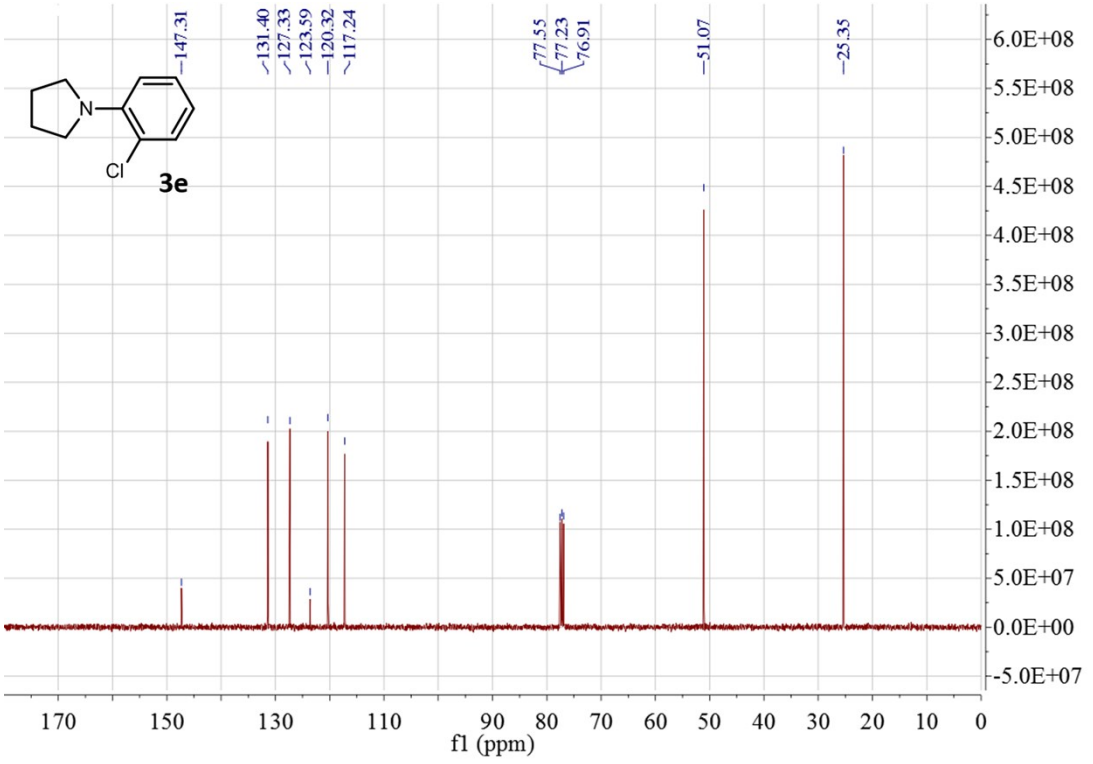
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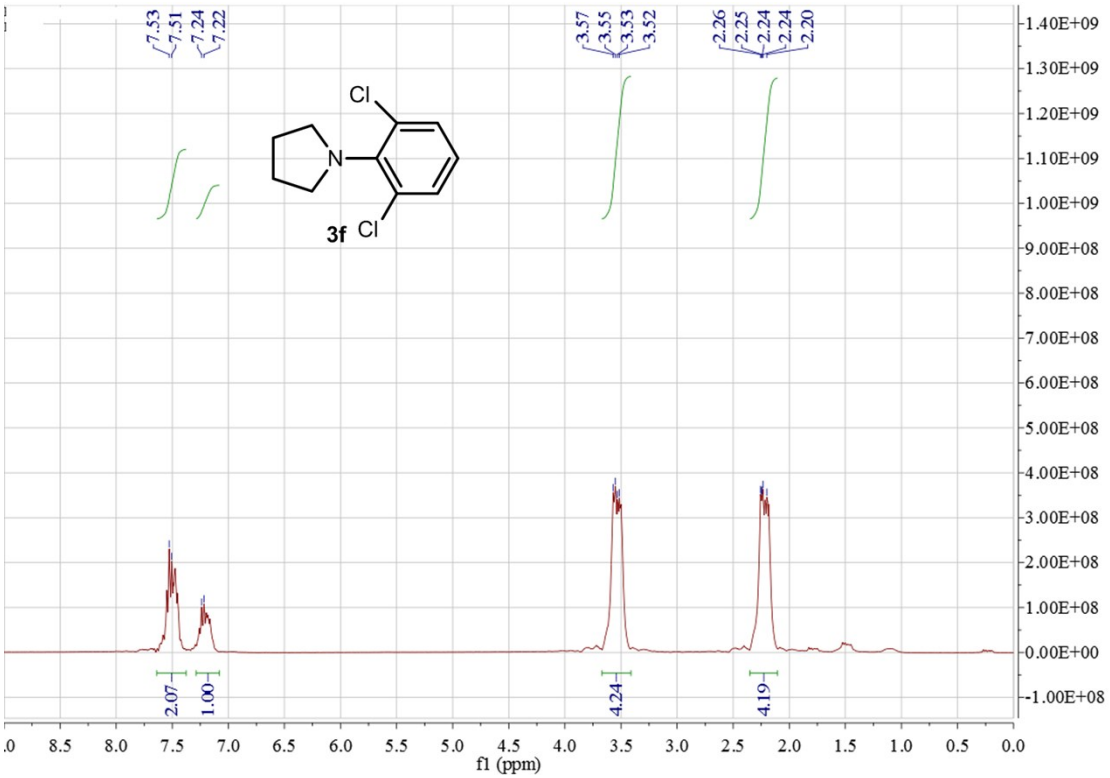
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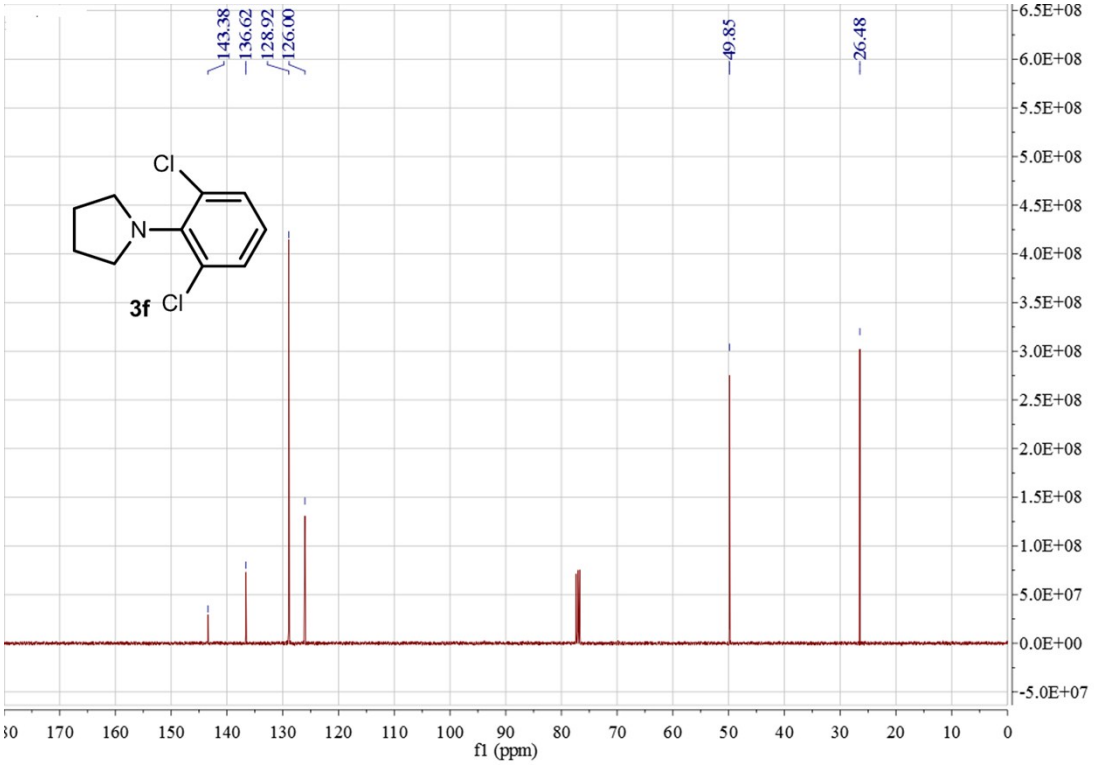
f1 (ppm)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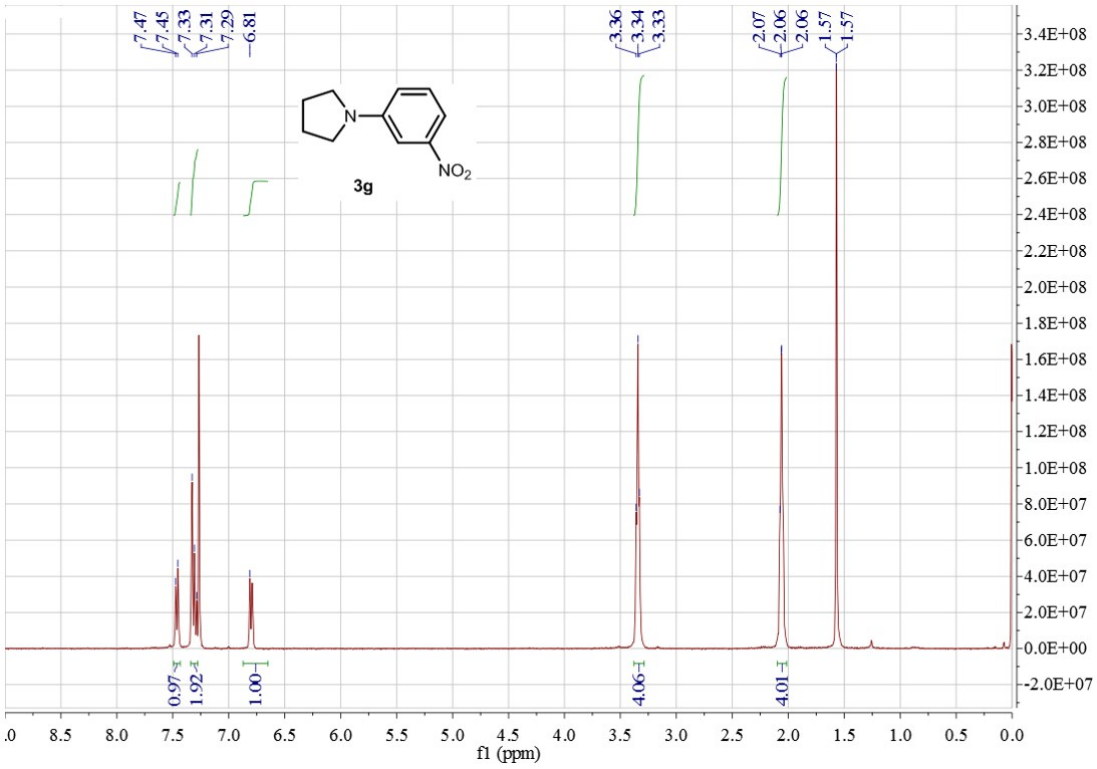
Cl
3f
f1 (ppm)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7.33
7.31
7.29
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3.36
3.34
3.33
2.07
2.06
2.06
1.57
1.57
N
NO2
3g
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1.92
1.00
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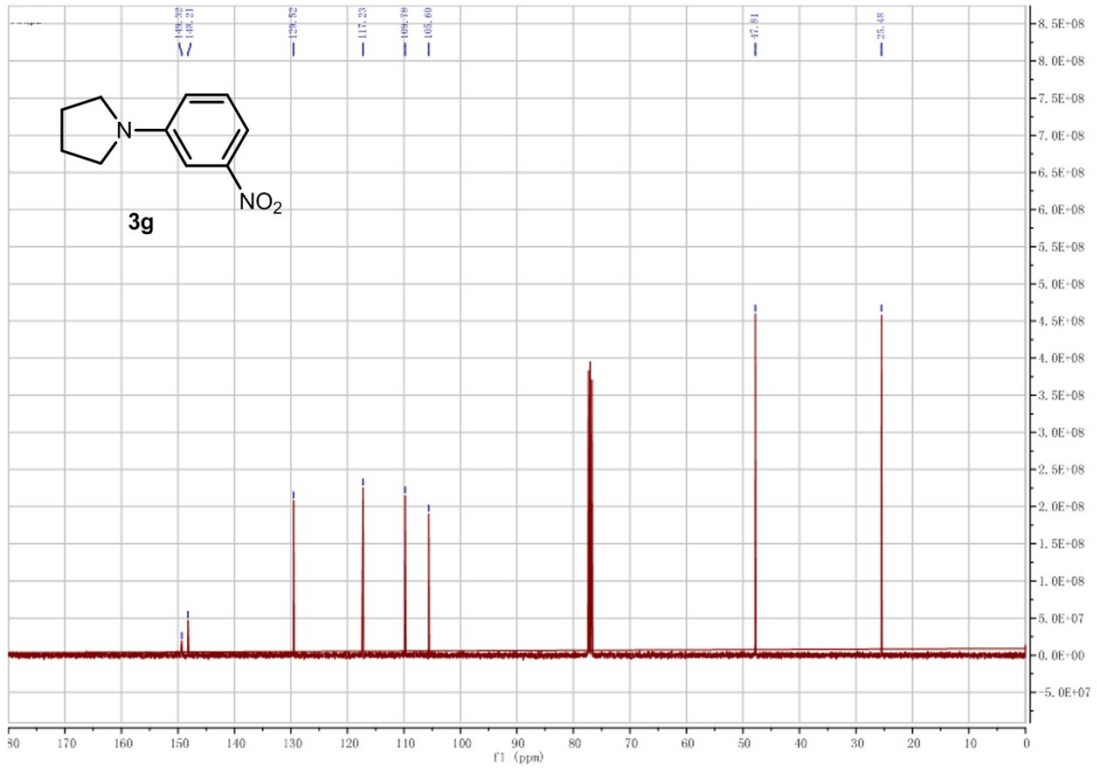
4.01
f1 (ppm)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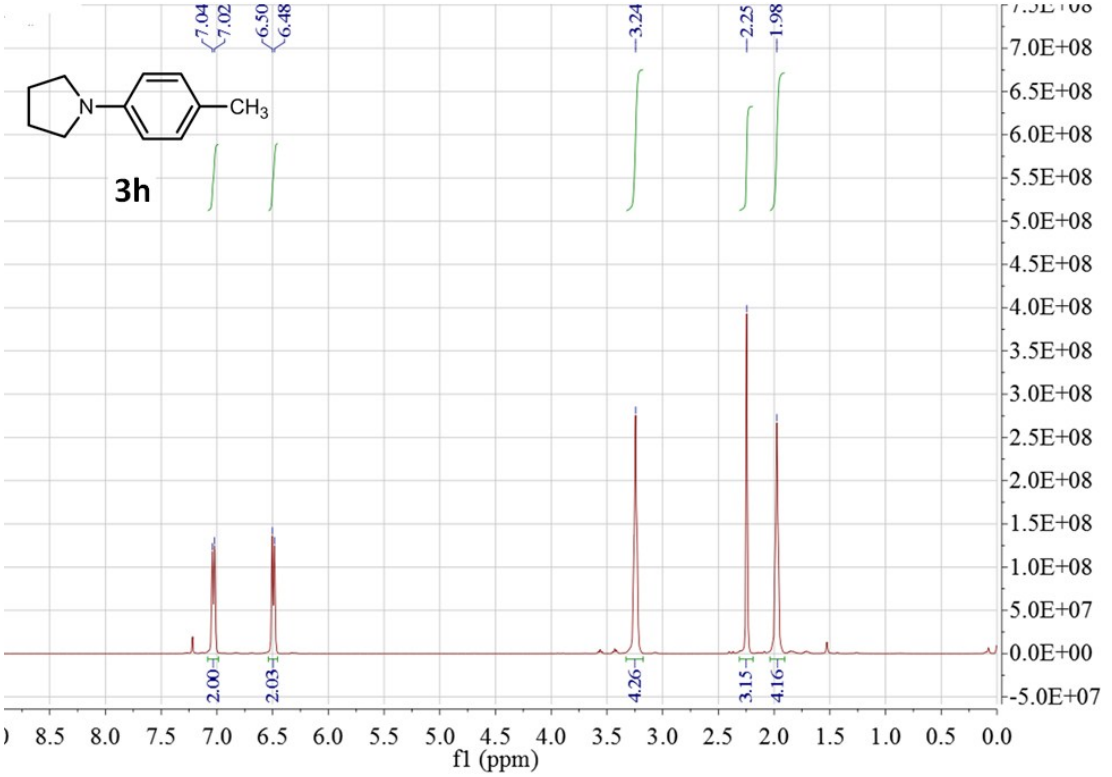
NO2
3g
f1 (ppm)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7.02
6.50
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3h
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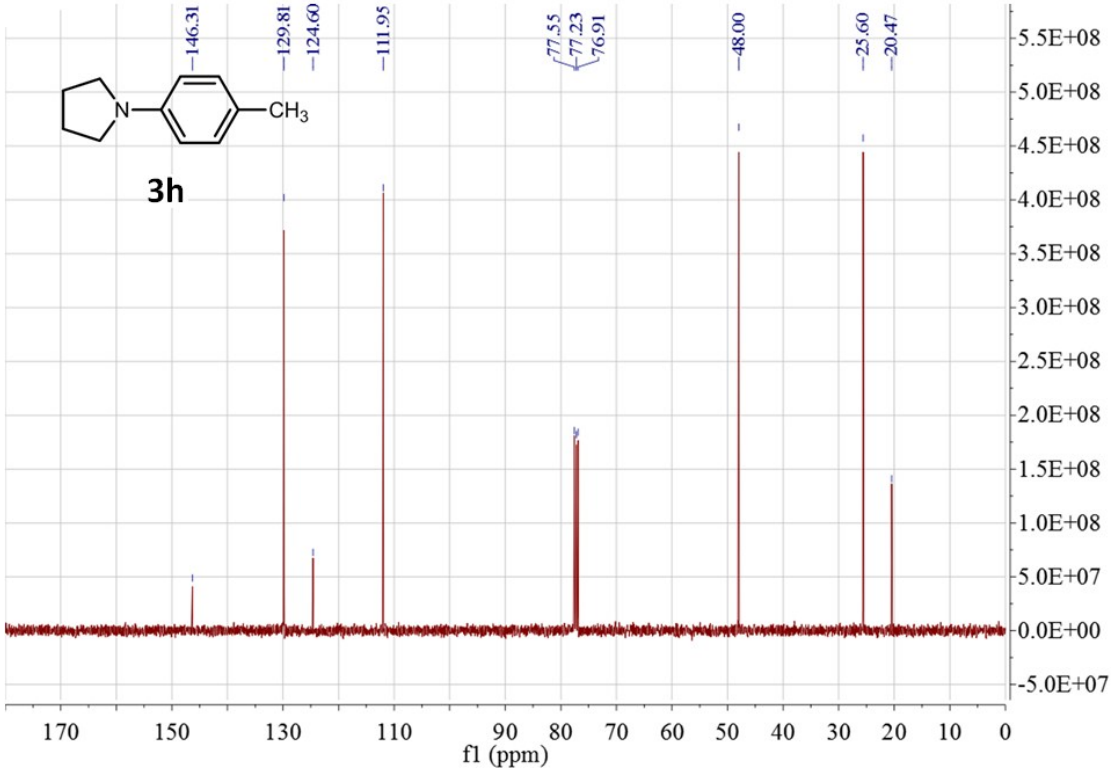
3.15
4.16
f1 (ppm)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48.00
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20.47
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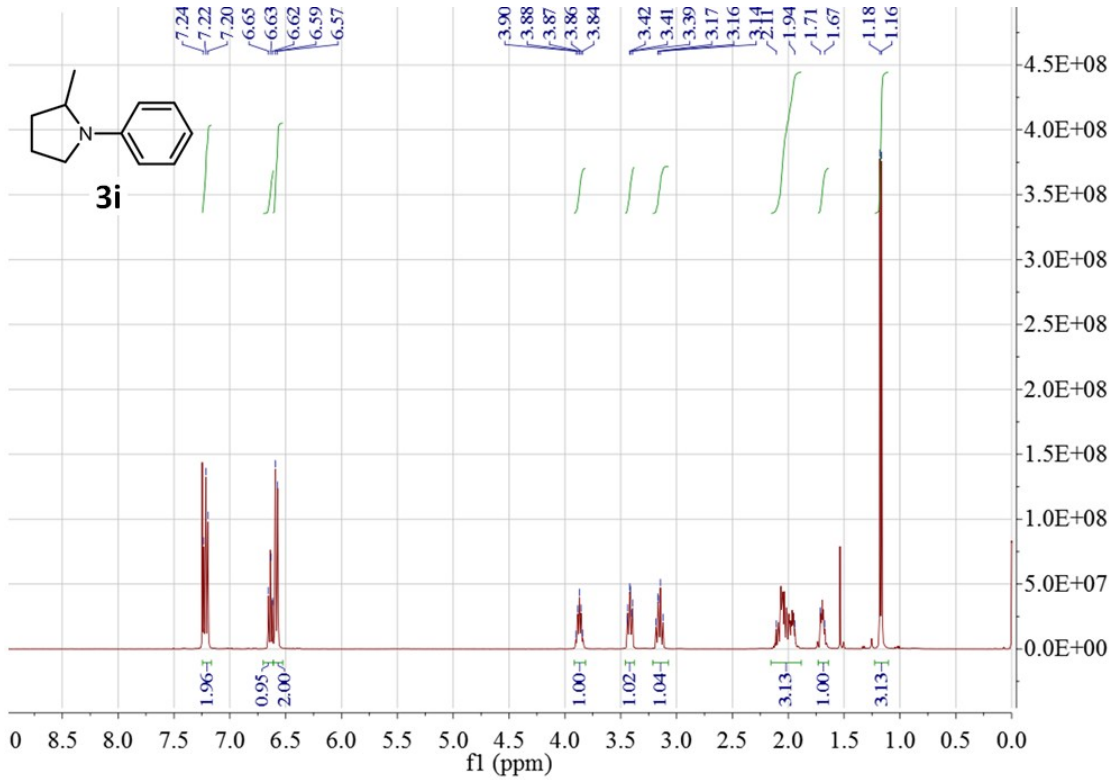
CH3
3h
f1 (ppm)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7.20
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6.62
6.59
6.57
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3.88
3.87
3.86
3.84
3.42
3.41
3.39
3.17
3.16
3.14
2.11
1.94
1.71
1.67
1.18
1.16
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0.95
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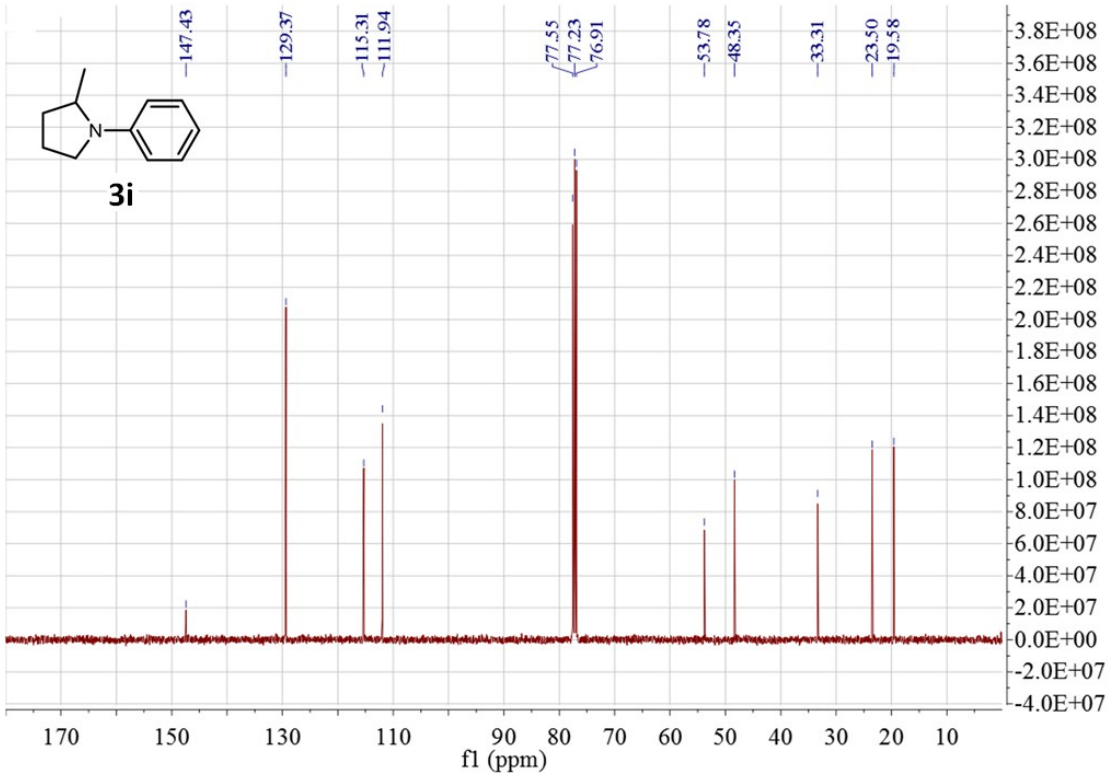
1.00
1.02
1.04
3.13
1.00
3.13
f1 (ppm)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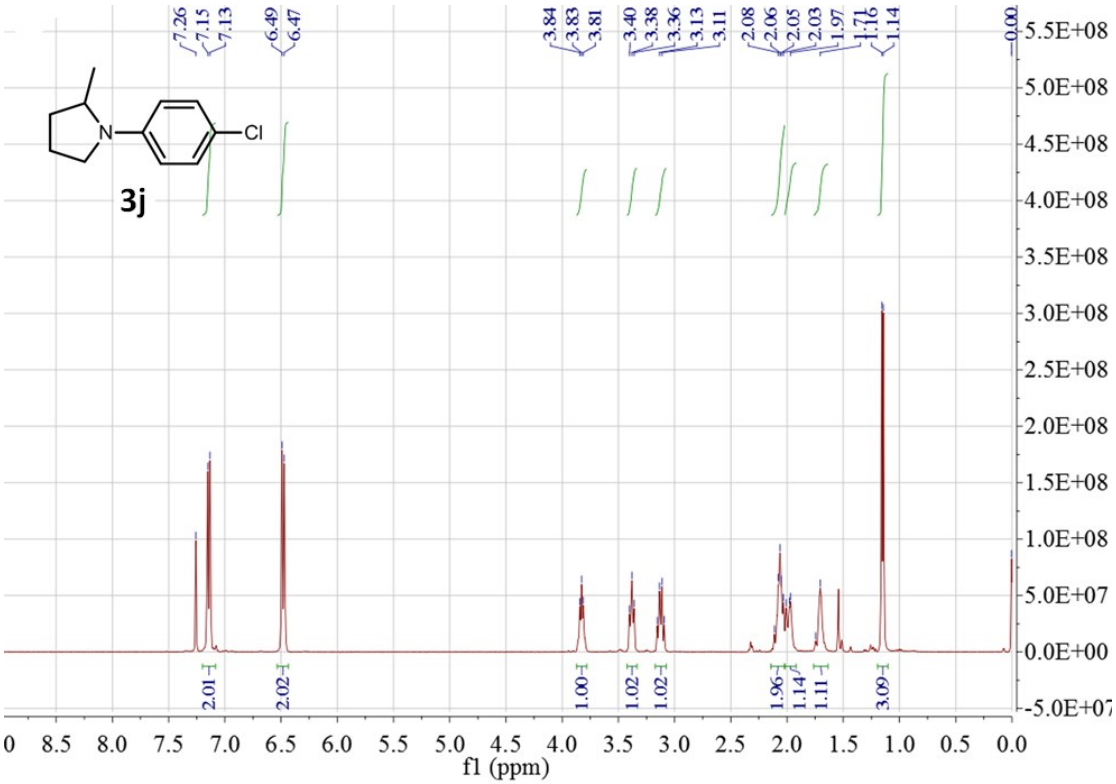
f1 (ppm)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7.15
7.13
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6.47
3.84
3.83
3.81
3.40
3.38
3.36
3.13
3.11
2.08
2.06
2.05
2.03
1.97
1.71
1.16
1.14
0.00
N
Cl
3j
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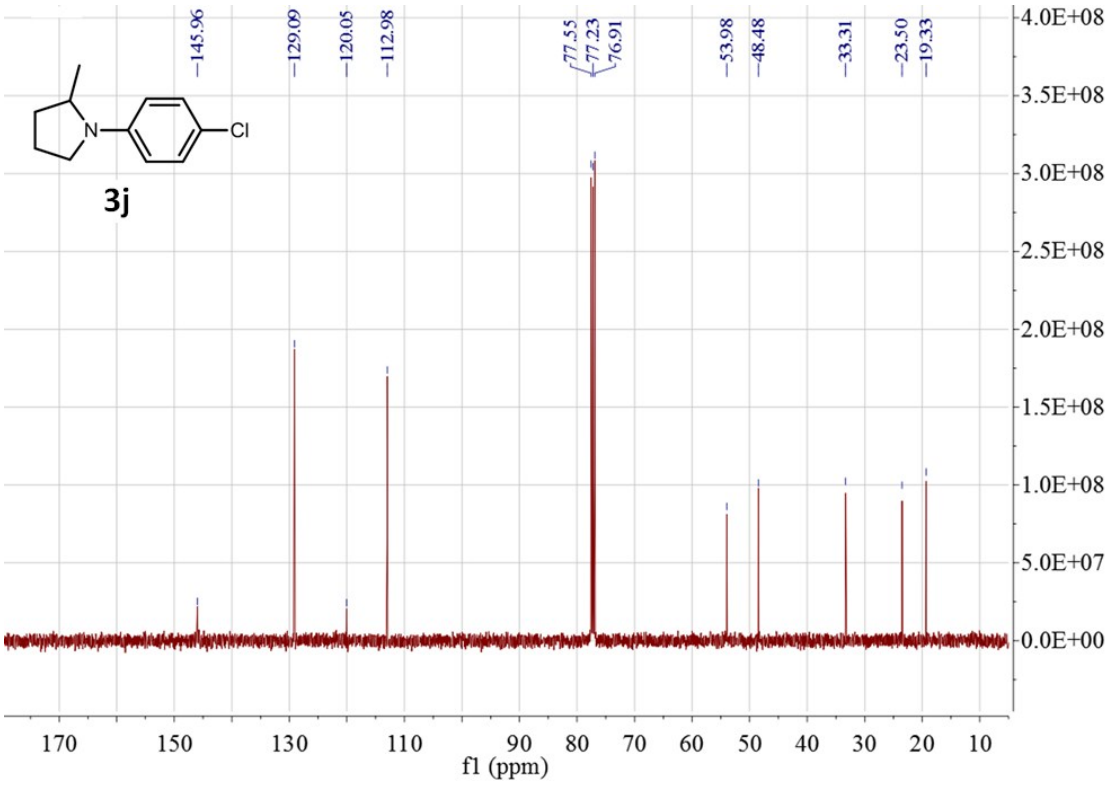
2.02
1.00
1.02
1.02
1.96
1.14
1.11
3.09
f1 (ppm)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120.05
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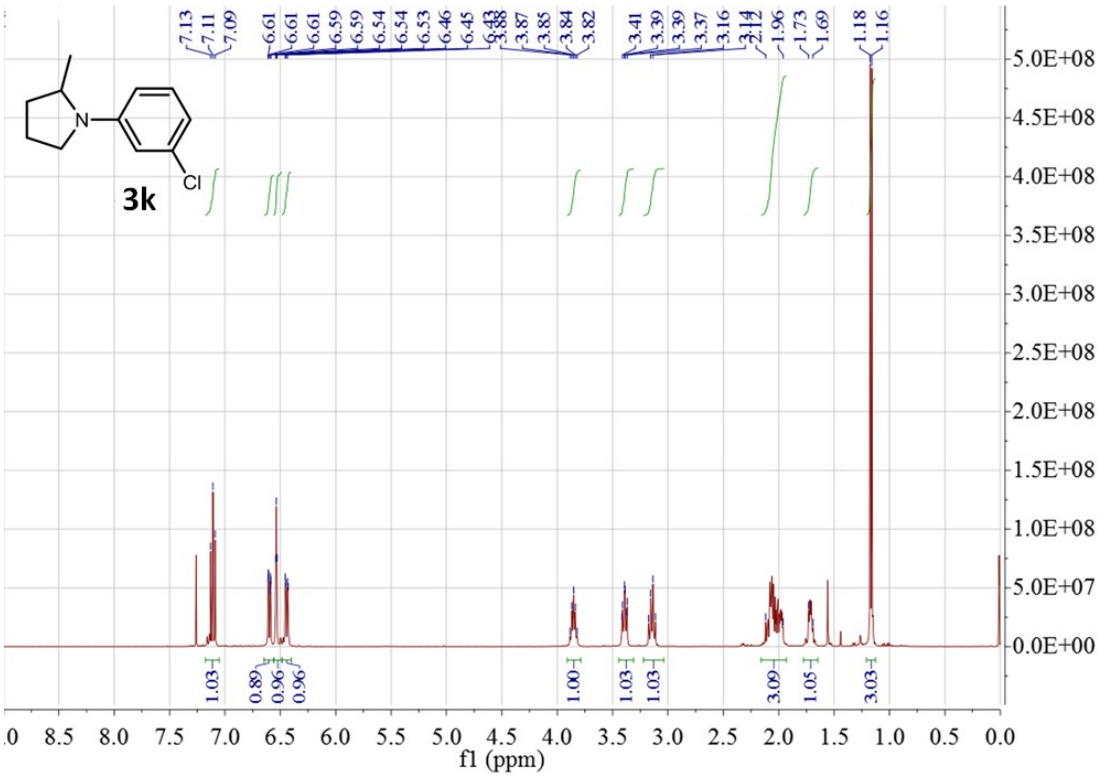
76.91
53.98
48.48
33.31
23.50
19.33
N
Cl
3j
f1 (ppm)


3k
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7.11
7.09
6.61
6.61
6.61
6.59
6.59
6.54
6.54
6.53
6.46
6.45
3.87
3.85
3.84
3.82
3.41
3.39
3.39
3.37
3.16
1.96
1.73
1.69
1.18
1.16
1.03
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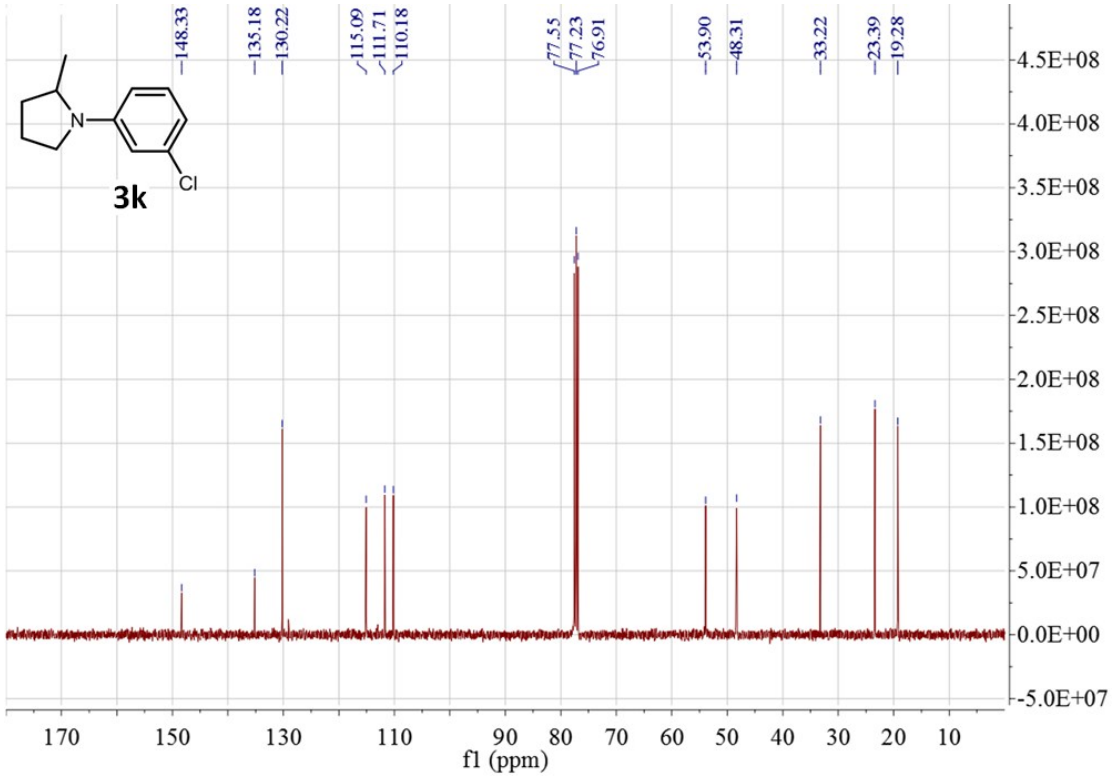
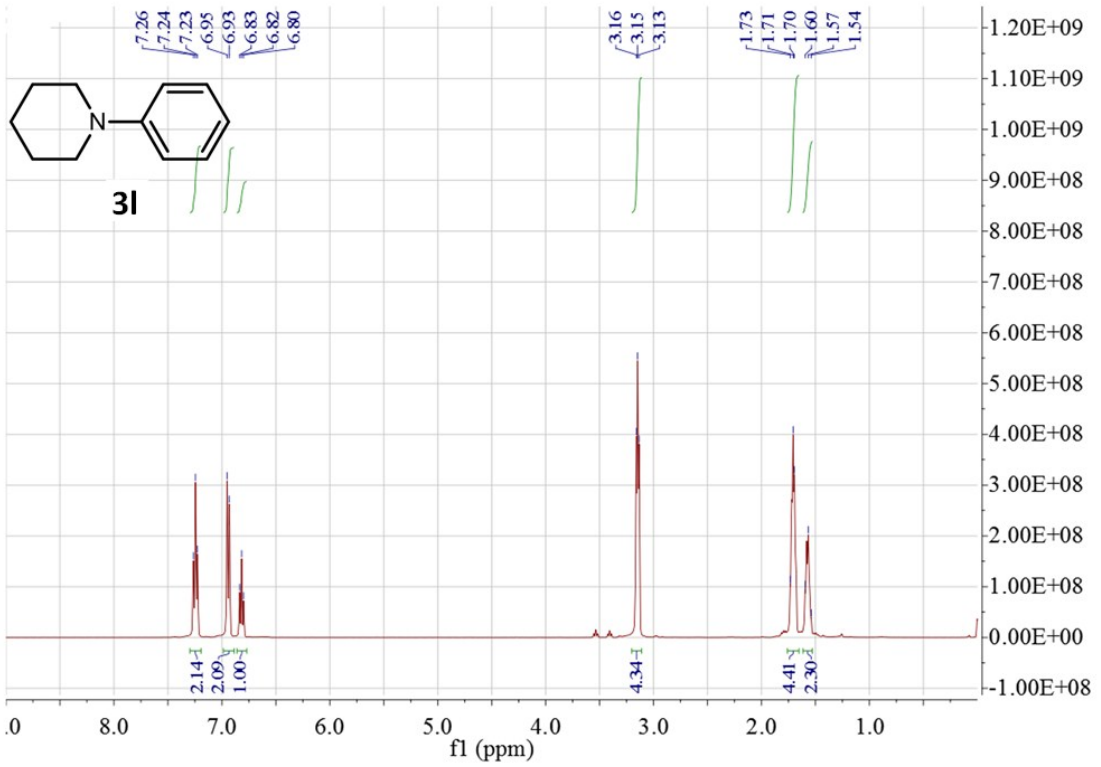
0.96
0.96
1.00
1.03
1.03
3.09
1.05
3.03
f1 (ppm)


3k
148.33
135.18
130.22
115.09
111.71
110.18
77.55
77.23
76.91
53.90
48.31
33.22
23.39
19.28
f1 (ppm)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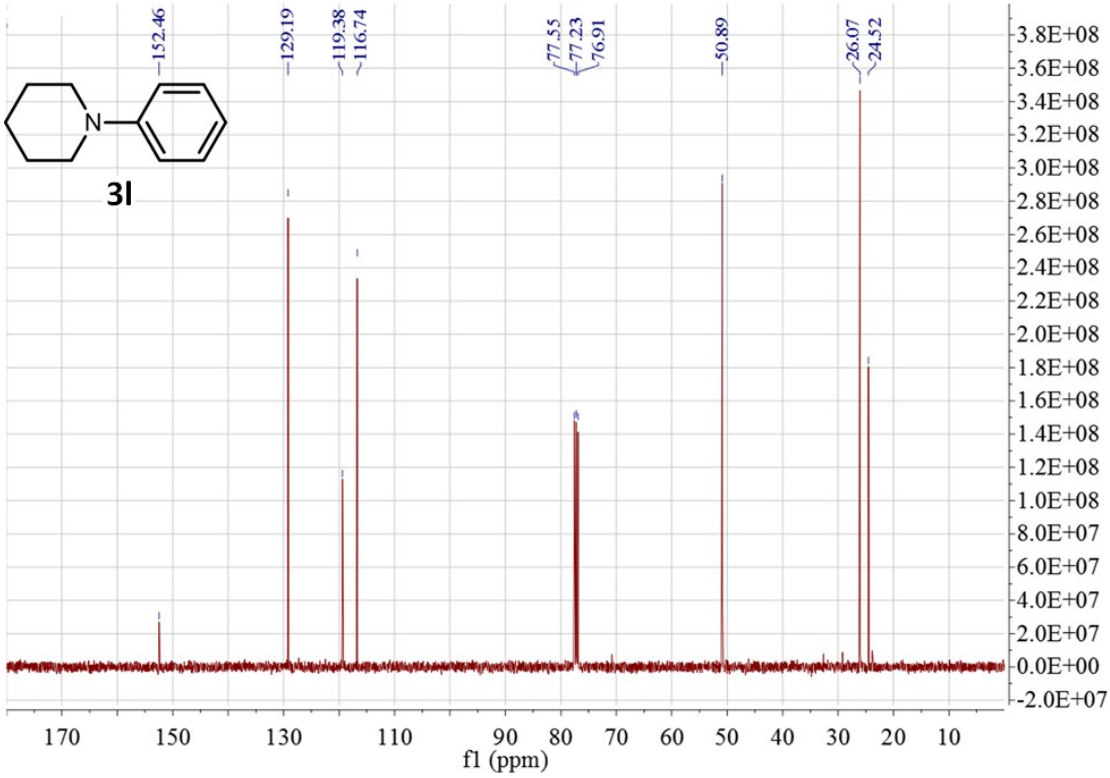
7.24
7.23
6.95
6.93
6.83
6.82
6.80
3.16
3.15
3.13
1.73
1.71
1.70
1.60
1.57
1.54
3l
2.14
2.09
1.00
4.34
4.41
2.30
f1 (ppm)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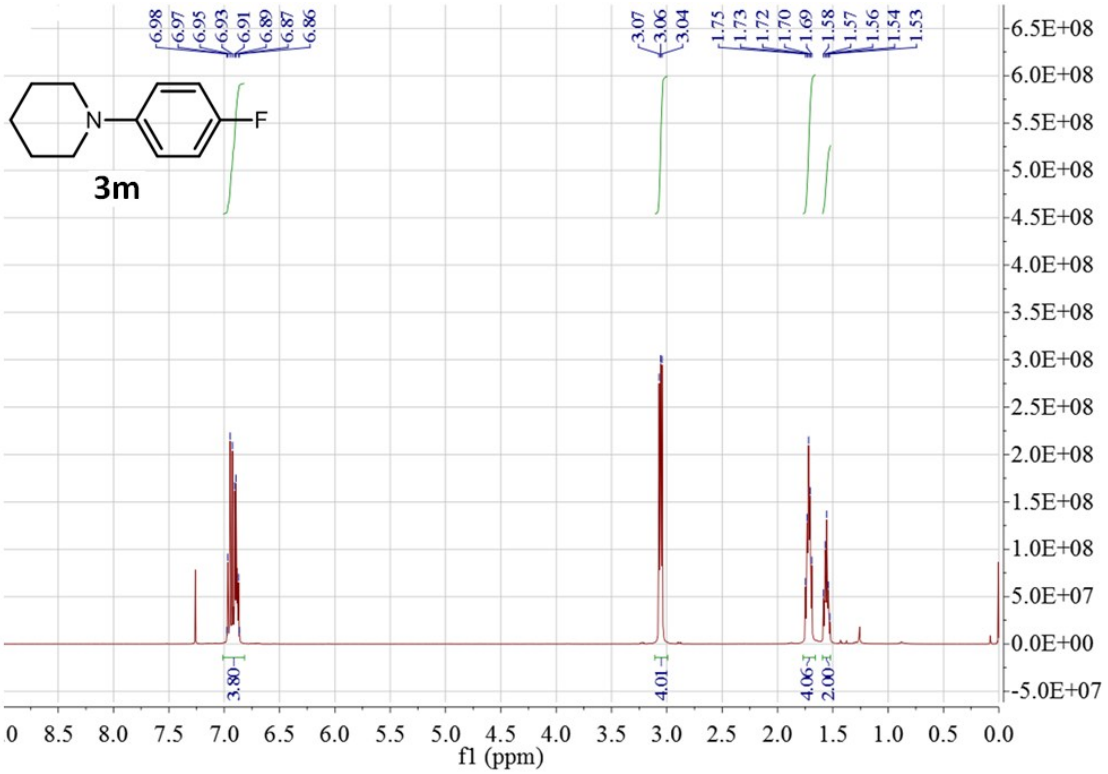
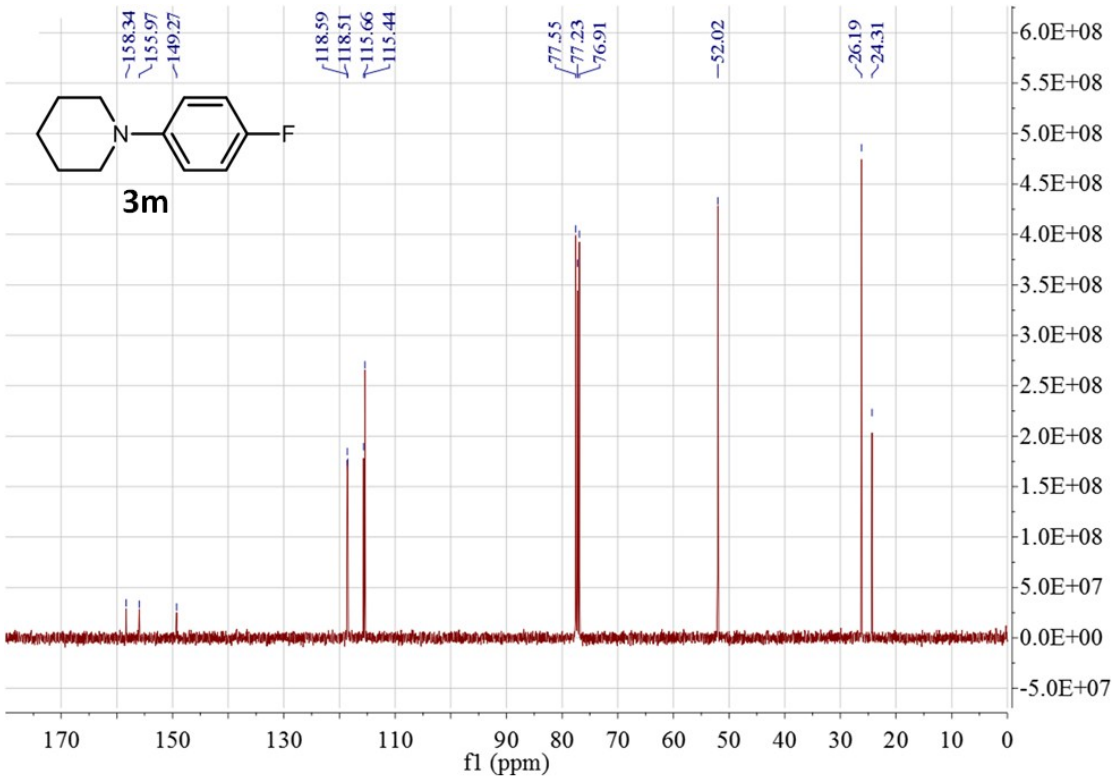
116.74
77.55
77.23
76.91
50.89
26.07
24.52
3l
f1 (ppm)


6.98
6.97
6.95
6.93
6.91
6.89
6.87
6.86
3.07
3.06
3.04
1.75
1.73
1.72
1.70
1.69
1.58
1.57
1.56
1.54
1.53
N
F
3m
3.80
4.01
4.06
2.00
f1 (ppm)


158.34
155.97
149.27
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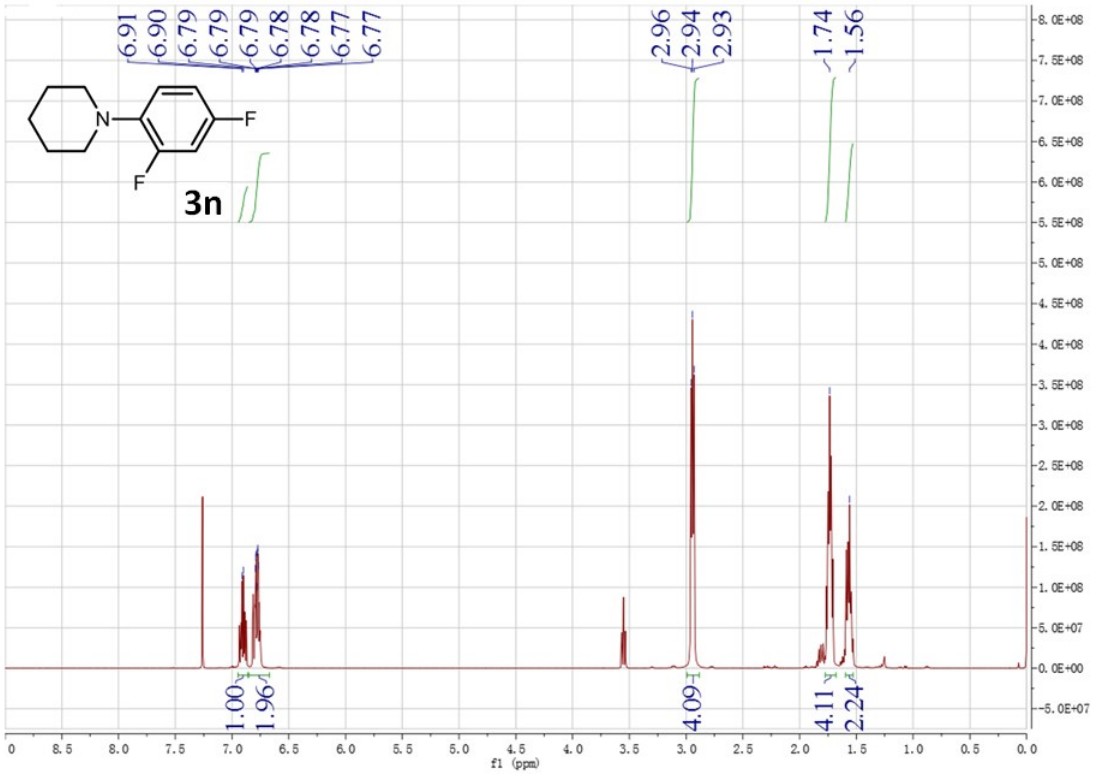
76.91
52.02
26.19
24.31
N
F
3m
f1 (ppm)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6.90
6.79
6.79
6.79
6.78
6.78
6.77
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2.94
2.93
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1.56
N
F
F
3n
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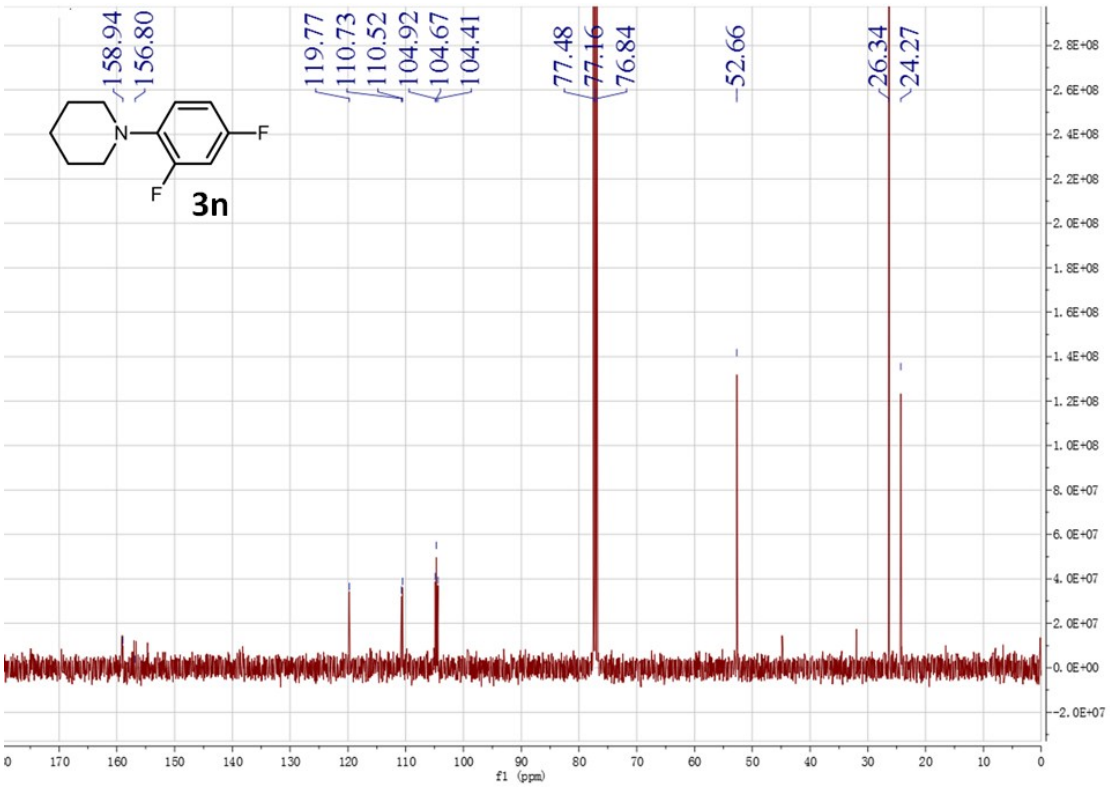
1.96
4.09
4.11
2.24
f1 (ppm)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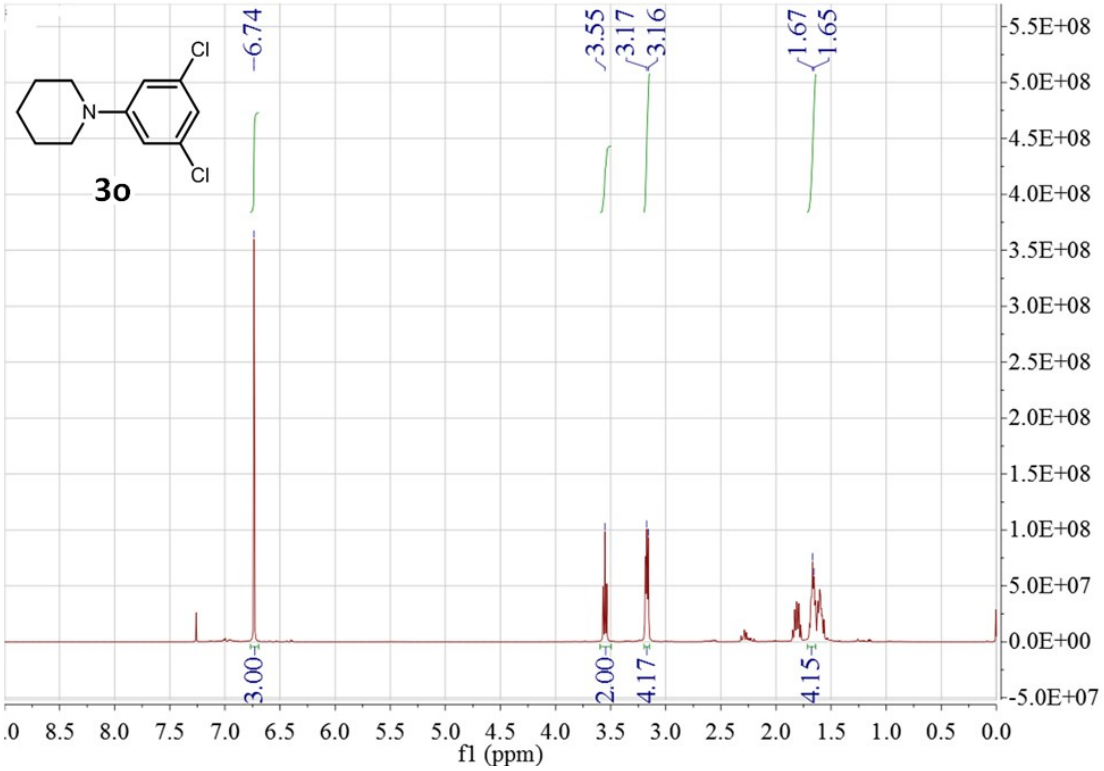
104.41
77.48
77.16
76.84
52.66
26.34
24.27
N
F
F
3n
f1 (ppm)


Cl
N
Cl
3o
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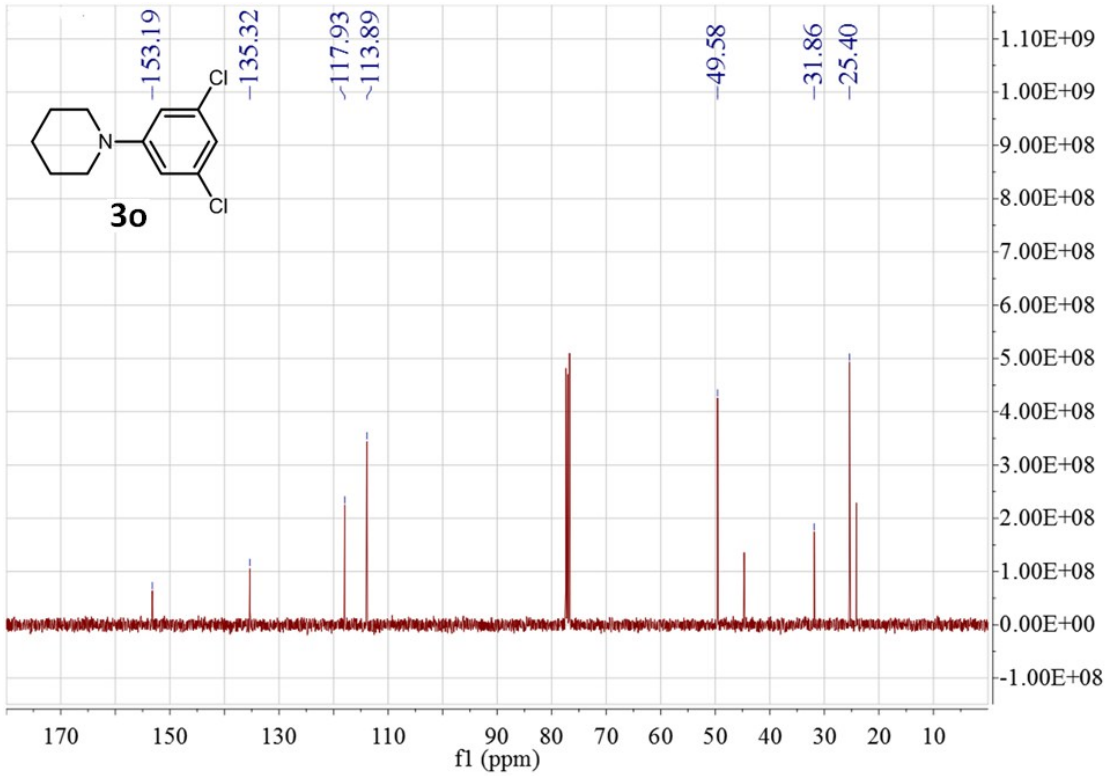
3.55
3.17
3.16
1.67
1.65
3.00
2.00
4.17
4.15
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Cl
N
Cl
3o
153.19
135.32
117.93
113.89
49.58
31.86
25.40
1.10E+09
1.00E+09
9.00E+08
8.00E+08
7.00E+08
6.00E+08
5.00E+08
4.00E+08
3.00E+08
2.00E+08
1.00E+08
0.00E+00
-1.00E+08
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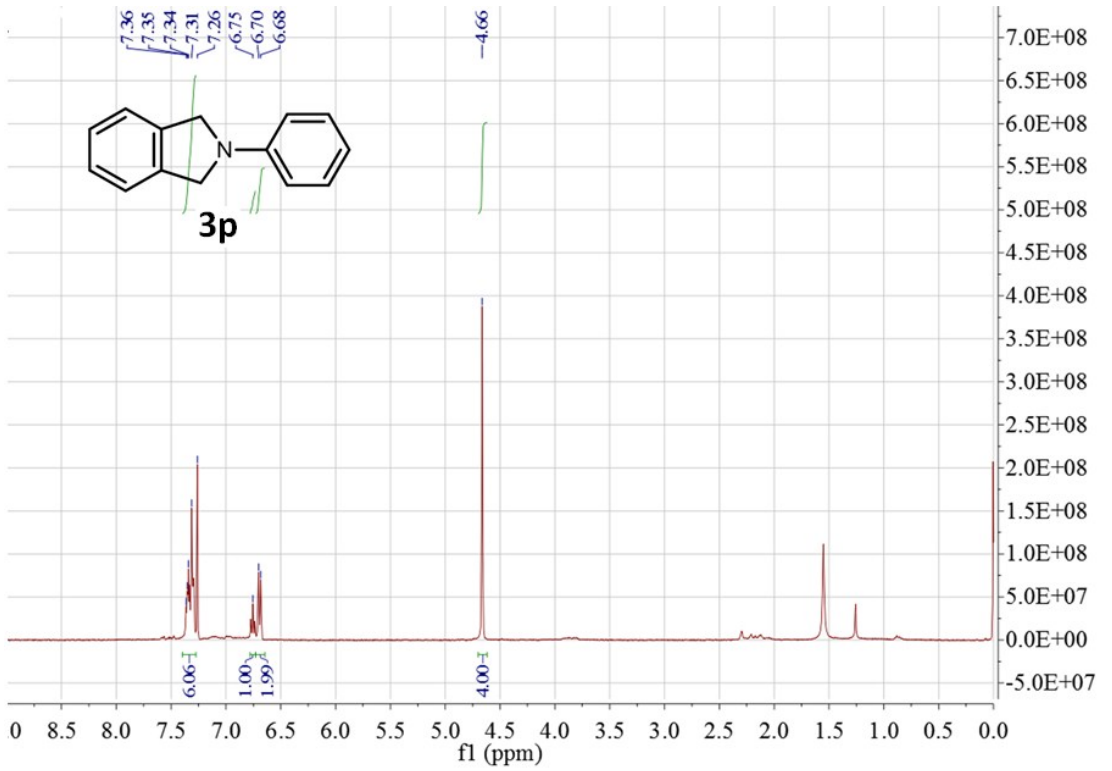
f1 (ppm)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7.35
7.34
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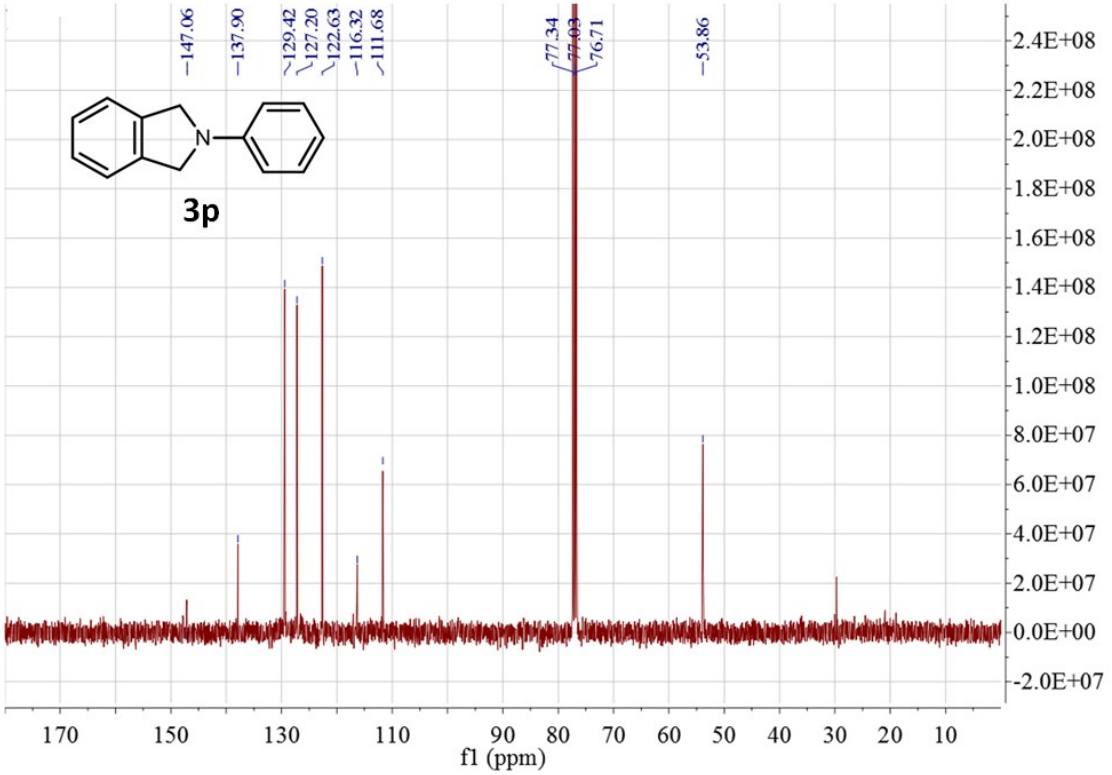
6.70
6.68
4.66
3p
6.06
1.00
1.99
4.00
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.06
137.90
129.42
127.20
122.63
116.32
111.68
77.34
77.03
76.71
53.86
3p
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
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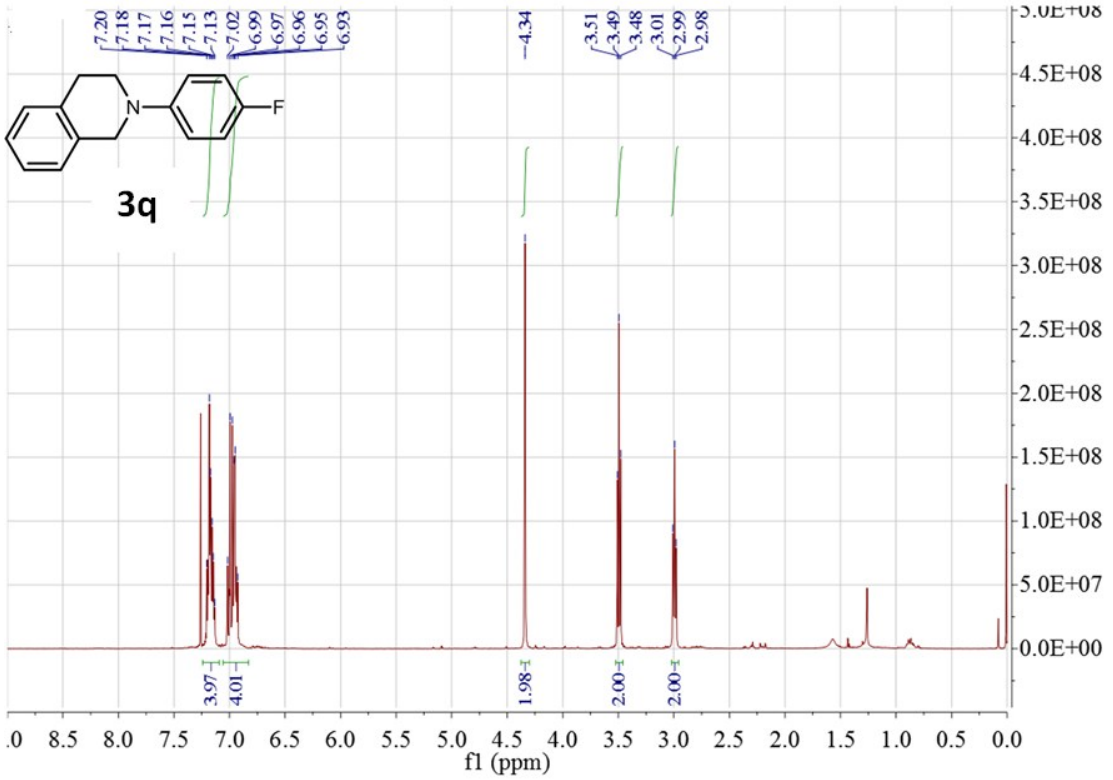
-2.0E+07
170 150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.20
7.18
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7.16
7.15
7.13
7.02
6.99
6.97
6.96
6.95
6.93
4.34
3.51
3.49
3.48
3.01
2.99
2.98
N
F
3q
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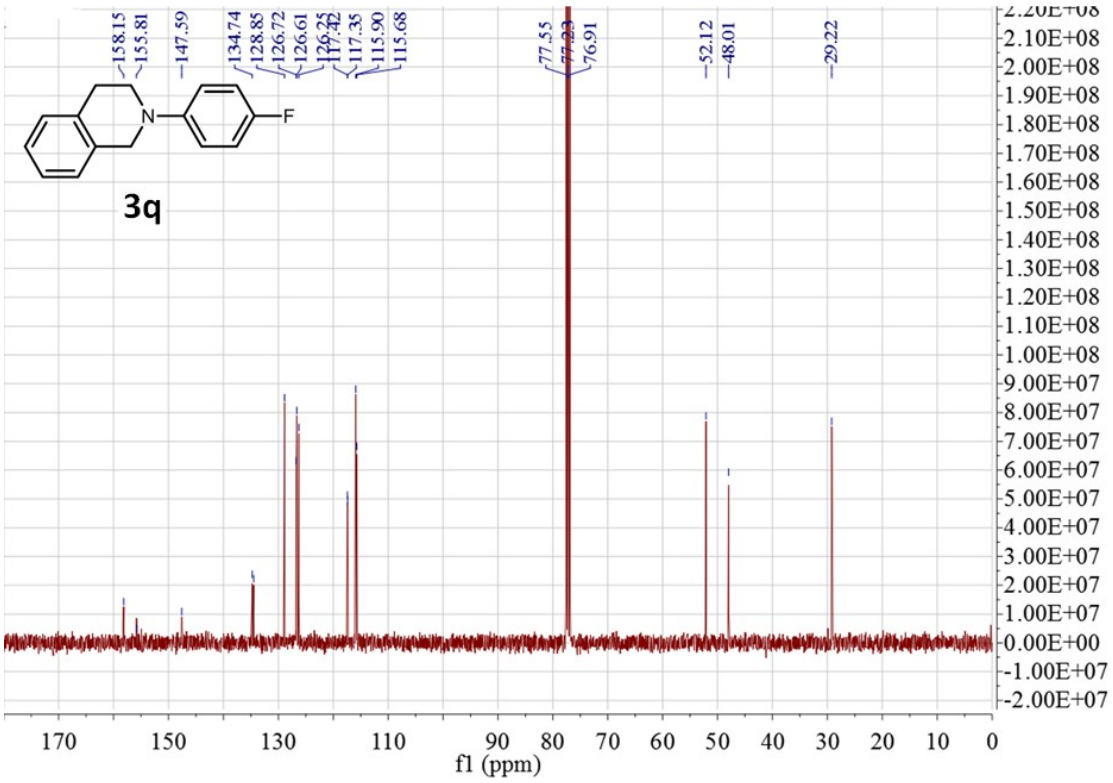
4.01
1.98
2.00
2.00
f1 (ppm)


158.15
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126.25
117.42
117.35
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77.55
76.91
52.12
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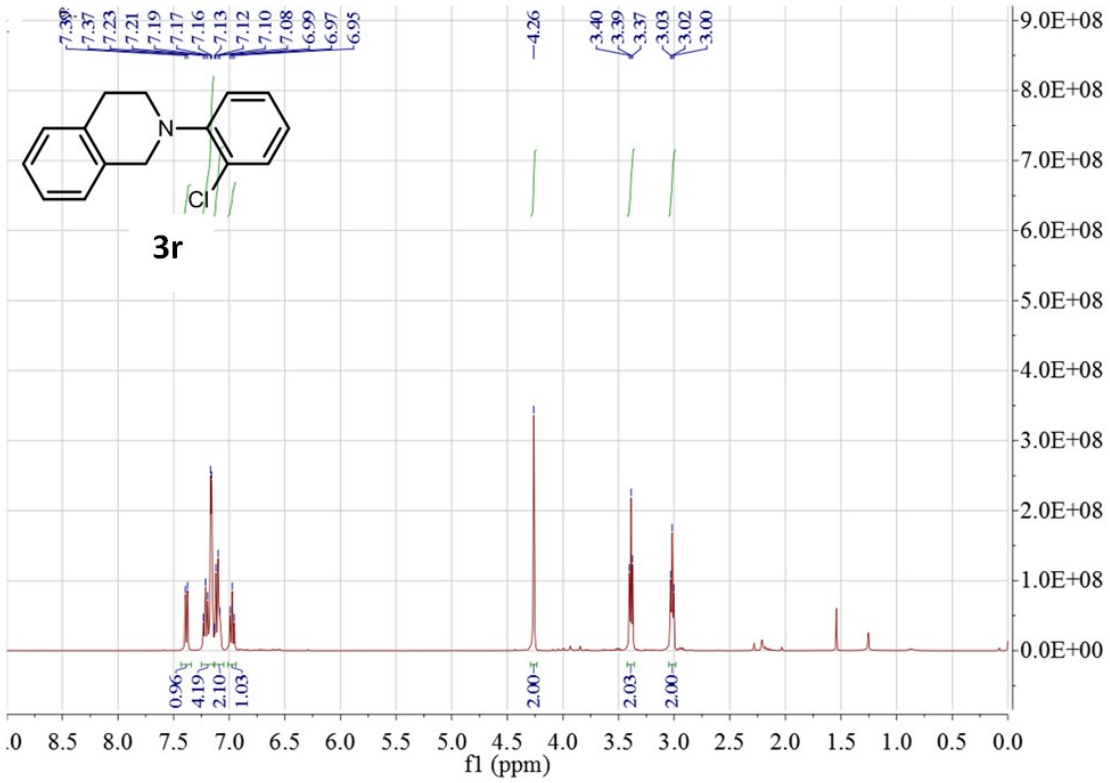
29.22
N
F
3q
f1 (ppm)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7.19
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7.13
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6.99
6.97
6.95
4.26
3.40
3.39
3.37
3.03
3.02
3.00
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Cl
3r
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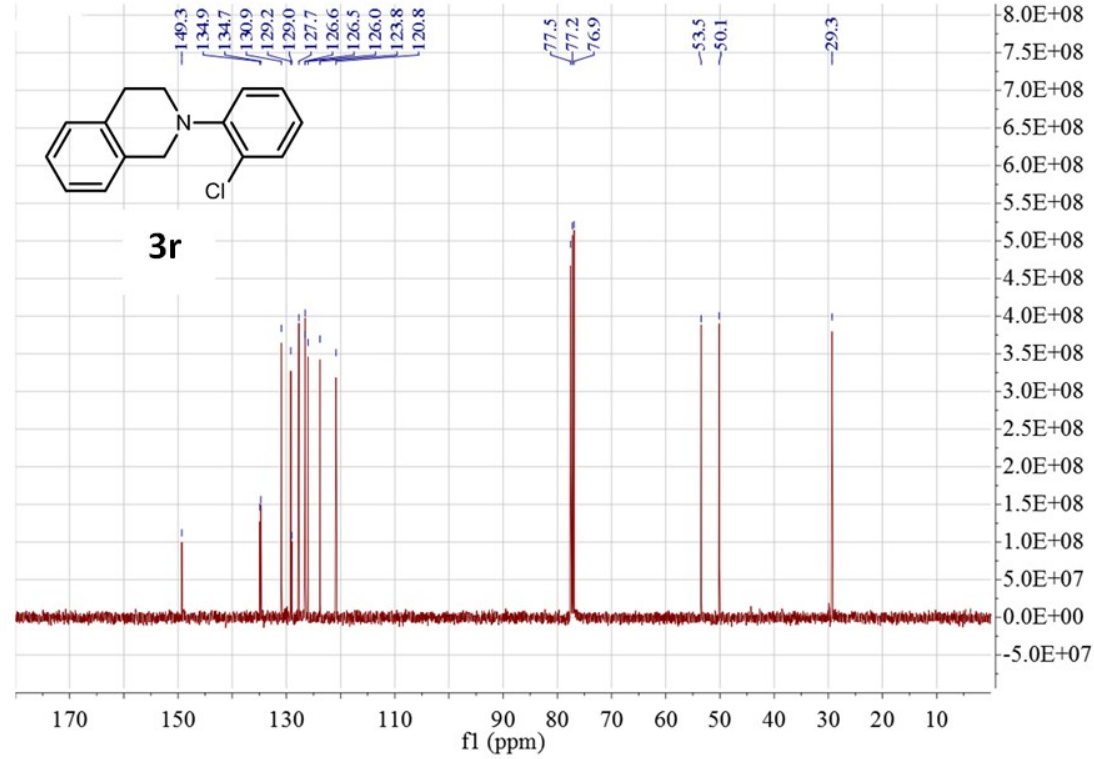
4.19
2.10
1.03
2.00
2.03
2.00
f1 (ppm)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134.7
130.9
129.2
129.0
127.7
126.6
126.5
126.0
123.8
120.8
77.5
77.2
76.9
53.5
50.1
29.3
N
Cl
3r
f1 (ppm)

Kinetic experiments

The reaction of 4-fluoroaniline with THF was selected in the kinetic study for the simplification of NMR. Diphenylmethane was added into the reaction mixture as an internal standard for integral. To a solution of 0.13 mL (1.2 mmol) of $TiCl_4$ in 8 mL of dry toluene was added 0.10 mL (1.0 mmol) of 4-fluoroaniline. The mixture was stirred at room temperature for 0.5 h and 2.0 mL (20 mmol) of THF was added to gain a condition of pseudo-first order reaction. The well-mixed solution was then divided into four portions for parallel experiments that were terminated after 1 h, 2 h, 3 h and 4 h respectively. After refluxing for a certain period of time, the solution was quenched with saturated $NaHCO_3$ solution, extracted with dichloromethane and dried over Na_2SO_4, and the solvent was removed under reduced pressure. Proton spectra were obtained under consistent conditions and the integral of the signals at 6.95 and 6.48 ppm were adopted to measure the amount of unreacted 4-fluoroaniline, using diphenylmethane as the internal standard for integral. The concentration of 4-fluoroaniline at different reaction time were listed in Table S1 and the data were used to gain the first order rate constant (Figure S1).

Table S1.

Time (h)	1	2	3	4
Concentration (mol/L)	0.081	0.066	0.059	0.046

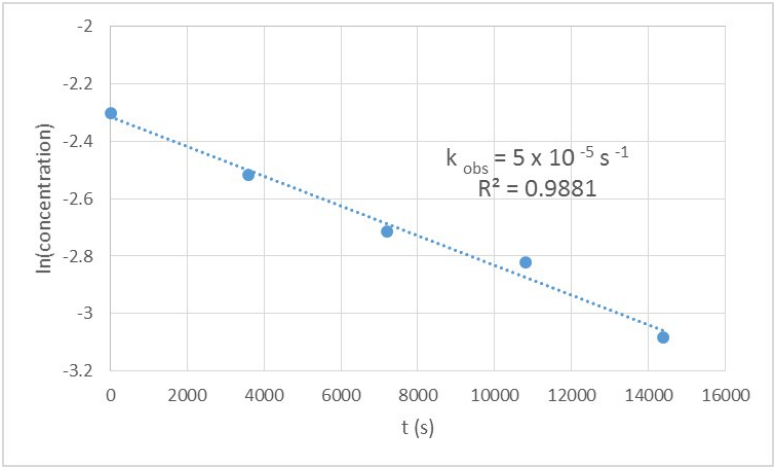
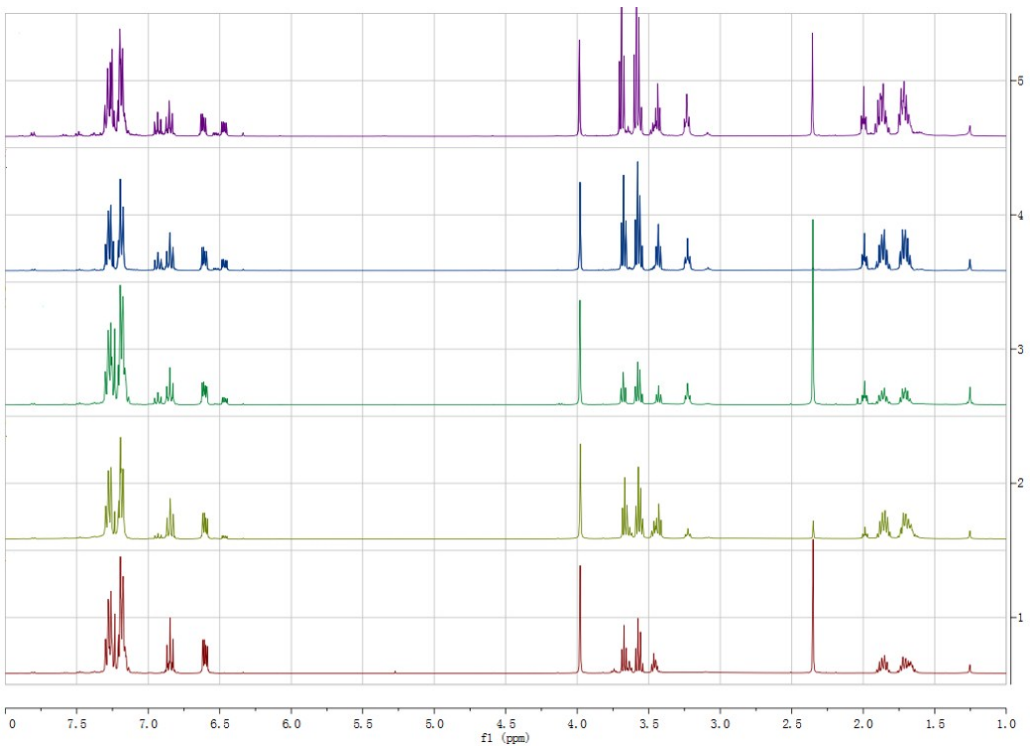


Figure S1. Change of 4-fluoroaniline concentration over time.

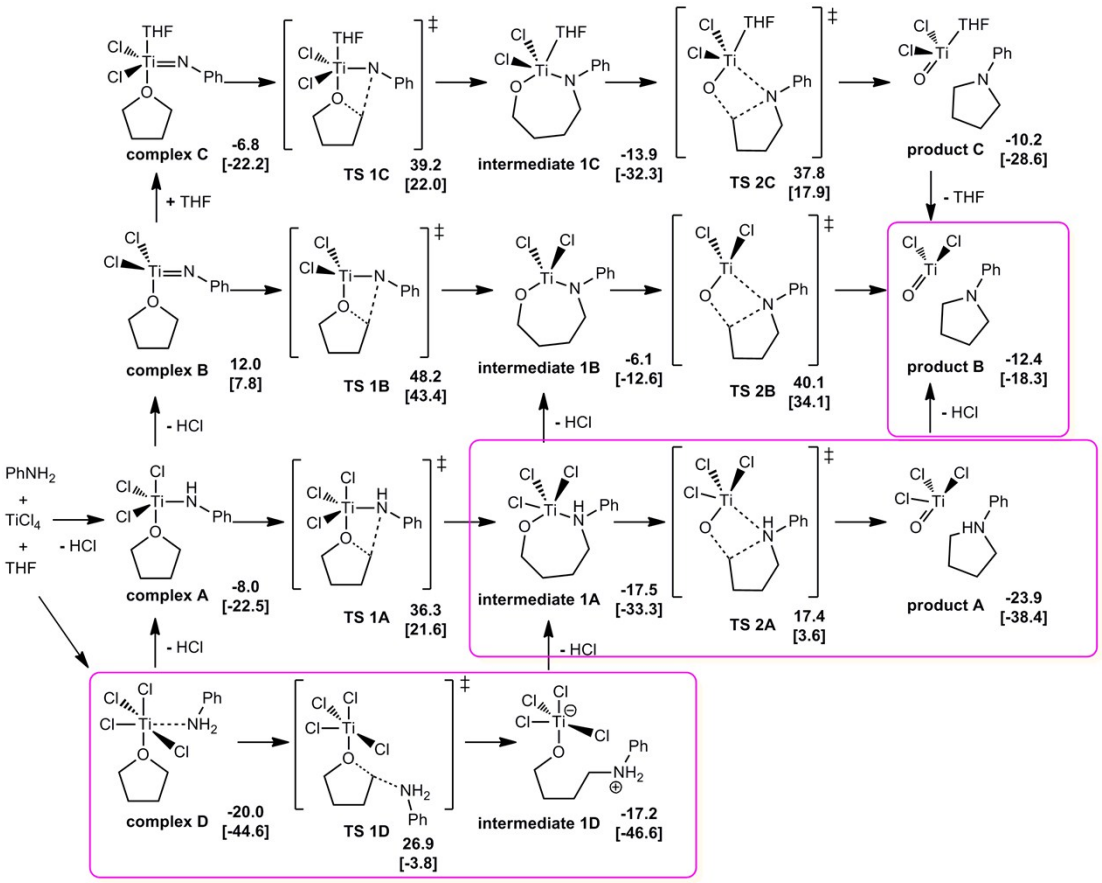

5
4
3
2
1
0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

Computational Details

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

Full geometrical optimizations were carried out using Gaussian 09 suite of programs, employing the Minnesota density functional M06. The 6-31+G** basis set was used on nonmetallic atoms while the SDD basis set was employed on Ti. The solvent effect was dealt with using conductor-like polarizable continuum model (CPCM) in toluene. Frequency calculations were performed at the same level to identify all of the stationary points as minima (zero imaginary frequency) or transition states (one imaginary frequency) and intrinsic reaction coordinates (IRC) were calculated for each transition state to confirm that the structure indeed connects the two relevant minima.

Cartesian coordinates and energetics for all stationary points are given below.



$TiCl_4$

Zero-point correction=	0.005671
(Hartree/Particle)	
Thermal correction to Energy=	0.012978
Thermal correction to Enthalpy=	0.013922
Thermal correction to Gibbs Free Energy=	-0.027445
Sum of electronic and zero-point Energies=	-1899.235308
Sum of electronic and thermal Energies=	-1899.228001
Sum of electronic and thermal Enthalpies=	-1899.227057
Sum of electronic and thermal Free Energies=	-1899.268424

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	8.144	20.869	87.064

Ti	0.00000	0.00000	0.00000
Cl	0.00000	1.76958	1.24876
Cl	1.76958	0.00000	-1.24876
Cl	-1.76958	0.00000	-1.24876
Cl	0.00000	-1.76958	1.24876

Aniline

Zero-point correction=	0.116880
(Hartree/Particle)	
Thermal correction to Energy=	0.122696
Thermal correction to Enthalpy=	0.123640
Thermal correction to Gibbs Free Energy=	0.087731
Sum of electronic and zero-point Energies=	-287.267089
Sum of electronic and thermal Energies=	-287.261273
Sum of electronic and thermal Enthalpies=	-287.260328
Sum of electronic and thermal Free Energies=	-287.296238

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	76.869	23.261	75.541

C	1.16732	-1.19891	0.00347
C	-0.22126	-1.20472	-0.00574
C	-0.93620	0.00002	-0.01086
C	-0.22122	1.20475	-0.00573
C	1.16736	1.19889	0.00346
C	1.87579	-0.00002	0.00838
H	1.70228	-2.14779	0.00959
H	-0.76789	-2.14848	-0.01226
H	-0.76782	2.14853	-0.01222
H	1.70235	2.14775	0.00958
H	2.96366	-0.00004	0.01741
N	-2.32648	0.00000	-0.07717
H	-2.76899	-0.83617	0.28515
H	-2.76899	0.83622	0.28501

THF

Zero-point correction=	0.116894
(Hartree/Particle)	
Thermal correction to Energy=	0.120947
Thermal correction to Enthalpy=	0.121891
Thermal correction to Gibbs Free Energy=	0.089977
Sum of electronic and zero-point Energies=	-232.170612
Sum of electronic and thermal Energies=	-232.166559
Sum of electronic and thermal Enthalpies=	-232.165615
Sum of electronic and thermal Free Energies=	-232.197528

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	76.045	16.880	71.592

C	-1.15379	-0.41196	0.11000
O	-0.04745	-1.19641	-0.29246
C	1.08621	-0.51429	0.20224
C	0.82477	0.95431	-0.11334
C	-0.70598	1.05643	0.00968
H	-2.00168	-0.66738	-0.53513
H	-1.42906	-0.65967	1.15146
H	1.17833	-0.66715	1.29484
H	1.97623	-0.93238	-0.28074
H	1.35857	1.63281	0.56136
H	1.14614	1.17969	-1.13744
H	-1.01257	1.62353	0.89633
H	-1.14363	1.55496	-0.86244

HCl

Zero-point correction=	0.006691
(Hartree/Particle)	
Thermal correction to Energy=	0.009051
Thermal correction to Enthalpy=	0.009996
Thermal correction to Gibbs Free Energy=	-0.011200
Sum of electronic and zero-point Energies=	-460.760851
Sum of electronic and thermal Energies=	-460.758490
Sum of electronic and thermal Enthalpies=	-460.757546
Sum of electronic and thermal Free Energies=	-460.778742

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	5.680	4.968	44.611

Cl	0.00000	0.00000	0.07159
H	0.00000	0.00000	-1.21697

Complex A

Zero-point correction=	0.229168
(Hartree/Particle)	
Thermal correction to Energy=	0.247284
Thermal correction to Enthalpy=	0.248228
Thermal correction to Gibbs Free Energy=	0.181007

Sum of electronic and zero-point Energies= -1957.948002
Sum of electronic and thermal Energies= -1957.929886
Sum of electronic and thermal Enthalpies= -1957.928941
Sum of electronic and thermal Free Energies= -1957.996162

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	155.173	64.565	141.478

C	-2.69462	-1.35218	-1.28904
C	-1.72796	-1.10345	-0.30410
C	-2.13641	-0.65212	0.95859
C	-3.48317	-0.42921	1.21211
C	-4.44058	-0.65969	0.22598
C	-4.03895	-1.12960	-1.02185
H	-2.37894	-1.70797	-2.27012
H	-1.38950	-0.48168	1.73283
H	-3.78887	-0.07880	2.19650
H	-5.49405	-0.48263	0.43286
H	-4.77795	-1.32073	-1.79798
C	0.62506	2.40212	1.02703
H	0.42119	2.13761	2.06869
H	1.71099	2.50118	0.88362
C	-0.60167	1.83139	-0.92916
H	-0.30227	1.28606	-1.82897
H	-1.66371	1.63844	-0.71997
O	0.16411	1.30253	0.19264
C	-0.27636	3.30699	-0.95708
H	0.67217	3.47853	-1.48495
H	-1.05966	3.89110	-1.45122
C	-0.12456	3.61818	0.52598
H	0.42284	4.54483	0.72708
H	-1.10966	3.68868	1.00690
Cl	2.41813	0.54069	-1.57662
Ti	1.24384	-0.58301	0.01946
Cl	2.43467	-2.47259	-0.23433
Cl	1.39935	-0.47409	2.25177
N	-0.37197	-1.27359	-0.60333
H	-0.22749	-1.86600	-1.42585

TS 1A

Zero-point correction= 0.224877
(Hartree/Particle)

Thermal correction to Energy=	0.242750
Thermal correction to Enthalpy=	0.243694
Thermal correction to Gibbs Free Energy=	0.176995
Sum of electronic and zero-point Energies=	-1957.877666
Sum of electronic and thermal Energies=	-1957.859793
Sum of electronic and thermal Enthalpies=	-1957.858849
Sum of electronic and thermal Free Energies=	-1957.925547

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	152.328	64.886	140.379

C	-2.49675	0.06459	0.85150
C	-2.05404	0.29511	-0.46267
C	-3.00010	0.61712	-1.45004
C	-4.35082	0.67621	-1.13717
C	-4.78423	0.43028	0.16402
C	-3.84983	0.12877	1.15308
H	-1.76825	-0.17624	1.62624
H	-2.66265	0.80433	-2.47019
H	-5.07192	0.91435	-1.91723
H	-5.84381	0.47563	0.40712
H	-4.17785	-0.05954	2.17387
Cl	2.47817	-2.02271	-1.08773
Ti	0.86426	-0.76796	-0.10278
Cl	-0.50022	-2.58047	0.24715
Cl	1.31086	-0.37686	2.05516
N	-0.69624	0.27837	-0.75547
H	-0.51650	0.58803	-1.71368
C	0.23152	2.39009	0.05101
H	-0.02796	2.67478	-0.96746
H	-0.60318	2.13851	0.70399
C	2.97083	1.37972	-0.48324
H	3.44571	0.94608	0.41392
H	3.64777	1.22507	-1.33707
O	1.74010	0.77546	-0.72449
C	2.67669	2.86351	-0.26353
H	2.45779	3.34878	-1.22573
H	3.53340	3.37813	0.18664
C	1.45765	2.93081	0.63865
H	1.16404	3.98900	0.81625
H	1.64725	2.49925	1.63115

Intermediate 1A

Zero-point correction= 0.232008
(Hartree/Particle)
Thermal correction to Energy= 0.249255
Thermal correction to Enthalpy= 0.250200
Thermal correction to Gibbs Free Energy= 0.185897
Sum of electronic and zero-point Energies= -1957.965141
Sum of electronic and thermal Energies= -1957.947894
Sum of electronic and thermal Enthalpies= -1957.946950
Sum of electronic and thermal Free Energies= -1958.011253

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.410	63.087	135.337
C	2.77798	0.95150	-0.22329
C	1.96155	0.07572	0.48814
C	2.37463	-1.24377	0.69042
C	3.58174	-1.68539	0.16658
C	4.39218	-0.81735	-0.56199
C	3.98623	0.49842	-0.74757
H	2.48375	1.98539	-0.38690
H	1.73751	-1.92647	1.25453
H	3.89020	-2.71612	0.33083
H	5.33627	-1.16518	-0.97610
H	4.61320	1.18971	-1.30784
C	0.50639	1.91040	1.31766
H	-0.26248	1.95798	2.09951
H	1.44425	2.26214	1.77189
C	-2.28878	2.21961	-0.42877
H	-2.11879	2.11001	-1.51094
H	-3.34440	2.47235	-0.26724
O	-2.05267	0.95953	0.17663
C	-1.35943	3.25889	0.16085
H	-1.67182	3.50015	1.18794
H	-1.48597	4.17824	-0.42781
C	0.10651	2.82553	0.15136
H	0.73354	3.72604	0.20058
H	0.33993	2.34864	-0.81213
Cl	-1.21189	-1.73639	1.90936
Cl	-0.01368	-0.39615	-1.91029
Ti	-1.23758	-0.54989	-0.04461
Cl	-2.86557	-1.79061	-0.97471
N	0.67326	0.46580	1.00408
H	0.55551	-0.02998	1.88906

TS 2A

Zero-point correction= (Hartree/Particle)	0.226303
Thermal correction to Energy=	0.244346
Thermal correction to Enthalpy=	0.245290
Thermal correction to Gibbs Free Energy=	0.178036
Sum of electronic and zero-point Energies=	-1957.906442
Sum of electronic and thermal Energies=	-1957.888399
Sum of electronic and thermal Enthalpies=	-1957.887455
Sum of electronic and thermal Free Energies=	-1957.954709

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	153.329	64.650	141.548
C	3.78536	0.43879	0.39539
C	2.56788	-0.22694	0.20807
C	2.57356	-1.54354	-0.28017
C	3.77228	-2.18286	-0.55188
C	4.98621	-1.52307	-0.35619
C	4.98168	-0.21571	0.11615
H	3.80867	1.45590	0.78163
H	1.62070	-2.05403	-0.43185
H	3.76016	-3.20762	-0.91857
H	5.92654	-2.02702	-0.56923
H	5.92221	0.30853	0.27730
C	1.19112	1.65773	1.09508
H	0.18967	1.69024	1.54402
H	1.92008	1.77606	1.91047
C	0.54892	1.31824	-1.80931
H	1.52191	0.83491	-1.89348
H	-0.17537	1.06442	-2.57620
O	-1.01586	-0.22003	-1.09650
C	0.36878	2.55441	-1.06861
H	-0.68899	2.64701	-0.76634
H	0.48812	3.33239	-1.85419
C	1.32905	2.79170	0.07690
H	1.12126	3.75545	0.55644
H	2.35862	2.83695	-0.30665
Cl	-2.72666	1.66947	0.73109
Cl	-1.33919	-1.58398	1.67109
Ti	-2.24540	-0.40458	-0.03401

Cl	-3.98042	-1.40980	-1.04110
N	1.33297	0.37636	0.43932
H	0.57868	-0.28582	0.60074

Product A

Zero-point correction= 0.232349
(Hartree/Particle)
Thermal correction to Energy= 0.250096
Thermal correction to Enthalpy= 0.251041
Thermal correction to Gibbs Free Energy= 0.184190
Sum of electronic and zero-point Energies= -1957.973381
Sum of electronic and thermal Energies= -1957.955633
Sum of electronic and thermal Enthalpies= -1957.954689
Sum of electronic and thermal Free Energies= -1958.021540

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	156.938	62.746	140.700

C	3.76478	0.09938	-0.24724
C	2.46734	-0.21765	0.13993
C	2.09994	-1.50918	0.48756
C	3.06409	-2.51271	0.44390
C	4.36700	-2.21582	0.05952
C	4.71664	-0.91160	-0.28453
H	4.03323	1.12083	-0.51726
H	1.07588	-1.73168	0.78815
H	2.78915	-3.52995	0.71255
H	5.11629	-3.00367	0.02575
H	5.73581	-0.67810	-0.58414
C	1.76183	2.05495	1.04383
H	1.00185	2.06067	1.83283
H	2.74525	1.91067	1.49708
C	1.06104	1.37175	-1.20689
H	1.96518	1.33221	-1.82439
H	0.30097	0.70484	-1.62808
O	-2.30220	1.29887	-0.81478
C	0.62058	2.78970	-0.92285
H	-0.40002	2.78808	-0.51500
H	0.62038	3.39858	-1.83249
C	1.63858	3.25082	0.11497
H	1.32734	4.14680	0.66110
H	2.60375	3.46799	-0.36450

Cl	-4.61566	-0.63125	0.27183
Cl	-1.20058	-0.03686	1.83353
Ti	-2.44695	-0.14525	-0.12229
Cl	-1.28712	-1.60533	-1.43339
N	1.44706	0.83560	0.16899
H	0.59234	0.41854	0.58140

Complex B

Zero-point correction= (Hartree/Particle)	0.215576
Thermal correction to Energy=	0.231256
Thermal correction to Enthalpy=	0.232200
Thermal correction to Gibbs Free Energy=	0.168776
Sum of electronic and zero-point Energies=	-1497.138823
Sum of electronic and thermal Energies=	-1497.123143
Sum of electronic and thermal Enthalpies=	-1497.122199
Sum of electronic and thermal Free Energies=	-1497.185622

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	145.115	55.763	133.486

C	2.74553	0.51061	1.11924
C	2.15455	-0.08757	-0.00601
C	2.90844	-0.23410	-1.18215
C	4.22375	0.20826	-1.22501
C	4.80644	0.79923	-0.10506
C	4.06235	0.94746	1.06433
H	2.15090	0.61298	2.02712
H	2.44049	-0.70180	-2.04759
H	4.80031	0.08994	-2.14120
H	5.83867	1.14222	-0.14300
H	4.51378	1.40627	1.94277
N	0.84504	-0.51256	0.04372
C	-3.10011	0.89774	-0.36017
H	-3.48333	0.14814	-1.06048
H	-3.48748	0.69854	0.64834
Ti	-0.74903	-1.00437	0.14354
C	-0.99339	2.05246	-0.28336
H	-0.26274	2.03310	0.53099
H	-0.47325	2.16735	-1.24157

O	-1.64925	0.74421	-0.31524
C	-2.12929	3.03568	-0.09649
H	-2.34239	3.17624	0.97142
H	-1.89619	4.01304	-0.53061
C	-3.29833	2.33592	-0.78404
H	-4.27454	2.72111	-0.47335
H	-3.21981	2.42822	-1.87516
Cl	-1.24880	-2.47529	-1.51962
Cl	-1.38806	-1.23054	2.31979

TS 1B

Zero-point correction= 0.211353
(Hartree/Particle)
Thermal correction to Energy= 0.227381
Thermal correction to Enthalpy= 0.228325
Thermal correction to Gibbs Free Energy= 0.165568
Sum of electronic and zero-point Energies= -1497.082124
Sum of electronic and thermal Energies= -1497.066097
Sum of electronic and thermal Enthalpies= -1497.065153
Sum of electronic and thermal Free Energies= -1497.127910

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	142.684	58.248	132.083

C	-2.67737	-0.28484	1.08354
C	-2.00513	-0.27562	-0.15677
C	-2.72082	0.08831	-1.31586
C	-4.06763	0.40885	-1.23372
C	-4.72454	0.38972	-0.00297
C	-4.02342	0.04593	1.15204
H	-2.11566	-0.56621	1.97472
H	-2.19476	0.09657	-2.26993
H	-4.61319	0.67955	-2.13639
H	-5.78112	0.64400	0.05525
H	-4.53240	0.03163	2.11453
N	-0.67350	-0.56736	-0.21932
C	0.17990	1.89776	0.07644
H	-0.26655	1.94014	-0.91606
H	-0.45805	1.52744	0.87821
C	2.90724	1.38988	-0.83387
H	3.50873	1.07647	0.03696
H	3.53979	1.32170	-1.73081

Ti	1.01335	-0.83546	-0.05632
O	1.78986	0.57028	-1.00135
C	2.39639	2.81348	-0.64826
H	1.97445	3.17806	-1.59538
H	3.20537	3.49128	-0.35228
C	1.31379	2.75485	0.41519
H	0.83517	3.75149	0.52809
H	1.71421	2.49825	1.40551
Cl	1.59466	-2.87474	-0.85569
Cl	1.57096	-0.49296	2.12499

Intermediate 1B

Zero-point correction= 0.216336
(Hartree/Particle)
Thermal correction to Energy= 0.231088
Thermal correction to Enthalpy= 0.232032
Thermal correction to Gibbs Free Energy= 0.173291
Sum of electronic and zero-point Energies= -1497.171405
Sum of electronic and thermal Energies= -1497.156653
Sum of electronic and thermal Enthalpies= -1497.155709
Sum of electronic and thermal Free Energies= -1497.214451

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	145.010	55.063	123.632

C	2.03307	-1.59961	0.33687
C	1.46277	-0.57370	-0.43476
C	2.27389	0.46780	-0.89719
C	3.62939	0.49472	-0.57531
C	4.18851	-0.52179	0.18829
C	3.38534	-1.57263	0.63598
H	1.40359	-2.40753	0.71042
H	1.83733	1.24128	-1.52691
H	4.24957	1.31162	-0.94028
H	5.24840	-0.50331	0.43414
H	3.81928	-2.37199	1.23404
C	-0.54020	-1.77023	-1.26104
H	-0.99612	-1.50597	-2.22771
H	0.27425	-2.47302	-1.48617
C	-3.29929	-0.67624	0.28741
H	-3.14873	-0.84805	1.36565
H	-4.33209	-0.33651	0.13522

O	-2.43522	0.37183	-0.11275
C	-3.01652	-1.93543	-0.50323
H	-3.25796	-1.76264	-1.56364
H	-3.71965	-2.70139	-0.14358
C	-1.58601	-2.46732	-0.38283
H	-1.59519	-3.52562	-0.67901
H	-1.26156	-2.44584	0.67061
Cl	-0.38112	0.72447	2.30483
Ti	-0.78285	0.88451	0.10798
Cl	-0.41255	2.84673	-0.94653
N	0.07004	-0.55553	-0.70182

TS 2B

Zero-point correction= (Hartree/Particle)	0.212439
Thermal correction to Energy=	0.227958
Thermal correction to Enthalpy=	0.228902
Thermal correction to Gibbs Free Energy=	0.168630
Sum of electronic and zero-point Energies=	-1497.097027
Sum of electronic and thermal Energies=	-1497.081508
Sum of electronic and thermal Enthalpies=	-1497.080564
Sum of electronic and thermal Free Energies=	-1497.140836

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	143.046	57.715	126.853

C	-2.68484	0.74688	-0.82727
C	-1.60509	-0.00918	-0.33293
C	-1.90247	-1.12712	0.47306
C	-3.21390	-1.46003	0.77527
C	-4.27355	-0.70110	0.28202
C	-3.99593	0.39690	-0.52431
H	-2.51234	1.60702	-1.46953
H	-1.09228	-1.74288	0.86112
H	-3.40937	-2.33068	1.39881
H	-5.30162	-0.96624	0.51967
H	-4.80892	0.99920	-0.92676
C	0.02853	1.47295	-1.39985
H	1.06337	1.40370	-1.76710
H	-0.61054	1.53285	-2.29281
C	0.32541	1.57604	1.67203
H	-0.70096	1.22033	1.75891

H	0.95591	1.44000	2.54564
O	1.01115	-0.61649	1.73119
C	0.67207	2.64197	0.73623
H	1.75892	2.69688	0.58487
H	0.44625	3.52558	1.37998
C	-0.12131	2.74614	-0.54916
H	0.21586	3.61779	-1.12299
H	-1.18147	2.90626	-0.30973
Cl	3.29031	0.51654	-0.22439
Ti	1.33422	-0.60109	0.11472
Cl	1.42950	-2.72068	-0.66103
N	-0.26788	0.28797	-0.61598

Product B

Zero-point correction= 0.217825
(Hartree/Particle)
Thermal correction to Energy= 0.233394
Thermal correction to Enthalpy= 0.234338
Thermal correction to Gibbs Free Energy= 0.173749
Sum of electronic and zero-point Energies= -1497.180461
Sum of electronic and thermal Energies= -1497.164892
Sum of electronic and thermal Enthalpies= -1497.163948
Sum of electronic and thermal Free Energies= -1497.224537

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	146.457	56.765	127.520

C	1.59430	-0.96357	-1.32955
C	0.94451	-1.05915	-0.08968
C	1.69750	-1.00487	1.09308
C	3.07915	-0.86135	1.02673
C	3.72003	-0.76624	-0.20323
C	2.97336	-0.81875	-1.37720
H	1.02693	-0.98963	-2.25621
H	1.21161	-1.07536	2.06252
H	3.65356	-0.82508	1.94941
H	4.80046	-0.65069	-0.24955
H	3.46548	-0.74148	-2.34417
C	-1.21792	-1.52856	-1.24564
H	-1.17849	-0.74690	-2.01387
H	-0.70672	-2.42340	-1.63263
C	-1.09506	-1.92023	1.07022

H	-0.68832	-2.94033	0.97442
H	-0.84278	-1.51764	2.05347
O	-0.67638	1.06129	1.92796
C	-2.57578	-1.85813	0.75630
H	-2.99477	-0.93008	1.16774
H	-3.11783	-2.69676	1.20475
C	-2.64164	-1.84561	-0.77975
H	-3.34935	-1.09146	-1.13950
H	-2.95629	-2.81478	-1.18199
Cl	-2.34394	1.68955	-0.69914
Ti	-0.43756	1.05503	0.34260
Cl	1.24403	2.49385	-0.18224
N	-0.49404	-1.08805	-0.01419

Complex C

Zero-point correction= (Hartree/Particle)	0.334809
Thermal correction to Energy=	0.357045
Thermal correction to Enthalpy=	0.357989
Thermal correction to Gibbs Free Energy=	0.279188
Sum of electronic and zero-point Energies=	-1729.357365
Sum of electronic and thermal Energies=	-1729.335129
Sum of electronic and thermal Enthalpies=	-1729.334185
Sum of electronic and thermal Free Energies=	-1729.412986

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	224.049	79.850	165.851

C	2.88538	-0.31634	-0.96684
C	2.30710	-0.21469	0.31181
C	3.14378	-0.23648	1.44076
C	4.51905	-0.35463	1.28780
C	5.08469	-0.45374	0.01804
C	4.26189	-0.43498	-1.10640
H	2.22872	-0.29922	-1.83740
H	2.69045	-0.16095	2.42766
H	5.15621	-0.36889	2.17036
H	6.16340	-0.54590	-0.09445
H	4.69733	-0.51112	-2.10154
N	0.94300	-0.09882	0.43909
C	0.35270	2.86362	-0.49225
H	1.09633	3.18841	0.24689

H	0.81547	2.15403	-1.18545
C	-1.91929	2.94443	0.22781
H	-2.60241	2.48606	-0.50395
H	-2.35544	2.87387	1.22915
C	-2.46004	-2.52736	0.16992
H	-2.92234	-2.31460	1.13891
H	-3.00937	-2.00005	-0.62483
Ti	-0.72069	0.06550	0.31365
C	-0.19461	-2.88372	-0.47907
H	0.37209	-2.29176	-1.20503
H	0.49248	-3.28347	0.27787
O	-1.11391	-1.99249	0.21334
C	-1.07936	-3.94192	-1.10675
H	-1.41061	-3.61494	-2.10247
H	-0.56097	-4.90044	-1.21507
C	-2.26557	-3.99300	-0.15032
H	-3.16157	-4.44279	-0.59042
H	-2.00729	-4.55189	0.75942
O	-0.69534	2.16664	0.23798
C	-1.48185	4.33025	-0.19357
H	-1.09969	4.89145	0.67014
H	-2.30133	4.90188	-0.64111
C	-0.35564	4.01614	-1.17209
H	0.31514	4.86159	-1.35656
H	-0.77057	3.68533	-2.13461
Cl	-1.87912	0.17018	2.32744
Cl	-1.34953	0.14250	-1.95361

TS 1C

Zero-point correction=	0.329809
(Hartree/Particle)	
Thermal correction to Energy=	0.351701
Thermal correction to Enthalpy=	0.352645
Thermal correction to Gibbs Free Energy=	0.276812
Sum of electronic and zero-point Energies=	-1729.286829
Sum of electronic and thermal Energies=	-1729.264938
Sum of electronic and thermal Enthalpies=	-1729.263994
Sum of electronic and thermal Free Energies=	-1729.339827

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	220.695	80.706	159.604

C	2.40838	-1.75454	-1.10782
C	2.01192	-1.05260	0.04890
C	2.88871	-1.01740	1.15473
C	4.10326	-1.68434	1.10509
C	4.48238	-2.38180	-0.04279
C	3.63262	-2.40942	-1.14679
H	1.73001	-1.77980	-1.96133
H	2.57452	-0.46936	2.04353
H	4.76449	-1.66072	1.97013
H	5.43822	-2.90131	-0.07547
H	3.92421	-2.95205	-2.04492
N	0.81942	-0.39323	0.09253
C	1.61466	1.71497	-1.03764
H	2.31147	1.58947	-0.21041
H	1.53646	0.88789	-1.74037
C	-0.19493	3.54808	0.39789
H	-1.11639	3.62833	-0.20548
H	-0.33102	4.14412	1.31412
C	-3.29436	-1.22298	0.46910
H	-3.37144	-1.15206	1.55807
H	-3.74902	-0.33034	0.01039
Ti	-0.60872	0.49587	0.45836
C	-1.64313	-2.12761	-0.97359
H	-1.09865	-1.57321	-1.74502
H	-1.01215	-2.94524	-0.59982
O	-1.88777	-1.23623	0.14209
C	-3.01690	-2.59195	-1.42118
H	-3.42016	-1.89734	-2.17150
H	-2.99307	-3.59586	-1.85822
C	-3.83108	-2.50149	-0.13564
H	-4.91200	-2.45956	-0.30562
H	-3.61518	-3.35480	0.52170
O	0.05762	2.22837	0.73276
C	1.00115	4.06391	-0.39334
H	1.87658	4.13500	0.26816
H	0.80707	5.05963	-0.80990
C	1.26879	3.05661	-1.49640
H	2.19286	3.33384	-2.05172
H	0.46525	3.02568	-2.24397
Cl	-1.11723	0.14896	2.70492
Cl	-1.72358	1.22383	-1.52350

Intermediate 1C

Zero-point correction=	0.335522
(Hartree/Particle)	
Thermal correction to Energy=	0.356687
Thermal correction to Enthalpy=	0.357631
Thermal correction to Gibbs Free Energy=	0.284659
Sum of electronic and zero-point Energies=	-1729.373460
Sum of electronic and thermal Energies=	-1729.352294
Sum of electronic and thermal Enthalpies=	-1729.351350
Sum of electronic and thermal Free Energies=	-1729.424323

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	223.825	79.176	153.584

C	1.35039	2.38473	-1.00666
C	0.81008	1.73726	0.11365
C	1.59249	1.60582	1.26368
C	2.89619	2.09372	1.28580
C	3.42851	2.73262	0.17017
C	2.64703	2.88051	-0.97511
H	0.74637	2.47381	-1.91061
H	1.16826	1.11042	2.13637
H	3.49342	1.98301	2.18940
H	4.44589	3.11868	0.19241
H	3.05462	3.37619	-1.85482
N	-0.51607	1.22155	0.06792
C	-1.54382	2.25569	-0.17140
H	-1.95281	2.56778	0.80519
H	-1.02310	3.13451	-0.57511
C	-3.79928	-0.14911	-0.08149
H	-3.75870	-0.78131	-0.98525
H	-4.64028	-0.48721	0.54006
C	1.62254	-2.53728	0.44719
H	1.82104	-2.46615	1.51982
H	0.79222	-3.23935	0.27803
Ti	-0.87726	-0.59010	0.43396
C	1.88001	-0.90147	-1.25127
H	1.14450	-0.47408	-1.94088
H	2.64610	-0.14880	-1.02000
O	1.19864	-1.22433	-0.00937
C	2.48008	-2.20745	-1.72325
H	1.72771	-2.79294	-2.26934
H	3.34419	-2.05149	-2.37765
C	2.82554	-2.88443	-0.40340

H	2.96615	-3.96700	-0.48915
H	3.73958	-2.45088	0.02524
O	-2.60447	-0.34585	0.62690
C	-3.94025	1.31269	-0.45470
H	-4.18140	1.90091	0.44459
H	-4.80342	1.40386	-1.12981
C	-2.69543	1.89997	-1.11742
H	-2.99302	2.83339	-1.61545
H	-2.32654	1.23386	-1.91412
Cl	-0.40391	-1.16155	2.60176
Cl	-1.27705	-1.81634	-1.51861

TS 2C

Zero-point correction= (Hartree/Particle)	0.331866
Thermal correction to Energy=	0.352706
Thermal correction to Enthalpy=	0.353650
Thermal correction to Gibbs Free Energy=	0.283194
Sum of electronic and zero-point Energies=	-1729.293328
Sum of electronic and thermal Energies=	-1729.272488
Sum of electronic and thermal Enthalpies=	-1729.271544
Sum of electronic and thermal Free Energies=	-1729.342000

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	221.326	79.714	148.286

C	1.98457	-1.92679	-1.22992
C	1.12096	-1.32996	-0.29153
C	1.66630	-1.03099	0.97139
C	2.99263	-1.31204	1.27711
C	3.83032	-1.90284	0.33563
C	3.31135	-2.20351	-0.92003
H	1.62757	-2.15088	-2.23338
H	1.03926	-0.54544	1.71727
H	3.37096	-1.06433	2.26866
H	4.86886	-2.12318	0.57475
H	3.94839	-2.65492	-1.67975
C	-0.90568	-2.03243	-1.38416
H	-1.82854	-1.62198	-1.80397
H	-0.31222	-2.39378	-2.23545
C	-1.49784	-1.91588	1.71089
H	-0.44024	-1.99385	1.95903

H	-2.15273	-1.52723	2.48571
O	-1.17199	0.30871	1.74346
C	-2.07102	-2.80362	0.71150
H	-3.08912	-2.50278	0.43785
H	-2.20866	-3.68157	1.39303
C	-1.22635	-3.22442	-0.47366
H	-1.75680	-4.00129	-1.03922
H	-0.28185	-3.66601	-0.12074
Cl	-3.36575	-0.03751	-0.50818
Ti	-1.21528	0.60773	0.11425
Cl	-1.79064	2.85706	-0.36519
N	-0.21425	-1.00173	-0.62248
C	1.25525	2.33145	1.10724
H	0.41265	2.85311	1.57387
H	1.72486	1.66234	1.84135
C	1.38486	1.81849	-1.20404
H	1.47313	0.89112	-1.77980
H	0.74778	2.53352	-1.74684
O	0.74040	1.49176	0.04428
C	2.69691	2.43320	-0.77550
H	3.40111	1.64262	-0.47701
H	3.15876	3.03378	-1.56590
C	2.25776	3.25216	0.43390
H	3.08075	3.52370	1.10321
H	1.76345	4.17625	0.10353

Product C

Zero-point correction= (Hartree/Particle)	0.336190
Thermal correction to Energy=	0.356944
Thermal correction to Enthalpy=	0.357889
Thermal correction to Gibbs Free Energy=	0.285227
Sum of electronic and zero-point Energies=	-1729.367508
Sum of electronic and thermal Energies=	-1729.346754
Sum of electronic and thermal Enthalpies=	-1729.345810
Sum of electronic and thermal Free Energies=	-1729.418471

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	223.986	77.055	152.929

C	0.06047	2.33167	1.14010
C	0.45658	1.67784	-0.02851

C	-0.19958	1.97995	-1.22650
C	-1.17729	2.96509	-1.26429
C	-1.52898	3.65878	-0.10880
C	-0.91613	3.32406	1.09175
H	0.49871	2.07699	2.10182
H	0.03461	1.42813	-2.13562
H	-1.66627	3.18966	-2.21075
H	-2.28464	4.44061	-0.14442
H	-1.19523	3.83492	2.01141
N	1.50313	0.66771	-0.00909
C	2.40865	0.69362	-1.23533
H	2.35700	-0.27836	-1.73969
H	2.05874	1.45901	-1.93135
C	2.42472	0.76188	1.18867
H	2.43180	1.80391	1.53397
H	2.05604	0.13039	2.00699
C	-2.60423	-0.51848	-1.21699
H	-2.59949	0.45066	-1.74321
H	-2.25348	-1.29160	-1.90286
Ti	0.63634	-1.38667	0.05634
C	-2.42016	0.09361	0.96177
H	-1.83055	-0.01839	1.87530
H	-2.60020	1.16544	0.77118
O	-1.66690	-0.44756	-0.13062
C	-3.70672	-0.70216	0.92551
H	-3.53126	-1.69391	1.36315
H	-4.52196	-0.22122	1.47720
C	-3.97345	-0.80655	-0.58243
H	-4.35553	-1.79374	-0.86401
H	-4.71089	-0.06315	-0.90866
O	2.10091	-2.02935	0.16729
C	3.80183	0.38319	0.68479
H	3.91513	-0.70472	0.64532
H	4.58180	0.79507	1.33464
C	3.80636	0.98253	-0.71234
H	4.57693	0.56302	-1.36781
H	3.96514	2.06918	-0.65752
Cl	0.10013	-2.22073	-2.02268
Cl	-0.18909	-2.05244	2.09981

Complex D

Zero-point correction= 0.244498
(Hartree/Particle)

Thermal correction to Energy= 0.264411
Thermal correction to Enthalpy= 0.265355
Thermal correction to Gibbs Free Energy= 0.194420
Sum of electronic and zero-point Energies= -2418.744019
Sum of electronic and thermal Energies= -2418.724105
Sum of electronic and thermal Enthalpies= -2418.723161
Sum of electronic and thermal Free Energies= -2418.794096

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.920	70.728	149.295

C	-3.24180	-0.64481	0.51428
C	-2.28691	0.34122	0.74807
C	-2.57682	1.67645	0.48571
C	-3.82314	2.02577	-0.02262
C	-4.78087	1.04605	-0.26465
C	-4.48621	-0.28702	0.00916
H	-3.00526	-1.68856	0.71890
H	-1.82781	2.44529	0.67697
H	-4.04490	3.07155	-0.22684
H	-5.75574	1.32041	-0.66227
H	-5.23139	-1.05952	-0.17063
C	2.96416	1.28397	0.45490
H	3.14867	0.76899	1.40208
H	3.54284	0.79624	-0.33934
C	0.97134	2.39796	-0.19603
H	0.26399	2.25796	-1.01803
H	0.43472	2.75783	0.69658
O	1.55162	1.10647	0.12074
C	2.15390	3.28283	-0.51120
H	2.49611	3.10401	-1.53948
H	1.91368	4.34572	-0.40450
C	3.18118	2.78203	0.49438
H	4.21222	3.04679	0.23811
H	2.96386	3.18156	1.49441
Cl	2.48593	-1.53856	-1.26107
Cl	-0.46617	-0.01690	-1.85751
Ti	0.67664	-0.90634	-0.11826
Cl	-0.44105	-2.83553	-0.14327
Cl	1.57707	-1.27975	1.98066
N	-0.98580	-0.03473	1.23295
H	-0.53881	0.74224	1.72388
H	-1.06780	-0.78383	1.92371

TS 1D

Zero-point correction=	0.241759
(Hartree/Particle)	
Thermal correction to Energy=	0.261652
Thermal correction to Enthalpy=	0.262596
Thermal correction to Gibbs Free Energy=	0.191253
Sum of electronic and zero-point Energies=	-2418.683458
Sum of electronic and thermal Energies=	-2418.657565
Sum of electronic and thermal Enthalpies=	-2418.656621
Sum of electronic and thermal Free Energies=	-2418.727963

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	164.189	70.700	150.153

C	-0.59627	1.80561	-0.00113
H	-0.73665	1.14598	0.84922
H	-0.8834	1.40249	-0.97006
C	2.04145	2.31067	-0.24876
H	2.46041	2.46219	0.75756
H	2.86772	2.14833	-0.95217
O	1.21182	1.15239	-0.22507
C	1.11802	3.43307	-0.65896
H	0.89918	3.36632	-1.73367
H	1.55873	4.41702	-0.46278
C	-0.16674	3.22925	0.14536
H	-0.95056	3.89437	-0.23409
H	-0.00193	3.46774	1.20418
C	-3.29176	-0.09581	1.30502
C	-3.32553	0.74639	0.19342
C	-3.77814	0.26698	-1.03549
C	-4.1976	-1.05349	-1.14723
C	-4.16603	-1.89931	-0.04177
C	-3.71005	-1.41587	1.18143
H	-2.92959	0.28197	2.26227
H	-3.79104	0.92636	-1.90412
H	-4.55005	-1.42364	-2.10806
H	-4.49114	-2.93319	-0.1342
H	-3.67837	-2.06952	2.05092
Cl	3.12056	-1.58902	-1.40855
Cl	-0.09771	-1.15658	-1.50787
Ti	1.61602	-0.66435	-0.02835

Cl	0.44581	-1.60378	1.65052
Cl	3.30162	-0.07644	1.43213
N	-2.79625	2.05978	0.28991
H	-3.17252	2.68909	-0.4169
H	-2.93271	2.4766	1.20937

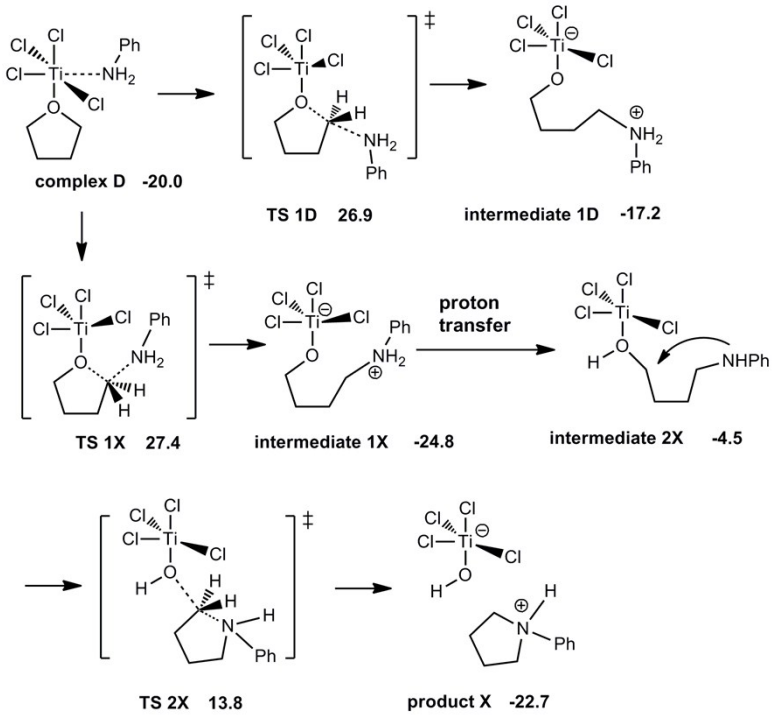
Intermediate 1D

Zero-point correction= 0.244711
(Hartree/Particle)
Thermal correction to Energy= 0.264670
Thermal correction to Enthalpy= 0.265614
Thermal correction to Gibbs Free Energy= 0.193777
Sum of electronic and zero-point Energies= -2418.747224
Sum of electronic and thermal Energies= -2418.727265
Sum of electronic and thermal Enthalpies= -2418.726321
Sum of electronic and thermal Free Energies= -2418.798158

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.083	70.154	151.194

C	-1.31798	1.8062	0.69726
H	-2.20473	1.90459	1.33165
H	-0.57499	1.21043	1.23956
C	1.57555	2.43561	-0.26
H	1.82249	2.59849	0.80259
H	2.45806	2.7063	-0.85576
O	1.31344	1.06306	-0.45716
C	0.36497	3.24372	-0.68076
H	0.07312	2.92439	-1.69364
H	0.66382	4.29642	-0.77603
C	-0.81239	3.17744	0.28973
H	-1.65274	3.75932	-0.11915
H	-0.5322	3.67861	1.22796
C	-4.1722	0.57235	-0.69699
C	-2.94142	0.13655	-0.22862
C	-2.79542	-1.02407	0.51808
C	-3.93392	-1.77527	0.7915
C	-5.17991	-1.36217	0.32725
C	-5.30023	-0.1909	-0.41472
H	-4.25334	1.49158	-1.27674

H	-1.81257	-1.33951	0.86968
H	-3.84135	-2.69259	1.36812
H	-6.0636	-1.95798	0.54532
H	-6.27255	0.13282	-0.77897
Cl	3.37326	-1.43334	-1.46362
Cl	0.11508	-1.5084	-1.34681
Ti	1.88834	-0.54198	-0.01869
Cl	0.73602	-1.22555	1.84484
Cl	3.56423	0.28166	1.29864
N	-1.75308	0.9621	-0.49231
H	-0.9708	0.33482	-0.79621
H	-1.94631	1.57561	-1.29205



TS 1X

Zero-point correction=	0.238038
(Hartree/Particle)	
Thermal correction to Energy=	0.258661
Thermal correction to Enthalpy=	0.259605
Thermal correction to Gibbs Free Energy=	0.185274
Sum of electronic and zero-point Energies=	-2418.674335
Sum of electronic and thermal Energies=	-2418.653712
Sum of electronic and thermal Enthalpies=	-2418.652968
Sum of electronic and thermal Free Energies=	-2418.727098

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	162.312	72.885	156.442

C	-1.05234	1.65384	0.26894
H	-1.77952	1.63723	-0.53990
H	-1.13833	0.87516	1.02891
C	1.62015	2.19074	-1.03102
H	2.44747	2.40352	-0.33776
H	2.00682	2.19796	-2.05908
O	1.10157	0.90525	-0.75191
C	0.50569	3.20901	-0.84792
H	-0.18851	3.18995	-1.69934
H	0.92147	4.21978	-0.77342
C	-0.23185	2.83339	0.44234
H	-0.98169	3.62610	0.65385
H	0.44607	2.75816	1.30070
C	-4.00934	0.15924	-1.27458
C	-3.03726	-0.50392	-0.50857
C	-3.36359	-0.93747	0.78711
C	-4.64567	-0.74408	1.28195
C	-5.61549	-0.10460	0.51190
C	-5.28761	0.34564	-0.76553
H	-3.75646	0.50275	-2.27849
H	-2.60559	-1.44436	1.38542
H	-4.88932	-1.09858	2.28181
H	-6.61900	0.04240	0.90521
H	-6.03698	0.84701	-1.37550
Cl	3.96740	-0.67225	-0.68128
Cl	1.18278	-2.10793	-1.45400
Ti	1.85760	-0.50214	0.07676
Cl	0.35130	-1.43361	1.57602
Cl	2.62460	0.78953	1.85269
N	-1.74075	-0.63046	-0.97477
H	-1.15732	-1.34212	-0.53887
H	-1.60301	-0.59477	-1.97972

Intermediate 1X

Zero-point correction=	0.244896
(Hartree/Particle)	
Thermal correction to Energy=	0.264735
Thermal correction to Enthalpy=	0.265679
Thermal correction to Gibbs Free Energy=	0.194081

Sum of electronic and zero-point Energies=	-2418.750803
Sum of electronic and thermal Energies=	-2418.730964
Sum of electronic and thermal Enthalpies=	-2418.730020
Sum of electronic and thermal Free Energies=	-2418.801618

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	166.123	70.015	150.691

C	-1.59348	2.32794	0.27762
H	-2.27474	2.69925	-0.49830
H	-2.08725	2.44217	1.24966
C	1.64151	2.10550	-1.20581
H	2.41593	2.41943	-0.48797
H	2.08154	2.10815	-2.21196
O	1.26942	0.77753	-0.89234
C	0.43697	3.02325	-1.13686
H	-0.27955	2.75002	-1.92892
H	0.78756	4.03215	-1.39122
C	-0.25335	3.03605	0.23626
H	-0.45637	4.06925	0.54502
H	0.41281	2.61995	1.00841
C	-3.43011	0.07032	-1.21392
C	-2.76138	0.14752	-0.00115
C	-3.27631	-0.39132	1.16829
C	-4.51047	-1.03104	1.11544
C	-5.20096	-1.11949	-0.08998
C	-4.66250	-0.57230	-1.25191
H	-2.99114	0.49535	-2.11661
H	-2.71507	-0.32603	2.10038
H	-4.92760	-1.46716	2.02011
H	-6.16369	-1.62460	-0.12649
H	-5.19918	-0.64998	-2.19459
Cl	3.25856	-1.83483	-1.17577
Cl	0.02452	-1.97438	-0.68970
Ti	1.79877	-0.62658	0.03438
Cl	0.60391	-0.47365	2.09526
Cl	3.49281	0.48516	1.09824
N	-1.47397	0.84278	0.05833
H	-0.89690	0.43420	0.82726
H	-0.91293	0.64518	-0.78532

Intermediate 2X

Zero-point correction=	0.243340
(Hartree/Particle)	
Thermal correction to Energy=	0.263598
Thermal correction to Enthalpy=	0.264542
Thermal correction to Gibbs Free Energy=	0.191396
Sum of electronic and zero-point Energies=	-2418.725993
Sum of electronic and thermal Energies=	-2418.705735
Sum of electronic and thermal Enthalpies=	-2418.704790
Sum of electronic and thermal Free Energies=	-2418.777936

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	165.410	71.952	153.948

C	-1.34538	1.28605	0.85261
H	-1.25916	0.89618	1.87986
H	-0.8778	0.529	0.19347
C	1.09403	2.55388	-1.17119
H	1.88978	2.90741	-0.51101
H	1.30983	2.89246	-2.19154
C	-0.26712	3.01374	-0.69869
H	-1.04279	2.65251	-1.39487
H	-0.26333	4.10838	-0.8008
C	-0.60477	2.611	0.74038
H	-1.22374	3.38703	1.21376
H	0.31982	2.55965	1.33304
C	-3.18163	-0.94543	0.6152
C	-3.55871	0.35933	0.26258
C	-4.81826	0.55682	-0.32857
C	-5.66858	-0.51354	-0.55639
C	-5.29307	-1.80975	-0.20323
C	-4.04774	-2.00997	0.38173
H	-2.21542	-1.13347	1.08125
H	-5.12185	1.56834	-0.60315
H	-6.63946	-0.33301	-1.0165
H	-5.9627	-2.64828	-0.38281
H	-3.73447	-3.01416	0.66483
Cl	3.9801	-1.26039	-0.83738
Cl	0.66282	-1.60924	-1.41365
Ti	2.11084	-0.47853	-0.05426
Cl	1.63556	-1.69809	1.7062
Cl	2.91895	1.24721	1.1361
N	-2.74051	1.44869	0.50982

H	-2.97289	2.28632	-0.01025
O	1.21587	1.10471	-1.17675
H	0.60345	0.72682	-1.8345

TS 2X

Zero-point correction= 0.241328
(Hartree/Particle)
Thermal correction to Energy= 0.261223
Thermal correction to Enthalpy= 0.262167
Thermal correction to Gibbs Free Energy= 0.189373
Sum of electronic and zero-point Energies= -2418.696814
Sum of electronic and thermal Energies= -2418.676920
Sum of electronic and thermal Enthalpies= -2418.675975
Sum of electronic and thermal Free Energies= -2418.748770

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.920	70.822	153.208

C	2.8901	2.27178	-0.41926
H	3.48066	3.07886	0.03502
H	3.35819	2.02023	-1.37861
C	0.90604	0.28489	-0.05062
H	0.63429	0.44635	0.98829
H	1.43458	-0.63202	-0.28917
C	0.6936	1.37983	-1.04801
H	-0.37877	1.59719	-1.11564
H	1.02609	1.05444	-2.04382
C	1.43656	2.6428	-0.61828
H	1.00513	3.01599	0.32393
H	1.31948	3.43736	-1.36454
C	4.19425	-0.44239	-0.99852
C	3.9385	0.10677	0.2606
C	4.65498	-0.34501	1.36923
C	5.62702	-1.32754	1.21765
C	5.89408	-1.86494	-0.03773
C	5.17346	-1.41854	-1.14211
H	3.6228	-0.11577	-1.86744
H	4.45408	0.08088	2.35264
H	6.18304	-1.66838	2.08891
H	6.6571	-2.63137	-0.15561
H	5.36561	-1.83999	-2.12702

Cl	-4.06898	-1.17708	1.52322
Cl	-3.01994	-1.95296	-1.46495
Ti	-2.61459	-0.28992	0.08974
Cl	-3.4687	1.32691	-1.1456
Cl	-1.75965	1.14451	1.68195
N	2.90416	1.06801	0.42769
H	2.81807	1.3262	1.41
O	-0.77314	-0.67922	-0.27224
H	-0.66131	-1.36349	-0.95341

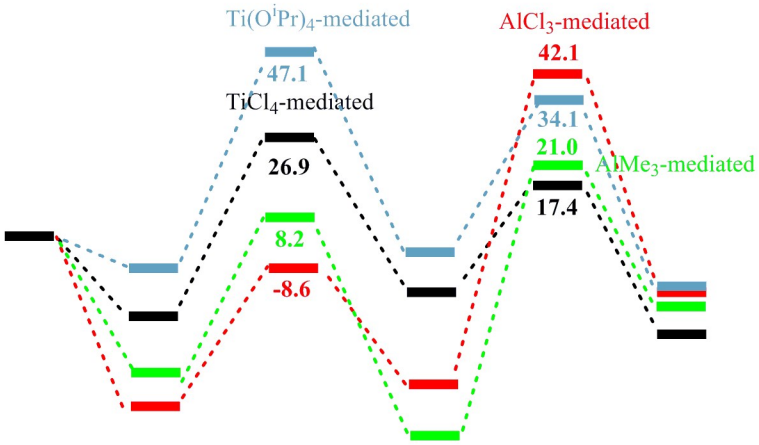
Product X

Zero-point correction= (Hartree/Particle)	0.243708
Thermal correction to Energy=	0.263889
Thermal correction to Enthalpy=	0.264833
Thermal correction to Gibbs Free Energy=	0.191538
Sum of electronic and zero-point Energies=	-2418.754840
Sum of electronic and thermal Energies=	-2418.734659
Sum of electronic and thermal Enthalpies=	-2418.733715
Sum of electronic and thermal Free Energies=	-2418.807011

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	165.593	71.073	154.264

C	2.29074	1.80976	1.15757
H	1.56287	1.73656	1.97295
H	3.27812	1.5372	1.53638
C	1.53403	1.52444	-1.15335
H	0.73911	0.97644	-1.66753
H	2.44233	1.52994	-1.76704
C	1.17486	2.90573	-0.65262
H	0.15999	2.90089	-0.22798
H	1.20418	3.64836	-1.45619
C	2.22125	3.14381	0.43121
H	1.95975	3.95741	1.11475
H	3.19218	3.38532	-0.02437
C	4.09976	-0.13326	-0.39576
C	2.77232	-0.36858	-0.05412
C	2.27884	-1.65234	0.12843
C	3.14507	-2.73026	-0.03633

C	4.47647	-2.5154	-0.37532
C	4.95282	-1.21823	-0.55455
H	4.47044	0.88296	-0.53252
H	1.23248	-1.80432	0.39013
H	2.77063	-3.74157	0.10548
H	5.14935	-3.36113	-0.4993
H	5.99449	-1.04791	-0.8173
Cl	-3.19756	-1.84596	1.19963
Cl	-3.49725	-0.6455	-1.82747
Ti	-2.15576	-0.27513	-0.01616
Cl	-2.5142	1.95655	-0.10778
Cl	-0.67998	0.10215	1.8606
N	1.86052	0.76579	0.12171
H	0.95878	0.38244	0.47762
O	-0.6813	-0.79526	-0.92342
H	-0.82535	-1.16544	-1.80997



$AlCl_3$

Zero-point correction=	0.004722
(Hartree/Particle)	
Thermal correction to Energy=	0.010086
Thermal correction to Enthalpy=	0.011030
Thermal correction to Gibbs Free Energy=	-0.025709
Sum of electronic and zero-point Energies=	-1623.117811
Sum of electronic and thermal Energies=	-1623.112447
Sum of electronic and thermal Enthalpies=	-1623.111503
Sum of electronic and thermal Free Energies=	-1623.148242

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	6.329	15.172	77.324

Al	0.	0.	0.00186
Cl	0.	0.	2.08099
Cl	0.	1.79668	-1.0412
Cl	0.	-1.79668	-1.0412

$AlCl_3$ starting complex

Zero-point correction= 0.243824
(Hartree/Particle)
Thermal correction to Energy= 0.261721
Thermal correction to Enthalpy= 0.262666
Thermal correction to Gibbs Free Energy= 0.195999
Sum of electronic and zero-point Energies= -2142.664983
Sum of electronic and thermal Energies= -2142.647085
Sum of electronic and thermal Enthalpies= -2142.646141
Sum of electronic and thermal Free Energies= -2142.712808

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	164.233	64.475	140.311

C	2.40413	-0.98281	0.41667
C	1.90765	-0.38176	-0.7361
C	2.62194	0.61843	-1.38498
C	3.83984	1.04018	-0.86159
C	4.34179	0.45524	0.29623
C	3.62595	-0.55809	0.92706
H	1.84084	-1.77674	0.90682
H	2.22468	1.071	-2.29415
H	4.39588	1.82804	-1.36527
H	5.29311	0.78791	0.70585
H	4.01596	-1.02206	1.83032
C	-2.25071	1.91326	-0.39703
H	-2.69975	1.77357	-1.38353
H	-2.89877	1.45358	0.36133
C	0.0336	2.05846	0.22351
H	0.641	1.45312	0.90581
H	0.67493	2.4394	-0.58365
O	-0.97572	1.20436	-0.38498
C	-0.73586	3.16907	0.90107
H	-1.08472	2.83747	1.88789
H	-0.131	4.07261	1.02858
C	-1.91162	3.34581	-0.04905
H	-2.76347	3.86594	0.4009

H	-1.60441	3.90228	-0.94495
N	0.60571	-0.7892	-1.24952
H	0.33353	-0.17735	-2.0236
H	0.66746	-1.73907	-1.63245
Al	-1.00972	-0.92128	-0.00554
Cl	-0.51511	-3.07438	0.31855
Cl	-1.22124	-0.36294	2.08166
Cl	-2.70326	-1.09034	-1.33646

$AlCl_3$ TS 1

Zero-point correction= 0.238322
(Hartree/Particle)
Thermal correction to Energy= 0.256586
Thermal correction to Enthalpy= 0.257530
Thermal correction to Gibbs Free Energy= 0.189314
Sum of electronic and zero-point Energies= -2142.606667
Sum of electronic and thermal Energies= -2142.588403
Sum of electronic and thermal Enthalpies= -2142.587458
Sum of electronic and thermal Free Energies= -2142.655675

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	161.010	66.017	143.574

C	0.38875	0.95344	-1.64507
H	1.45337	0.75405	-1.72368
H	-0.27181	0.2603	-2.16597
C	-0.73434	1.71928	1.02238
H	-1.71926	2.21728	0.9755
H	-0.44346	1.65825	2.08323
O	-0.77712	0.43867	0.45711
C	0.27676	2.54716	0.24371
H	1.30479	2.2311	0.47903
H	0.19061	3.61586	0.46958
C	-0.03043	2.28613	-1.24225
H	0.58959	2.97551	-1.8442
H	-1.09264	2.46316	-1.44905
C	3.05787	0.05847	1.11482
C	2.75128	-0.71408	-0.01475
C	3.78426	-1.10468	-0.87716
C	5.09589	-0.73937	-0.60298
C	5.39951	0.02645	0.51962
C	4.37222	0.42085	1.37452

H	2.25801	0.34779	1.79809
H	3.54778	-1.70235	-1.75774
H	5.88964	-1.05732	-1.27668
H	6.42835	0.31002	0.7299
H	4.59787	1.01171	2.26051
N	1.43083	-1.01028	-0.32177
H	1.2567	-1.84377	-0.87486
H	0.72789	-0.85747	0.39763
Al	-2.31032	-0.40618	0.14301
Cl	-3.41932	-0.57338	1.96518
Cl	-3.38386	0.74423	-1.33419
Cl	-1.70581	-2.30396	-0.67345

$AlCl_3$ intermediate 1

Zero-point correction=	0.230786
(Hartree/Particle)	
Thermal correction to Energy=	0.245217
Thermal correction to Enthalpy=	0.246161
Thermal correction to Gibbs Free Energy=	0.188932
Sum of electronic and zero-point Energies=	-1681.883637
Sum of electronic and thermal Energies=	-1681.869206
Sum of electronic and thermal Enthalpies=	-1681.868262
Sum of electronic and thermal Free Energies=	-1681.925491

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	153.876	55.051	120.450

C	1.97267	-1.52932	0.02588
C	1.47499	-0.37049	-0.55857
C	2.28305	0.75705	-0.69011
C	3.59316	0.72285	-0.23177
C	4.10072	-0.43162	0.35707
C	3.28839	-1.55119	0.48186
H	1.35652	-2.41804	0.13444
H	1.88459	1.66383	-1.1462
H	4.21906	1.60609	-0.33792
H	5.12703	-0.45738	0.71634
H	3.67506	-2.4602	0.93791
C	-0.56891	-1.56487	-1.40218
H	-1.31869	-1.31057	-2.15967
H	0.19471	-2.18057	-1.89412
C	-3.17886	-0.8667	0.53239

H	-2.87087	-0.8995	1.59498
H	-4.2773	-0.79506	0.52843
O	-2.64835	0.26043	-0.10981
C	-2.7511	-2.15609	-0.14378
H	-3.19322	-2.20868	-1.15114
H	-3.16956	-2.9995	0.42457
C	-1.23423	-2.32473	-0.24891
H	-1.00953	-3.39033	-0.3946
H	-0.76527	-2.0589	0.71223
N	0.09452	-0.27027	-1.02911
H	0.13438	0.28601	-1.88944
Al	-1.0818	0.90986	0.12488
Cl	-0.82726	2.80275	-0.83759
Cl	-0.30673	0.81452	2.11122

$AlCl_3$ TS 2

Zero-point correction= 0.225240
(Hartree/Particle)
Thermal correction to Energy= 0.241096
Thermal correction to Enthalpy= 0.242040
Thermal correction to Gibbs Free Energy= 0.179417
Sum of electronic and zero-point Energies= -1681.750402
Sum of electronic and thermal Energies= -1681.734546
Sum of electronic and thermal Enthalpies= -1681.733602
Sum of electronic and thermal Free Energies= -1681.796225

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	151.290	58.227	131.801

C	-3.49782	0.44501	-0.64034
C	-2.31162	-0.23683	-0.34288
C	-2.38271	-1.52235	0.21978
C	-3.6128	-2.11669	0.4491
C	-4.79467	-1.4447	0.13627
C	-4.72571	-0.16611	-0.40545
H	-3.46794	1.4458	-1.06747
H	-1.45088	-2.03147	0.46847
H	-3.6513	-3.11635	0.87856
H	-5.75952	-1.91402	0.31645
H	-5.63999	0.37168	-0.6513
C	-0.82024	1.5919	-1.15811
H	0.18753	1.57025	-1.5957

H	-1.52901	1.7703	-1.97816
C	-0.20487	0.95838	1.57006
H	-1.22777	0.65365	1.79104
H	0.55721	0.48256	2.17269
O	1.05171	-0.77105	0.55061
C	0.0513	2.29453	1.02053
H	1.10545	2.3797	0.71787
H	-0.06593	2.97193	1.8902
C	-0.89252	2.69277	-0.09721
H	-0.62247	3.66898	-0.51667
H	-1.92101	2.77032	0.28623
Cl	3.52607	1.32524	-0.17769
Cl	3.98729	-2.15229	-0.32792
N	-1.0524	0.3144	-0.5314
H	-0.23568	-0.31568	-0.41554
Al	2.62287	-0.5889	0.08485

$AlMe_3$

Zero-point correction=	0.104969
(Hartree/Particle)	
Thermal correction to Energy=	0.112784
Thermal correction to Enthalpy=	0.113728
Thermal correction to Gibbs Free Energy=	0.072638
Sum of electronic and zero-point Energies=	-361.963175
Sum of electronic and thermal Energies=	-361.955360
Sum of electronic and thermal Enthalpies=	-361.954415
Sum of electronic and thermal Free Energies=	-361.995506

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	70.773	25.599	86.482

Al	0.00258	-0.00217	-0.00345
C	-0.5457	1.88111	0.00503
H	0.11324	2.50092	0.62784
H	-0.49377	2.30014	-1.01091
H	-1.57539	2.026	0.35585
C	-1.36262	-1.41072	-0.00046
H	-0.94821	-2.41721	-0.13776
H	-1.91847	-1.41272	0.94849
H	-2.10955	-1.24744	-0.78994
C	1.9073	-0.46943	-0.00271
H	2.2254	-0.77502	1.00533

H	2.12546	-1.31803	-0.66483
H	2.55388	0.36577	-0.30046

$AlMe_3$ starting complex

Zero-point correction= 0.295673
(Hartree/Particle)
Thermal correction to Energy= 0.312805
Thermal correction to Enthalpy= 0.313749
Thermal correction to Gibbs Free Energy= 0.250109
Sum of electronic and zero-point Energies= -841.083319
Sum of electronic and thermal Energies= -841.066188
Sum of electronic and thermal Enthalpies= -841.065244
Sum of electronic and thermal Free Energies= -841.128884

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	196.288	64.518	133.942

C	3.10435	0.46186	-1.07266
C	1.89828	0.39667	-0.34878
C	1.86234	-0.46713	0.76478
C	2.97737	-1.20718	1.13312
C	4.16572	-1.12839	0.4101
C	4.21191	-0.28627	-0.69863
H	3.15882	1.12068	-1.94145
H	0.93975	-0.55652	1.34031
H	2.91405	-1.86134	2.00282
H	5.03606	-1.71237	0.70286
H	5.12757	-0.20723	-1.28469
C	-2.78239	-0.64493	0.88248
H	-2.57157	-0.64401	1.95628
H	-3.46453	0.18562	0.64493
C	-1.4173	-1.28802	-0.96522
H	-1.08555	-0.68307	-1.81514
H	-0.6451	-2.03312	-0.73571
O	-1.52825	-0.41246	0.19164
C	-2.79617	-1.89515	-1.11735
H	-3.44213	-1.23044	-1.70789
H	-2.76526	-2.87075	-1.61276
C	-3.28109	-1.9612	0.32692
H	-4.36687	-2.06349	0.41975

H	-2.80928	-2.80176	0.85288
N	0.79105	1.13307	-0.71718
H	0.95972	1.65847	-1.57102
Al	-0.82566	1.44119	0.12658
C	-2.09187	2.29847	-1.12204
H	-2.4446	1.58994	-1.88861
H	-2.98743	2.68644	-0.61582
H	-1.64828	3.14636	-1.66292
C	-0.84262	1.8813	2.04408
H	-1.8644	1.97446	2.44119
H	-0.3242	1.13214	2.65967
H	-0.34588	2.84259	2.2361

$AlMe_3$ TS1

Zero-point correction=	0.292558
(Hartree/Particle)	
Thermal correction to Energy=	0.309688
Thermal correction to Enthalpy=	0.310633
Thermal correction to Gibbs Free Energy=	0.248165
Sum of electronic and zero-point Energies=	-841.015473
Sum of electronic and thermal Energies=	-840.998343
Sum of electronic and thermal Enthalpies=	-840.997399
Sum of electronic and thermal Free Energies=	-841.059866

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	194.332	66.156	131.475

C	2.13131	0.33708	0.92569
C	1.70397	0.1302	-0.401
C	2.6288	-0.4134	-1.31366
C	3.93014	-0.70014	-0.92688
C	4.34539	-0.47433	0.38356
C	3.43343	0.04168	1.30263
H	1.42578	0.74681	1.64781
H	2.31046	-0.59183	-2.34224
H	4.62768	-1.10757	-1.65758
H	5.36606	-0.70028	0.68547
H	3.74181	0.22056	2.3319
N	0.40105	0.38645	-0.76846
H	0.27988	0.24956	-1.77264
C	-0.75701	-1.70209	-0.24261

H	-0.75251	-1.92271	-1.30794
H	0.2201	-1.65687	0.23394
C	-3.37868	-0.44554	-0.13984
H	-3.55656	-0.0093	0.86235
H	-4.25016	-0.19404	-0.76688
O	-2.20293	0.01926	-0.7101
C	-3.24181	-1.9607	-0.00955
H	-3.30592	-2.42401	-1.0052
H	-4.03398	-2.39121	0.61486
C	-1.87053	-2.2008	0.58015
H	-1.65602	-3.28639	0.65698
H	-1.79602	-1.81056	1.60631
Al	-1.10577	1.29467	-0.01129
C	-1.12739	1.23002	1.96908
H	-2.12494	1.46206	2.37258
H	-0.83988	0.25279	2.38897
H	-0.44474	1.97308	2.40866
C	-1.40296	3.03883	-0.88521
H	-0.67392	3.79215	-0.55297
H	-1.3142	2.97123	-1.97933
H	-2.39973	3.45181	-0.67241

$AlMe_3$ intermediate 1

Zero-point correction=	0.298727
(Hartree/Particle)	
Thermal correction to Energy=	0.315408
Thermal correction to Enthalpy=	0.316352
Thermal correction to Gibbs Free Energy=	0.255617
Sum of electronic and zero-point Energies=	-841.095461
Sum of electronic and thermal Energies=	-841.078781
Sum of electronic and thermal Enthalpies=	-841.077837
Sum of electronic and thermal Free Energies=	-841.138572

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	197.921	64.706	127.828

C	1.75834	-1.38779	0.21153
C	1.35718	-0.26995	-0.51501
C	2.26377	0.76176	-0.76146
C	3.56038	0.67982	-0.27109

C	3.96388	-0.43034	0.4653
C	3.06048	-1.46022	0.69833
H	1.06618	-2.20289	0.40918
H	1.948	1.63237	-1.33752
H	4.25987	1.48925	-0.47016
H	4.97887	-0.49339	0.85164
H	3.36494	-2.33612	1.26803
C	-0.75194	-1.35026	-1.30891
H	-1.45949	-1.07507	-2.09965
H	-0.03498	-2.05925	-1.74651
C	-3.27798	-0.30422	0.60515
H	-2.96027	-0.37595	1.66661
H	-4.36903	-0.13595	0.62739
O	-2.65288	0.7555	-0.04503
C	-3.00362	-1.64187	-0.06307
H	-3.43941	-1.64071	-1.07533
H	-3.52994	-2.42655	0.50178
C	-1.51967	-2.00264	-0.15461
H	-1.43034	-3.09024	-0.2876
H	-1.03106	-1.7819	0.80725
Al	-1.01279	1.28496	0.26521
C	-0.29105	0.98111	2.07348
H	0.76705	1.27912	2.12601
H	-0.8275	1.58448	2.82024
H	-0.34033	-0.06247	2.41729
C	-0.61493	2.96453	-0.68742
H	-1.32636	3.74778	-0.38944
H	0.38849	3.35988	-0.4733
H	-0.70231	2.87529	-1.78144
N	-0.00063	-0.10433	-0.97756
H	0.04222	0.45461	-1.83239

$AlMe_3$ TS2

Zero-point correction=	0.246003
(Hartree/Particle)	
Thermal correction to Energy=	0.260353
Thermal correction to Enthalpy=	0.261297
Thermal correction to Gibbs Free Energy=	0.204645
Sum of electronic and zero-point Energies=	-800.546160
Sum of electronic and thermal Energies=	-800.531810
Sum of electronic and thermal Enthalpies=	-800.530865
Sum of electronic and thermal Free Energies=	-800.587517

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	163.374	55.484	119.233

C	1.87525	-0.99167	-0.72945
C	0.95281	-0.07954	-0.19207
C	1.44592	0.90774	0.6819
C	2.79619	1.00039	0.97915
C	3.70305	0.10058	0.42321
C	3.229	-0.89154	-0.42743
H	1.54524	-1.78076	-1.40135
H	0.75002	1.62121	1.13282
H	3.14198	1.7815	1.65391
H	4.76348	0.16979	0.65554
H	3.92181	-1.60775	-0.86677
C	-0.95124	-1.16548	-1.29507
H	-1.934	-0.84586	-1.67451
H	-0.315	-1.32555	-2.17704
C	-1.45347	-0.94514	1.46277
H	-0.40195	-0.95648	1.75584
H	-2.12541	-0.36462	2.08097
O	-2.84921	0.93024	0.70098
C	-1.98791	-2.09369	0.71703
H	-3.02988	-1.89292	0.43907
H	-2.00045	-2.93639	1.43428
C	-1.13792	-2.4489	-0.49059
H	-1.61106	-3.23254	-1.09515
H	-0.16066	-2.83191	-0.16163
Al	-1.54805	1.40779	-0.18596
C	-0.87852	3.08787	-0.91351
H	-0.73945	3.81685	-0.10394
H	0.08844	2.95797	-1.41602
H	-1.57911	3.53555	-1.62908
N	-0.4221	-0.105	-0.44471

$Ti(O^iPr)_4$

Zero-point correction= (Hartree/Particle)	0.391074
Thermal correction to Energy=	0.415141
Thermal correction to Enthalpy=	0.416085

Thermal correction to Gibbs Free Energy= 0.335812
Sum of electronic and zero-point Energies= -832.703851
Sum of electronic and thermal Energies= -832.679784
Sum of electronic and thermal Enthalpies= -832.678839
Sum of electronic and thermal Free Energies= -832.759112

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	260.505	86.358	168.948

Ti	0.07173	0.07684	-0.30361
O	1.38226	-0.82808	-1.13752
O	0.51174	1.79628	0.0235
O	-1.45378	-0.05112	-1.268
O	-0.20111	-0.71028	1.28401
C	2.77242	-1.07364	-1.11876
H	2.90558	-2.12487	-0.80418
C	3.47085	-0.16757	-0.12107
H	3.35605	0.88478	-0.41739
H	3.04634	-0.28768	0.88621
H	4.54297	-0.39785	-0.07011
C	3.32442	-0.90264	-2.52053
H	4.39522	-1.14261	-2.54999
H	2.80085	-1.55651	-3.22776
H	3.19274	0.13774	-2.8489
C	0.25149	2.78812	0.99245
H	0.59951	2.40749	1.97161
C	1.03773	4.03552	0.63907
H	0.69514	4.4348	-0.32571
H	0.90311	4.81195	1.40332
H	2.10782	3.80878	0.55716
C	-1.24037	3.05889	1.06673
H	-1.6094	3.38281	0.08283
H	-1.7938	2.15584	1.36241
H	-1.46262	3.84674	1.79864
C	-2.80062	-0.34383	-0.95158
H	-2.93653	-0.22977	0.14161
C	-3.70343	0.64212	-1.66607
H	-4.75712	0.45778	-1.41863
H	-3.45436	1.67254	-1.38447
H	-3.58005	0.54349	-2.75345
C	-3.10119	-1.77861	-1.33916
H	-2.9605	-1.91034	-2.42096

H	-2.42636	-2.4711	-0.81841
H	-4.13626	-2.04597	-1.08822
C	0.22656	-1.86368	1.98387
H	1.32772	-1.92568	1.89932
C	-0.38707	-3.09302	1.34335
H	-0.06463	-4.00779	1.85753
H	-1.48424	-3.03354	1.39813
H	-0.09358	-3.16509	0.28693
C	-0.15595	-1.72291	3.44317
H	-1.24864	-1.65795	3.53977
H	0.19177	-2.589	4.02085
H	0.28333	-0.81638	3.87655

$Ti(O^iPr)_4$ starting complex

Zero-point correction= 0.629457
(Hartree/Particle)
Thermal correction to Energy= 0.664551
Thermal correction to Enthalpy= 0.665496
Thermal correction to Gibbs Free Energy= 0.563315
Sum of electronic and zero-point Energies= -1352.199441
Sum of electronic and thermal Energies= -1352.164347
Sum of electronic and thermal Enthalpies= -1352.163403
Sum of electronic and thermal Free Energies= -1352.265583

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	417.012	133.688	215.057

C	-3.41624	0.65138	-1.4876
C	-2.5611	-0.44536	-1.38892
C	-3.05006	-1.6691	-0.93466
C	-4.38747	-1.79102	-0.57699
C	-5.24718	-0.69928	-0.67562
C	-4.75503	0.5198	-1.13507
H	-3.02464	1.60978	-1.83314
H	-2.36508	-2.51214	-0.84823
H	-4.76119	-2.74977	-0.22011
H	-6.29511	-0.79863	-0.3992
H	-5.41777	1.3797	-1.21891
C	2.92642	-0.71735	-1.85781
H	2.89004	-0.17688	-2.81169

H	3.20077	-0.0083	-1.06829
C	1.64801	-2.63526	-1.4576
H	0.85849	-2.93921	-0.76392
H	1.44533	-3.07231	-2.45092
O	1.6026	-1.20776	-1.55041
C	3.06247	-2.93888	-1.01743
H	3.17703	-2.70924	0.05296
H	3.35329	-3.98155	-1.18655
C	3.83815	-1.9398	-1.87041
H	4.83641	-1.71178	-1.47967
H	3.95785	-2.33261	-2.8898
Ti	0.37906	0.19557	0.0232
N	-1.18231	-0.30636	-1.69997
H	-0.77988	-1.17264	-2.05449
H	-1.01058	0.42215	-2.39132
O	-0.72844	1.36044	0.85624
O	0.97804	1.43056	-1.25232
O	1.88278	0.19384	1.06491
O	-0.25041	-1.44138	0.68031
C	-1.40904	1.42328	2.08964
H	-0.71807	1.06587	2.87807
C	-1.76349	2.8726	2.36859
H	-2.29403	2.97202	3.32522
H	-0.86323	3.50045	2.40529
H	-2.41561	3.25457	1.56925
C	-2.64046	0.53597	2.08087
H	-3.38574	0.91771	1.36831
H	-2.37666	-0.4861	1.77892
H	-3.09748	0.50715	3.08019
C	0.4892	2.61675	-1.79653
H	-0.62453	2.59237	-1.79901
C	0.91653	3.80462	-0.95001
H	2.01496	3.85594	-0.91
H	0.54005	4.74952	-1.36642
H	0.53499	3.69468	0.07291
C	0.97113	2.7515	-3.23281
H	0.56812	3.6538	-3.71276
H	2.0695	2.80996	-3.25079
H	0.67359	1.87794	-3.83047
C	2.82276	1.17395	1.41797
H	3.03771	1.79307	0.5229
C	2.25721	2.07637	2.50108
H	2.97038	2.86812	2.7683
H	1.32394	2.54385	2.16074

H	2.03685	1.48842	3.40484
C	4.09815	0.48657	1.87321
H	3.88751	-0.13547	2.7559
H	4.49457	-0.16737	1.08451
H	4.87267	1.21792	2.14059
C	0.15208	-2.35701	1.66076
H	1.19304	-2.68145	1.43961
C	-0.75526	-3.57698	1.61524
H	-0.73688	-4.05472	0.62585
H	-0.45658	-4.32518	2.36225
H	-1.79215	-3.27356	1.82477
C	0.15191	-1.73903	3.051
H	0.81499	-0.86563	3.07767
H	-0.86493	-1.42016	3.32497
H	0.49621	-2.46615	3.79989

$Ti(O^iPr)_4$ TS1

Zero-point correction=	0.625231
(Hartree/Particle)	
Thermal correction to Energy=	0.660755
Thermal correction to Enthalpy=	0.661699
Thermal correction to Gibbs Free Energy=	0.559456
Sum of electronic and zero-point Energies=	-1352.112094
Sum of electronic and thermal Energies=	-1352.076570
Sum of electronic and thermal Enthalpies=	-1352.075626
Sum of electronic and thermal Free Energies=	-1352.177869

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	414.630	135.908	215.189

C	1.51824	-2.14518	-0.58742
H	2.52895	-2.20001	-0.98493
H	1.3775	-1.55476	0.32042
C	-0.81859	-1.86751	-2.41304
H	-1.77975	-2.19679	-1.98093
H	-1.00375	-1.52611	-3.44736
O	-0.24915	-0.8557	-1.66068
C	0.13772	-3.05607	-2.42889
H	1.00396	-2.8528	-3.0772
H	-0.34882	-3.97187	-2.78707

C	0.59732	-3.21408	-0.97278
H	1.17875	-4.14975	-0.88452
H	-0.28005	-3.24887	-0.31262
C	4.77721	-0.22471	-1.27008
C	3.55088	0.07063	-0.65923
C	3.51193	0.30192	0.72536
C	4.68557	0.27857	1.46591
C	5.90835	0.00741	0.85303
C	5.94394	-0.24877	-0.51585
H	4.80865	-0.41711	-2.34328
H	2.5431	0.48326	1.19432
H	4.64217	0.46833	2.53795
H	6.82517	-0.01013	1.43896
H	6.89227	-0.46626	-1.00501
Ti	-0.97936	0.14989	-0.15556
N	2.36465	0.01861	-1.37679
H	1.58841	0.64176	-1.10978
H	2.45529	-0.03503	-2.38634
O	0.19264	0.0905	1.27305
O	-0.06366	1.62533	-1.00041
O	-1.9689	-1.38606	0.29244
O	-2.40999	1.21861	0.27832
C	-0.16282	-0.15446	2.6166
H	-1.26579	-0.20396	2.69982
C	0.33134	0.99739	3.47255
H	1.42765	1.07348	3.41138
H	-0.09731	1.94598	3.12133
H	0.05362	0.85811	4.52609
C	0.41421	-1.48819	3.05344
H	1.5123	-1.46893	2.97323
H	0.15075	-1.71635	4.09546
H	0.02594	-2.29486	2.41601
C	0.03055	2.94517	-0.54161
H	-0.75805	3.12816	0.21884
C	1.37895	3.18411	0.12098
H	2.19192	3.03147	-0.60604
H	1.45621	4.21104	0.50477
H	1.52523	2.48872	0.95737
C	-0.17637	3.90833	-1.70082
H	0.61769	3.76704	-2.44905
H	-1.1396	3.72505	-2.19593
H	-0.15126	4.95455	-1.36498
C	-3.30484	2.041	-0.41886
H	-2.73947	2.86757	-0.89205

C	-4.00603	1.26101	-1.51955
H	-4.67414	1.91041	-2.10172
H	-3.27367	0.81872	-2.21277
H	-4.60657	0.44741	-1.08645
C	-4.29563	2.63823	0.56327
H	-4.99196	3.32118	0.05829
H	-4.87846	1.83861	1.04313
H	-3.76845	3.19532	1.3482
C	-3.23987	-1.70673	0.75921
H	-3.77194	-0.76564	1.01678
C	-4.03147	-2.43185	-0.31954
H	-3.53236	-3.37975	-0.57532
H	-5.05244	-2.66051	0.0165
H	-4.09487	-1.82407	-1.2327
C	-3.13455	-2.56721	2.01012
H	-4.12814	-2.84074	2.39161
H	-2.58641	-3.49402	1.77975
H	-2.59274	-2.04151	2.80711

$Ti(O^iPr)_4$ intermediate1

Zero-point correction=	0.519874
(Hartree/Particle)	
Thermal correction to Energy=	0.549831
Thermal correction to Enthalpy=	0.550775
Thermal correction to Gibbs Free Energy=	0.459414
Sum of electronic and zero-point Energies=	-1158.057713
Sum of electronic and thermal Energies=	-1158.027757
Sum of electronic and thermal Enthalpies=	-1158.026813
Sum of electronic and thermal Free Energies=	-1158.118173

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	345.024	112.483	192.284

C	-4.01403	-0.38399	0.29333
C	-2.71045	-0.24131	0.7899
C	-2.41872	0.88219	1.58473
C	-3.39295	1.82925	1.85843
C	-4.68513	1.69263	1.34867
C	-4.98169	0.57941	0.57116
H	-4.28169	-1.24782	-0.31277

H	-1.40811	1.00195	1.97767
H	-3.13824	2.68904	2.47806
H	-5.4471	2.44002	1.56089
H	-5.98617	0.44716	0.17018
C	-1.98208	-2.47018	-0.00393
H	-1.12456	-3.10634	0.25983
H	-2.85919	-2.89127	0.51938
C	0.01222	-1.77649	-2.58215
H	-0.50672	-0.85846	-2.91759
H	0.7118	-2.06201	-3.38424
O	0.75956	-1.50964	-1.42694
C	-1.00346	-2.88465	-2.37898
H	-0.48665	-3.76578	-1.96475
H	-1.35839	-3.17741	-3.37938
C	-2.21541	-2.53383	-1.51971
H	-2.99465	-3.28694	-1.71158
H	-2.63214	-1.5725	-1.86203
Ti	1.14392	-0.19168	-0.26795
N	-1.69164	-1.14286	0.50862
H	-0.93569	-1.11594	1.18833
O	0.19851	1.29784	-0.48029
O	2.87189	0.23124	-0.59465
O	1.04393	-0.73719	1.47795
C	1.80822	-1.57986	2.31812
H	1.10547	-2.03351	3.03988
C	2.46698	-2.68728	1.5149
H	3.0277	-3.36751	2.16932
H	1.71624	-3.2733	0.96802
H	3.16977	-2.2581	0.78416
C	2.82282	-0.74911	3.07944
H	3.38264	-1.36662	3.79404
H	3.54019	-0.30072	2.37663
H	2.32745	0.06043	3.62902
C	3.6417	1.35143	-0.19606
H	3.22098	1.75496	0.74696
C	5.06769	0.89783	0.04963
H	5.49517	0.49675	-0.87978
H	5.69196	1.73567	0.38631
H	5.10656	0.10744	0.81064
C	3.567	2.4239	-1.26607
H	3.97424	2.03956	-2.21157
H	2.52672	2.72934	-1.43902
H	4.14488	3.31063	-0.97397
C	-0.28949	2.39404	-1.22085

H	0.41009	2.57207	-2.0593
C	-1.66017	2.0627	-1.77986
H	-2.37536	1.91153	-0.96011
H	-2.02177	2.87905	-2.41895
H	-1.6242	1.14182	-2.3782
C	-0.31714	3.61813	-0.32574
H	0.67861	3.81763	0.09192
H	-0.64367	4.50286	-0.88757
H	-1.01747	3.4565	0.50581

$Ti(O^iPr)_4$ TS2

Zero-point correction= (Hartree/Particle)	0.515105
Thermal correction to Energy=	0.545180
Thermal correction to Enthalpy=	0.546124
Thermal correction to Gibbs Free Energy=	0.453229
Sum of electronic and zero-point Energies=	-1157.973232
Sum of electronic and thermal Energies=	-1157.943158
Sum of electronic and thermal Enthalpies=	-1157.942214
Sum of electronic and thermal Free Energies=	-1158.035108

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	342.106	113.037	195.514

C	4.47133	0.40434	-0.23605
C	3.25758	-0.27919	-0.09976
C	3.2639	-1.68248	-0.04687
C	4.4596	-2.37968	-0.111
C	5.6707	-1.69785	-0.23791
C	5.66572	-0.30934	-0.29988
H	4.49453	1.49187	-0.27183
H	2.3124	-2.20722	0.051
H	4.44744	-3.46708	-0.06012
H	6.60858	-2.24726	-0.28815
H	6.60393	0.23473	-0.39756
C	1.89231	1.78399	0.20227
H	0.90939	1.93012	0.6729
H	2.66074	2.13128	0.91025
C	1.27778	0.55287	-2.39683
H	2.30524	0.18985	-2.39248

H	0.57427	-0.01704	-2.9904
O	-0.34754	-0.92316	-1.42468
C	0.96951	1.9394	-2.07344
H	-0.07337	1.98896	-1.70539
H	0.96026	2.46121	-3.05183
C	1.93782	2.5806	-1.10242
H	1.67199	3.62815	-0.9123
H	2.95287	2.57763	-1.52665
Ti	-1.30102	-0.48847	-0.11104
N	2.01858	0.36334	-0.06278
H	1.2967	-0.20422	0.39905
O	-0.1911	-0.87616	1.35273
O	-2.89562	-1.40192	-0.11836
O	-1.54876	1.34915	-0.22009
C	-3.59108	-2.09149	-1.12896
H	-2.86592	-2.67654	-1.72755
C	-4.58597	-3.0463	-0.4954
H	-5.31469	-2.4828	0.10468
H	-5.13242	-3.61235	-1.26177
H	-4.07577	-3.75781	0.16523
C	-4.28268	-1.09572	-2.0462
H	-5.03757	-0.52648	-1.48326
H	-3.55654	-0.38236	-2.46208
H	-4.78618	-1.6036	-2.88013
C	-0.26452	-0.78198	2.75085
H	-0.2102	-1.80639	3.16566
C	0.928	0.00774	3.26443
H	0.9479	0.03753	4.36193
H	1.86991	-0.43477	2.91182
H	0.87397	1.04381	2.89421
C	-1.57155	-0.15215	3.20129
H	-1.62985	0.88795	2.8447
H	-2.43575	-0.7012	2.80155
H	-1.65268	-0.13967	4.29673
C	-2.46948	2.39949	-0.14085
H	-2.7909	2.6584	-1.17027
C	-3.70132	1.99989	0.6525
H	-4.16808	1.10728	0.21574
H	-3.42334	1.76242	1.6901
H	-4.44069	2.81201	0.67261
C	-1.78288	3.61285	0.46442
H	-0.89607	3.88991	-0.12282
H	-2.45572	4.48009	0.50056
H	-1.45648	3.38327	1.49023