Supporting Information

(83 Pages including the cover page)

Understanding Cyclic(alkyl)(amino)carbene-Copper Complex Catalysed N-H and O-H Bond Addition to Electron Deficient Olefin

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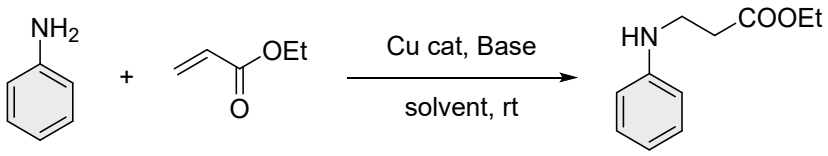
Contents

1. Optimisation of reaction conditions

Table S1: Optimization studies.[a]



Entry	Base	1 (mol%)	Solvent	Yield (%)[b]
1.	^{t}BuOK	10	Toluene	98
2.	^{t}BuOK	5	Toluene	98
3.	^{t}BuOK	4	Toluene	80
4.	Cs_2CO_3	5	Toluene	92
5.	Na_2CO_3	5	Toluene	70
6.	Et_3N	5	Toluene	88
7.	NaOAc	5	Toluene	75
8.	^{t}BuOK	5	THF	90
9.	^{t}BuOK	5	CH_3CN	88
10.	^{t}BuOK	5	CH_2Cl_2	80
11.	^{t}BuOK	—	Toluene	—
12.	—	5		—
13.	—	—	Toluene	—

[a]Reaction conditions: Aniline/ethyl acrylate/base/catalyst = 1.1/1/0.05/0.05 mmol), solvent (2 mL) at RT. [b]Determined by GC–MS using *mesitylene* as an internal standard.

2. Experimental Section

2a. Instrumentation and metarials

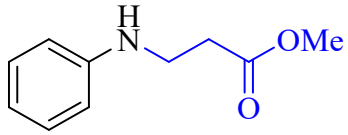
Unless otherwise stated, all reactions were performed under an open atmosphere. The ligand precursor CAAC.HCl (ref1) and Cu-CAAC complex **1(**ref2**)** were synthesized according to the literature procedure. Solvents for synthesis were dried by following the conventional procedures. All other chemicals were purchased from Sigma–Aldrich and Spectrochem chemicals Pvt. Ltd. ^{1}H-NMR spectra were recorded using Bruker 400 & 500 MHz NMR spectrometers, and ^{13}C-NMR were recorded at 75.47 and 100 & 125 MHz respectively. All chemical shifts (δ) re reported in ppm. All chemical shifts are related to residual solvent peaks [$CDCl_3$: 7.26 (^{1}H), 77.16 (^{13}C)]. Chromatographic purification of products was undertaken on silica gel (230-400 mesh) using a proper eluent system. The GC-MS

experiments were performed by using an Agilent 7890A GC and 5977B MS system. *We thank Central Research Facility, IIT Delhi for providing the access to GC-MS Instrument.*

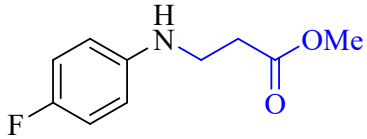
2b. General procedure for catalytic alkene hydroamination/hydroaryloxylation

An oven-dried reaction vessel was charged with **1** (0.05 mmol), alkene (1 mmol), aniline/alcohol (1.1 mmol), ^{t}BuOK (0.05 mmol) and mesitylene (1 mmol) in 2 mL of toluene stirred at room temperature for 6 h. The reaction mixture was cooled, diluted with ethyl acetate and washed with aqueous NH_4Cl solution. Organic phase was combined and passed through a short column of silica for GC–MS analysis to determine the yield. For NMR characterization of the product, the solvent was evaporated under vacuum and the residue was purified by column chromatography on silica gel (by petroleum ether/ethyl acetate).

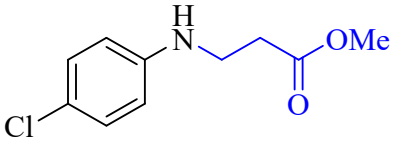
3. Spectroscopic Characterizations of Products



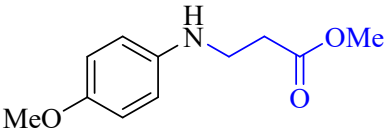
4a: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (dd, J = 8, 7.3 Hz, 2H), 6.77 – 6.74 (m, 1H), 6.65 (d, J = 8.9, 1.7 Hz, 2H), 4.05 (br, 1H), 3.73 (s, 3H), 3.49 (t, J = 6.2 Hz, 2H), 2.66 (t, J = 6.4 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.85, 147.58, 129.34, 117.77, 113.06, 51.77, 39.42, 33.7



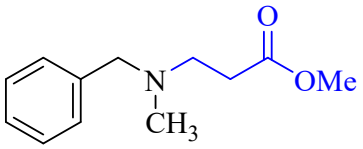
4b: ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.91 (t, J = 8.7 Hz, 2H), 6.58 (dd, J = 9.0, 4.4 Hz, 2H), 3.93 (br, 1H), 3.73 (s, 3H), 3.43 (t, J = 6.3 Hz, 2H), 2.64 (t, J = 6.3 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.78, 156.98, 155.10, 143.92, 115.74, 114.0, 51.77, 33.64.



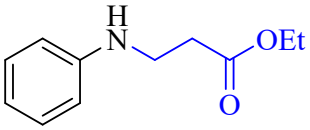
4c: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (d, *J* = 8.9 Hz, 2H), 6.54 (d, *J* = 8.9 Hz, 2H), 4.04 (br, 1H), 3.70 (s, 3H), 3.42 (q, *J* = 5.9 Hz, 2H), 2.61 (t, *J* = 6.3 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.13, 145.73, 129.14, 122.32, 115.82, 114.10, 51.84, 39.51, 33.51.



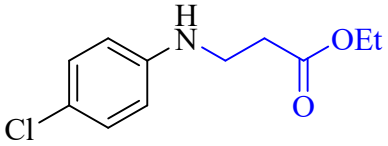
4d: ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.81 (d, *J* = 8.9 Hz, 2H), 6.63 (d, *J* = 8.9 Hz, 2H), 3.77 (s, 3H), 3.72 (s, 3H), 3.43 (t, *J* = 6.4 Hz, 2H), 2.64 (t, *J* = 6.3 Hz, 2H), 1.63 (br, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.13, 152.44, 141.73, 114.94, 114.62, 55.80, 51.77, 40.52, 33.76



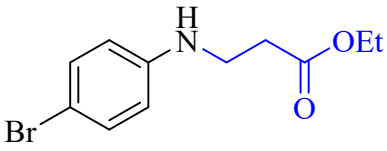
4e: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.13 (m, 5H), 3.60 (s, 3H), 3.44 (s, 2H), 2.68 (t, *J* = 7.2 Hz, 2H), 2.46 (t, *J* = 7.2 Hz, 2H), 2.14 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.17, 128.98, 128.24, 127.06, 77.30, 77.04, 76.79, 62.10, 52.68, 51.64, 41.91, 32.68



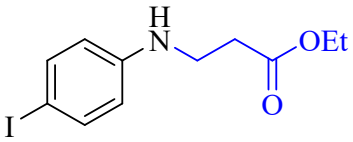
4f: 1H NMR (400 MHz, CDCl3) δ 7.18 (dd, J = 8.5, 7.4 Hz, 2H), 6.71 (t, J = 7.3 Hz, 1H), 6.62 (d, J = 7.7 Hz, 2H), 4.15 (q, J = 7.1 Hz, 2H), 4.02 (s, 1H), 3.45 (t, J = 6.2 Hz, 2H), 2.61 (t, J = 6.4 Hz, 2H), 1.26 (t, J = 7.1 Hz, 3H), ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.42, 147.22, 129.33, 117.72, 113.06, 60.68, 39.42, 33.94, 14.23



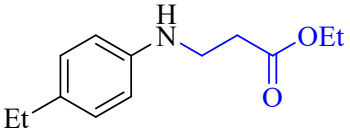
4g: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.9 Hz, 2H), 6.56 (d, *J* = 8.9 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 4.08 (br, 1H), 3.44 (d, *J* = 10.6, 4.2 Hz, 2H), 2.62 (t, *J* = 6.3 Hz, 2H), 1.29 (t, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.42, 146.19, 129.13, 121.94, 114.11, 60.75, 39.54, 33.74, 14.21.



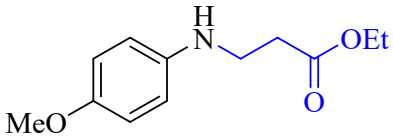
4h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, *J* = 9.0 Hz, 2H), 6.42 (d, *J* = 8.9 Hz, 2H), 4.08 (q, *J* = 7.1 Hz, 2H), 4.01 (br, 1H), 3.34 (t, *J* = 6.3 Hz, 2H), 2.5(t, J= 6.3Hz, 2H), 1.02 (d, *J* = 6.8 Hz, 3H)



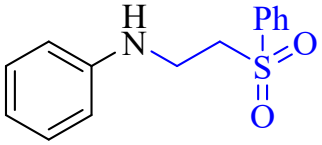
4i: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.8 Hz, 2H), 6.43 (d, *J* = 8.8 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.43 (t, *J* = 6.3 Hz, 2H), 2.61 (t, *J* = 6.3 Hz, 2H), 1.62 (br, 1H), 1.28 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.24, 147.21, 137.86, 115.22, 78.25, 60.73, 39.26, 33.71, 14.20.



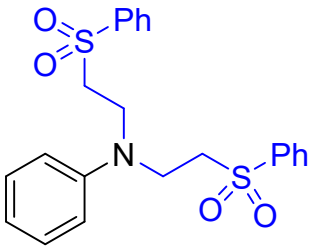
4j: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (d, *J* = 8.3 Hz, 2H), 6.60 (d, *J* = 8.4 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.93 (s, 1H), 3.46 (t, *J* = 6.4 Hz, 2H), 2.63 (t, *J* = 6.4 Hz, 2H), 2.57 (q, *J* = 7.6 Hz, 2H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.22 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.47, 145.56, 133.65, 128.61, 113.28, 60.59, 39.83, 34.04, 27.92, 15.94, 14.21.



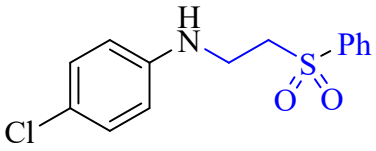
4k: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 (d, *J* = 5.2, 2H), 6.5 (d, *J* = 5.2 Hz, 2H), 4.17 (q, *J* = 6 Hz, 2H), 3.7 (s, 3H), 3.4 (t, *J* = 7.3 Hz, 2H), 2.5 (t, *J* = 7.3 Hz, 2H), 1.2 (t, J= 6.5, 3H), ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.42, 152.22, 141.75, 114.94, 114.67, 60.61, 55.80, 40.62, 33.99, 18.63, 14.21.



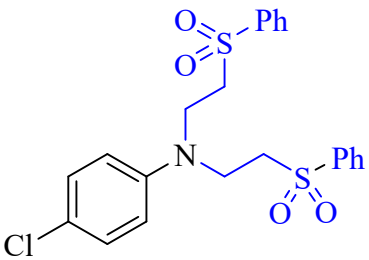
4l: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 5.2, 3.4 Hz, 2H), 7.68 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.58 (t, *J* = 7.6 Hz, 2H), 7.16 (dd, *J* = 8.5, 7.4 Hz, 2H), 6.74 (t, *J* = 7.3 Hz, 1H), 6.58 – 6.49 (m, 2H), 4.14 (br, 1H), 3.60 (t, J = 6.2Hz, 2H), 3.37 (t, *J* = 6.2 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.48, 134.01, 129.50, 129.43, 127.99, 118.42, 113.12, 54.83, 37.70.



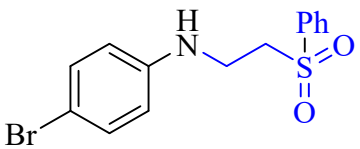
4l':^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.2 Hz, 4H), 7.61 (t, *J* = 7.4 Hz, 2H), 7.51 (t, *J* = 7.7 Hz, 4H), 7.12 – 7.06 (t, J = 7.3 Hz, 2H), 6.70 (t, *J* = 7.3 Hz, 1H), 6.37 (d, *J* = 8.1 Hz, 2H), 3.66 – 3.60 (t, J = 7Hz, 4H), 3.23 – 3.17 (t, J = 7 Hz, 4H).^{13}C NMR (126 MHz, $CDCl_3$) δ 144.96, 139.21, 134.02, 131.72, 129.80, 129.48, 127.82, 118.72, 113.07, 52.86, 44.98.



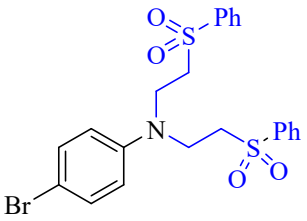
4m: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.3 Hz, 2H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 8.8 Hz, 2H), 6.46 (d, *J* = 8.8 Hz, 2H), 4.22 (br, 1H), 3.58 (t, *J* = 6.1 Hz, 2H), 3.35 (t, *J* = 6.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.15, 138.96, 134.09, 129.54, 129.25, 127.94, 123.02, 114.20, 54.63, 37.84.



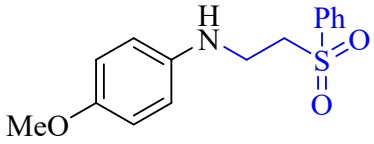
4m′: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.2 Hz, 4H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.7 Hz, 5H), 7.04 (d, *J* = 9.0 Hz, 2H), 6.30 (d, *J* = 9.1 Hz, 2H), 3.62(t, J = 8 Hz, 4H), 3.18 (t, J = 8 Hz, 4H).



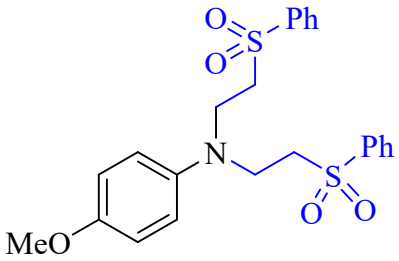
4n: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.2 Hz, 2H), 7.72 – 7.66 (m, 1H), 7.61 – 7.56 (m, 2H), 7.24 (d, *J* = 8.9 Hz, 2H), 6.41 (d, *J* = 8.9 Hz, 2H), 4.24 (s, 1H), 3.57 (dd, *J* = 12.4, 6.2 Hz, 2H), 3.35 (t, *J* = 6.2 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.96, 138.84, 134.15, 132.13, 129.57, 127.96, 114.66, 54.55, 37.89.



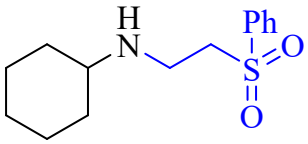
4n´: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.2 Hz, 4H), 7.62 (t, *J* = 7.5 Hz, 2H), 7.52 (t, *J* = 7.7 Hz, 4H), 7.17 (d, *J* = 9.1 Hz, 2H), 6.25 (d, *J* = 9.1 Hz, 2H), 3.62 (t, J = 8 Hz 4H), 3.18 (t, J = 8 Hz, 4H)



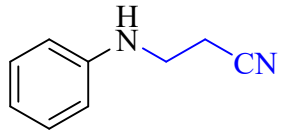
4o: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 – 7.84 (m, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 2H), 6.70 (d, *J* = 8.9 Hz, 2H), 6.46 (d, *J* = 8.9 Hz, 2H), 3.84 (s, 1H), 3.68 (s, 3H), 3.49 (t, *J* = 6.2 Hz, 2H), 3.28 (t, *J* = 6.2 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.83, 140.53, 139.12, 133.96, 129.47, 127.97, 115.00, 114.78, 55.75, 54.84, 38.79



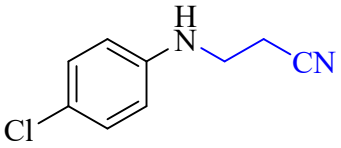
4o´: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.2 Hz, 4H), 7.63 – 7.57 (m, 2H), 7.50 (t, *J* = 7.7 Hz, 4H), 6.66 (d, *J* = 9.1 Hz, 2H), 6.41 (d, J = 9.1 Hz, 2H), 3.67 (s, 3H), 3.48 (t, J = 8 Hz, 4H), 3.12 (t, J = 8 Hz, 4H).^{13}C NMR (126 MHz, $CDCl_3$) δ 153.71, 139.61, 133.50, 129.42, 127.83, 117.62, 114.34, 55.22, 52.30, 45.82.



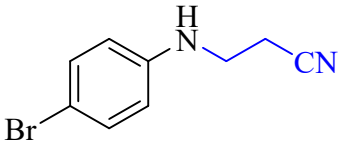
4p :^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.4 Hz, 2H), 7.70 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.7 Hz, 2H), 3.40 (t, *J* = 6.5 Hz, 2H), 3.14 (t, *J* = 6.5 Hz, 2H), 2.53-2.50 (m, 1H), 1.90-1.62 (m, 2H), 1.30-1.14 (m, 9H), ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.96, 134.04, 129.46, 128.00, 56.65, 54.65, 39.20, 31.82, 25.60, 24.73.



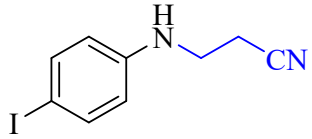
4q :^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 – 7.11 (t, *J* = 8.0 Hz, 2H), 6.71 (t, *J* = 7.4 Hz, 1H), 6.59 – 6.51 (d, *J* = 8.0 Hz, 2H), 3.90 (br, 1H), 3.45 (t, *J* = 6.5 Hz, 2H), 2.56 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.13, 129.56, 118.68, 113.10, 39.83, 18.16.



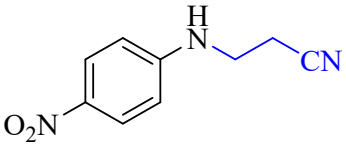
4r: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18 (d, *J* = 8.9 Hz, 2H), 6.57 (d, *J* = 8.8 Hz, 2H), 4.03 (br, 1), 3.51 (t, *J* = 6.3 Hz, 2H), 2.65 (t, *J* = 6.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.76, 129.40, 123.32, 117.99, 114.19, 39.87, 18.09.



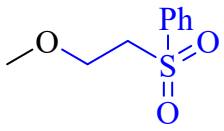
4s: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.9 Hz, 2H), 6.44 (d, *J* = 8.9 Hz, 2H), 3.93 (s, 1H), 3.43 (t, *J* = 6.6 Hz, 2H), 2.56 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.10, 139.29, 132.29, 114.65, 110.35, 39.79, 18.08.



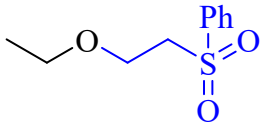
4t: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.8 Hz, 2H), 6.43 (d, *J* = 8.8 Hz, 2H), 4.05 (br, 1H), 3.52 (t, *J* = 6.4 Hz, 2H), 2.65 (t, *J* = 6.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.79, 138.15, 117.77, 115.22, 39.69, 18.05.



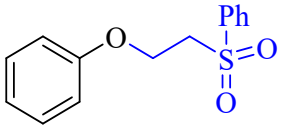
4u: ^{1}H NMR (500 MHz, DMSO) δ 8.07 (d, *J* = 9.0 Hz, 2H), 7.02 (d, *J* = 9.0 Hz, 2H), 3.86 (t, *J* = 6.8 Hz, 2H), 2.83 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (126 MHz, DMSO) δ 152.09, 137.52, 126.29, 119.48, 112.12, 46.04, 15.67.



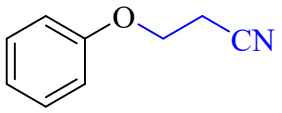
6a: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.3 Hz, 2H), 7.68 (t, *J* = 7.5 Hz, 2H), 7.59 (t, *J* = 7.7 Hz, 2H), 3.76 (t, *J* = 6.3 Hz, 2H), 3.41 (t, *J* = 6.3 Hz, 2H), 3.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 133.72, 129.15, 128.03, 65.68, 58.71, 56.17



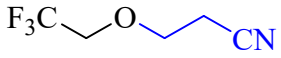
6b: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.7 Hz, 2H), 3.80 (t, *J* = 6.3 Hz, 2H), 3.42 (t, *J* = 6.3 Hz, 2H), 3.38 (q, *J* = 7.0 Hz, 2H), 1.04 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 133.63, 129.07, 128.11, 66.53, 63.72, 56.34, 14.77.



6c: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 – 7.67 (m, 2H), 7.55 (s, 1H), 7.42 (d, *J* = 17.8 Hz, 2H), 7.09 (d, *J* = 17.6 Hz, 2H), 6.83 (s, 1H), 6.67 – 6.37 (m, 2H), 4.24 (t, J = 6.4 Hz, 2H), 3.47 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.42, 139.87, 133.84, 129.53, 129.23, 128.22, 121.55, 114.32, 61.36, 55.84.

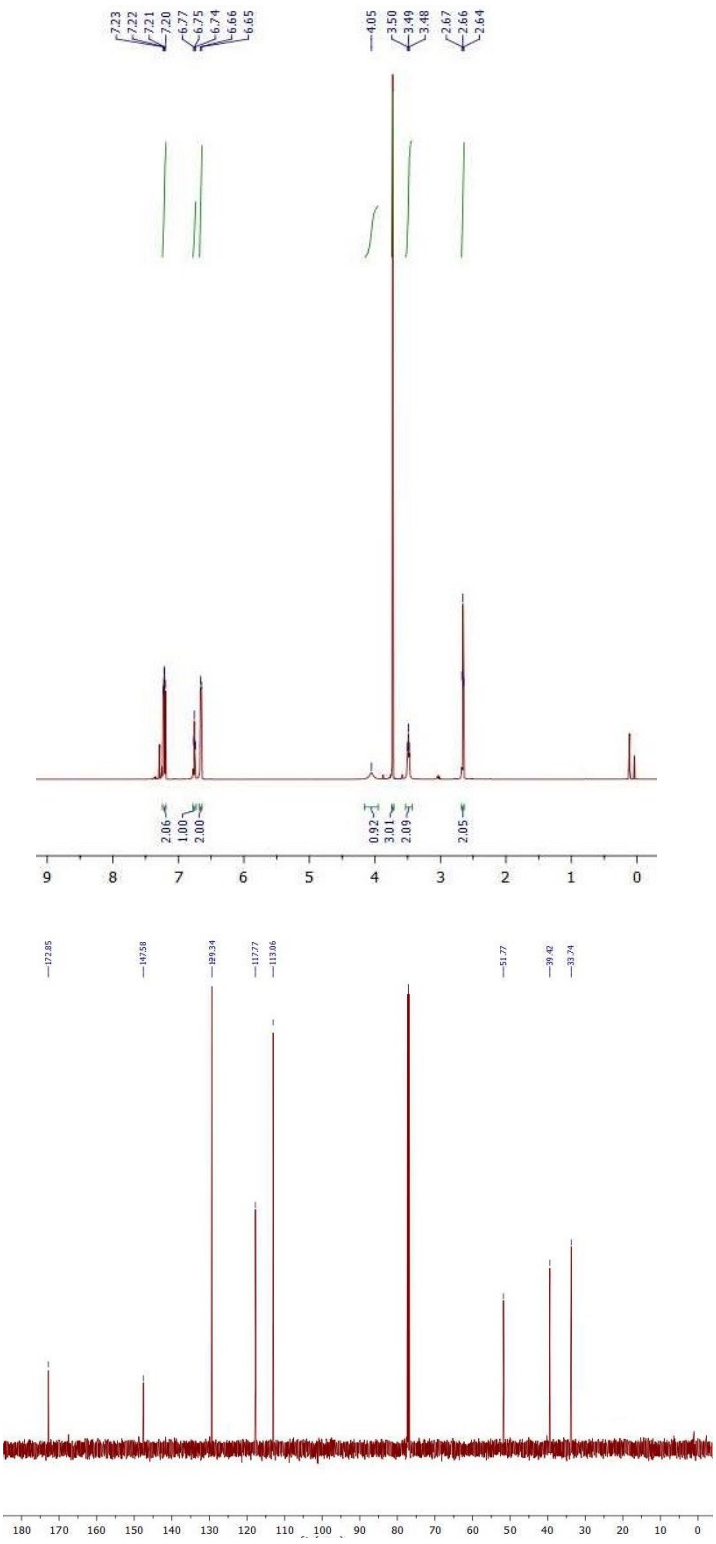


6d: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 – 7.32 (m, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.94 (d, *J* = 7.8 Hz, 2H), 4.23 (t, *J* = 6.4 Hz, 2H), 2.86 (t, *J* = 6.4 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.29, 129.67, 121.86, 114.71, 62.60, 18.63.

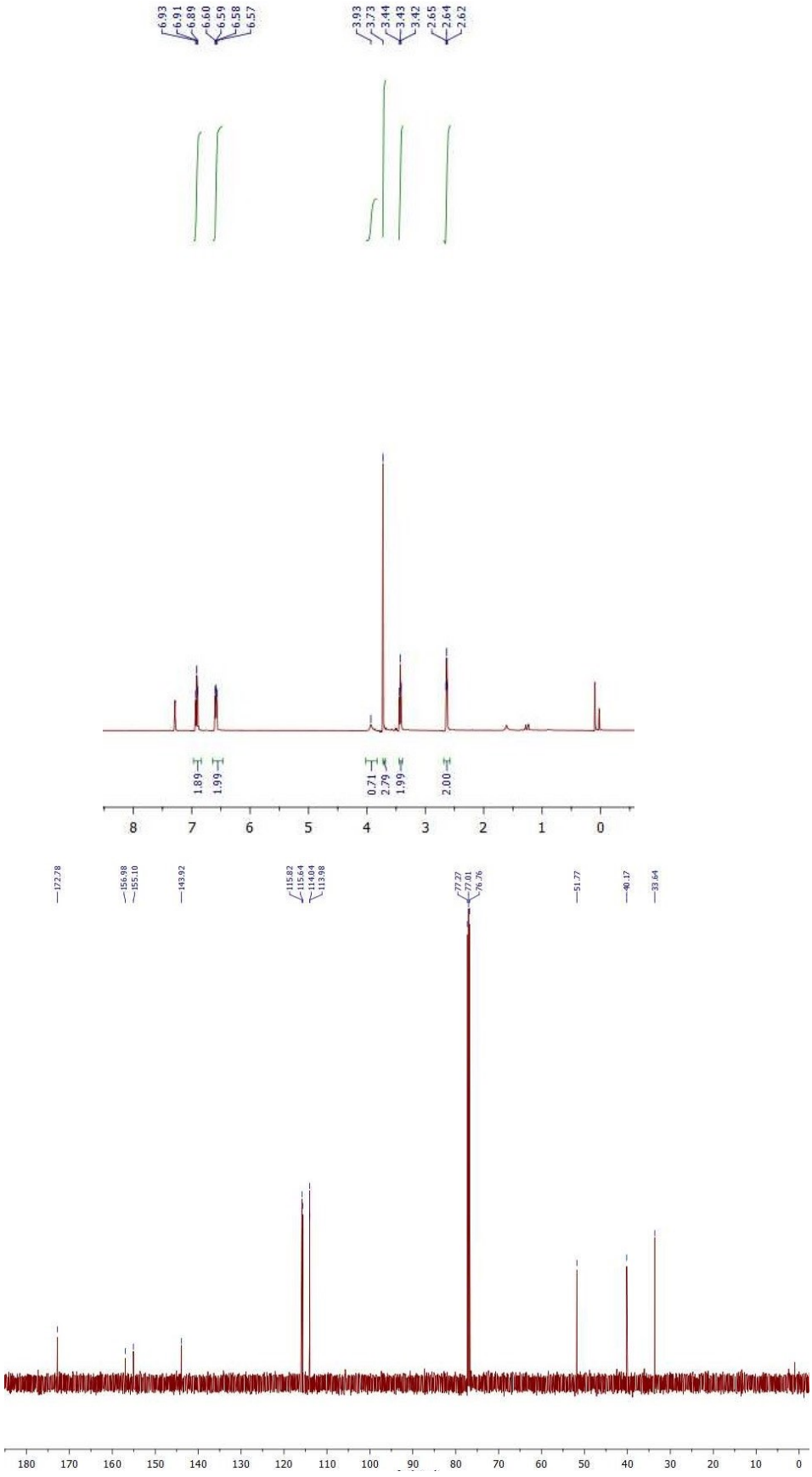


6e: ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.94 (q, *J* = 7.8 Hz, 2H), 3.88 (t, *J* = 5.1 Hz, 2H), 2.69 (t, *J* = 5.6 Hz, 2H).

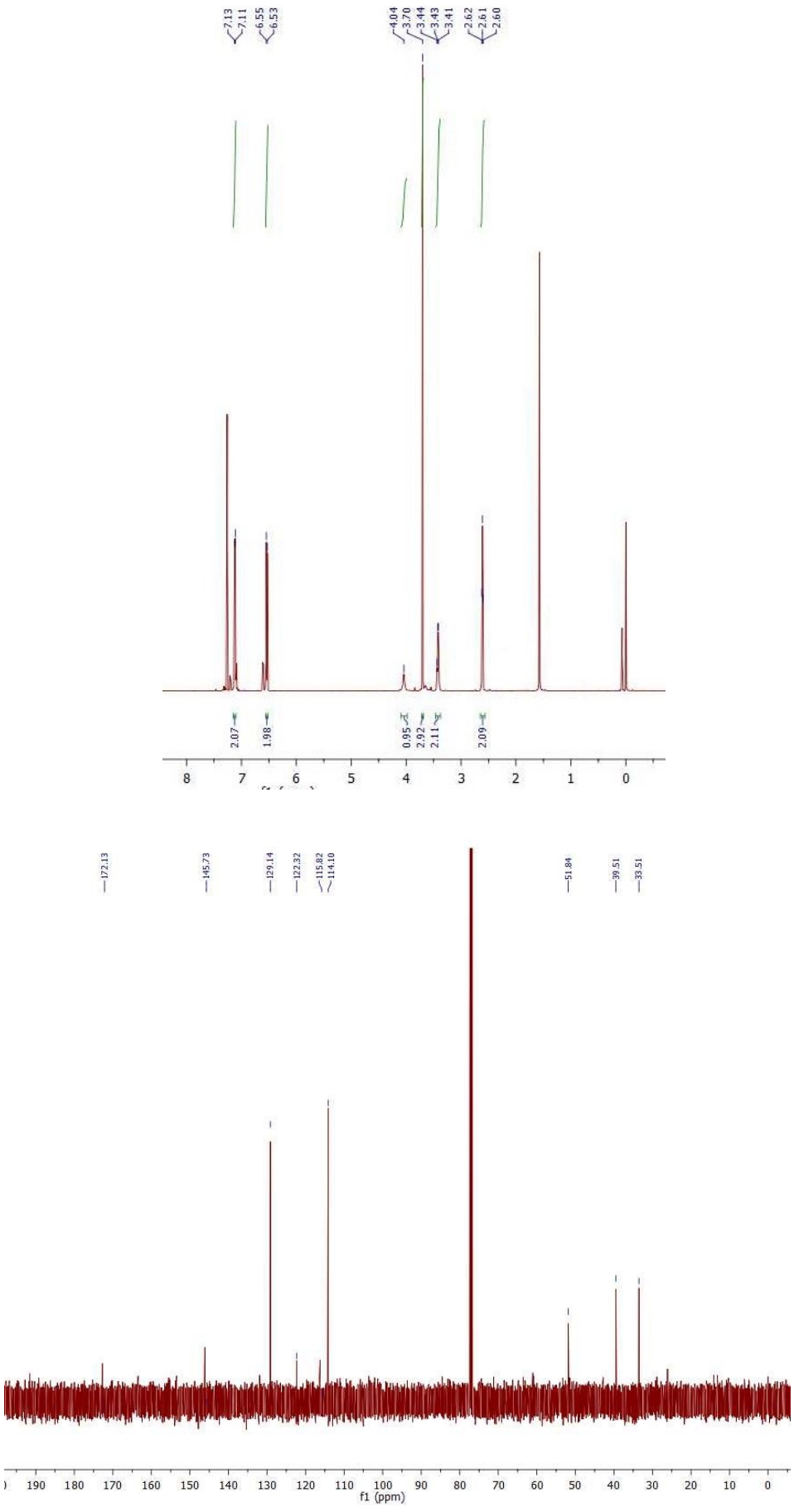
4. NMR Spectra of The Products



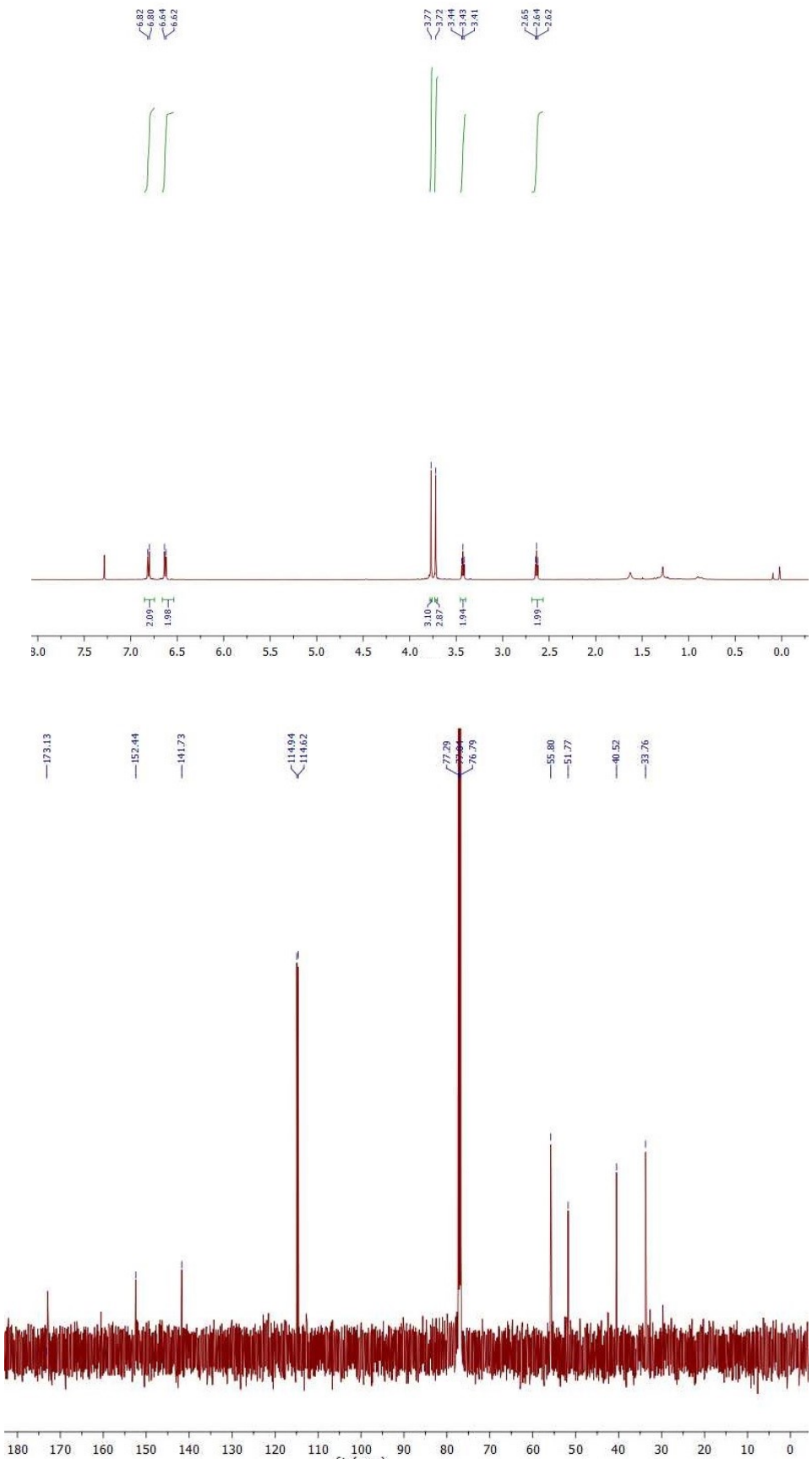
^{1}H and ^{13}C-NMR of 4a



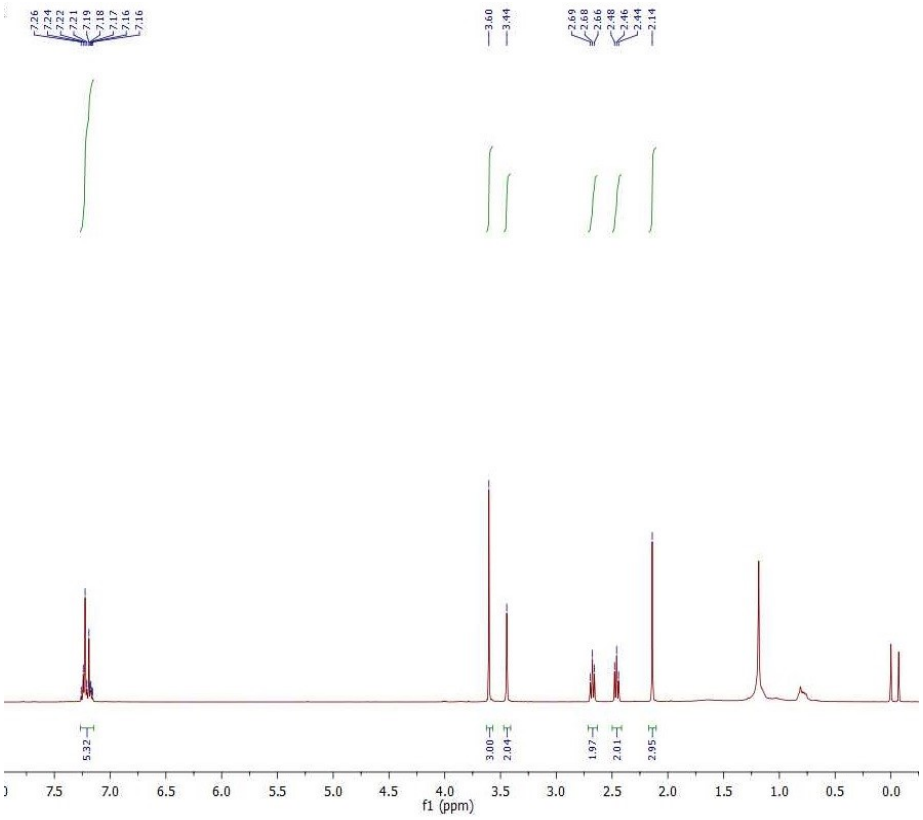
^{1}H and ^{13}C-NMR of 4b

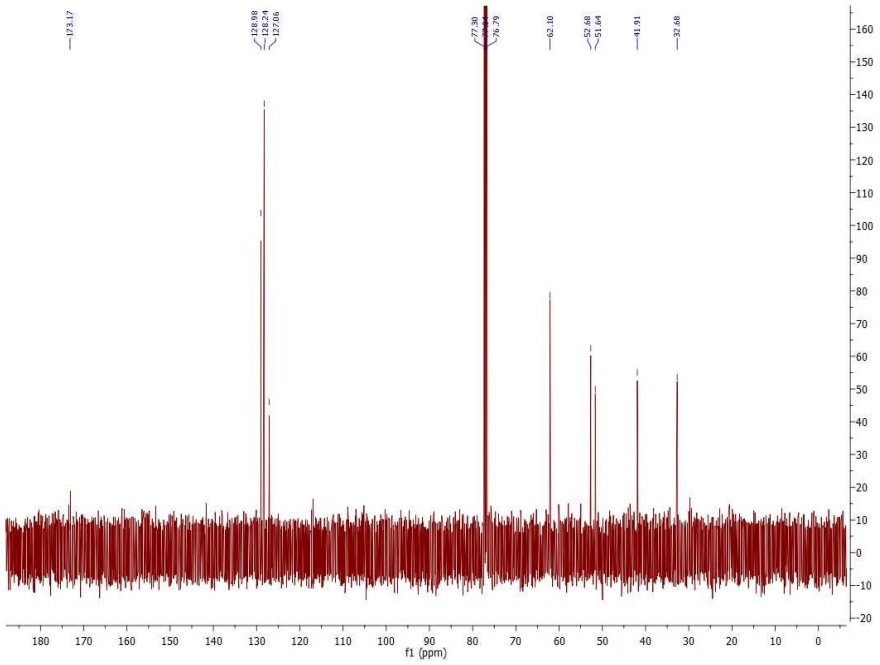


^{1}H and ^{13}C-NMR of 4c

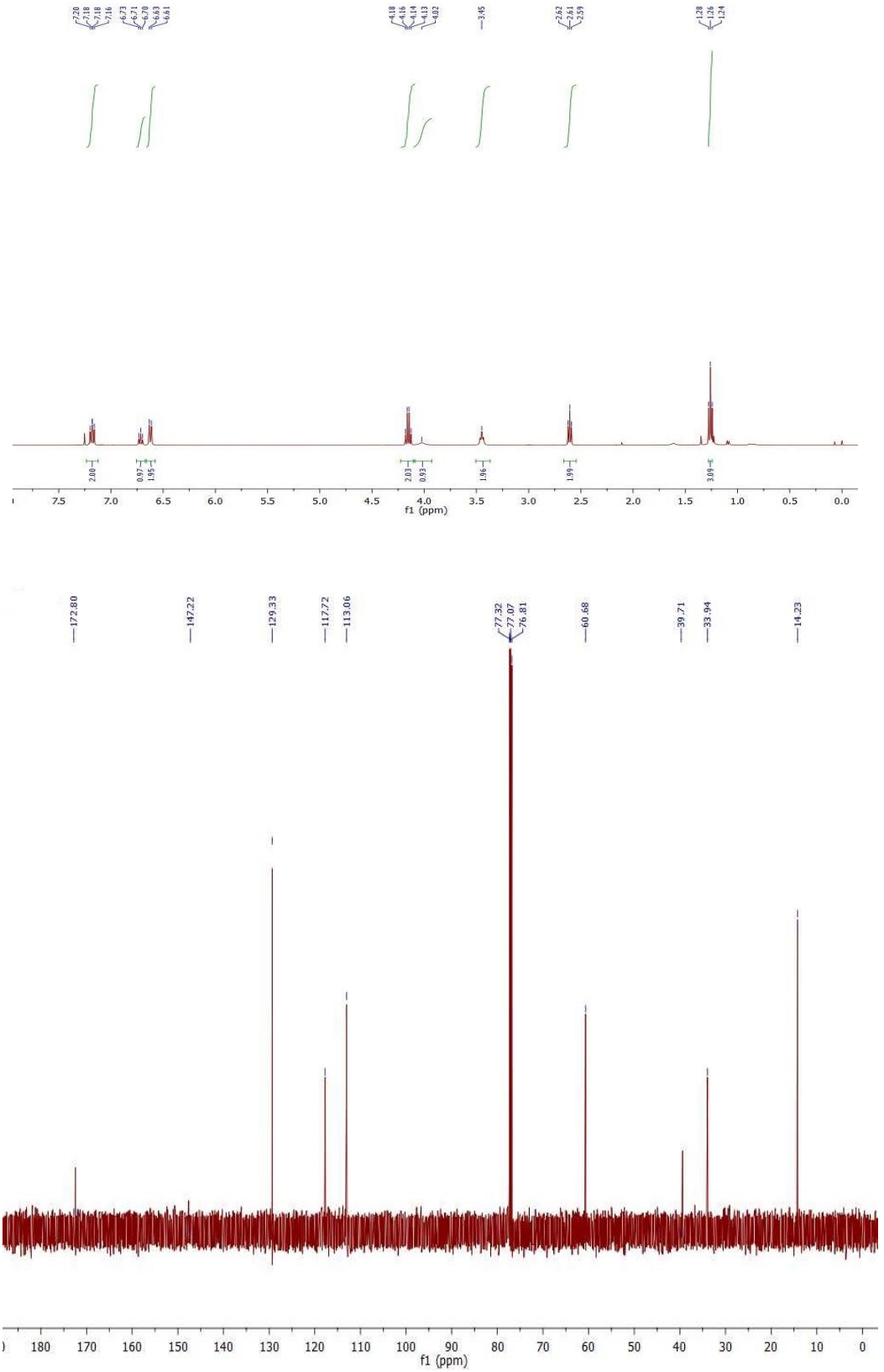


^{1}H and ^{13}C-NMR of 4d

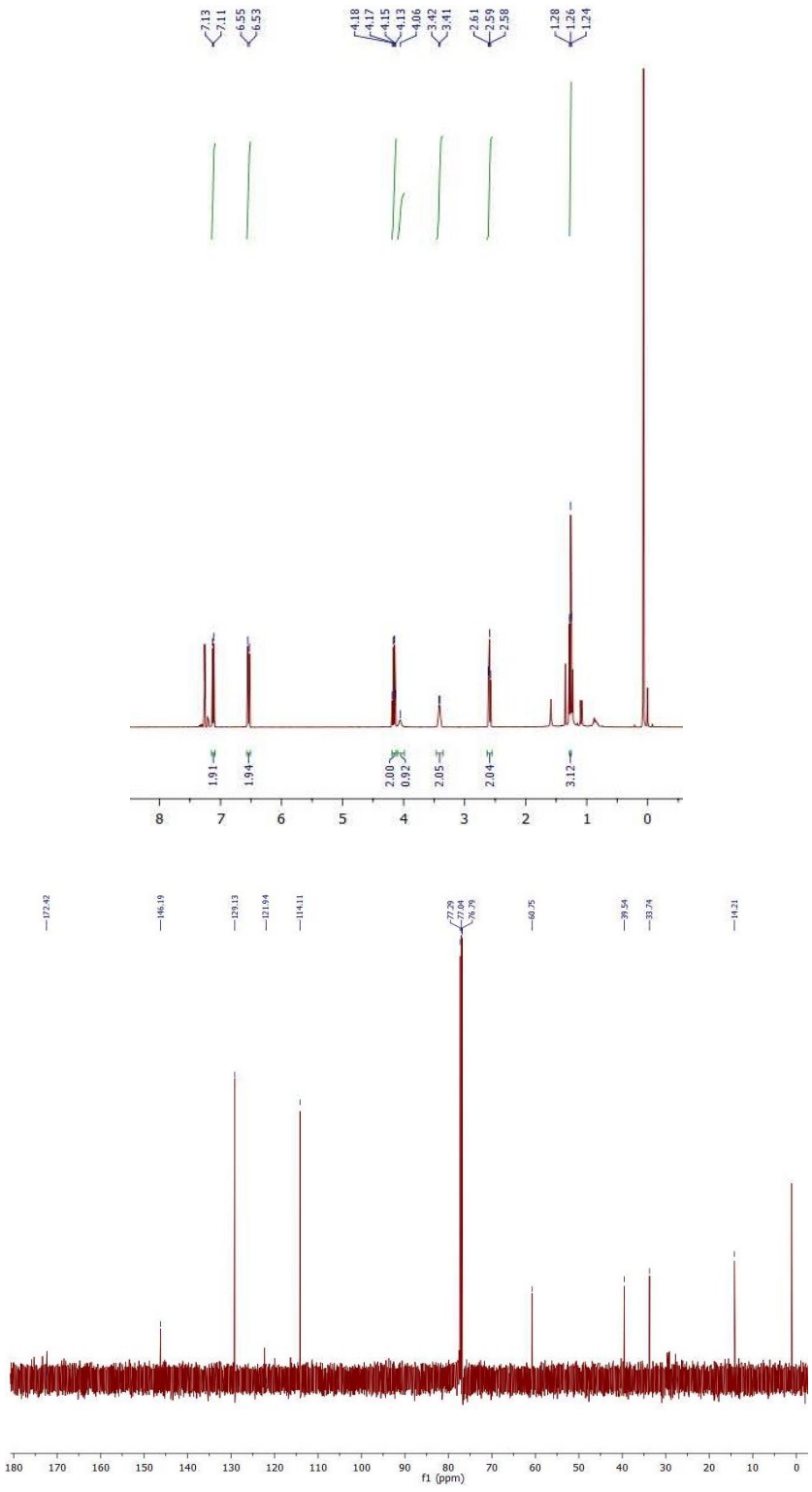




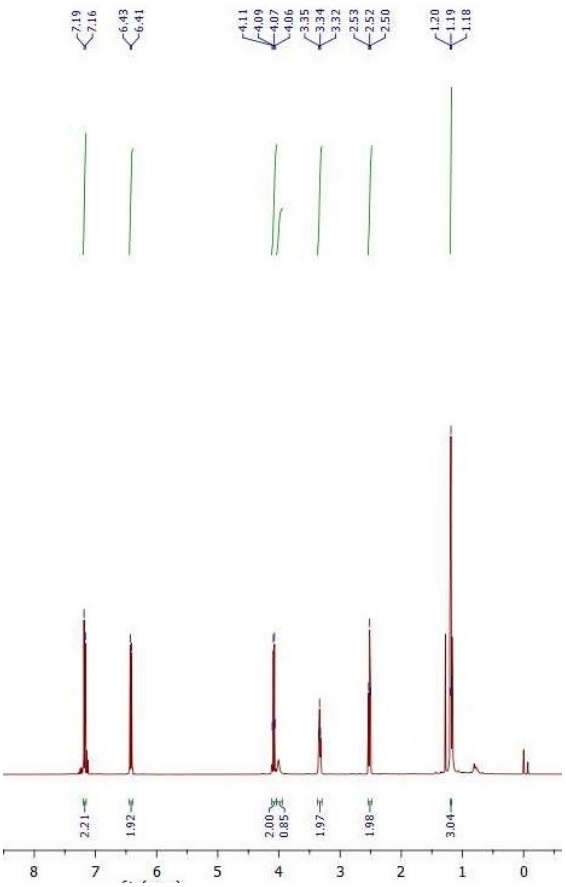
^{1}H and ^{13}C-NMR of 4e



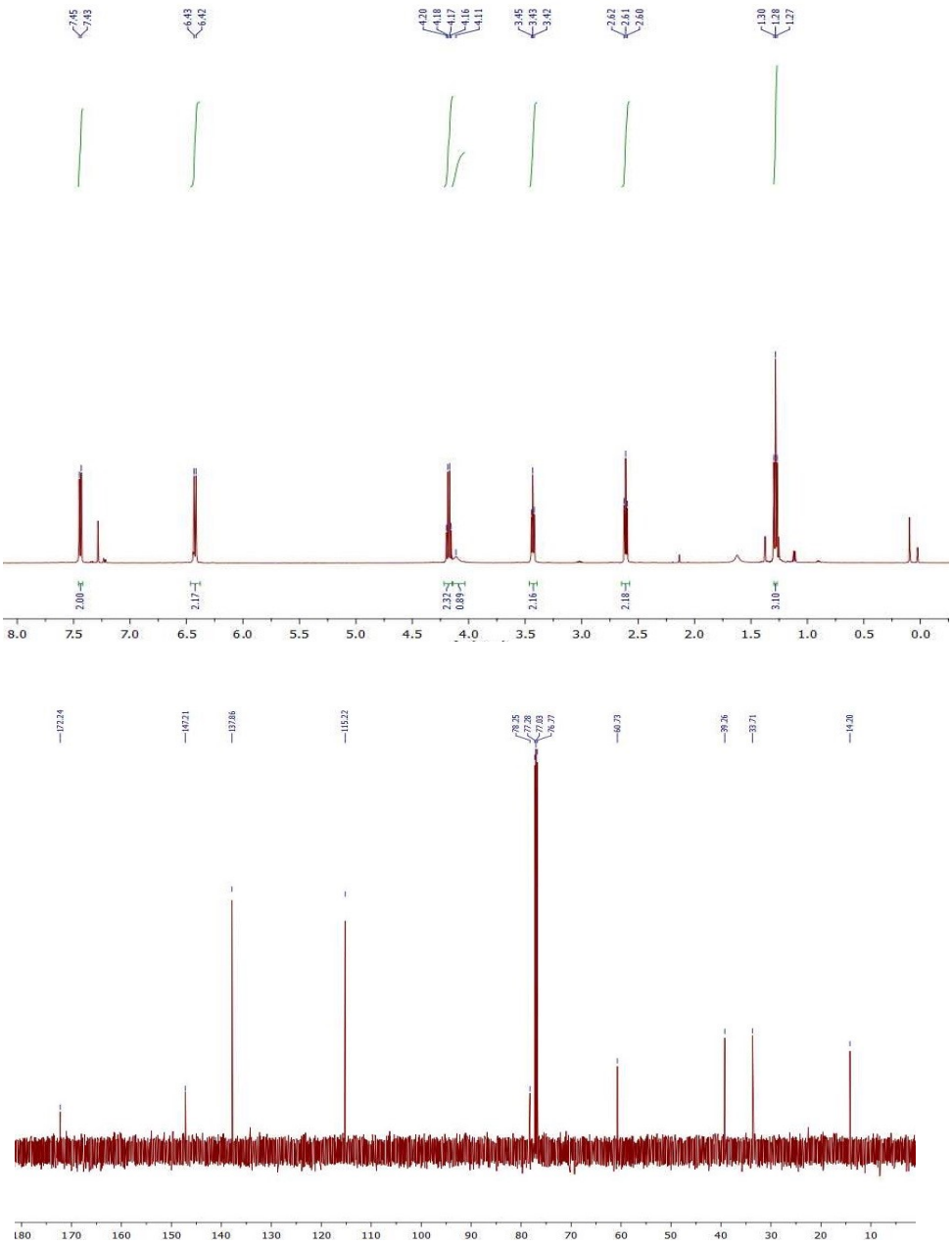
^{1}H and ^{13}C-NMR of 4f



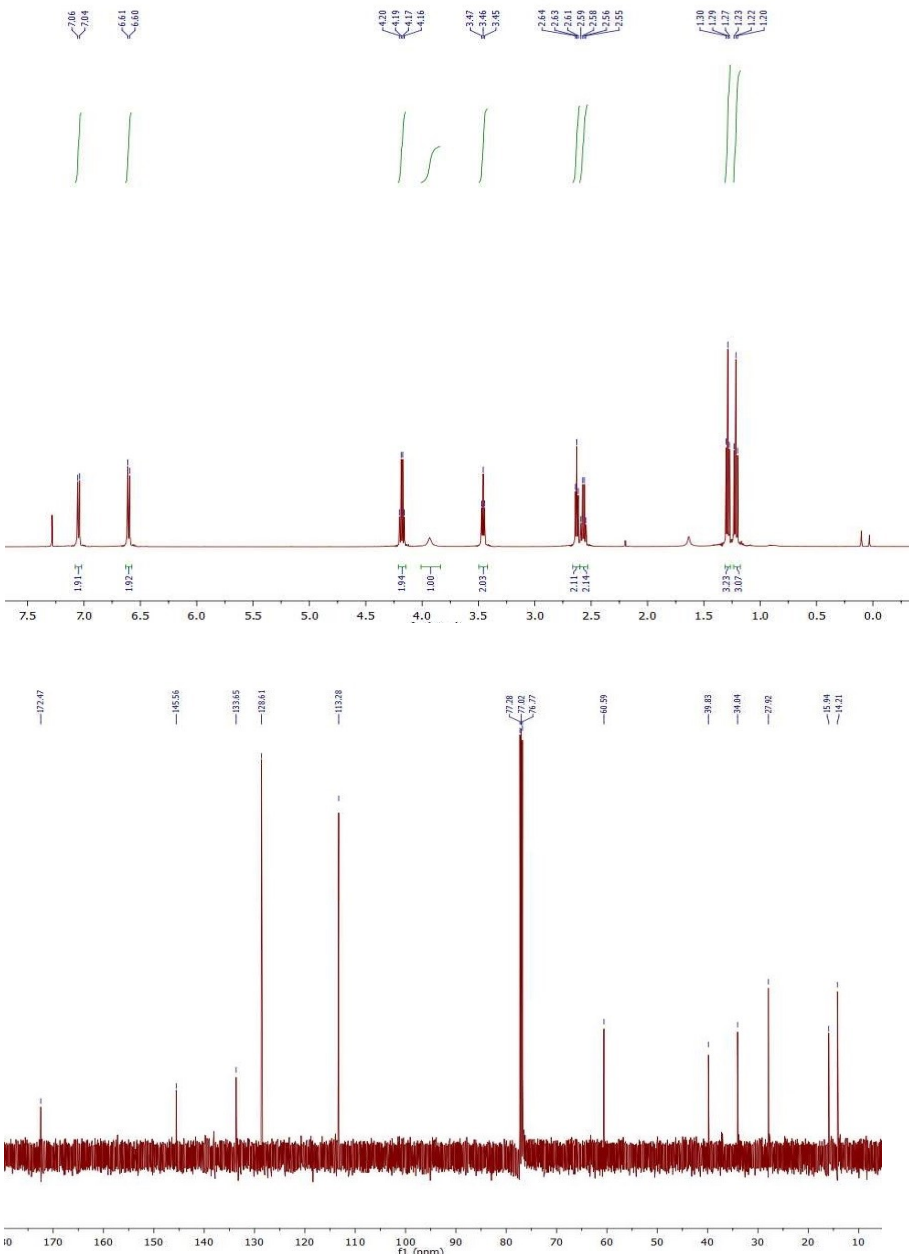
^{1}H and ^{13}C-NMR of 4g


7.19
7.16
6.43
6.41
4.11
4.09
4.07
4.06
3.35
3.34
3.32
2.53
2.52
2.50
1.20
1.19
1.18
2.21
1.92
2.00
0.85
1.97
1.98
3.04
8
7
6
5
4
3
2
1
0

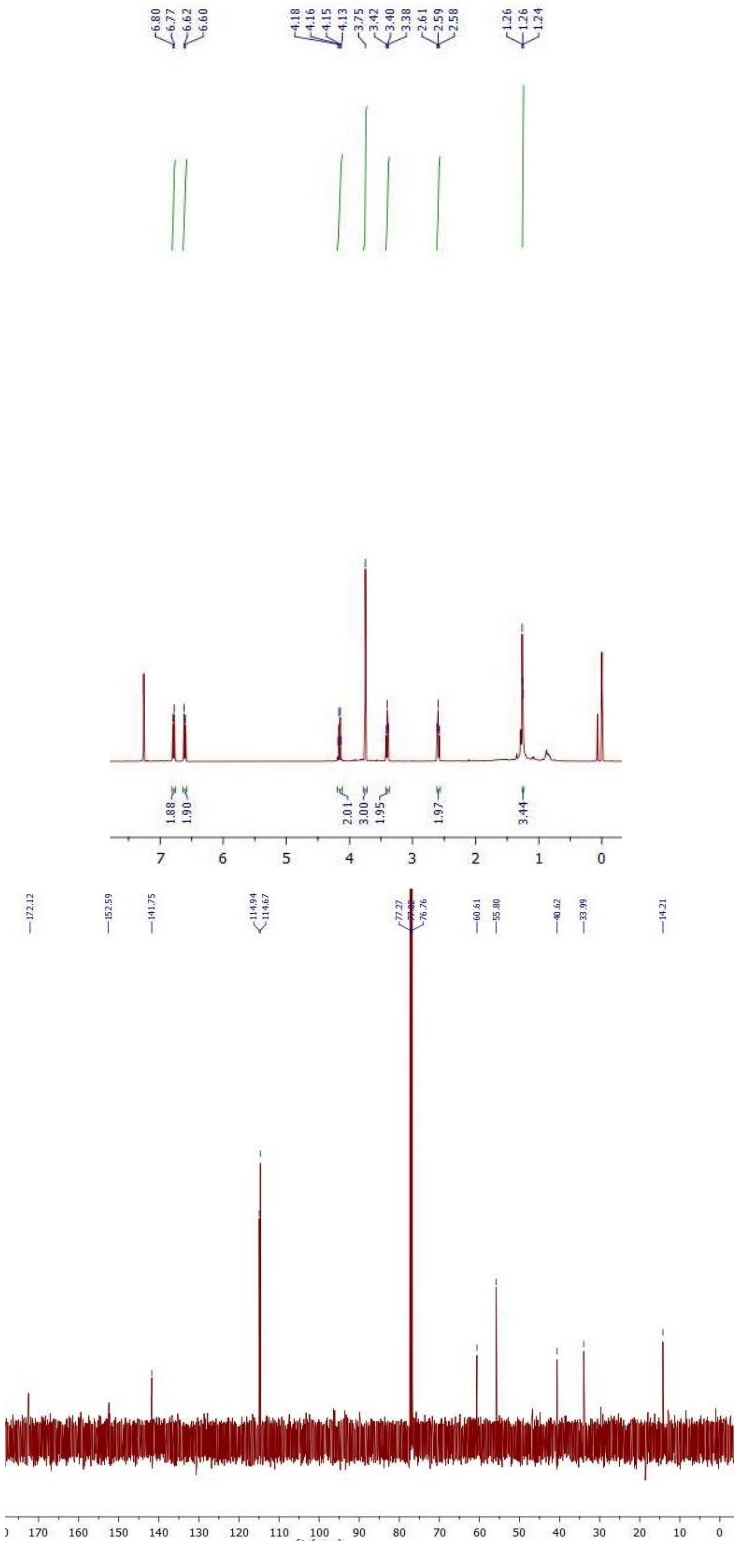
^{1}H -NMR of 4h



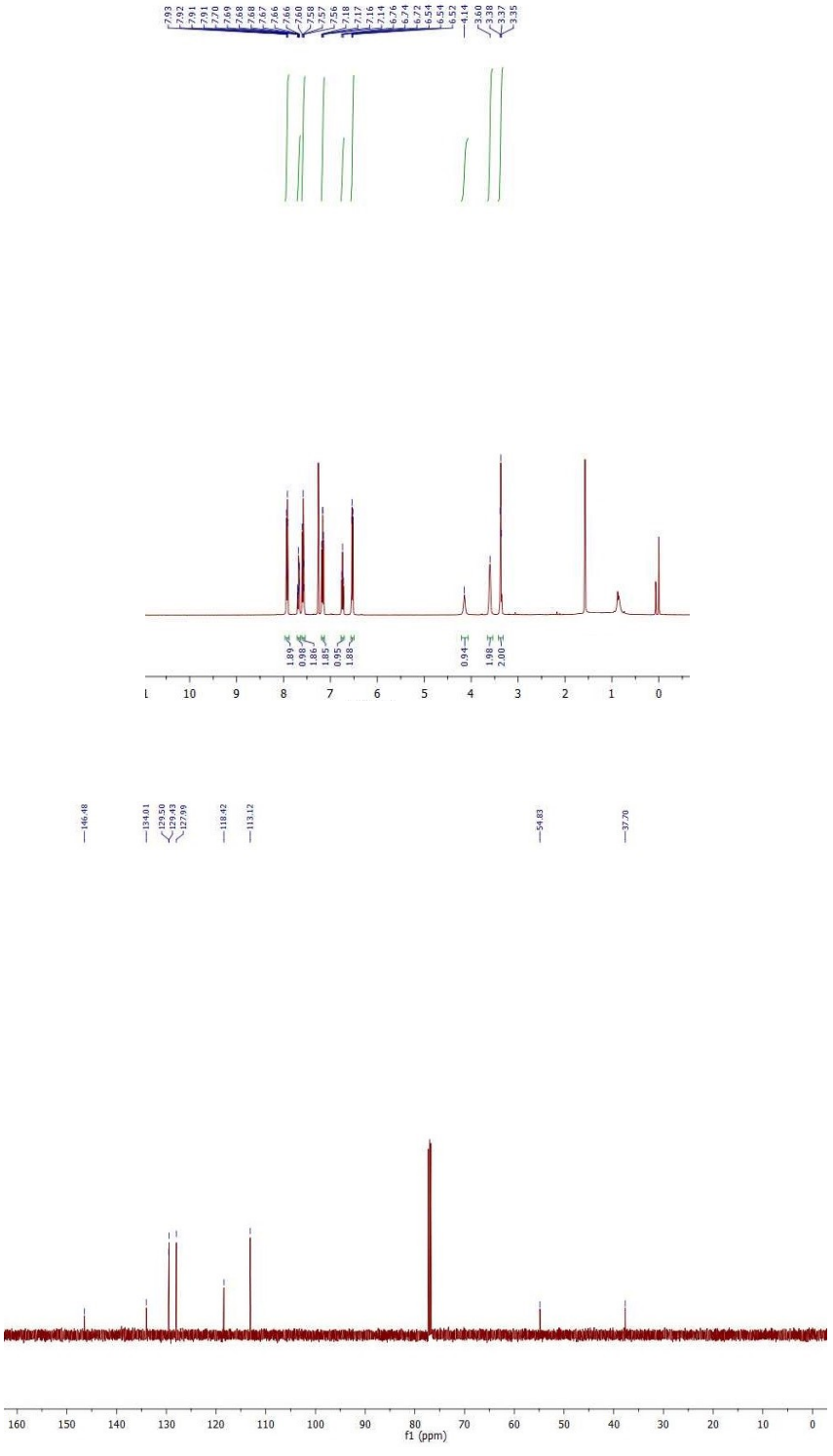
^{1}H and ^{13}C-NMR of 4i



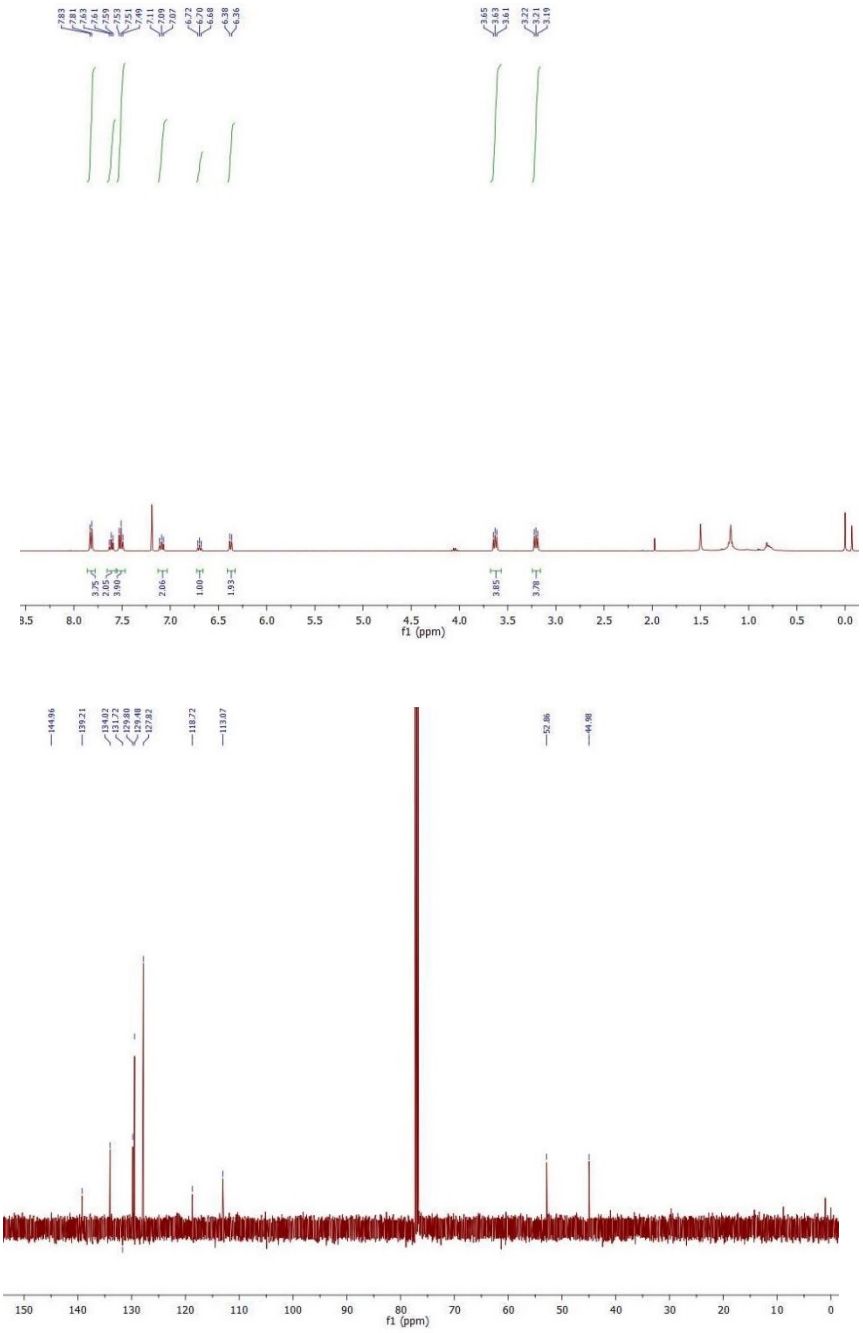
^{1}H and ^{13}C-NMR of 4j



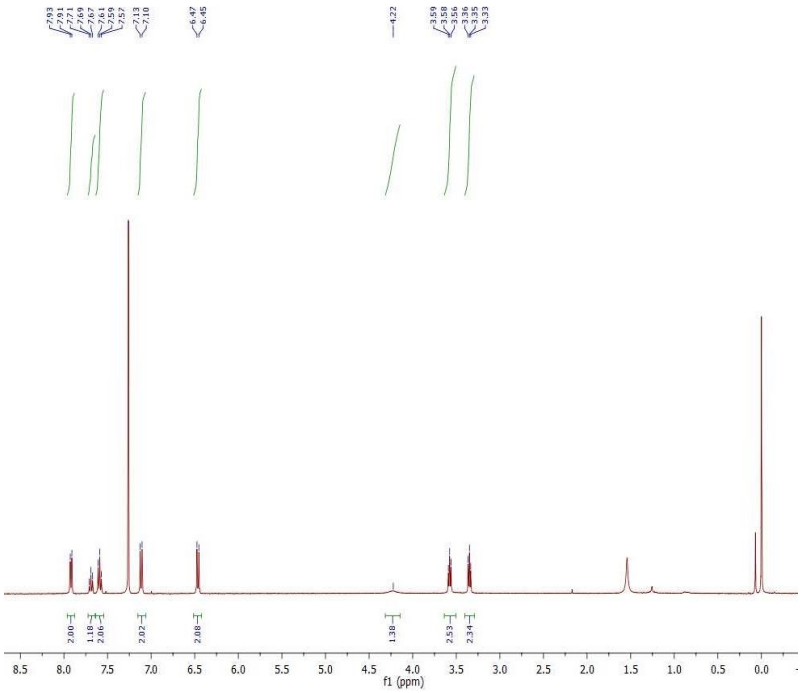
^{1}H NMR and ^{13}C NMR of 4k

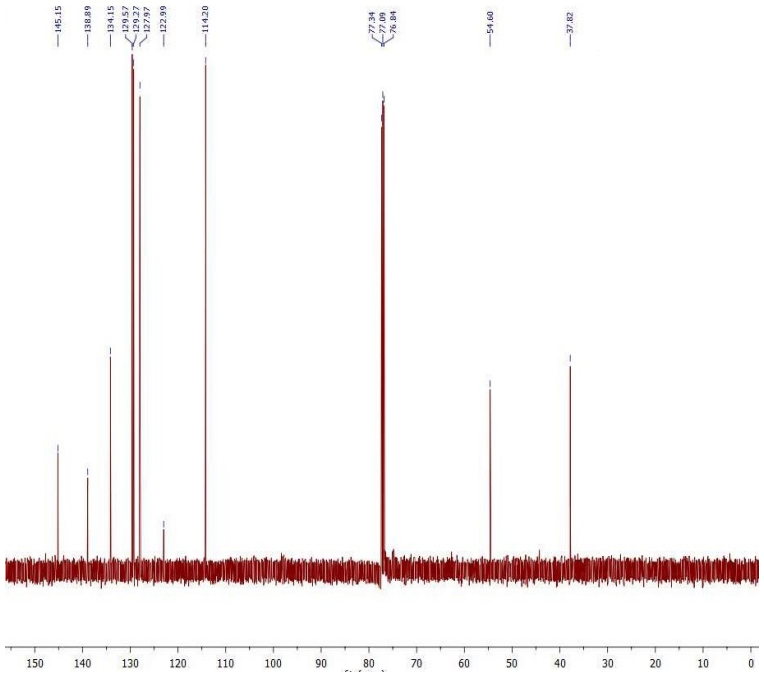


^{1}H and ^{13}C NMR of 4l

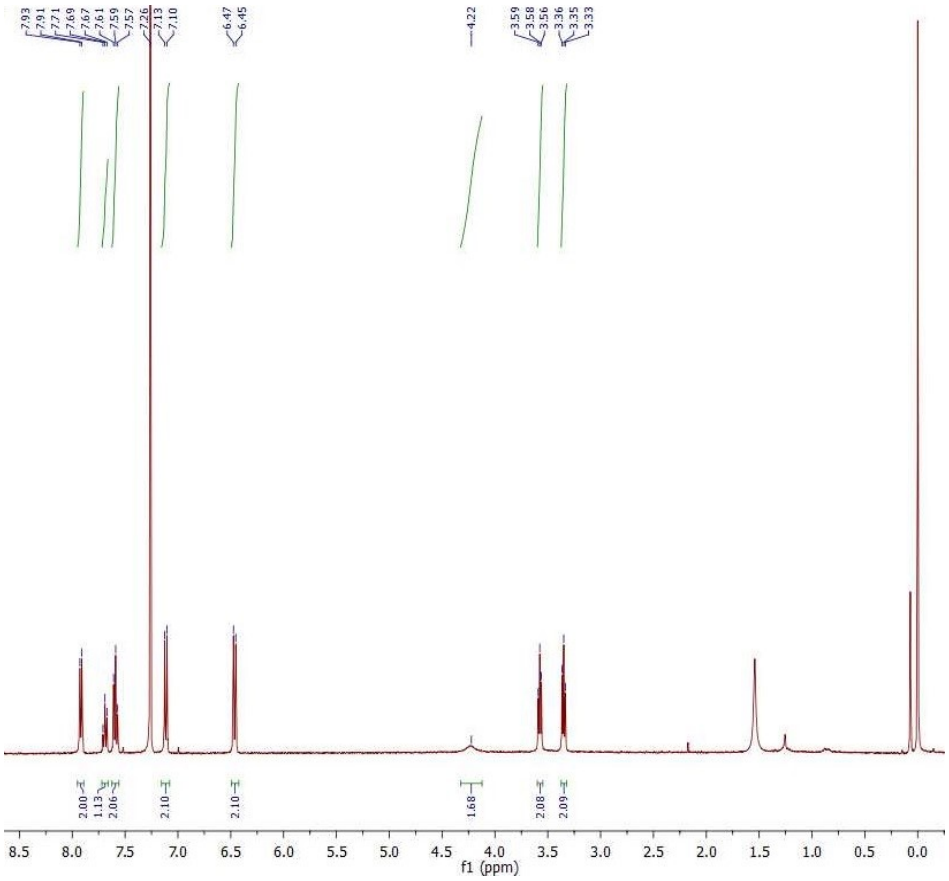


^{1}H and ^{13}C NMR of 4l’

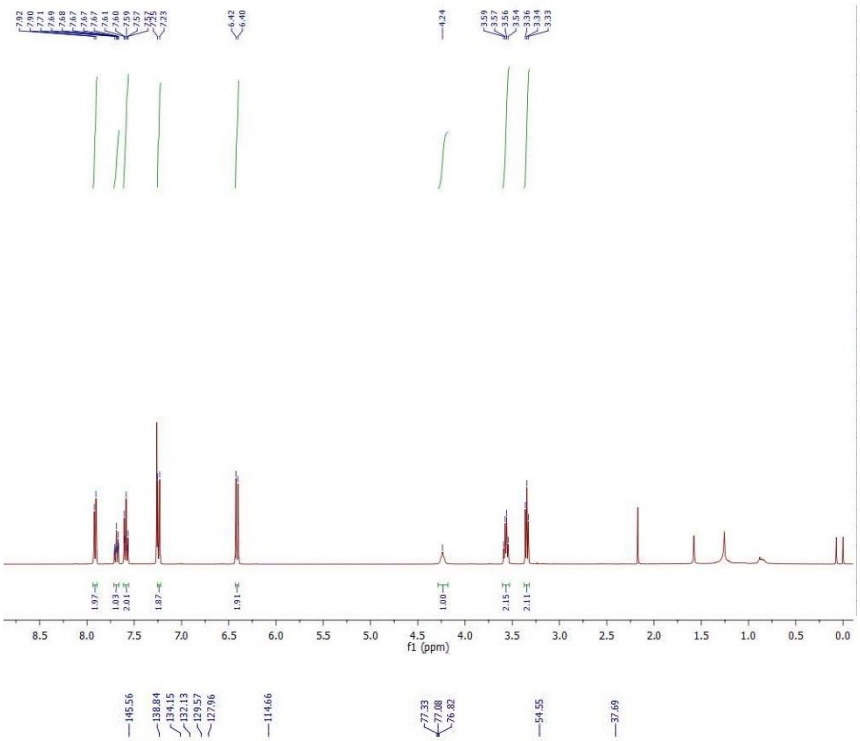


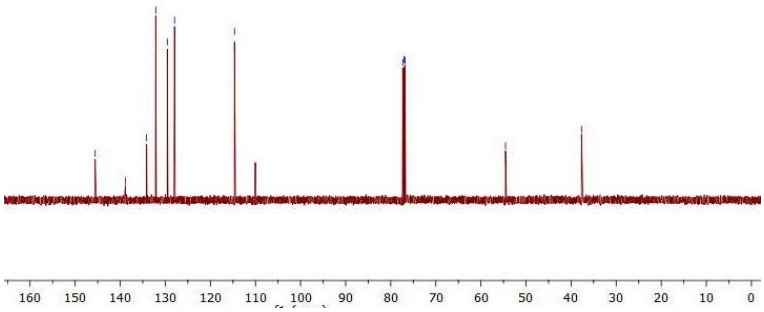


^{1}H and ^{13}C-NMR of 4m

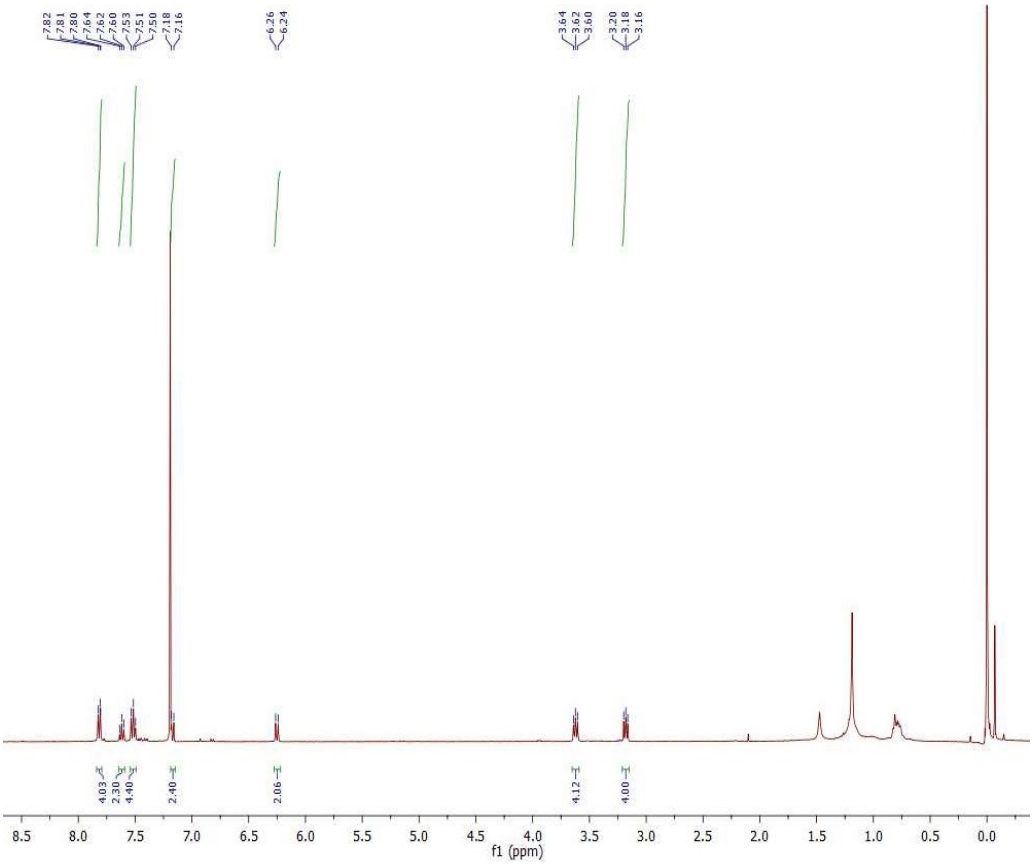

7.93
7.91
7.71
7.69
7.67
7.61
7.59
7.57
7.26
7.13
7.10
6.47
6.45
4.22
3.59
3.58
3.56
3.36
3.35
3.33
2.00
1.13
2.06
2.10
2.10
1.68
2.08
2.09
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

^{1}H-NMR of 4m’

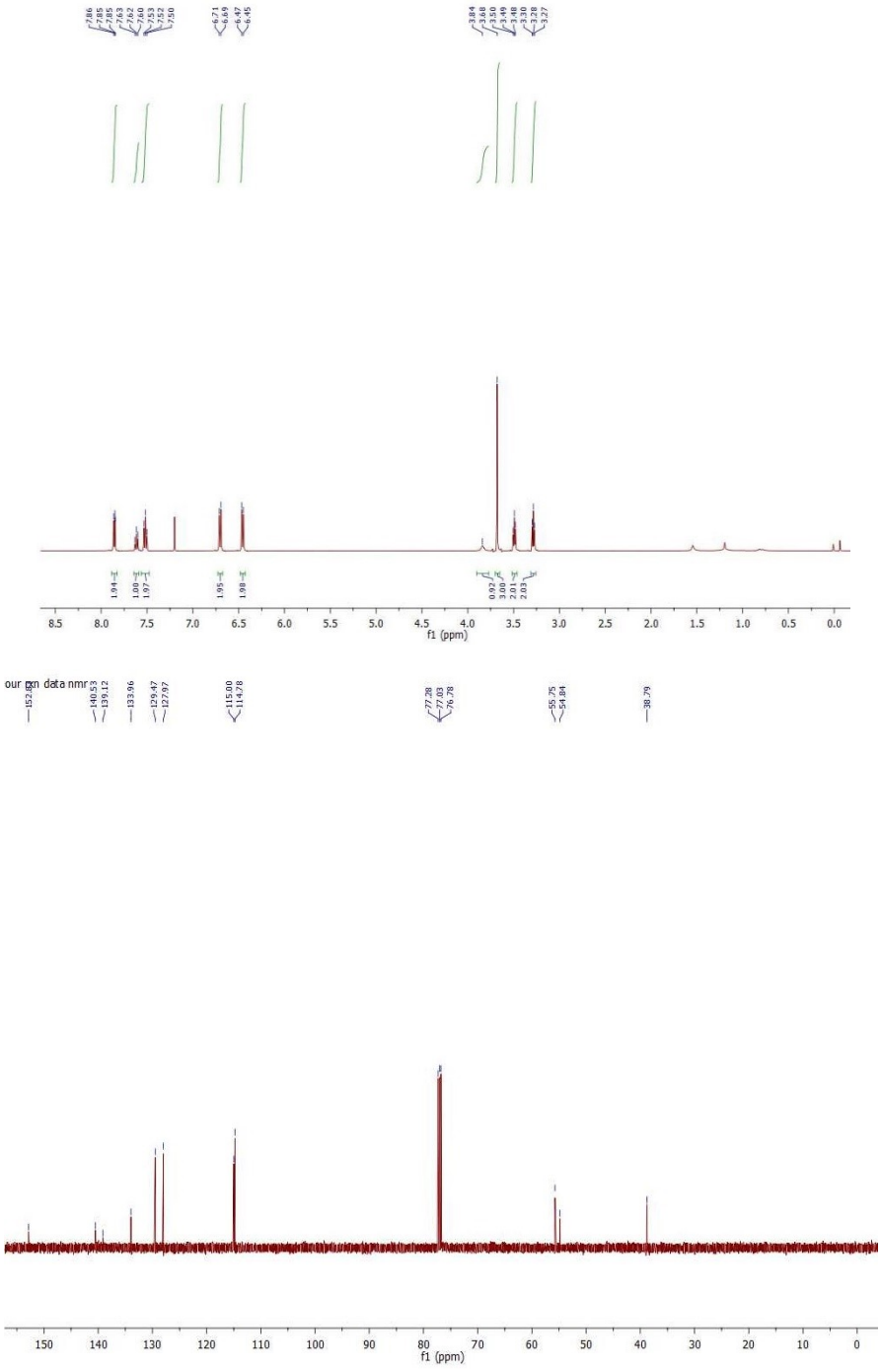




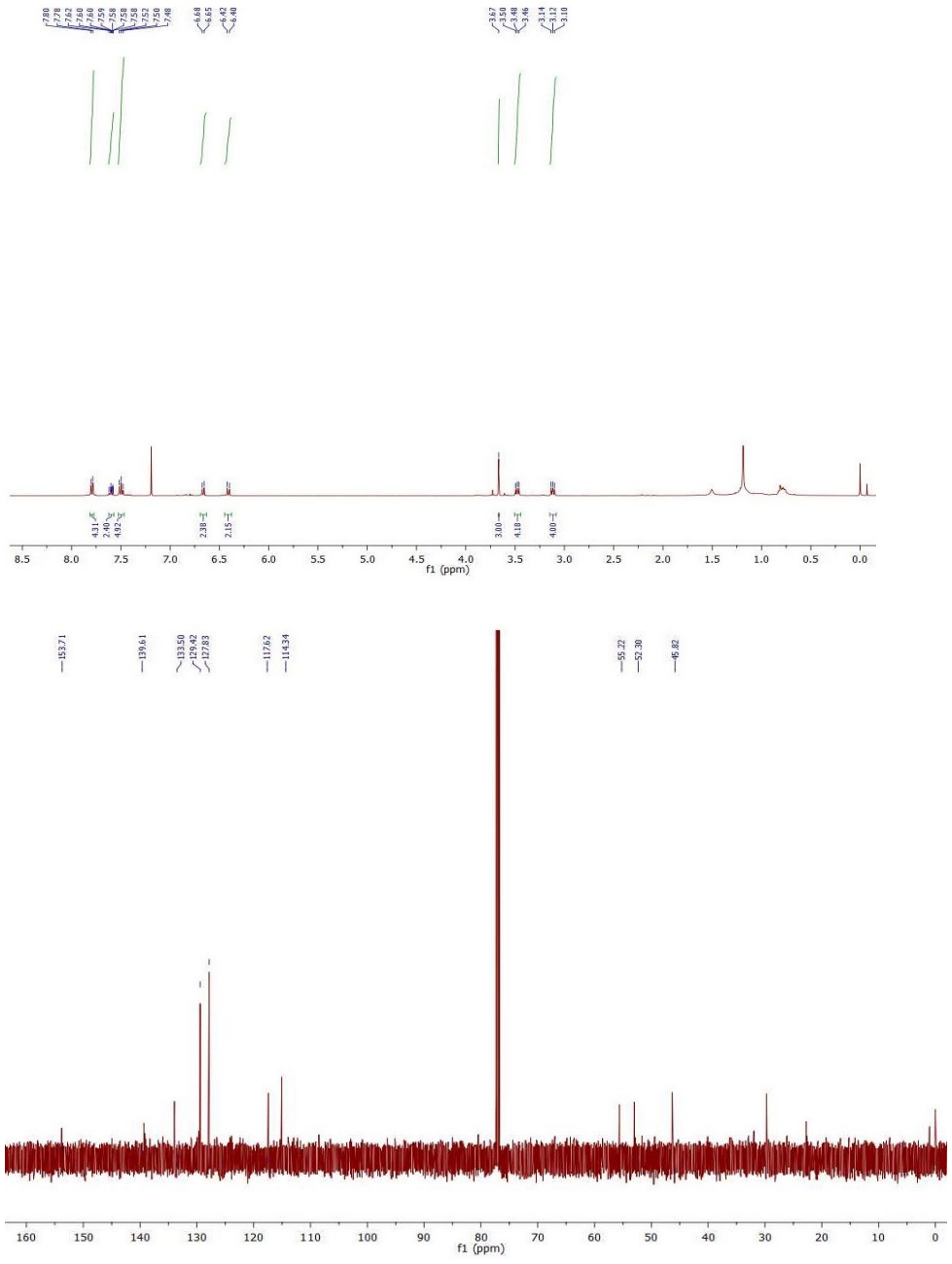
^{1}H and ^{13}C-NMR of 4n



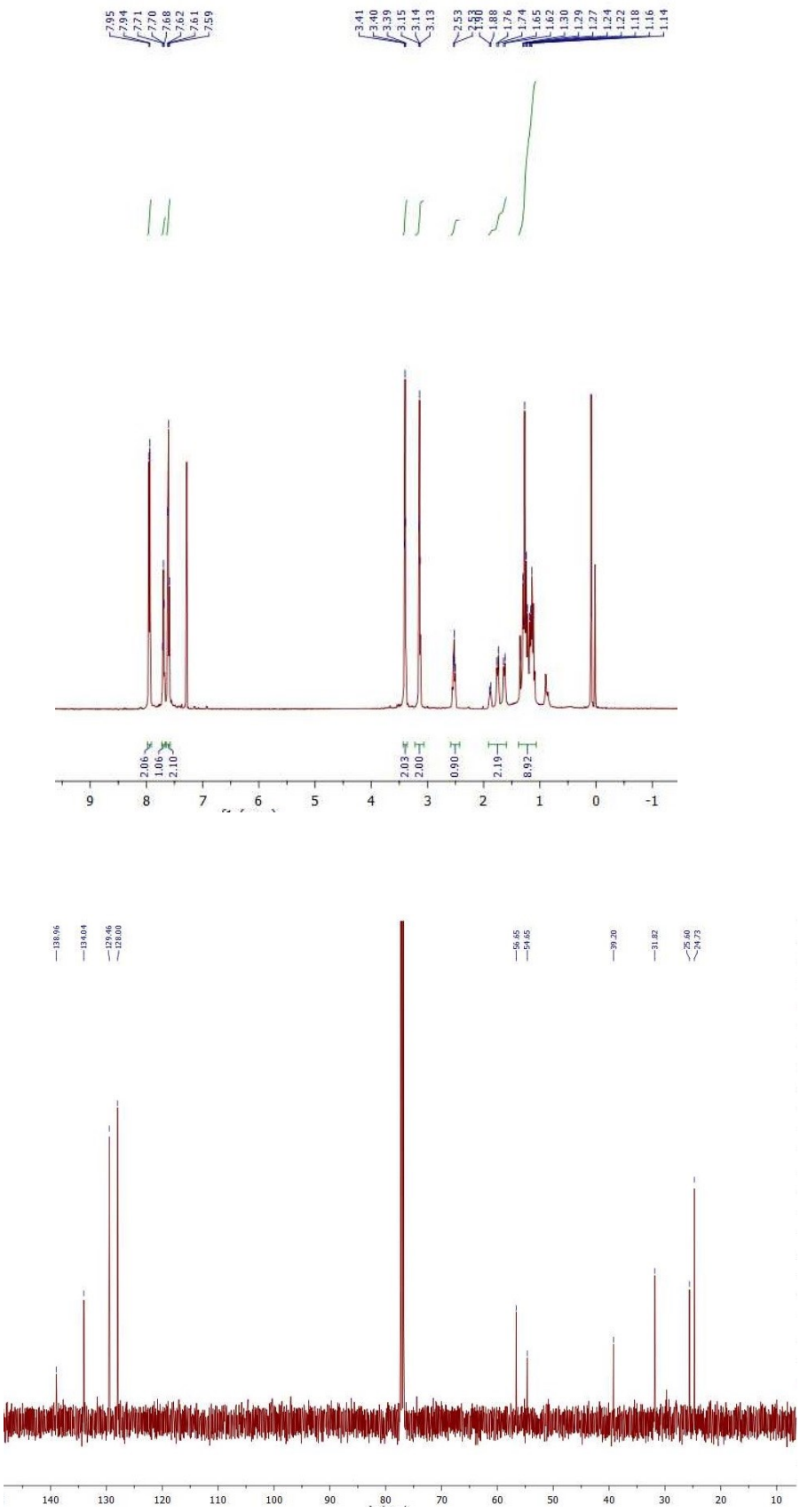
^{1}H and ^{13}C-NMR of 4n’



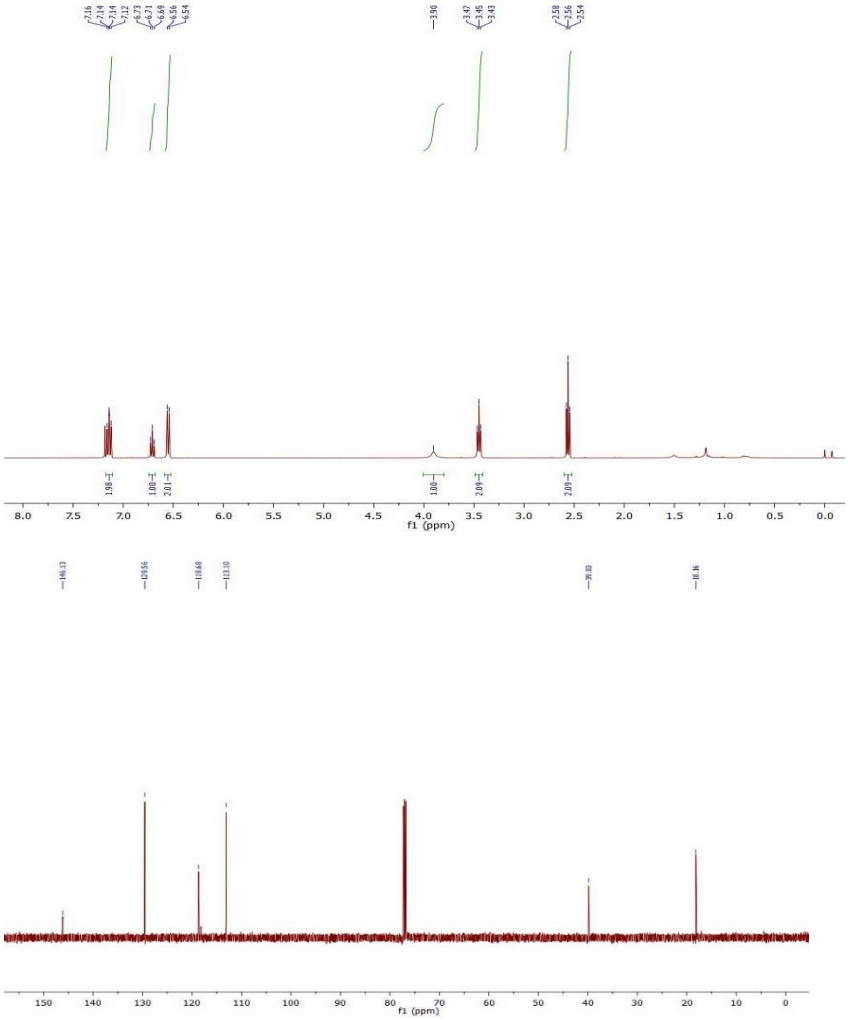
^{1}H and ^{13}C NMR of 4o



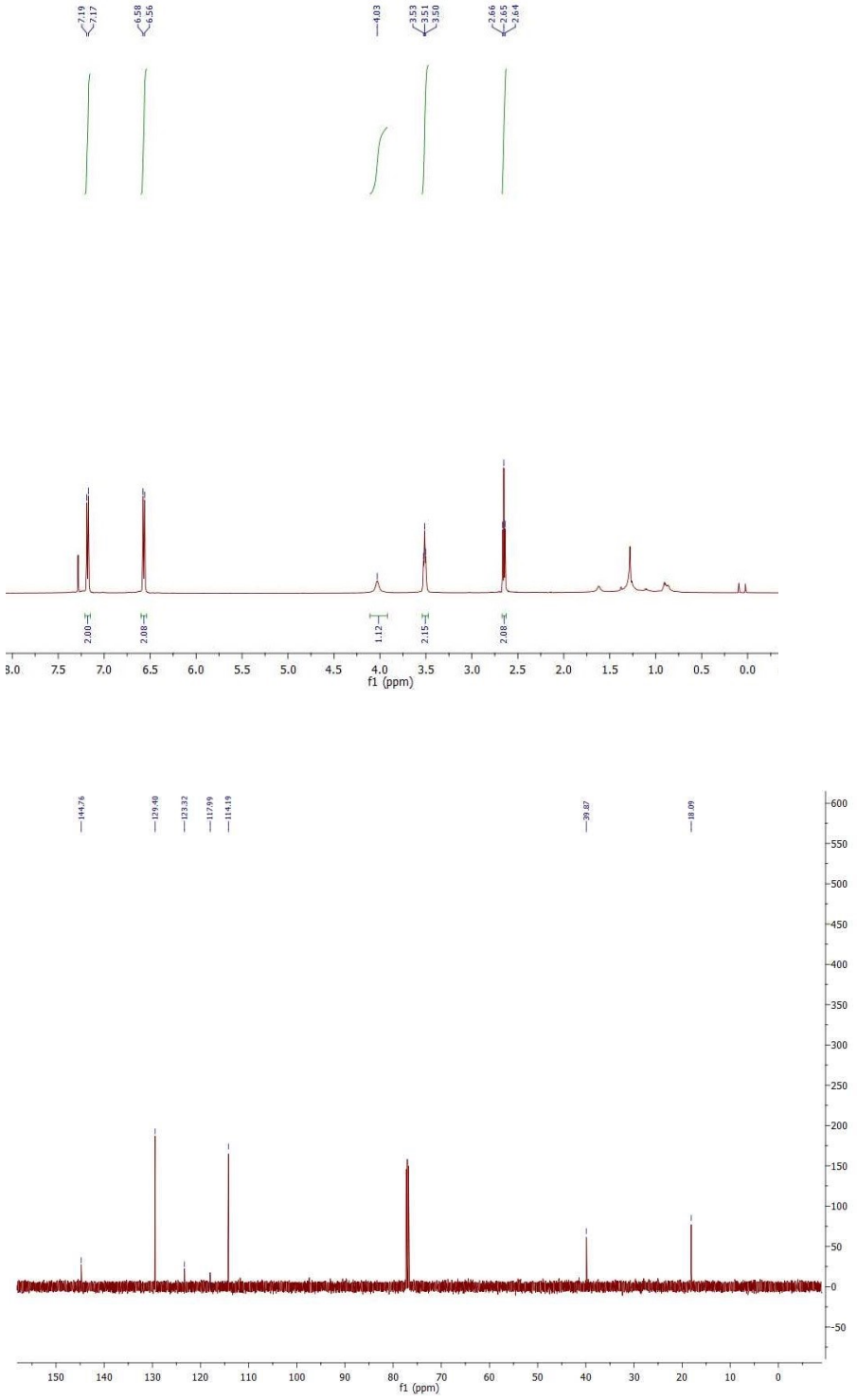
^{1}H and ^{13}C NMR of 4o’



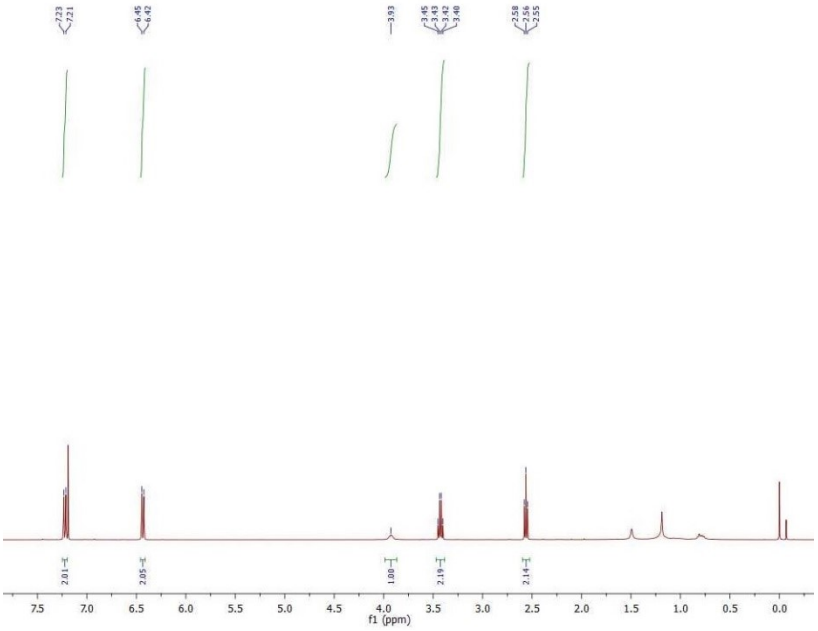
^{1}H and ^{13}C NMR of 4p

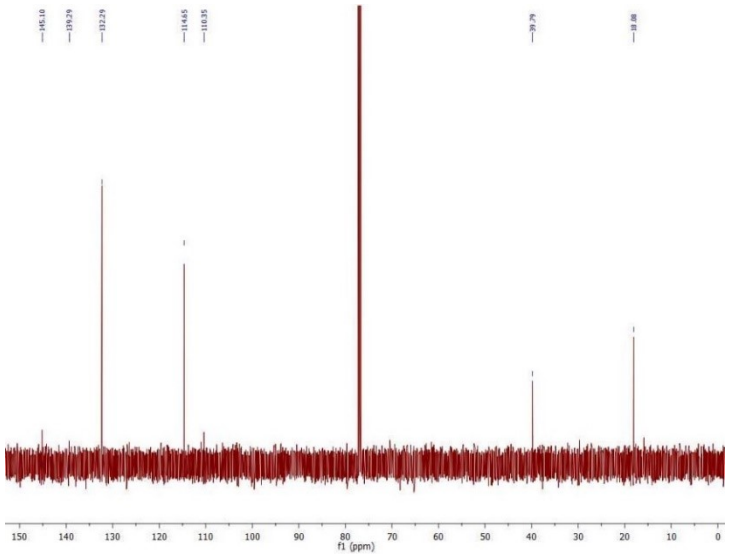


^{1}H and ^{13}C NMR of 4q

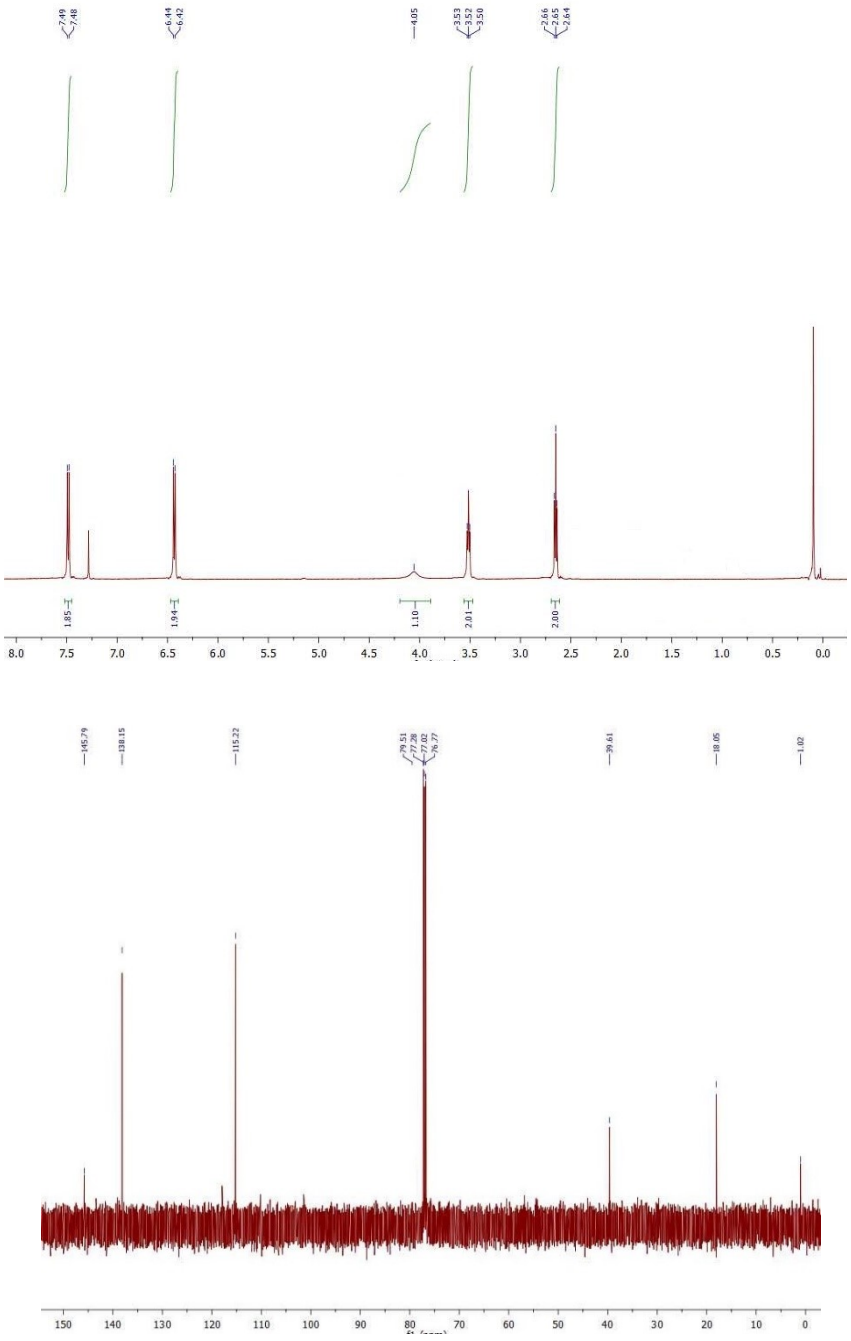


^{1}H and ^{13}C NMR of 4r

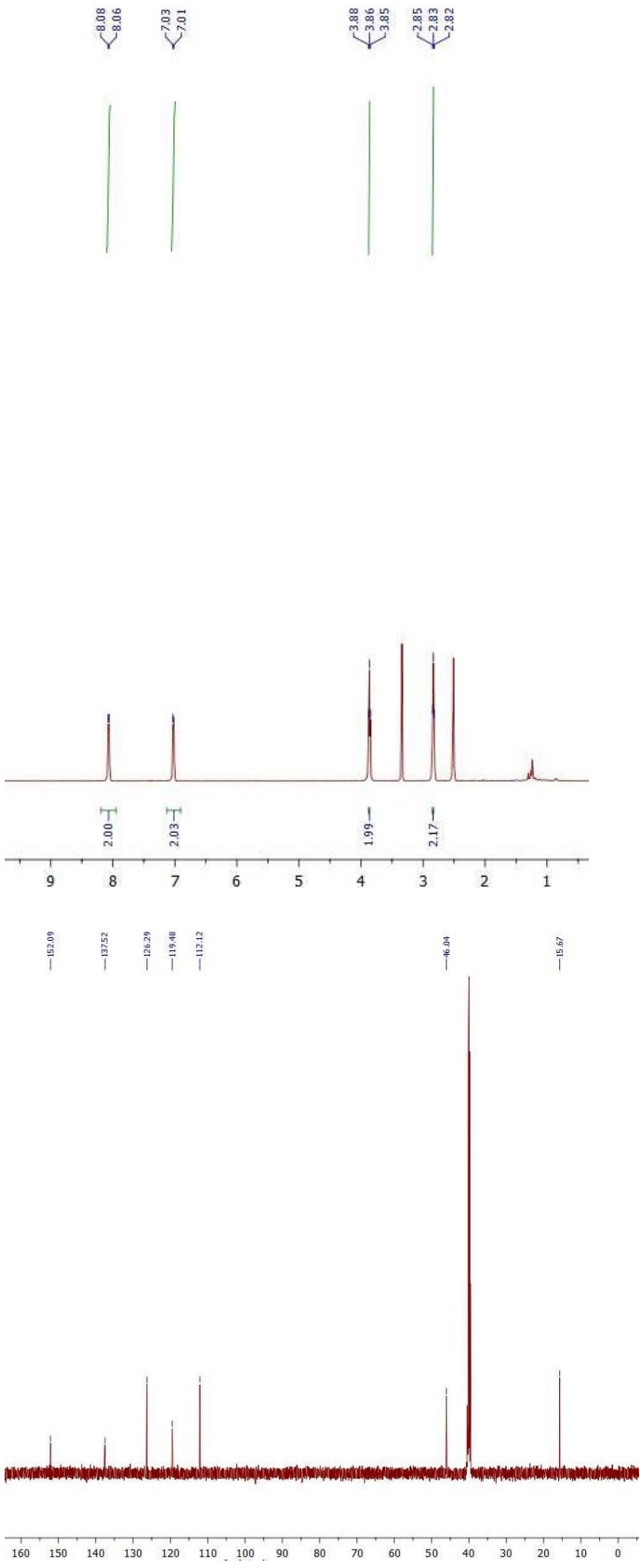




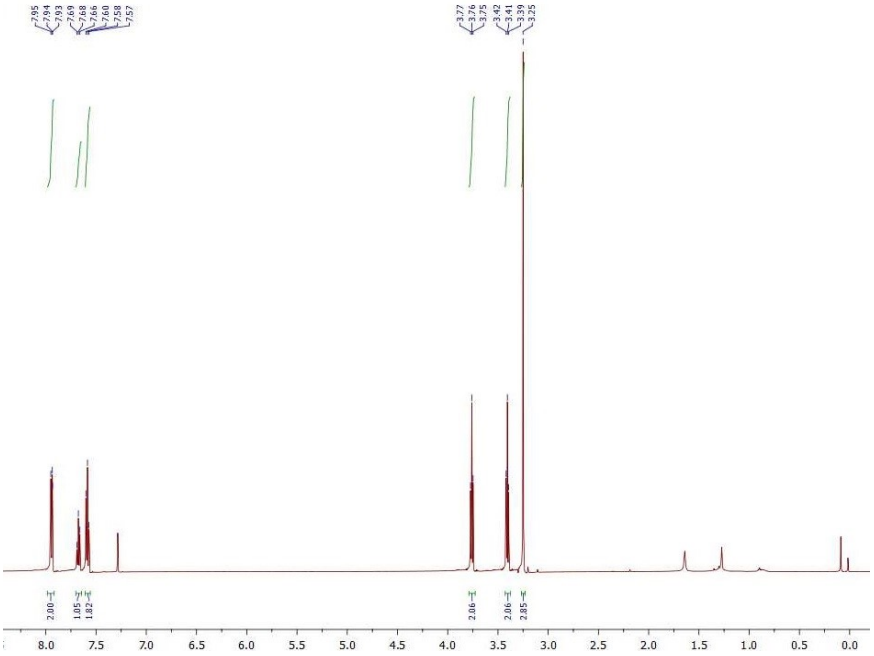
^{1}H and ^{13}C NMR of 4s

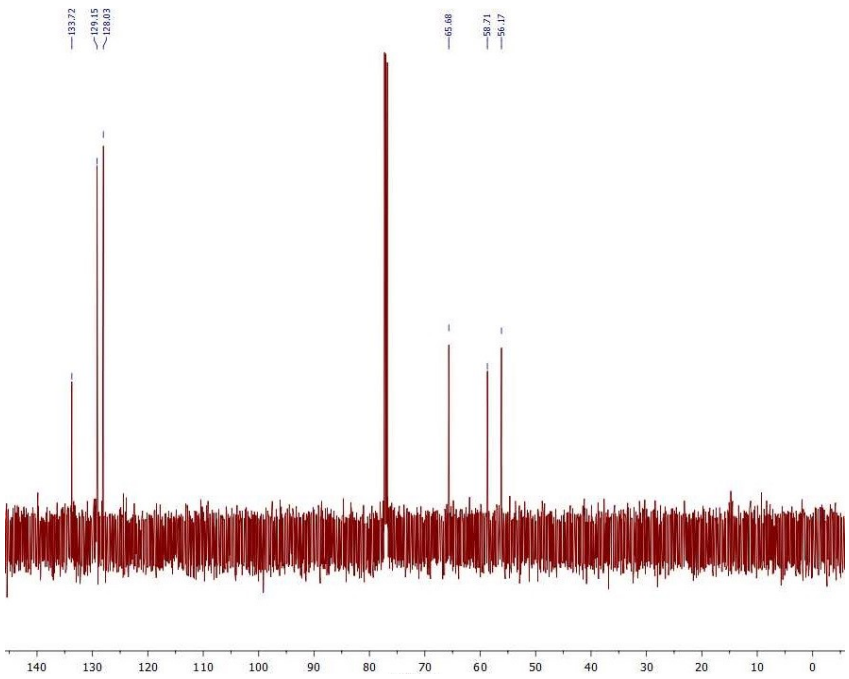


^{1}H and ^{13}C NMR of 4t

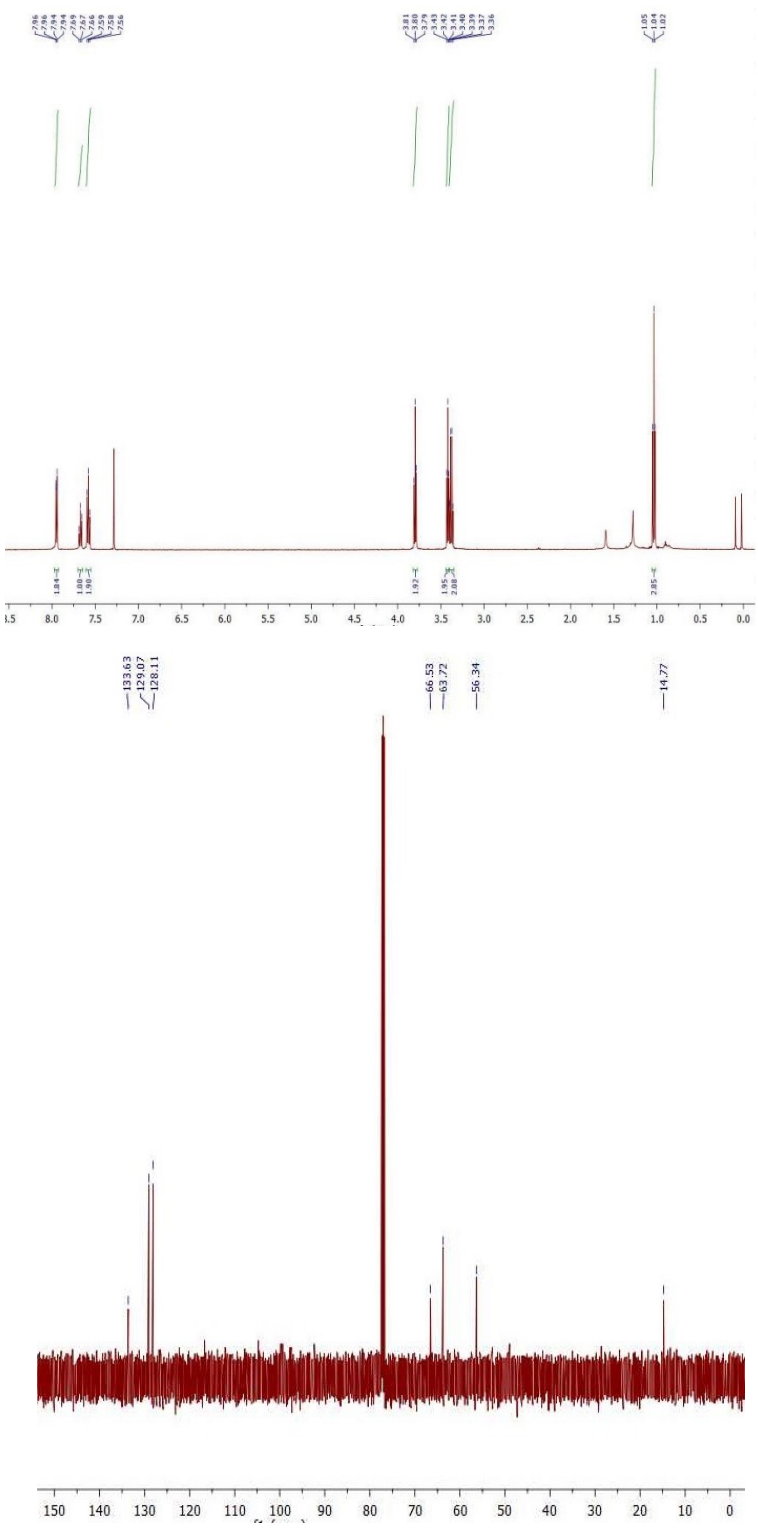


^{1}H and ^{13}C NMR of 4u

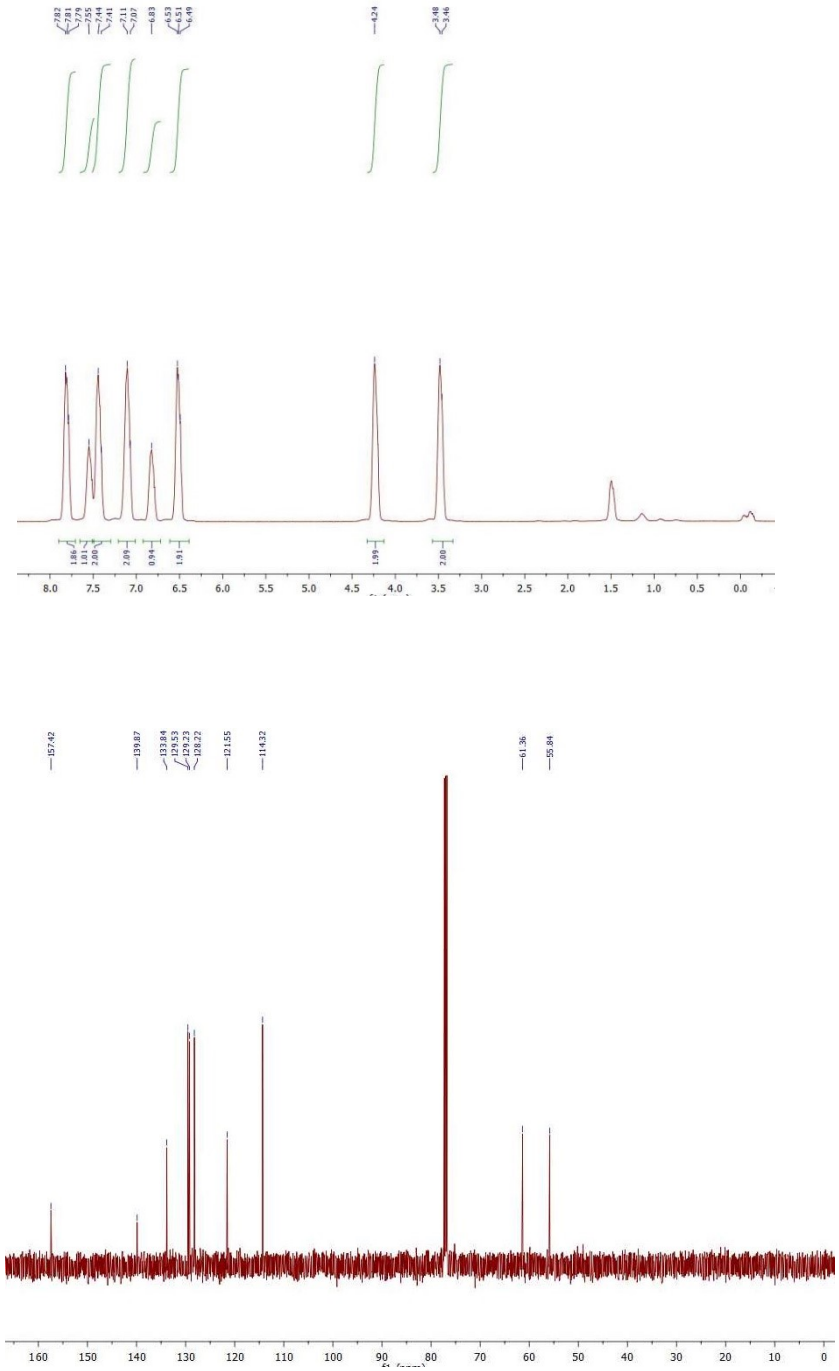




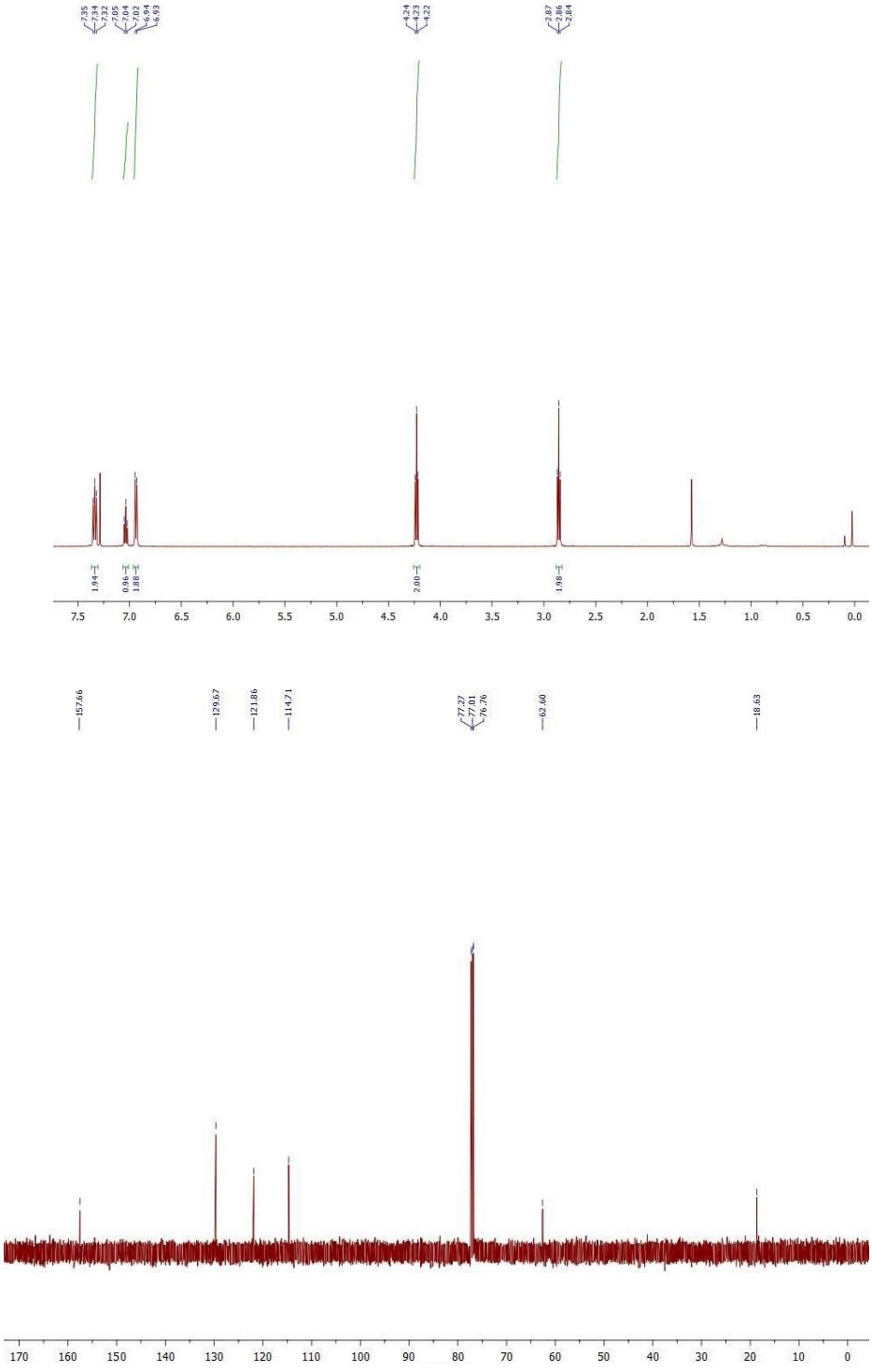
^{1}H and ^{13}C NMR of 6a



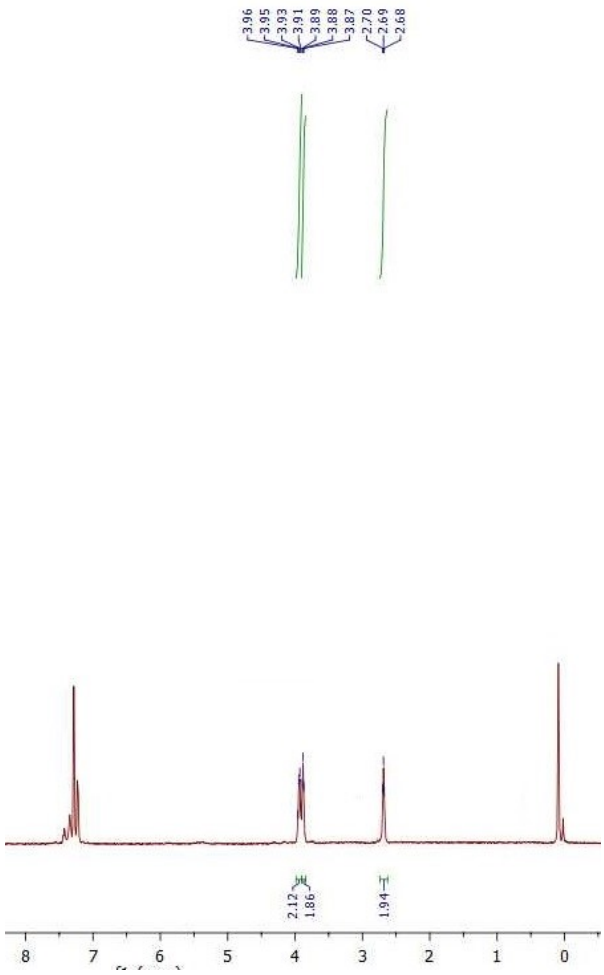
^{1}H and ^{13}C NMR of 6b



^{1}H and ^{13}C NMR of 6c



^{1}H and ^{13}C NMR of 6d



^{1}H NMR of 6e

5. Computational details

All the density functional theory (DFT) calculations were performed using *Gaussian 09 Revision D.01*.[1] The geometry optimisation of all the stationary points in gas phase was performed using B3LYP[2] hybrid density functional with a combination of a double zeta (DZ) and Stuttgart-Dresden effective core potential (ECP) basis set, SDD[3] for copper and a Pople type basis set with double polarisation 6-31g (d, p)[4] for all other atoms. To confirm the nature of the stationary points, the harmonic vibrational frequencies of normal modes were computed using the same level of theory. From the vibrational frequency analysis, it was confirmed that all the intermediates are at minimum with no imaginary frequencies, whereas all the transition states were accompanied with exactly one imaginary frequency corresponding to the stretching of the bond involved which is expected to form or break during that step of the reaction. Further, the single point energy correction was performed using SDD basis set for Cu and a higher basis set def2-TZVP[5], having a valance triple zeta polarisation was used for all other atoms along with Grimme's dispersion[6] and Becke–Johnson[7] damping correction (GD3BJ). To incorporate the effect of solvent, a continuum solvation model SMD[8] was used with toluene as the solvent where the continuous quantum mechanical charge density of the solute serves as the basis for this model. All the 3D structures were illustrated using CYLview[9] software and 2D structure were obtained using ChemDraw software.

6. Proton assisted olefin activation (PAOA)

In this pathway, the olefin is activated by the proton attached to the nitrogen in the active catalyst rather than copper. The nitrogen interacts with the carbon of the olefin and the hydrogen interacts with the carbon of the olefin to form a four-membered TS (TS_1B) at a cost of 35.7 kcal/mol of Gibbs free energy. This requirement of a high activation energy makes this pathway kinetically less feasible. This four-membered TS generates Int_2B which is feasible by 4.8 kcal/mol, in this intermediate nitrogen is covalently bound to copper. This intermediate reacts with upcoming aniline molecule to give the final product via a new four-membered TS (TS_2B) having a low Gibbs free energy barrier of 13.9 kcal/mol. In this transition state, the metal atom interacts with the aniline's nitrogen atom and the nitrogen bonded to β carbon. This transition state results in the formation of the product through the transfer of a proton from aniline to the nitrogen bonded to the carbon and the active catalyst is regenerated. The product is feasible by 1.9 kcal/mol which is less than the Int_2B, making this step thermodynamically less feasible.

Our mechanistic investigation indicates that the MAOA pathway is the most likely pathway for this reaction which is favoured over the PAOA pathway both kinetically and thermodynamically. The TS_1B in PAOA has an energy barrier of 35.7 kcal/mol, approximately 16 kcal higher than TS_1A in MAOA which shows its kinetic favourability. In the product in the PAOA is less feasible than the Int_2B, whereas in MAOA the product is more feasible which shows thermodynamic favourability of MAOA pathway. Therefore, it follows the four-membered MAOA pathway. In addition, the intermediate formed in pathway B, Int 2B, is more stable than both the starting material and the product, necessitating a higher reaction temperature for the formation of the product due to the thermodynamics favouring Int 2B over the product.

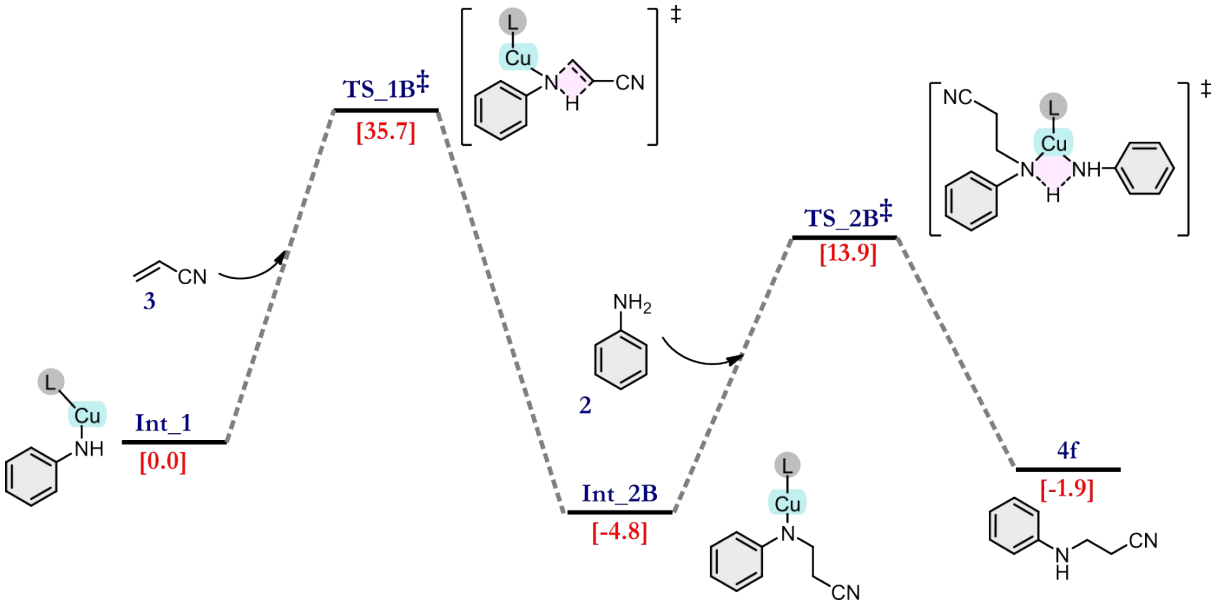


Figure S1: Proton assisted olefin activation pathway for the hydroamination reaction.

7. Energy profile diagram for hydroalkoxylation reaction of vinyl cyanide and phenol (MAOA has been shown)

Hydroalkoxylation of vinyl cyanide occurs in the same way that hydroamination of vinyl cyanide with aniline does. Since the active catalyst lacks a proton on oxygen, the PAOA pathway is unreliable for this reaction. This reaction also goes through two transition states: the olefin activation transition state, which has four members, and the product leading transition state, which has six members. The activation energy is slightly higher than the hydroamination reaction, which is in accordance with the experimental data (less yield is obtained as compared to the hydroamination reaction). The higher activation energy can be attributed to the higher electronegativity of oxygen as compared to nitrogen.

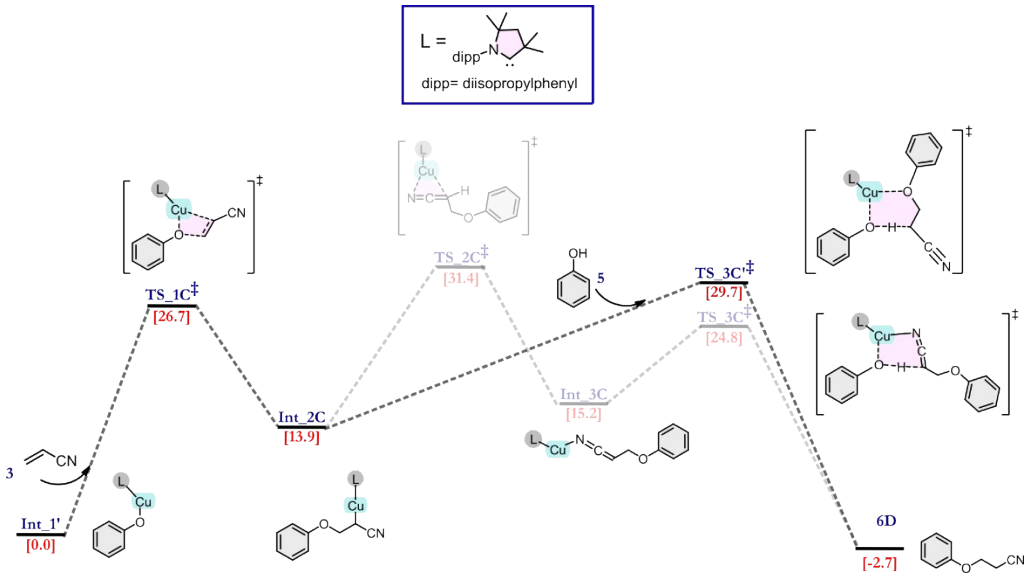


Figure S2: Copper assisted olefin activation pathway for the hydroalkoxylation reaction.

8. NBO charge analysis

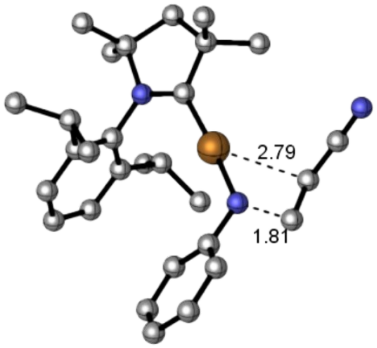
The following table summarises the NBO charges on the atoms directly or indirectly involved in the MAOA pathway and PAOA pathway for vinyl cyanide hydroamination reaction.

Table S2: NBO charge analysis

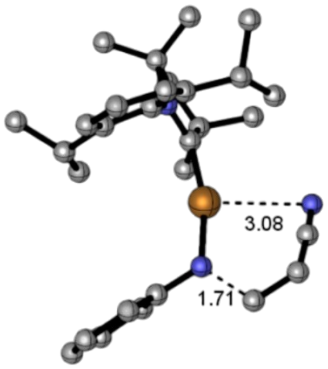
	N- β-C/Cu	*α-C*	*β-C*	*C-CN*	*N-CN*	*Cu*	*N(Aniline)*
INT_1	-0.979					0.533	
TS_1A	-0.52282	-0.6548	-0.18069	0.28076	-0.78568	0.5418	
TS_1A'	-0.75578	-0.65515	-0.18878	0.28471	-0.55091	0.55679	
INT_2A	-0.57804	-0.78493	-0.19959	0.30001	-0.4725	0.48087	
TS_2A	-0.570	-0.585	-0.218	0.185	-0.602	0.617	
INT_3A	-0.570	-0.592	-0.210	0.382	-0.747	0.590	
TS_3A	-0.57318	-0.66369	-0.20553	0.32999	-0.55351	0.57391	-0.93786
TS_3A'	-0.64876	-0.70089	-0.19466	0.30831	-0.50164	0.60998	-0.94856
TS_1B	-0.81	-0.708	-0.207	0.288	-0.509	0.538	
INT_2B	-0.755	-0.526	-0.755	0.323	-0.399	0.536	
TS_2B	-0.727	-0.519	0.186	0.319	-0.389	0.589	-0.96
Aniline							-0.785
Olefin		-0.332	-0.269	0.273	-0.343		

Investigation of the data obtained from NBO charge analysis provides useful insights into the two mechanisms. As we can see from the charge analysis of the olefin activation TS for the PAOA pathway, i.e., TS_1B, the charge on the α carbon (-0.708) is comparatively much more negative than the N-CN (-0.509), but in the case of MAOA olefin activation (TS_1A), there is a significantly greater negative charge on the N-CN (-0.7857) as compared to the α carbon (-0.6548). This observation shows that if the reaction was going through the proton-assisted pathway, the electron withdrawing group has no role to play. Contrary to this conclusion, only electron-deficient olefins undergo this reaction. In addition to the kinetic and thermodynamic viability of the PAOA pathway, data from charge analysis also supports the MAOA pathway. One additional observation that can be withdrawn from the NBO analysis is the fact that when olefin interacts with the catalyst, there is a significant increase in negative charge on the α carbon (-0.6548) as compared to free olefin α carbon (-0.332). As we can see in TS_1A, apart from the electron withdrawing cyano group, metal also plays a role in stabilising this incipient carbanion as there is a slight increase of positive charge on the copper.

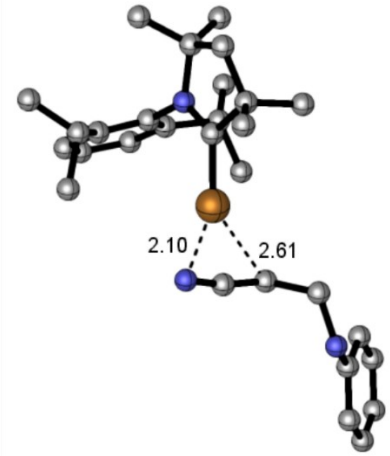
9. 3D Images of the TS involved in MAOA Pathway



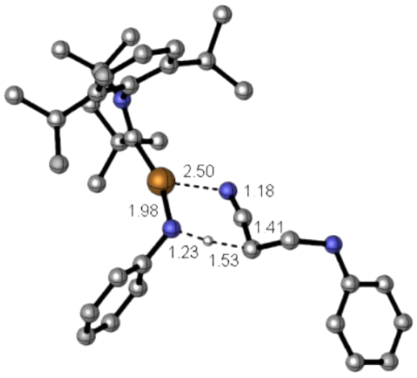
TS_1A‡



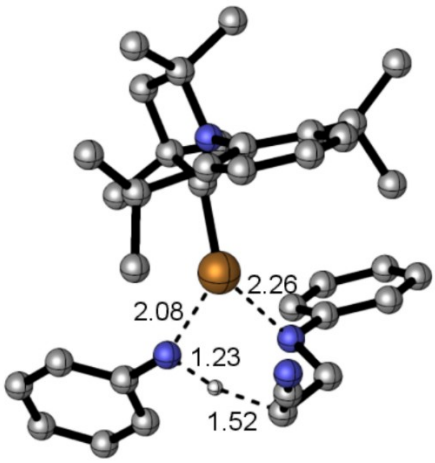
TS_1A'‡



TS_2A‡



TS_3A‡



TS_3A'‡

10. TS_1A energy comparison of different olefinic substrates in MAOA pathway

Figure S3 depicts the olefin activation transition states, both 4-membered as well as 6-membered and their corresponding free energies of activation of MAOA pathway for olefins with different electron withdrawing groups (EWGs). Here, four different olefins were used: vinyl cyanide (CH_2CHCN), methyl vinyl ketone ($CH_2CHCOMe$), methyl acrylate ($CH_2CHCOOMe$), and vinyl sulphone ($CH_2CHSOOPh$). In the case of vinyl cyanide, the 4-membered TS is much lower in energy than the 6-membered TS which gives direct indication that the reaction proceeds via 4-membered TS. The high energy of 6-membered TS is expected because of a geometrical constraint due to linear structure of cyanide (CN) group. In contrast to this 6-membered TS of other olefins have a lower activation energy barrier due to geometrically feasible triangular structures of EWGs. As a result, the energy of a six-membered TS is similar to that of a four-membered TS. In the case of methyl vinyl ketone, the energy of 6-membered TS is in fact lower than the 4-membered transition state. Hence, in this case reaction must be happening via this 6-membered TS. Whereas in other two cases, i.e., methyl acrylate and vinyl sulphone both transition states are feasibly equally, hence reaction can proceed via any of these two transition states.

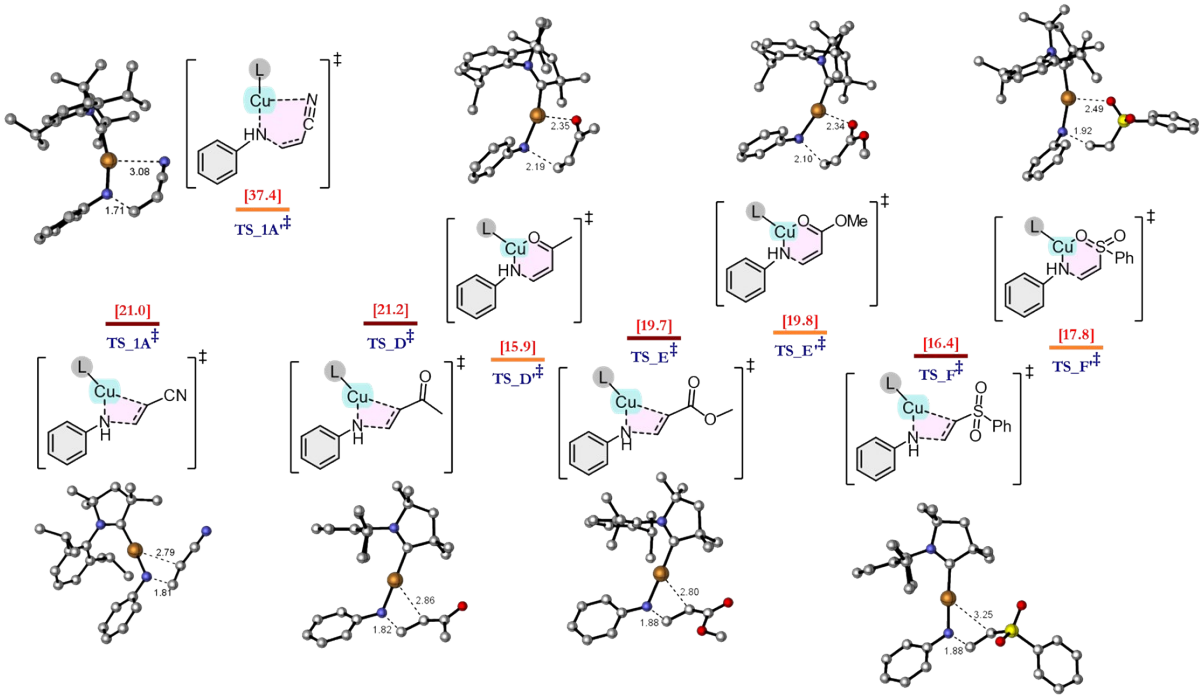
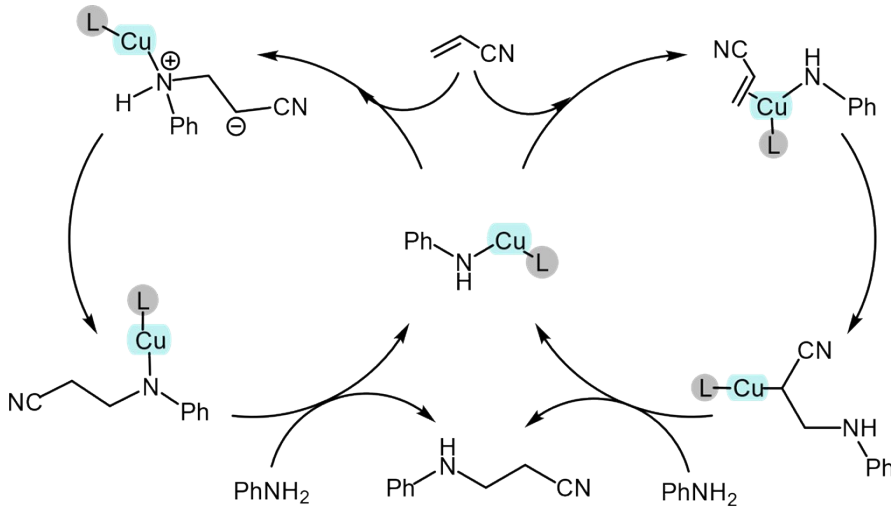


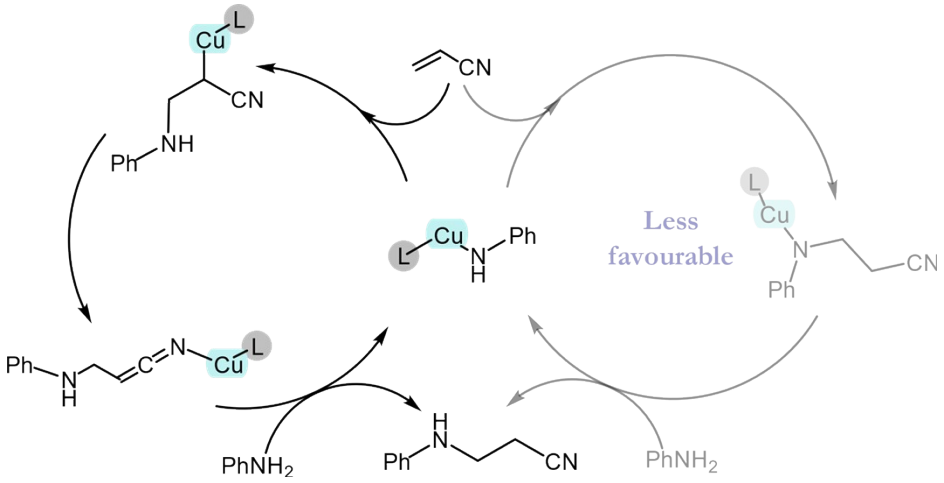
Figure S3: Comparison of Gibbs free energy of activation of 4 and 6-membered transition states (TS_1A) formed in the MAOA mechanism for different withdrawing groups on olefin such as CN, COMe, COOMe and SO_2Ph.

11. Comparison from Previous Literature



Previously, Gunnoe and co-workers had presented these two pathways. The first pathway is the Zwitter ionic pathway. The second pathway relies on the conventional organometallic catalytic mechanism, which involves the formation of metal olefin or cation-complexes. They have suggested that the hydroamination reaction proceeds via pathway one that is a zwitter ionic pathway to yield the product. Initially, they proposed both of these mechanisms without any mechanistic investigation, neither experimentally nor computationally. Later, they performed kinetic studies to support their hypothesis, but they have not provided convincing evidence for the mechanistic pathway. In this communication, we have done an exhaustive search and an ab-initio calculation to determine the mechanistic route. The proposed pathway is distinct and provides a different understanding of the reaction's mechanism. As previously described, we propose that the reaction proceeds via the MAOA pathway, and copper plays a crucial role in this reaction. It should also be noted that the MAOA pathway and the second pathway should not be confused. In the second pathway, the olefin forms a metal olefin complex, which is then followed by migratory insertion to generate the product-leading intermediate. However, in the MAOA, the olefin interacts with copper and nitrogen simultaneously and generates the same intermediate via a four-membered TS, as described previously.

DFT computed pathway



12. Single Point Energy of Stationary Points

Single point energy of all the transition states, intermediates and molecules involved in reaction pathways.

STATIONARY POINT/MOLECULE	SINGLE POINT ENERGY (HARTREE)
INT_1	-1320.536684
TS_1A	-1491.443306
TS_1A'	-1491.417264
INT_2A	-1491.470283
INT_3A	-1491.461739
TS_2A	-1491.441508
TS_3A	-1779.204693
TS_3A'	-1779.210811
TS_1B	-1491.407265
INT_2B	-1491.482684
TS_2B	-1779.219799
INT_1'	-1340.422078
TS_1C	-1511.316996
INT_2C	-1511.338449
TS_2C	-1511.311423
INT_3C	-1511.333427
TS_3C	-1818.955651
TS_3C'	-1818.949349
TS_D	-1551.879423
TS_D'	-1551.887291
TS_E	-1627.145274
TS_E'	-1627.146633
TS_F	-2179.053128
TS_F'	-2179.050705
Aniline	-287.750234
Phenol	-307.61676
Vinyl Cynaide	-170.913669
Methyl Vinyl Ketone	-231.352399
Methyl Acrylatre	-306.616372
Vinyl Sulphone	-858.518101
Product (4p)	-458.690104
Product (6d)	-478.558787

13. Coordinates for Optimised Structure

INT_1

Zero-point correction = 0.575517 (Hartree/Particle)

Thermal correction to Energy = 0.607185

Thermal correction to Enthalpy = 0.608129

Thermal correction to Gibbs Free Energy = 0.512074

Sum of electronic and zero-point Energies =-1319.402114

Sum of electronic and thermal Energies =-1319.370446

Sum of electronic and thermal Enthalpies =-1319.369502

Sum of electronic and thermal Free Energies =-1319.465557

Cartesian coordinates

Cu	1.17193900	0.07520600	-0.02377900
N	-1.61506300	0.73110900	-0.03218000
C	-2.69083800	1.81876800	-0.04092600
C	-1.83831700	3.05894500	-0.39052800
H	-2.15543800	3.93428000	0.18347700
H	-1.96694400	3.30393600	-1.44994300
C	-0.36233000	1.15435500	-0.06206200
C	-0.35704700	2.67841800	-0.11802700
C	-2.12265600	-1.39112000	-1.19456600
C	-1.95025100	-0.68590200	0.02149000
C	-1.81173900	-0.79952300	-2.56950400
H	-1.63645300	0.27220300	-2.45137700
C	-3.77647600	1.54393000	-1.08778800
H	-4.30551400	0.60845100	-0.88563400
H	-3.36854800	1.50550400	-2.09898300
H	-4.50937200	2.35624000	-1.05521200
C	-3.36218200	1.93714400	1.33655600
H	-3.87639800	1.01202100	1.60718100
H	-4.11083700	2.73461800	1.29807700
H	-2.65000100	2.18553300	2.12606200
C	0.15414100	3.22211700	1.23696700
H	1.17005000	2.87057300	1.43844700
H	-0.47924100	2.90941700	2.07251500
H	0.16762300	4.31744000	1.21403800
C	-2.50781300	-2.73568900	-1.12324800
H	-2.64660500	-3.29514600	-2.04293000
C	-2.45141300	-2.68206500	1.27870300
H	-2.54605300	-3.20009500	2.22781600
C	-0.50693400	-1.40480900	-3.13064500
H	0.33527700	-1.23602700	-2.45257400
H	-0.26295700	-0.94979000	-4.09702500
H	-0.60748100	-2.48472700	-3.28423500
C	-2.06185400	-1.33595000	1.27390000
C	-2.69398000	-3.37372500	0.09793900
H	-2.99855800	-4.41593700	0.12847500
C	-0.36479300	-1.30359100	3.13985100
H	0.45214500	-1.18428800	2.42166200
H	-0.48137700	-2.37273900	3.34779300
H	-0.07086800	-0.81101900	4.07334900
C	0.57281000	3.17614600	-1.24109200
H	1.60923100	2.87928500	-1.05634400
H	0.53482600	4.26983200	-1.30214900
H	0.27633100	2.77131000	-2.21406600
C	-1.67908600	-0.69297100	2.60669000
H	-1.48694200	0.36721700	2.43445600
C	-2.78824000	-0.80522900	3.67033500
H	-3.74088800	-0.39510400	3.32205800
H	-2.49664800	-0.26170000	4.57518800
H	-2.96391300	-1.84609400	3.96086400
C	-2.96380700	-0.98021300	-3.57641700
H	-3.90768000	-0.57582000	-3.19928500

H	-3.12807300	-2.03565100	-3.81638700
H	-2.72532300	-0.46943100	-4.51539600
N	2.66821300	-0.99105200	0.01519600
H	2.53016100	-1.99634700	0.02982100
C	4.00876900	-0.67711200	0.00181600
C	5.01352800	-1.67697000	-0.00453700
C	4.45371100	0.66893600	-0.00414300
C	6.36616700	-1.34913300	-0.01829700
H	4.71114800	-2.72309700	0.00020700
C	5.80671300	0.98616800	-0.01867300
H	3.70794900	1.46147000	0.00598500
C	6.78398300	-0.01570000	-0.02617800
H	7.10381700	-2.14878400	-0.02317900
H	6.10508500	2.03253100	-0.02298000
H	7.83979200	0.23722300	-0.03696700

TS_1A

Zero-point correction = 0.630341 (Hartree/Particle)

Thermal correction to Energy = 0.665808

Thermal correction to Enthalpy = 0.666752

Thermal correction to Gibbs Free Energy = 0.563512

Sum of electronic and zero-point Energies =-1490.163158

Sum of electronic and thermal Energies =-1490.127691

Sum of electronic and thermal Enthalpies =-1490.126747

Sum of electronic and thermal Free Energies =-1490.229987

Cartesian coordinates

Cu	-0.69495000	1.13329700	-0.65580700
N	1.89198100	-0.09596000	-0.25504500
C	3.40893800	-0.00944200	-0.48513700
C	3.51514000	1.35790200	-1.19307800
H	4.23119000	1.32338400	-2.01940800
H	3.87051000	2.11071500	-0.48328600
C	1.17307700	0.83998400	-0.83588800
C	2.08715500	1.73569100	-1.66529900
C	1.18457600	-1.11539000	1.90446300
C	1.31615500	-1.20715200	0.49762100
C	1.36361900	0.17285300	2.70790500
H	1.69917900	0.97207400	2.04392900
C	4.17449900	-0.02461500	0.84073600
H	4.04518800	-0.97059000	1.37312600
H	3.86640000	0.79521800	1.49115300
H	5.24155300	0.09677700	0.62806900
C	3.90381500	-1.17439400	-1.35500500
H	3.70773200	-2.13755100	-0.87727500
H	4.98672500	-1.08083900	-1.48225900
H	3.45158100	-1.17641900	-2.34866100
C	1.85263800	1.38857100	-3.15686800
H	0.81272000	1.57746700	-3.44053400
H	2.08128700	0.34355600	-3.38802900
H	2.49473000	2.02053500	-3.77987300
C	0.74821300	-2.25779700	2.59155200
H	0.64929600	-2.21220700	3.67140600
C	0.47391900	-3.47053400	0.53699500
H	0.16019000	-4.36962500	0.01620000
C	0.00073200	0.63009300	3.27049600
H	-0.74434600	0.71419600	2.47536600
H	0.09952200	1.62067200	3.71991000
H	-0.37494900	-0.07236600	4.02365700
C	0.91131200	-2.36875900	-0.20822700
C	0.41805700	-3.43129300	1.92566300
H	0.08865400	-4.30305400	2.48405000
C	-0.65389800	-2.39588600	-2.18259300
H	-1.14244300	-1.48638700	-1.82077400
H	-1.21779500	-3.25343900	-1.80064100
H	-0.71899400	-2.40976000	-3.27647800
C	1.79339800	3.23012400	-1.44800100
H	0.78861100	3.48689400	-1.79600500

H	2.51798300	3.82864700	-2.01257700
H	1.84725100	3.49699500	-0.39005200
C	0.82159400	-2.45342600	-1.73252300
H	1.31450200	-1.57793700	-2.15717400
C	1.50754000	-3.70334200	-2.31594100
H	2.55347900	-3.78224200	-2.00632400
H	1.48054700	-3.66860200	-3.41032800
H	1.00048700	-4.62410400	-2.01015800
C	2.37402000	0.03567000	3.86376300
H	3.35765600	-0.30039300	3.52559100
H	2.02448200	-0.67572100	4.62008600
H	2.49808300	1.00376000	4.35922500
H	-2.89257600	1.80297500	-1.41318900
N	-2.67699400	1.34882000	-0.52464900
C	-3.60008900	0.25590500	-0.33697700
C	-4.74184100	0.12860500	-1.13740700
C	-3.37211400	-0.67405700	0.68558800
C	-5.63513600	-0.92359200	-0.92968400
H	-4.92898900	0.85311200	-1.92690500
C	-4.27555600	-1.71403800	0.89984600
H	-2.48087900	-0.58492600	1.29961400
C	-5.40801000	-1.84622600	0.09246700
H	-6.51139500	-1.01660400	-1.56497700
H	-4.08737200	-2.42967800	1.69509200
H	-6.10537000	-2.66203400	0.25758200
C	-2.79278700	2.53741100	0.53300200
H	-3.80857300	2.93223900	0.40669900
H	-2.73850800	2.02523500	1.49799600
C	-1.73906300	3.53821200	0.32400900
H	-1.96960500	4.44486700	-0.22498200
C	-0.56929000	3.50910700	1.07935800
N	0.43674600	3.45262800	1.69891200

TS_1A'

Zero-point correction = 0.630155 (Hartree/Particle)

Thermal correction to Energy = 0.665657

Thermal correction to Enthalpy = 0.666602

Thermal correction to Gibbs Free Energy = 0.563548

Sum of electronic and zero-point Energies =-1490.131673

Sum of electronic and thermal Energies =-1490.096171

Sum of electronic and thermal Enthalpies =-1490.095226

Sum of electronic and thermal Free Energies =-1490.198280

Cartesian coordinates

Cu	-0.77854700	-1.03937600	-0.04215300
N	1.71385200	0.25889000	-0.55079700
C	2.92992500	0.47622700	-1.47010900
C	2.46163600	-0.28368600	-2.73103800
H	3.29079000	-0.81535400	-3.20582100
H	2.07276100	0.43050100	-3.46482300
C	0.85806500	-0.65856500	-0.95376700
C	1.33255800	-1.24922200	-2.27824100
C	1.84703000	-2.69617400	-2.07192200
H	1.11041200	-3.31281800	-1.54973400
H	2.77762200	-2.72270800	-1.49948000
H	2.05452700	-3.13462800	-3.05474800
C	0.16883400	-1.29842400	-3.28849300
H	-0.60575900	-1.99160800	-2.94746000
H	0.53817500	-1.65502900	-4.25639700
H	-0.28639600	-0.31547200	-3.44143600
N	-2.52987600	-0.93142400	0.86160700
C	-3.23381200	-2.48294600	1.03259400
H	-3.54260700	-2.64896700	-0.00180300
H	-4.10661600	-2.28096000	1.65875300
C	-2.31127600	-3.43936500	1.57504500
H	-2.25487900	-3.62040400	2.64258900
C	-1.25663800	-3.82804800	0.75645800
N	-0.39220700	-4.09014100	-0.00658000

C	1.51410200	1.03196200	0.67672200
C	0.81058100	2.27249900	0.60626400
C	1.99046300	0.53450200	1.92612800
C	0.70947000	3.03047900	1.78363900
C	1.85575900	1.36996000	3.04811500
C	1.25077500	2.61344300	2.98804800
H	0.15995000	3.96652700	1.74908300
H	2.21512700	1.00359000	4.00557900
H	1.15670100	3.22699000	3.87918800
C	2.58298300	-0.84358000	2.32937800
C	0.01695900	2.93671200	-0.55386400
C	4.20524300	-0.11683500	-0.85588600
H	5.02721700	0.00848300	-1.56750300
H	4.47789800	0.41248600	0.05945100
H	4.11443700	-1.17990100	-0.63506700
C	3.19836900	1.95788800	-1.74575100
H	4.08530500	2.03639500	-2.38232500
H	2.37293900	2.43279900	-2.27284500
H	3.39836100	2.51339500	-0.82548000
H	2.08632400	-1.02573100	3.29092600
H	-0.92910200	3.19793500	-0.06199300
C	2.28102200	-2.10148600	1.50875200
H	2.81479100	-2.13732000	0.56075100
H	2.60688800	-2.97295400	2.08675400
H	1.21843500	-2.23845300	1.30027700
C	4.08941700	-0.76031000	2.66774200
H	4.31772400	0.09831700	3.30616700
H	4.39438800	-1.66674500	3.20129500
H	4.71030100	-0.68652500	1.77256500
C	-0.41692300	2.12800100	-1.78297600
H	-0.94078500	1.21323000	-1.49988300
H	-1.11461000	2.74016200	-2.36452400
H	0.40725300	1.86340600	-2.44761600
C	0.63583500	4.28639600	-0.98939800
H	0.84371400	4.93595000	-0.13521700
H	1.57201900	4.15745700	-1.53663500
H	-0.06245400	4.81429700	-1.64754200
H	-2.29028900	-0.71700700	1.83045600
C	-3.44455900	0.06123500	0.38709300
C	-3.99319300	1.02789700	1.24491800
C	-3.86487400	0.03111100	-0.95336700
C	-4.92026700	1.95479500	0.76833300
H	-3.68444500	1.05444800	2.28768000
C	-4.80246900	0.95087800	-1.42020500
H	-3.44464100	-0.71361000	-1.62361200
C	-5.33270300	1.92073100	-0.56554900
H	-5.32538200	2.70213900	1.44520200
H	-5.11620100	0.91238800	-2.45981200
H	-6.05828900	2.63949500	-0.93408300

INT_2A

Zero-point correction = 0.631338 (Hartree/Particle)

Thermal correction to Energy = 0.667561

Thermal correction to Enthalpy = 0.668505

Thermal correction to Gibbs Free Energy = 0.560157

Sum of electronic and zero-point Energies =-1490.194857

Sum of electronic and thermal Energies =-1490.158634

Sum of electronic and thermal Enthalpies =-1490.157689

Sum of electronic and thermal Free Energies =-1490.266038

Cartesian coordinates

Cu	0.46145200	0.37397900	0.46283500
N	-2.39846500	0.68145100	0.07771400
C	-3.65338500	1.54905000	0.25020800
C	-3.01411100	2.89703100	0.65119200
H	-3.58499300	3.38684300	1.44502200
H	-3.01337500	3.57318400	-0.20991600
C	-1.27408000	1.20338400	0.51374300

C	-1.55232100	2.59051800	1.07850400
C	-2.28638400	-0.76273800	-1.92629900
C	-2.46195400	-0.64682700	-0.52639500
C	-1.85608400	0.39504000	-2.82731500
H	-1.91892000	1.32274800	-2.25343200
C	-4.46111600	1.64769900	-1.04835500
H	-4.81908600	0.66831500	-1.37694300
H	-3.88383100	2.10031000	-1.85601300
H	-5.33547100	2.28109500	-0.86878600
C	-4.56157600	0.97794400	1.34939900
H	-4.92036100	-0.01987100	1.08775600
H	-5.43506600	1.62838600	1.45735900
H	-4.06081000	0.92690600	2.31835400
C	-1.38105400	2.53655300	2.61476500
H	-0.36539800	2.23016200	2.88219300
H	-2.07715000	1.83456600	3.08336100
H	-1.56302700	3.52904900	3.04110500
C	-2.41657200	-2.03459000	-2.49671400
H	-2.28232900	-2.15042300	-3.56738900
C	-2.78742500	-3.02605900	-0.33904600
H	-2.93736500	-3.91295300	0.26783100
C	-0.37847000	0.22684500	-3.24126900
H	0.27437300	0.16020800	-2.36529600
H	-0.05323900	1.07899500	-3.84848300
H	-0.23526300	-0.68327700	-3.83283800
C	-2.66532200	-1.78174700	0.29315500
C	-2.68611800	-3.15468600	-1.71857600
H	-2.78185500	-4.13141800	-2.18343500
C	-1.35379800	-2.41084300	2.35097800
H	-0.45753900	-1.95123600	1.92667400
H	-1.31894300	-3.47462200	2.09626800
H	-1.30696500	-2.32375400	3.44244100
C	-0.56049600	3.61632600	0.49761800
H	0.46749800	3.37552400	0.78424600
H	-0.79569600	4.61868500	0.87281000
H	-0.60789100	3.64413800	-0.59589600
C	-2.64418900	-1.74969000	1.82096300
H	-2.62409900	-0.70706000	2.14400600
C	-3.88071900	-2.41504600	2.45551400
H	-4.81890000	-1.98195400	2.09576400
H	-3.85087200	-2.30036200	3.54421500
H	-3.91072400	-3.48871600	2.24449900
C	-2.74831100	0.55471200	-4.07295800
H	-3.80512300	0.66069700	-3.81090000
H	-2.65847100	-0.30366000	-4.74612600
H	-2.44717500	1.44215900	-4.63976400
C	2.26013500	-0.42547300	0.39588300
H	2.69477000	-0.12756700	-0.56807200
C	3.21863300	-0.00164300	1.53513300
H	3.28520100	1.08925700	1.56993100
H	2.80593400	-0.31376100	2.50021500
N	4.57683600	-0.54260700	1.46795200
H	4.60542600	-1.53965400	1.64310600
C	5.49965900	-0.13585600	0.50674000
C	5.41570500	1.10403100	-0.15777200
C	6.60319600	-0.96585300	0.21583400
C	6.40508200	1.49193500	-1.06185700
H	4.58152900	1.77056900	0.03262700
C	7.58112800	-0.56801400	-0.68846200
H	6.68388400	-1.92950300	0.71401100
C	7.49520200	0.66714900	-1.33844300
H	6.31379800	2.45485600	-1.55854300
H	8.41773200	-1.23224500	-0.88977100
H	8.25855700	0.97527400	-2.04614700
C	2.07488200	-1.86101600	0.38347200
N	1.89567500	-3.01514500	0.42346200

TS_2A

Zero-point correction = 0.630555 (Hartree/Particle)

Thermal correction to Energy = 0.666016

Thermal correction to Enthalpy = 0.666961

Thermal correction to Gibbs Free Energy = 0.561373

Sum of electronic and zero-point Energies =-1490.169132

Sum of electronic and thermal Energies =-1490.133671

Sum of electronic and thermal Enthalpies =-1490.132727

Sum of electronic and thermal Free Energies =-1490.238315

Cartesian coordinates

Cu	-0.04477900	-1.08379000	0.50789800
N	2.42547300	-0.17299900	-0.62137300
C	3.55790900	-0.43334700	-1.61811600
C	3.24309500	-1.88773900	-2.03313400
H	3.90701400	-2.57241400	-1.49521300
H	3.41561200	-2.04360100	-3.10186300
C	1.45913400	-1.07608000	-0.60091600
C	1.77065700	-2.16324200	-1.62525700
C	1.80267300	2.18875800	-0.15509600
C	2.41813800	0.98499400	0.26489200
C	1.00206300	2.33836200	-1.44859100
H	1.11939400	1.42541200	-2.03423800
C	1.86092200	3.28966600	0.70992400
H	1.39576500	4.22261600	0.40765700
C	3.02243900	1.99865100	2.36963100
H	3.46139900	1.92647700	3.35958500
C	-0.50446200	2.48105300	-1.14497200
H	-0.88751000	1.61042700	-0.60560000
H	-1.06897000	2.57463200	-2.07961500
H	-0.70534500	3.37374900	-0.54305100
C	2.99931400	0.86208300	1.55161400
C	2.47782000	3.20731800	1.95212300
H	2.51074600	4.07538100	2.60420100
C	2.60715600	-0.95561800	3.26583000
H	1.58032000	-1.10447700	2.92184800
H	2.58624600	-0.24702400	4.10098600
H	2.97913600	-1.91185700	3.65072900
C	3.52704800	-0.44995200	2.13353800
H	3.50790000	-1.20833500	1.34710300
C	-2.60468100	-0.56891400	0.48968700
H	-2.83780500	0.49002900	0.55506500
C	-3.52689300	-1.44335100	-0.33560800
H	-3.55802700	-1.09246200	-1.37199700
H	-3.13267200	-2.46441900	-0.37261800
N	-4.91631500	-1.54913700	0.13153900
H	-4.99539400	-2.06971300	0.99643700
C	-5.81247900	-0.48447200	0.06099600
C	-5.64500900	0.60003100	-0.82279400
C	-6.97061700	-0.50519700	0.86706300
C	-6.60821800	1.60646900	-0.89918000
H	-4.76419600	0.66133200	-1.45242600
C	-7.92129800	0.50560600	0.78306000
H	-7.11765300	-1.33261400	1.55801400
C	-7.75283600	1.57418400	-0.10291800
H	-6.45218600	2.43055500	-1.59100100
H	-8.80200100	0.45859700	1.41849700
H	-8.49518900	2.36367700	-0.16636000
C	-1.85842300	-1.09774100	1.51512900
N	-1.05534200	-1.56131900	2.28628600
C	4.97790900	-0.33065700	2.64147400
H	5.04644200	0.34218200	3.50237800
H	5.34265800	-1.31040100	2.96804900
H	5.65800500	0.04706200	1.87256000
C	1.48133700	3.52163500	-2.31257500
H	0.94464200	3.53204100	-3.26712600
H	1.28761100	4.48085100	-1.82162800

H	2.55299000	3.47376000	-2.52752700
C	1.60665100	-3.56294600	-1.00384000
H	0.57206200	-3.73804400	-0.69389100
H	1.88017300	-4.33249400	-1.73482100
H	2.24505700	-3.68653300	-0.12347700
C	0.79050200	-2.02257100	-2.81371500
H	1.00349400	-2.79464700	-3.56128200
H	-0.24365700	-2.14336000	-2.47904100
H	0.87014400	-1.04710300	-3.30232300
C	4.93653300	-0.30172700	-0.96181900
H	5.10610000	0.70777800	-0.57732300
H	5.07000700	-1.01483500	-0.14733100
H	5.70464500	-0.50690300	-1.71411800
C	3.49026600	0.54054400	-2.80497800
H	2.54783100	0.46768400	-3.35143500
H	3.62725400	1.57370200	-2.47873100
H	4.29991800	0.30258600	-3.50199500

INT_3A

Zero-point correction = 0.630238 (Hartree/Particle)

Thermal correction to Energy = 0.666891

Thermal correction to Enthalpy = 0.667835

Thermal correction to Gibbs Free Energy = 0.557255

Sum of electronic and zero-point Energies =-1490.191041

Sum of electronic and thermal Energies =-1490.154388

Sum of electronic and thermal Enthalpies =-1490.153444

Sum of electronic and thermal Free Energies =-1490.264024

Cartesian coordinates

Cu	-0.15220200	0.43228400	0.32737000
N	-2.93205600	0.65461900	-0.29774700
C	-4.10393900	1.55922800	-0.68946800
C	-3.34954000	2.85051800	-1.07812700
H	-3.87793200	3.74075600	-0.72566200
H	-3.28665400	2.92310800	-2.16874800
C	-1.76297300	1.25256700	-0.16839600
C	-1.92124100	2.73617700	-0.47842100
C	-2.94381200	-1.66519500	-1.15425100
C	-3.10383400	-0.77471500	-0.06496200
C	-2.42703900	-1.24111300	-2.52911400
H	-2.40233400	-0.14948800	-2.56675800
C	-4.90832600	0.97920500	-1.85803500
H	-5.35252100	0.01320000	-1.60289700
H	-4.29855900	0.86016300	-2.75490500
H	-5.72323600	1.66902900	-2.09876200
C	-5.05315500	1.76782700	0.50082300
H	-5.49779500	0.82341300	0.82296300
H	-5.86735200	2.43019800	0.19089200
H	-4.55401000	2.22948200	1.35518700
C	-1.76399500	3.53611600	0.83649300
H	-0.77638000	3.37047400	1.27671800
H	-2.51430300	3.25718600	1.58231900
H	-1.87256400	4.60669400	0.63126800
C	-3.17976400	-3.02643200	-0.92546900
H	-3.06336300	-3.72798600	-1.74531200
C	-3.61784400	-2.61725900	1.40195100
H	-3.84160000	-3.00067500	2.39232600
C	-0.97519800	-1.72759400	-2.72788800
H	-0.31435100	-1.34914500	-1.94215700
H	-0.58928800	-1.38418900	-3.69404400
H	-0.92071200	-2.82133400	-2.71401800
C	-3.39165300	-1.24407500	1.23879500
C	-3.53595700	-3.50030400	0.33205400
H	-3.71847900	-4.56012900	0.48413000
C	-2.11668300	-0.69662400	3.34383300
H	-1.19189800	-0.57495100	2.77195900
H	-2.15160200	-1.72818500	3.70994200
H	-2.06897700	-0.03320600	4.21441400

C	-0.84373600	3.19884000	-1.47793200
H	0.15965000	3.08750000	-1.05632000
H	-0.99462100	4.25495200	-1.72839400
H	-0.88484400	2.62083100	-2.40672100
C	-3.35976700	-0.36601700	2.48940900
H	-3.26098600	0.67503900	2.17730000
C	-4.63801000	-0.48279800	3.34167200
H	-5.54273600	-0.26860400	2.76499400
H	-4.59605300	0.22151500	4.17911200
H	-4.74787500	-1.48529400	3.76757300
C	-3.31970600	-1.73119400	-3.68526400
H	-4.36035700	-1.41658500	-3.56431600
H	-3.31105700	-2.82281400	-3.76639300
H	-2.95223700	-1.33417100	-4.63745200
C	3.70160400	-1.31944900	1.33309700
H	3.75524000	-2.38491800	1.53252300
C	4.96207300	-0.50448700	1.33919100
H	5.62977900	-0.86144400	2.14009100
C	2.49987000	-0.78849200	1.04483300
N	1.42917800	-0.31114700	0.80744800
N	5.67093100	-0.57314100	0.05035100
H	4.73659900	0.54635200	1.56789800
C	6.99777700	-0.23540800	-0.11268000
C	7.69812400	0.53150600	0.84371900
C	7.69272400	-0.63231900	-1.27833600
C	9.03254300	0.87842400	0.63206300
H	7.19468400	0.86250100	1.74537500
C	9.02156300	-0.27693400	-1.47401700
H	7.17064100	-1.22377300	-2.02766200
C	9.71018600	0.48212300	-0.52116800
H	9.54674400	1.46987300	1.38597500
H	9.52760200	-0.59960800	-2.38080800
H	10.74901600	0.75648000	-0.67676600
H	5.30046700	-1.27355100	-0.57538000

TS_3A

Zero-point correction = 0.745493 (Hartree/Particle)

Thermal correction to Energy = 0.788352

Thermal correction to Enthalpy = 0.789297

Thermal correction to Gibbs Free Energy = 0.665065

Sum of electronic and zero-point Energies =-1777.679510

Sum of electronic and thermal Energies =-1777.636651

Sum of electronic and thermal Enthalpies =-1777.635706

Sum of electronic and thermal Free Energies =-1777.759938

Cartesian coordinates

Cu	0.27392000	0.37366400	-0.36823800
N	2.97364600	-0.63423300	-0.65446600
C	4.12764400	-0.99342000	-1.60078400
C	3.65050700	-0.29873800	-2.89354400
H	3.88969900	-0.89381500	-3.77935900
H	4.16359600	0.66329600	-2.99982300
C	1.88716500	-0.15359700	-1.22971100
C	2.12373500	-0.06598900	-2.73473500
C	3.57908900	0.25448100	1.57197200
C	3.07714600	-0.81444900	0.78858600
C	3.89190200	1.64487900	1.01754900
H	3.83343900	1.60241800	-0.07229800
C	1.28334600	-1.15488800	-3.44483600
H	0.22465900	-1.05560700	-3.19889000
H	1.59046900	-2.16383900	-3.15462200
H	1.41628700	-1.06204200	-4.52868900
C	3.71913400	0.04795300	2.94983800
H	4.10142900	0.85379900	3.56845400
C	2.82356400	-2.17367300	2.76491300
H	2.50797300	-3.09753500	3.23927700
C	2.82968900	2.66466200	1.47793500
H	1.82858400	2.36553800	1.15725700

H	3.04035500	3.65167700	1.05212000
H	2.82545200	2.76432000	2.56904200
C	2.65500800	-2.02819500	1.38076600
C	3.36431300	-1.15822700	3.54381100
H	3.48782200	-1.29728500	4.61405300
C	1.70009900	1.31703400	-3.26403600
H	0.62548000	1.47381200	-3.13356500
H	1.92866300	1.39353600	-4.33315200
H	2.22554300	2.12579900	-2.74545900
C	5.30224900	2.13649100	1.39767600
H	6.08008900	1.42412600	1.10851800
H	5.39258200	2.30510900	2.47564100
H	5.51297000	3.09077100	0.90326100
C	-3.83159500	-0.88525400	1.25967600
H	-4.23615000	-0.19737600	2.00906500
C	-3.22156500	-0.07651000	0.11583000
C	1.94520800	-3.15049600	0.62442800
C	-1.06938800	5.14325100	1.05429500
C	-1.49726300	5.51642800	-0.22116100
C	-1.75443300	4.52206000	-1.16883700
C	-1.57965800	3.17600400	-0.85359000
C	-1.14317700	2.79414200	0.42779800
C	-0.89908700	3.79768100	1.37971700
H	-0.86954500	5.90256000	1.80581100
H	-1.63196200	6.56415400	-0.47203700
H	-2.09557700	4.79533700	-2.16388400
H	-1.78213000	2.40704200	-1.59412600
H	-0.57182300	3.51761500	2.37884400
N	-1.00244400	1.41281700	0.73424700
H	-0.76695900	1.30959200	1.72047300
H	-2.07024000	0.82311100	0.56205700
C	2.62540800	-4.52041100	0.81508300
H	2.13743800	-5.27167600	0.18546900
H	3.68746600	-4.49803200	0.55328500
H	2.54950200	-4.86657100	1.85114800
C	5.47280600	-0.44965300	-1.10762600
H	5.47684200	0.63906100	-1.04287000
H	5.74459100	-0.86280700	-0.13226400
H	6.24924600	-0.74182300	-1.82161500
C	4.25210200	-2.51733800	-1.75754900
H	4.51409700	-2.99200400	-0.80921900
H	3.33659800	-2.97456900	-2.13643800
H	5.05461900	-2.73402400	-2.46954400
H	1.95777600	-2.91300400	-0.44009600
C	0.46194300	-3.23169100	1.04178000
H	0.36176800	-3.45464200	2.10973600
H	-0.06116100	-2.29622600	0.82939500
H	-0.04364200	-4.02505100	0.48140800
C	-2.34326600	-0.75759800	-0.74837300
N	-1.42452500	-1.17485400	-1.36196000
H	-3.94722400	0.54106700	-0.41822700
H	-3.04510800	-1.45545500	1.76747400
N	-4.88586700	-1.84959400	0.92491400
H	-4.53108400	-2.65820600	0.42988900
C	-6.14640500	-1.45712600	0.48053600
C	-6.95827700	-2.38926500	-0.20008900
C	-6.67824600	-0.17557200	0.72548900
C	-8.24593100	-2.05737500	-0.60572200
H	-6.56496200	-3.38357500	-0.40145500
C	-7.97282400	0.14368900	0.31495700
H	-6.08456700	0.57430600	1.23646500
C	-8.77027700	-0.78623400	-0.35197300
H	-8.84476300	-2.79936200	-1.12784800
H	-8.35635400	1.14051300	0.51781200
H	-9.77511700	-0.52757200	-0.67111200

TS_3A'

Zero-point correction = 0.745974 (Hartree/Particle)

Thermal correction to Energy = 0.788591

Thermal correction to Enthalpy = 0.789535

Thermal correction to Gibbs Free Energy = 0.668519

Sum of electronic and zero-point Energies = -1777.661561

Sum of electronic and thermal Energies =-1777.618944

Sum of electronic and thermal Enthalpies =-1777.618000

Sum of electronic and thermal Free Energies =-1777.739016

Cartesian coordinates

Cu	0.72272700	-0.21986600	0.12270700
N	-1.96227400	-0.17264200	-1.11010500
C	-2.71726900	-0.22007600	-2.44726700
C	-1.54637800	-0.38703500	-3.43646300
H	-1.69706500	0.21194500	-4.33926200
H	-1.47976900	-1.43392100	-3.75071100
C	-0.64447100	-0.08238600	-1.19344700
C	-0.25802400	0.00992300	-2.67320300
C	-3.02446600	-1.41730500	0.76690700
C	-2.70653700	-0.18422700	0.14626600
C	-2.43326700	-2.76521800	0.35545400
H	-1.82496200	-2.61462600	-0.54102100
C	0.16783000	1.46761200	-2.97060200
H	1.02983100	1.75977900	-2.36493400
H	-0.63617600	2.18188800	-2.77057300
H	0.44380300	1.55889500	-4.02722800
C	-3.84833400	-1.38929000	1.89930200
H	-4.09593700	-2.32291100	2.39363100
C	-3.94390500	1.00769300	1.84417300
H	-4.27049600	1.94066600	2.29224900
C	-1.50082700	-3.28891700	1.47160800
H	-0.83282800	-2.51188600	1.84985300
H	-0.91115700	-4.13859700	1.10724400
H	-2.07905400	-3.63711800	2.33332900
C	-3.12455100	1.04697000	0.70918200
C	-4.32536900	-0.19555600	2.42425000
H	-4.96054700	-0.20134400	3.30493400
C	0.91016000	-0.93180900	-3.01384500
H	1.81808800	-0.65916800	-2.46805200
H	1.13111500	-0.88091100	-4.08631700
H	0.67455400	-1.97103200	-2.76492500
C	-3.50115300	-3.83269400	0.04287800
H	-4.19499200	-3.51918500	-0.74070200
H	-4.09326300	-4.06948100	0.93268300
H	-3.01959700	-4.76170200	-0.28169200
H	2.95268800	0.55116200	0.95353900
N	2.17247800	1.17322400	1.15032900
C	1.96187500	1.16848000	2.64552100
H	2.73278300	1.80967200	3.09704600
H	0.99617900	1.64474300	2.83262100
C	2.00189100	-0.25030800	3.20628000
H	2.86997400	-0.43556700	3.84228200
C	0.78881300	-0.67781800	3.82042600
N	-0.23592200	-1.07759400	4.22564400
C	-2.63778600	2.41209900	0.22516500
C	3.95898700	-3.83111200	-1.32434100
C	5.20550900	-3.21811300	-1.16879700
C	5.32289400	-2.14661400	-0.28259700
C	4.21489400	-1.68367000	0.42845300
C	2.94743400	-2.27607800	0.25973900
C	2.84721400	-3.36844200	-0.62444600
H	3.85005600	-4.67731900	-1.99794400
H	6.07019300	-3.57828200	-1.71756200
H	6.28921300	-1.67445500	-0.12535200
H	4.34643600	-0.89527500	1.16445300
H	1.88121200	-3.85048900	-0.75758800
N	1.82031000	-1.77932700	0.95263200

H	1.14850800	-2.52847100	1.10175700
H	2.02296700	-1.19626000	2.01379700
C	-3.77249400	3.43046500	0.00643600
H	-3.36657800	4.35865800	-0.40990900
H	-4.53758100	3.05874900	-0.68113100
H	-4.27020200	3.68940700	0.94637500
C	2.44734600	2.42631600	0.52315100
C	1.97282700	3.64338100	1.03218700
C	3.21500200	2.43899800	-0.65513200
C	2.24701200	4.83837700	0.36220400
H	1.39487100	3.66508600	1.94787000
C	3.48583900	3.63572100	-1.31363200
H	3.60499100	1.50160800	-1.04620000
C	2.99908700	4.84615100	-0.81177400
H	1.87252700	5.77173700	0.77367600
H	4.08618600	3.62182300	-2.21914400
H	3.21245500	5.77955500	-1.32342800
C	-3.68122600	-1.40904800	-2.50540700
H	-3.15746600	-2.35717500	-2.37440600
H	-4.46850900	-1.33189000	-1.75115000
H	-4.15958200	-1.42447700	-3.49001100
C	-3.51940500	1.06753900	-2.68838800
H	-4.27596100	1.21191700	-1.91387500
H	-2.88543900	1.95507900	-2.72967800
H	-4.03832600	0.98322900	-3.64838600
H	-2.12035500	2.27929600	-0.72612300
C	-1.60164600	2.97523900	1.21838700
H	-2.05160700	3.15098200	2.20133000
H	-0.77158000	2.27653800	1.34691600
H	-1.19586400	3.92411400	0.85194900

TS_1B

Zero-point correction = 0.625198 (Hartree/Particle)

Thermal correction to Energy = 0.661149

Thermal correction to Enthalpy = 0.662093

Thermal correction to Gibbs Free Energy = 0.555306

Sum of electronic and zero-point Energies =-1490.127739

Sum of electronic and thermal Energies =-1490.091788

Sum of electronic and thermal Enthalpies =-1490.090844

Sum of electronic and thermal Free Energies =-1490.197631

Cartesian coordinates

Cu	0.73681100	-0.89812800	-0.13255700
N	-2.11449300	-0.57674300	0.09106700
C	-3.49333200	-1.24497200	0.19171400
C	-3.07912000	-2.70601800	0.47625200
H	-3.70921700	-3.41109800	-0.07283000
H	-3.20581000	-2.92179200	1.54194700
C	-1.08679500	-1.39380200	0.02565700
C	-1.57909500	-2.83321500	0.09190600
C	-1.78135500	1.56226200	1.28573100
C	-1.95438100	0.87382900	0.06064400
C	-1.59994900	0.86681900	2.63538100
H	-1.82190900	-0.19540100	2.50935600
C	-4.33761400	-0.64356700	1.32018200
H	-4.53247300	0.41986300	1.15680200
H	-3.86738000	-0.76963200	2.29641400
H	-5.30220400	-1.15976200	1.34695200
C	-4.26586300	-1.09938400	-1.12820100
H	-4.45695700	-0.05000000	-1.36372900
H	-5.23433200	-1.59806500	-1.02423700
H	-3.74334000	-1.55897000	-1.96962300
C	-1.37292400	-3.49054000	-1.29322400
H	-0.31480500	-3.49089200	-1.57120400
H	-1.92811300	-2.97582000	-2.08318200
H	-1.71616000	-4.52999700	-1.26063900
C	-1.67825000	2.95822200	1.23944100
H	-1.54308600	3.50877800	2.16472000

C	-1.82915400	2.94759800	-1.16016300
H	-1.81156900	3.49004800	-2.09991700
C	-0.13075700	0.96315200	3.09905000
H	0.55288100	0.52729200	2.36442900
H	0.00311700	0.43057800	4.04673100
H	0.16912600	2.00476000	3.25301100
C	-1.93474100	1.55040800	-1.18227300
C	-1.72199400	3.65039200	0.03433100
H	-1.64490700	4.73367800	0.02458700
C	-0.52121300	0.96472400	-3.19065400
H	0.25805800	0.54429900	-2.54752300
H	-0.26122400	2.00951100	-3.38947500
H	-0.50273600	0.42674800	-4.14474300
C	-0.78347700	-3.62483400	1.14820400
H	0.27678100	-3.68393800	0.88517000
H	-1.17502200	-4.64544800	1.22134900
H	-0.85937300	-3.16175900	2.13728200
C	-1.91619300	0.84759900	-2.53975500
H	-2.10108600	-0.21577300	-2.38021700
C	-2.99856000	1.37263400	-3.50257500
H	-4.00094800	1.32127600	-3.06721000
H	-2.99914900	0.78173600	-4.42437300
H	-2.81501700	2.41392000	-3.78586500
C	-2.54285200	1.41554200	3.72345400
H	-3.59222300	1.37633300	3.41699400
H	-2.30884800	2.45525700	3.97303500
H	-2.43414500	0.83097300	4.64293200
N	2.62247100	-0.58112400	-0.21158100
H	3.11309700	-1.30371200	0.68264400
C	3.14246700	0.76097100	-0.18347000
C	2.26874700	1.85903000	-0.17135100
C	4.52520900	1.00807400	-0.08099800
C	2.75199900	3.16396500	-0.06189700
H	1.19922100	1.68671800	-0.26035900
C	5.00191300	2.31410600	0.02026500
H	5.23013500	0.18293400	-0.05346200
C	4.12331900	3.40050400	0.02978800
H	2.05030100	3.99410000	-0.06069600
H	6.07255900	2.47962600	0.10320200
H	4.50350900	4.41488800	0.10875900
C	3.41363300	-1.60868800	-1.02446300
H	4.18283400	-1.10807400	-1.61764500
H	2.74331300	-2.13548400	-1.71191300
C	3.94974000	-2.48197400	0.11293700
H	3.51252500	-3.47941300	0.18356900
C	5.35484900	-2.47181500	0.32557800
N	6.50652700	-2.39623500	0.52968000

INT_2B

Zero-point correction = 0.631205 (Hartree/Particle)

Thermal correction to Energy = 0.667247

Thermal correction to Enthalpy = 0.668192

Thermal correction to Gibbs Free Energy = 0.561677

Sum of electronic and zero-point Energies =-1490.205654

Sum of electronic and thermal Energies =-1490.169612

Sum of electronic and thermal Enthalpies =-1490.168668

Sum of electronic and thermal Free Energies =-1490.275182

Cartesian coordinates

Cu	0.81542600	-0.59608100	-0.02721500
N	-2.03862200	-0.76206200	-0.04776600
C	-3.29245200	-1.63555400	-0.14966100
C	-2.66906400	-3.04255200	-0.00999200
H	-3.14490000	-3.75735700	-0.68727400
H	-2.82380100	-3.41144900	1.00917700
C	-0.88426000	-1.39790600	-0.12562000
C	-1.14742100	-2.89072900	-0.28507200
C	-2.11273000	1.21738700	1.43354600

C	-2.10524700	0.68509000	0.12107100
C	-1.92242700	0.37582300	2.69603200
H	-1.96150900	-0.67947800	2.41647300
C	-4.29699000	-1.32679400	0.96612400
H	-4.64794600	-0.29222400	0.91829600
H	-3.87842100	-1.51059900	1.95663000
H	-5.16641900	-1.98062700	0.84598500
C	-3.99340100	-1.43707300	-1.50307500
H	-4.33660300	-0.40726100	-1.62593400
H	-4.87299600	-2.08706700	-1.54233500
H	-3.35059800	-1.69559800	-2.34703500
C	-0.75991000	-3.31205900	-1.72213800
H	0.29918600	-3.11621700	-1.91305500
H	-1.34065500	-2.77848400	-2.48042800
H	-0.93844300	-4.38499000	-1.85242600
C	-2.21255200	2.60732100	1.57452600
H	-2.21745100	3.03848100	2.57048700
C	-2.21375900	2.90695700	-0.80996600
H	-2.21819800	3.57146000	-1.66805400
C	-0.52650500	0.62205400	3.30737100
H	0.26943900	0.38589400	2.59430000
H	-0.38543100	-0.00619800	4.19378100
H	-0.40739300	1.66643900	3.61450200
C	-2.11175300	1.52506800	-1.01803500
C	-2.28135600	3.44721600	0.46874700
H	-2.35758100	4.52204300	0.60358100
C	-0.51300500	1.42372200	-2.96954400
H	0.27718100	1.01672800	-2.33082500
H	-0.39739000	2.51229300	-3.00357700
H	-0.36229500	1.03819300	-3.98396500
C	-0.30390300	-3.69835800	0.72009300
H	0.76626900	-3.56076400	0.54006000
H	-0.53268000	-4.76611900	0.62764900
H	-0.51251500	-3.39512000	1.75109700
C	-1.91046700	1.02560300	-2.44851100
H	-1.94307600	-0.06469800	-2.44025100
C	-3.00206500	1.52197900	-3.41602900
H	-4.00864900	1.27239100	-3.06721500
H	-2.86376500	1.06888200	-4.40330500
H	-2.95939400	2.60771500	-3.54900600
C	-3.01947300	0.62426600	3.74938300
H	-4.02328100	0.47361400	3.34173200
H	-2.97295900	1.64328500	4.14647200
H	-2.88923900	-0.05850800	4.59569600
N	2.48391900	0.21820600	0.15947300
C	3.68318300	-0.47910100	0.12957000
C	4.93200900	0.05382800	0.53887500
C	3.69735600	-1.82205300	-0.33108800
C	6.09639800	-0.71557700	0.50196800
H	5.00034700	1.07166000	0.90676000
C	4.86025300	-2.57849700	-0.36229600
H	2.76090900	-2.25473800	-0.67914700
C	6.08189300	-2.03556200	0.05525100
H	7.03033200	-0.26539300	0.83092000
H	4.81680400	-3.60320800	-0.72471200
H	6.99288600	-2.62522500	0.02568900
C	2.52738500	1.63276800	0.46859000
H	1.51512100	1.97944000	0.69814100
H	3.13620900	1.85686800	1.35801600
C	3.05954800	2.48703500	-0.72267000
H	4.07725600	2.17593900	-0.97993800
H	2.43326500	2.29786300	-1.60124900
C	3.05126800	3.92076500	-0.43375000
N	3.01580300	5.05215500	-0.17152000

TS_2B

Zero-point correction = 0.745107 (Hartree/Particle)

Thermal correction to Energy = 0.788004

Thermal correction to Enthalpy = 0.788948

Thermal correction to Gibbs Free Energy = 0.666607

Sum of electronic and zero-point Energies =-1777.682822

Sum of electronic and thermal Energies =-1777.639925

Sum of electronic and thermal Enthalpies =-1777.638981

Sum of electronic and thermal Free Energies =-1777.761322

Cartesian coordinates

Cu	0.67307800	-0.28237100	0.06778500
N	-2.08836400	-0.79802000	0.80890300
C	-3.03700600	-1.52118800	1.77340200
C	-2.06381300	-1.86297100	2.92075400
H	-2.27142100	-2.85150900	3.34001100
H	-2.18545300	-1.13605500	3.73080100
C	-0.79659200	-0.91103500	1.07457800
C	-0.62968400	-1.75830700	2.33679000
C	-2.86568300	1.33537400	-0.17258900
C	-2.57991700	-0.04259800	-0.33735400
C	-2.58559600	2.11969000	1.10968100
H	-2.28670900	1.41244900	1.88675200
C	-4.18949000	-0.62254700	2.23487600
H	-4.80816600	-0.29484900	1.39486700
H	-3.83420600	0.25611300	2.77443500
H	-4.82748000	-1.19453800	2.91584600
C	-3.63831600	-2.77701100	1.12243600
H	-4.25445200	-2.51924600	0.25843700
H	-4.28350100	-3.27609300	1.85215200
H	-2.87554800	-3.49206600	0.80890800
C	-0.05042600	-3.13694700	1.93834700
H	0.93081600	-3.03211700	1.46678000
H	-0.69932000	-3.67085800	1.23816000
H	0.06350100	-3.75859500	2.83335600
C	-3.36883100	2.03777700	-1.27474300
H	-3.58985000	3.09511500	-1.17032400
C	-3.24048600	0.07627700	-2.65532000
H	-3.36551000	-0.39460400	-3.62534700
C	-1.40267400	3.08891400	0.90977900
H	-0.49991800	2.55902800	0.59884100
H	-1.19019600	3.61943900	1.84507600
H	-1.62661300	3.83851200	0.14412500
C	-2.73188500	-0.68188900	-1.59196500
C	-3.57121800	1.41713000	-2.50171600
H	-3.96585000	1.98225500	-3.34120700
C	-1.07847900	-2.15888000	-2.81237200
H	-0.22866900	-1.64120500	-2.36027800
H	-1.29605300	-1.69159700	-3.77891900
H	-0.77896600	-3.19562900	-3.00086000
C	0.33189600	-1.08244200	3.33127600
H	1.33791900	-0.99332700	2.91065800
H	0.40222400	-1.67667400	4.24921100
H	-0.01391800	-0.08032300	3.60547600
C	-2.30878800	-2.12211400	-1.88222300
H	-2.00509500	-2.58795100	-0.94394000
C	-3.44976300	-2.96533700	-2.48559900
H	-4.35477200	-2.94202900	-1.87163900
H	-3.13404800	-4.00927000	-2.58406500
H	-3.72279600	-2.61314600	-3.48568900
C	-3.82181900	2.88755300	1.61817500
H	-4.69015900	2.23567900	1.74884000
H	-4.10890900	3.68680900	0.92743200
H	-3.60094000	3.35825200	2.58214200
N	2.17310600	1.41327800	-0.10825300
H	2.05318100	3.33610400	1.89477700
C	1.91265300	2.51652500	-0.93770100
C	0.98635500	2.35585800	-1.99571600
C	2.52570500	3.78225200	-0.81138300

C	0.70344900	3.39022200	-2.87991200
H	0.47227800	1.40307400	-2.10276000
C	2.23004600	4.81818200	-1.70034900
H	3.24911600	3.96660600	-0.02472800
C	1.32194700	4.63754000	-2.74204200
H	-0.01496300	3.22367500	-3.67876400
H	2.72339100	5.77839000	-1.57075100
H	1.09629600	5.44776100	-3.42859800
C	3.06454600	1.60585100	1.02086900
H	3.98398800	2.14696100	0.75175800
H	3.38527300	0.61820000	1.37134600
C	2.37952900	2.33842000	2.20638500
H	1.48015700	1.78301800	2.49312400
C	3.25149400	2.46535400	3.37451900
N	3.95897900	2.54287200	4.29242400
C	3.52463000	-2.30958600	0.14074700
C	4.32835900	-3.43615900	0.30084500
C	4.63007600	-4.25977600	-0.78687200
C	4.11410000	-3.93082700	-2.04209800
C	3.31300000	-2.80262200	-2.20988500
C	2.99817900	-1.96530100	-1.12144000
H	3.30248400	-1.67746400	0.99695800
H	4.72434000	-3.67024400	1.28583700
H	5.25662600	-5.13701200	-0.65877600
H	4.33874200	-4.55537500	-2.90308200
H	2.92495900	-2.55591900	-3.19609700
N	2.19031600	-0.82725300	-1.27232000
H	2.45436100	0.31887200	-0.77358500
H	1.94329800	-0.69828100	-2.25083500

INT_1'

Zero-point correction = 0.563097 (Hartree/Particle)

Thermal correction to Energy = 0.594691

Thermal correction to Enthalpy = 0.595635

Thermal correction to Gibbs Free Energy = 0.498182

Sum of electronic and zero-point Energies =-1339.291802

Sum of electronic and thermal Energies =-1339.260208

Sum of electronic and thermal Enthalpies =-1339.259264

Sum of electronic and thermal Free Energies =-1339.356717

Cartesian coordinates

Cu	-1.16683200	-0.20091700	-0.07771300
N	1.63273700	-0.70049500	-0.03530000
C	2.77251100	-1.72289600	-0.03672100
C	2.00433100	-3.00612000	-0.42561200
H	2.35570000	-3.86854400	0.14777300
H	2.17731100	-3.22956700	-1.48334400
C	0.41354800	-1.19801200	-0.10542500
C	0.49610200	-2.71696000	-0.19136200
C	2.05399700	1.47211700	-1.13758700
C	1.88559500	0.73294400	0.05809200
C	1.79565000	0.89945800	-2.53110100
H	1.67697500	-0.18310600	-2.44284600
C	3.86117400	-1.36375600	-1.05411000
H	4.32749000	-0.40181900	-0.82454400
H	3.47329900	-1.33196900	-2.07345500
H	4.64083600	-2.13108600	-1.01822100
C	3.41636000	-1.82062700	1.35503800
H	3.86446100	-0.86936900	1.65134000
H	4.21419700	-2.56909900	1.32343600
H	2.70227000	-2.12534200	2.12284600
C	-0.02290800	-3.31548800	1.13718600
H	-1.06152900	-3.02303500	1.31625200
H	0.56996800	-2.98856900	1.99668700
H	0.02270600	-4.40902000	1.09092900
C	2.37279400	2.83098000	-1.02595200
H	2.50627600	3.41850900	-1.92862100
C	2.25245000	2.71957600	1.37200700

H	2.29177500	3.22082200	2.33382200
C	0.46740500	1.45068900	-3.09381100
H	-0.37236100	1.23620700	-2.42580700
H	0.25316700	1.00091400	-4.06964200
H	0.51768500	2.53644500	-3.22788700
C	1.92725200	1.35739800	1.32719900
C	2.49640100	3.44783400	0.21385500
H	2.74911800	4.50235300	0.27565500
C	0.16035000	1.20697900	3.11697700
H	-0.61700900	1.08336100	2.35689200
H	0.22165400	2.27277800	3.36129100
H	-0.15604800	0.67348400	4.02013500
C	-0.37223600	-3.23978200	-1.35156800
H	-1.42829800	-3.00455300	-1.19084300
H	-0.27119100	-4.32791200	-1.43340300
H	-0.07092300	-2.79849500	-2.30711600
C	1.52416500	0.66900800	2.63089400
H	1.39235200	-0.39618000	2.43234100
C	2.58075100	0.81233900	3.74291500
H	3.56472100	0.45004500	3.43039700
H	2.27512500	0.24164300	4.62613000
H	2.69694400	1.85485000	4.05618900
C	2.94880600	1.16547900	-3.51728400
H	3.90756600	0.79917300	-3.13854200
H	3.06179600	2.23387300	-3.72722700
H	2.74773500	0.66890900	-4.47247000
O	-2.62845300	0.87835000	-0.04233700
C	-3.92704600	0.58431800	-0.03292900
C	-4.86853100	1.63685900	-0.10122400
C	-4.43074000	-0.73402700	0.04905600
C	-6.23635300	1.37841200	-0.09037400
H	-4.49116000	2.65370100	-0.16309600
C	-5.80225500	-0.98229500	0.05918000
H	-3.72118400	-1.55766700	0.10753300
C	-6.72037000	0.06855300	-0.01055200
H	-6.93475200	2.21078300	-0.14492900
H	-6.15684600	-2.00895100	0.12331100
H	-7.78843000	-0.12819000	-0.00223700

TS_1C

Zero-point correction = 0.615917 (Hartree/Particle)

Thermal correction to Energy = 0.651925

Thermal correction to Enthalpy = 0.652869

Thermal correction to Gibbs Free Energy = 0.547032

Sum of electronic and zero-point Energies =-1510.046869

Sum of electronic and thermal Energies =-1510.010861

Sum of electronic and thermal Enthalpies =-1510.009917

Sum of electronic and thermal Free Energies =-1510.115754

Cartesian coordinates

Cu	-0.78118300	0.89885700	0.26820400
N	1.71398900	-0.14282700	-0.79150400
C	2.68583800	-0.18067800	-1.97942000
C	1.86073700	0.57467500	-3.04173400
H	1.39516600	-0.14692400	-3.72166200
H	2.49253300	1.23009300	-3.64769600
C	0.66294800	0.64665700	-0.93151900
C	0.75970900	1.35799300	-2.28000600
C	2.71088300	-0.37906700	1.47155600
C	1.95794000	-0.93488600	0.40845900
C	3.14010300	1.08640100	1.54092600
H	2.92372600	1.55576600	0.58022000
C	4.00867900	0.52433900	-1.64350400
H	4.52832300	0.02057800	-0.82534900
H	3.86842200	1.57373300	-1.37869000
H	4.65969000	0.48640300	-2.52248000
C	3.00011500	-1.61825100	-2.40809300
H	3.49947100	-2.17961800	-1.61365900

H	3.67465500	-1.58590000	-3.26954100
H	2.10176300	-2.15826600	-2.71045900
C	-0.58396700	1.32518700	-3.03021000
H	-1.35057100	1.88332100	-2.48516100
H	-0.93756200	0.29879800	-3.17623700
H	-0.47045100	1.78710600	-4.01747400
C	2.99653300	-1.19856700	2.57160300
H	3.57362500	-0.79193200	3.39609600
C	1.74916600	-3.01468900	1.61572700
H	1.35424300	-4.02246400	1.69567900
C	2.30518300	1.83551900	2.60050100
H	1.23659100	1.74789500	2.38948800
H	2.56641100	2.89933400	2.60899400
H	2.48703900	1.43531200	3.60375700
C	1.43011500	-2.24695100	0.48831000
C	2.54104700	-2.50958400	2.64004000
H	2.77970600	-3.12684600	3.50140200
C	-0.95432800	-2.95343800	0.08898900
H	-1.30372200	-1.99328100	0.47546600
H	-0.96231100	-3.67210400	0.91586900
H	-1.67257800	-3.29899200	-0.66192100
C	1.15221300	2.83533400	-2.03022500
H	0.38105000	3.36220400	-1.46172400
H	1.26853600	3.34236400	-2.99460500
H	2.09932900	2.92500600	-1.48940500
C	0.45529300	-2.83905000	-0.52903100
H	0.37824900	-2.15016000	-1.37367600
C	0.90881400	-4.20840600	-1.07161100
H	1.91305900	-4.17292400	-1.50296300
H	0.21653500	-4.55137300	-1.84788600
H	0.91346600	-4.96961200	-0.28473400
C	4.64283800	1.26642900	1.82976300
H	5.27141400	0.73414100	1.11028600
H	4.90684100	0.90529000	2.82906700
H	4.90744700	2.32825600	1.78886700
C	-3.65592800	-0.31562800	0.48494100
C	-3.79541800	-0.43425000	-0.90871400
C	-4.68184400	-0.80423600	1.31404700
C	-4.92544600	-1.04249200	-1.45488600
H	-3.00814400	-0.04433900	-1.54743800
C	-5.81473500	-1.39635800	0.75774200
H	-4.56975100	-0.72404100	2.39131700
C	-5.94326300	-1.52388300	-0.62784100
H	-5.01563300	-1.13055200	-2.53464700
H	-6.59870800	-1.76861900	1.41220800
H	-6.82528500	-1.98973500	-1.05694300
C	-2.76556100	1.85737700	1.92317100
H	-3.68715900	2.14415000	1.42415600
H	-2.90109200	1.42184300	2.90723300
C	-1.59198600	2.60328200	1.69291000
H	-0.83188200	2.65181700	2.46595900
O	-2.56061200	0.26773700	1.03385600
C	-1.54554100	3.61168300	0.69508000
N	-1.48313600	4.42693400	-0.14311100

INT_2C

Zero-point correction = 0.618762 (Hartree/Particle)

Thermal correction to Energy = 0.654721

Thermal correction to Enthalpy = 0.655666

Thermal correction to Gibbs Free Energy = 0.547939

Sum of electronic and zero-point Energies =-1510.066941

Sum of electronic and thermal Energies =-1510.030982

Sum of electronic and thermal Enthalpies =-1510.030037

Sum of electronic and thermal Free Energies =-1510.137764

Cartesian coordinates

Cu	0.49402400	-0.33028000	-0.40800900
N	-2.36792500	-0.70218300	-0.12672000

C	-3.59893800	-1.59057600	-0.35747100
C	-2.91998800	-2.91820300	-0.76144300
H	-3.45351500	-3.40312400	-1.58372300
H	-2.93542600	-3.61094300	0.08622900
C	-1.21989800	-1.19475000	-0.53298300
C	-1.45068600	-2.57589400	-1.13227800
C	-2.35048000	0.70601600	1.90557200
C	-2.47758300	0.61348100	0.49875100
C	-1.92967400	-0.46101800	2.79911500
H	-1.95742500	-1.37878400	2.20668800
C	-4.44716900	-1.72902900	0.91126000
H	-4.83326400	-0.76264300	1.24632200
H	-3.88896100	-2.18740400	1.72903400
H	-5.30353600	-2.37381300	0.69038300
C	-4.48095800	-1.01614600	-1.47593100
H	-4.86825300	-0.03077400	-1.20804600
H	-5.33700100	-1.68136800	-1.62543100
H	-3.94911600	-0.93664400	-2.42621000
C	-1.22808300	-2.48976200	-2.66046600
H	-0.21009500	-2.15925700	-2.88732300
H	-1.92140200	-1.79248000	-3.14002400
H	-1.37575800	-3.47736400	-3.11070300
C	-2.52253700	1.96441000	2.49422800
H	-2.42532500	2.06282900	3.57062200
C	-2.84078900	2.98917700	0.34371800
H	-2.98625500	3.88461500	-0.25151700
C	-0.46976300	-0.27581800	3.26514600
H	0.21036200	-0.18249000	2.41265700
H	-0.15018800	-1.13314000	3.86813900
H	-0.36150900	0.62609000	3.87625700
C	-2.67555700	1.75936600	-0.30665600
C	-2.78655500	3.09384400	1.72783000
H	-2.91407700	4.06008400	2.20665800
C	-1.31429000	2.45341000	-2.31138600
H	-0.42202700	2.00669300	-1.86569100
H	-1.31001300	3.51303600	-2.03807600
H	-1.23161100	2.38582000	-3.40209300
C	-0.45942300	-3.59330800	-0.53591700
H	0.57287900	-3.32822300	-0.78302800
H	-0.66216600	-4.59285400	-0.93658700
H	-0.54350000	-3.64205400	0.55466700
C	-2.60607000	1.75633700	-1.83338400
H	-2.55461300	0.72054000	-2.17465400
C	-3.83602300	2.40841300	-2.49410400
H	-4.77582400	1.95008300	-2.17178300
H	-3.77017100	2.31487700	-3.58324100
H	-3.89449800	3.47706700	-2.26459100
C	-2.85960900	-0.65934700	4.01114700
H	-3.90503400	-0.77862400	3.71181200
H	-2.80766000	0.18776000	4.70230900
H	-2.56172300	-1.55191100	4.57162800
C	2.26844900	0.52171300	-0.26221300
H	2.68633200	0.18630600	0.69520100
C	3.21683400	0.16516700	-1.40410500
H	3.30980900	-0.92297100	-1.50252500
H	2.83972400	0.55643300	-2.35194700
C	5.44935900	0.20292000	-0.45122300
C	5.26030500	-0.95988300	0.31048000
C	6.67754500	0.88144800	-0.37520200
C	6.29506200	-1.42977700	1.12568900
H	4.32211700	-1.50128900	0.27910900
C	7.69584200	0.40209400	0.44045600
H	6.80233500	1.78172600	-0.96815600
C	7.51422900	-0.75997400	1.19895500
H	6.13444700	-2.33168400	1.71090400
H	8.63908200	0.93995200	0.48576000

H	8.30993200	-1.13171400	1.83728700
C	2.00230800	1.94286000	-0.17362700
N	1.71825500	3.07413600	-0.11841200
O	4.53359400	0.74613200	-1.30023600

TS_2C

Zero-point correction = 0.617957 (Hartree/Particle)

Thermal correction to Energy = 0.653174

Thermal correction to Enthalpy = 0.654118

Thermal correction to Gibbs Free Energy = 0.548833

Sum of electronic and zero-point Energies =-1510.042849

Sum of electronic and thermal Energies =-1510.007633

Sum of electronic and thermal Enthalpies =-1510.006688

Sum of electronic and thermal Free Energies =-1510.111973

Cartesian coordinates

Cu	-0.09579000	-0.97874900	0.51546300
N	2.45055000	-0.25551200	-0.57905500
C	3.60805400	-0.63286300	-1.50850700
C	3.24208500	-2.09697200	-1.83899100
H	3.85456200	-2.77225500	-1.23265500
H	3.44492900	-2.33117700	-2.88786200
C	1.44547000	-1.11231700	-0.53786400
C	1.74484100	-2.28086600	-1.47130900
C	1.91163700	2.15601000	-0.30314500
C	2.45931600	0.96187200	0.22450500
C	1.17033000	2.24508700	-1.63701900
H	1.27287700	1.28906300	-2.15263500
C	1.98171900	3.31180000	0.48593100
H	1.56823500	4.23862000	0.10100300
C	3.02316400	2.09660900	2.27752200
H	3.41999800	2.07726000	3.28743900
C	-0.33986600	2.46869800	-1.40972000
H	-0.78247900	1.65470500	-0.82895400
H	-0.86105600	2.51916100	-2.37245400
H	-0.52600100	3.40898100	-0.87977600
C	2.98478900	0.90693400	1.53942300
C	2.54563700	3.29300400	1.75567400
H	2.58903400	4.20275700	2.34747600
C	2.45424900	-0.76744400	3.35949400
H	1.43460900	-0.89790700	2.98792400
H	2.43437100	-0.00228300	4.14311500
H	2.77028600	-1.70891500	3.82265200
C	3.43499900	-0.38017800	2.23159500
H	3.41241400	-1.19142600	1.49988400
C	-2.63118200	-0.34399300	0.39928300
H	-2.81638600	0.72530000	0.41668100
C	-3.53733100	-1.21801900	-0.40907300
H	-3.64755000	-0.83422200	-1.43050200
H	-3.13968400	-2.23363300	-0.47206100
C	-5.79553900	-0.43586900	0.05384500
C	-5.61024800	0.79328600	-0.59670300
C	-7.03488800	-0.71215900	0.65684000
C	-6.65788400	1.71852700	-0.64221500
H	-4.66481800	1.03932900	-1.06525800
C	-8.06619000	0.21835400	0.60394300
H	-7.15857900	-1.66658300	1.15852600
C	-7.88742700	1.44391600	-0.04760600
H	-6.49949100	2.66684800	-1.14941700
H	-9.01749800	-0.01406200	1.07530300
H	-8.69320500	2.17057200	-0.08636200
C	-1.93839000	-0.85507500	1.47552600
N	-1.17520100	-1.29972400	2.29173400
C	4.87016300	-0.28223800	2.78657500
H	4.93536100	0.44739300	3.60014300
H	5.18100700	-1.24966400	3.19518400
H	5.59324800	0.01226800	2.02055900
C	1.73370400	3.34453400	-2.55907400

H	1.23737200	3.30823000	-3.53458100
H	1.56060400	4.34291200	-2.14449200
H	2.81024600	3.23975800	-2.72308400
C	1.49529400	-3.62478100	-0.76129400
H	0.44317500	-3.73454900	-0.48187900
H	1.76133100	-4.45472400	-1.42581300
H	2.09449500	-3.71257400	0.15037000
C	0.81537500	-2.18239500	-2.70394500
H	1.01892900	-3.01462900	-3.38664300
H	-0.23470600	-2.23404100	-2.40263900
H	0.95779100	-1.24889000	-3.25617700
C	4.96448100	-0.51663100	-0.80507500
H	5.16552300	0.50862100	-0.48240400
H	5.03320000	-1.17729400	0.06004600
H	5.75074800	-0.80619000	-1.50929300
C	3.63116100	0.26013000	-2.75885600
H	2.70880000	0.19019400	-3.33890500
H	3.80198600	1.30632500	-2.49636300
H	4.45603900	-0.05917100	-3.40346500
O	-4.86555100	-1.42443700	0.14770100

INT_3C

Zero-point correction = 0.618089 (Hartree/Particle)

Thermal correction to Energy = 0.654287

Thermal correction to Enthalpy = 0.655231

Thermal correction to Gibbs Free Energy = 0.545001

Sum of electronic and zero-point Energies =-1510.064542

Sum of electronic and thermal Energies =-1510.028344

Sum of electronic and thermal Enthalpies =-1510.027400

Sum of electronic and thermal Free Energies =-1510.137630

Cartesian coordinates

Cu	0.10703300	0.17691400	-0.68669000
N	2.77964200	0.77075500	0.13276500
C	3.86744700	1.82801300	0.34477600
C	3.03658900	3.12337100	0.20574500
H	3.58376300	3.88842000	-0.35215600
H	2.83044700	3.53389600	1.19948700
C	1.62390900	1.21852300	-0.31722400
C	1.70166000	2.73085900	-0.48488400
C	2.73919100	-1.15216000	1.68744400
C	3.01624900	-0.64445700	0.39497800
C	2.03863100	-0.34954800	2.78390800
H	1.98112000	0.69382400	2.46483300
C	4.52673400	1.70247700	1.72256000
H	5.02318300	0.73620900	1.84656200
H	3.80868500	1.83569700	2.53305500
H	5.28675100	2.48406300	1.81936100
C	4.95790300	1.70958300	-0.73141700
H	5.46400200	0.74290100	-0.67781500
H	5.70812800	2.48779800	-0.56049100
H	4.56260600	1.84265900	-1.74051200
C	1.69543600	3.06092600	-1.99631000
H	0.77855300	2.69792800	-2.46986200
H	2.54415100	2.61219300	-2.52108000
H	1.74660800	4.14617200	-2.13615900
C	3.03682900	-2.49742200	1.93793900
H	2.83262800	-2.90935800	2.92098300
C	3.76150800	-2.81868700	-0.33105300
H	4.12049100	-3.48074300	-1.11253400
C	0.58631800	-0.84254500	2.96257800
H	0.02220600	-0.77824400	2.02722000
H	0.06997300	-0.23623200	3.71482400
H	0.56201600	-1.88498800	3.29730900
C	3.48174800	-1.48237700	-0.64610400
C	3.56417300	-3.32077900	0.94965700
H	3.79093800	-4.36003300	1.16914700
C	2.47000600	-1.71053800	-2.94353300

H	1.47811500	-1.47307000	-2.54749300
H	2.57494500	-2.80058700	-2.95179000
H	2.51578200	-1.36111000	-3.98090500
C	0.49148700	3.41264200	0.18207900
H	-0.44534600	3.10761100	-0.29351900
H	0.58108600	4.50136100	0.09529600
H	0.42621200	3.16134400	1.24551600
C	3.58770900	-1.04932000	-2.10804200
H	3.42620600	0.02868400	-2.16114400
C	4.96559100	-1.34937400	-2.72852300
H	5.78463300	-0.90635900	-2.15415800
H	5.01293500	-0.95116100	-3.74751100
H	5.15252800	-2.42607600	-2.79315700
C	2.78734700	-0.38855600	4.12990500
H	3.82641900	-0.06032900	4.03370200
H	2.79646800	-1.39651500	4.55673600
H	2.28958000	0.26397600	4.85494700
C	-3.61644100	-2.00511200	-1.00385600
H	-3.61983800	-3.05693300	-0.73858600
C	-4.90389700	-1.29072700	-1.17190500
H	-5.63876900	-1.91960300	-1.69258900
C	-2.43677600	-1.35513900	-1.00770900
N	-1.38596600	-0.78759100	-1.06356300
H	-4.77453000	-0.36683800	-1.75037400
C	-6.68053500	-0.31261600	0.15903200
C	-7.43028000	0.05608800	-0.96997500
C	-7.18845400	-0.02541200	1.43996000
C	-8.66205300	0.69836700	-0.80588000
H	-7.06636800	-0.14950600	-1.96914500
C	-8.41350900	0.61382100	1.58555900
H	-6.59602700	-0.31829300	2.30113400
C	-9.16370900	0.98229100	0.46219600
H	-9.23072800	0.97722000	-1.68952400
H	-8.78825000	0.82634800	2.58364500
H	-10.12133500	1.48099300	0.57784100
O	-5.47556600	-0.93488900	0.12713800

TS_3C

Zero-point correction = 0.720826 (Hartree/Particle)

Thermal correction to Energy = 0.763111

Thermal correction to Enthalpy = 0.764055

Thermal correction to Gibbs Free Energy = 0.640845

Sum of electronic and zero-point Energies =-1817.435927

Sum of electronic and thermal Energies =-1817.393643

Sum of electronic and thermal Enthalpies =-1817.392698

Sum of electronic and thermal Free Energies =-1817.515909

Cartesian coordinates

Cu	0.43975300	0.52707400	-0.99728300
N	2.90117500	-0.83787700	-0.22042700
C	4.37113500	-1.10794700	-0.57185500
C	4.58683500	-0.09180300	-1.71383000
H	5.18538300	-0.52164000	-2.52205500
H	5.13485900	0.77632900	-1.33279000
C	2.24843800	-0.03634200	-1.04388700
C	3.17964400	0.34864900	-2.19292400
C	2.31847400	-0.75347600	2.18904400
C	2.28210100	-1.44671300	0.95350500
C	2.80164300	0.68764500	2.35133200
H	3.22792200	1.01859400	1.40099600
C	2.71778000	-0.42115100	-3.45482700
H	1.68767300	-0.16272900	-3.71428900
H	2.76098500	-1.50503300	-3.31473700
H	3.36624600	-0.16222300	-4.29919400
C	1.79373900	-1.39476000	3.31827400
H	1.81368000	-0.87964500	4.27340900
C	1.14722500	-3.29848200	2.00703800
H	0.66322500	-4.26757100	1.94060100

C	1.60785800	1.61614600	2.65978200
H	0.82603200	1.52941600	1.90201800
H	1.93437700	2.66072900	2.69090200
H	1.16534700	1.37413200	3.63226400
C	1.65450300	-2.71234900	0.83922200
C	1.23072300	-2.66263800	3.23912500
H	0.83417400	-3.14167900	4.12973100
C	3.12761200	1.85814100	-2.48505600
H	2.12429300	2.16850500	-2.79205300
H	3.82263700	2.10706500	-3.29503300
H	3.41205500	2.44615700	-1.60639300
C	3.88285000	0.84199500	3.43912600
H	4.74216800	0.18788100	3.26855800
H	3.48512200	0.61241100	4.43295200
H	4.24219100	1.87631500	3.46641500
C	-4.04463300	0.56773900	-0.28081800
H	-4.54887400	1.38537000	0.25199100
C	-3.03078700	1.13375400	-1.23316900
C	1.41463600	-3.44694100	-0.48061900
H	-1.79864200	1.79964600	-0.50566200
C	1.95862000	-4.89005500	-0.46867300
H	1.84807100	-5.33878800	-1.46145300
H	3.01505100	-4.94091100	-0.19069700
H	1.40306700	-5.51996600	0.23368900
C	5.29301200	-0.83408700	0.62155200
H	5.22218500	0.20078100	0.96002200
H	5.07398600	-1.49687700	1.46299400
H	6.32787000	-1.01449600	0.31370000
C	4.58568600	-2.55840700	-1.02706800
H	4.34698400	-3.26275500	-0.22770100
H	3.99337500	-2.81296100	-1.90776600
H	5.64122100	-2.69285400	-1.28345700
H	1.92077200	-2.90034000	-1.27815400
C	-0.08814700	-3.46076500	-0.83186800
H	-0.66719200	-3.98862100	-0.06631300
H	-0.48863200	-2.45096400	-0.93681700
H	-0.24438200	-3.97879700	-1.78438100
C	-2.09624900	0.25363100	-1.79172700
N	-1.13637700	-0.35378000	-2.12687000
H	-3.43488600	1.84804000	-1.95230200
H	-3.56259100	-0.07770000	0.46625700
O	-5.03640100	-0.20134200	-0.99452100
O	-0.75854300	2.04115600	-0.18275700
C	-0.57941800	3.36770300	0.07847800
C	-1.66105100	4.16140800	0.49110900
C	0.69038700	3.94758800	-0.04331000
C	-1.46765000	5.51447600	0.76763800
H	-2.64377700	3.71175200	0.59394300
C	0.87307700	5.29974400	0.24595800
H	1.52028100	3.32683400	-0.36379400
C	-0.20224700	6.09351200	0.65086000
H	-2.31476500	6.11770200	1.08313000
H	1.86401100	5.73575700	0.14829900
H	-0.05670500	7.14662300	0.87107800
C	-6.05815500	-0.76518500	-0.29190300
C	-6.22670300	-0.66641400	1.09673800
C	-6.99132000	-1.49187900	-1.05086000
C	-7.32012100	-1.29110000	1.70614200
H	-5.52160500	-0.11354700	1.70563600
C	-8.07192100	-2.10688800	-0.42995700
H	-6.84131900	-1.55622200	-2.12384300
C	-8.24627200	-2.01155000	0.95579400
H	-7.44041500	-1.20732900	2.78311800
H	-8.78460900	-2.66519100	-1.03113800
H	-9.09150700	-2.49245800	1.43861500

TS_D

Zero-point correction = 0.667882 (Hartree/Particle)

Thermal correction to Energy = 0.705593

Thermal correction to Enthalpy = 0.706537

Thermal correction to Gibbs Free Energy = 0.597128

Sum of electronic and zero-point Energies =-1550.528372

Sum of electronic and thermal Energies =-1550.490662

Sum of electronic and thermal Enthalpies =-1550.489717

Sum of electronic and thermal Free Energies =-1550.599126

Cartesian coordinates

Cu	0.79843800	0.72107600	-0.09266100
N	-2.03484200	0.34328500	0.12244600
C	-3.42874300	0.95956300	0.31446300
C	-3.15061600	2.40809600	-0.12724700
H	-3.68754600	3.12638100	0.49837800
H	-3.49937800	2.54982900	-1.15558600
C	-1.04810100	1.20137600	-0.04246100
C	-1.60993300	2.61764100	-0.07081500
C	-1.89475200	-1.77399100	-1.13281000
C	-1.82565900	-1.09989800	0.11111600
C	-2.03998000	-1.05789000	-2.47647800
H	-2.30062800	-0.01479700	-2.28605200
C	-4.49370900	0.26820700	-0.54330600
H	-4.59349700	-0.79152100	-0.29208400
H	-4.28580900	0.35934400	-1.61023400
H	-5.45857400	0.74853300	-0.35324300
C	-3.85611000	0.87364500	1.78813700
H	-3.96394500	-0.16284300	2.11500000
H	-4.83096900	1.35878600	1.89798800
H	-3.15424100	1.38297900	2.45181500
C	-1.14687900	3.37757600	1.19686600
H	-0.07114300	3.56814500	1.15727700
H	-1.39144400	2.84185700	2.12066700
H	-1.64718900	4.35141600	1.22952500
C	-1.74013700	-3.16539000	-1.13353600
H	-1.78754800	-3.70274800	-2.07533100
C	-1.39664600	-3.18327100	1.24492400
H	-1.17371500	-3.73422000	2.15311400
C	-0.69520300	-1.04453400	-3.23238200
H	0.08075200	-0.54382000	-2.64512200
H	-0.79687200	-0.51135600	-4.18389200
H	-0.35328400	-2.06207300	-3.45048300
C	-1.53761000	-1.79040300	1.31136700
C	-1.51120600	-3.87055600	0.04287900
H	-1.39844600	-4.95053000	0.01886200
C	0.21711200	-1.21458800	3.03201100
H	0.85707000	-0.79605400	2.24986100
H	0.51359600	-2.25787100	3.18271200
H	0.41084500	-0.67152400	3.96374600
C	-1.11245800	3.39137800	-1.31149900
H	-0.06159100	3.68070400	-1.21019800
H	-1.69939600	4.31266600	-1.40727400
H	-1.25677500	2.81008600	-2.22983600
C	-1.27464100	-1.10480000	2.65144800
H	-1.49625800	-0.04199200	2.54375600
C	-2.15244500	-1.65944600	3.79020200
H	-3.21887400	-1.62010800	3.54953000
H	-1.99084600	-1.08074800	4.70568000
H	-1.90486900	-2.70164100	4.01662500
C	-3.14778700	-1.66056000	-3.36133500
H	-4.10870100	-1.70432800	-2.84040900
H	-2.90015200	-2.67614400	-3.68636000
H	-3.27706100	-1.05515400	-4.26464000
H	2.97381800	0.61234800	0.97722100
N	2.68507300	0.20262000	0.08842300
C	3.20752400	-1.11707100	0.01679600
C	4.20351300	-1.56470000	0.90267100

C	2.78843900	-1.97955300	-1.01079600
C	4.74932800	-2.84123100	0.77449000
H	4.54475400	-0.90620100	1.69883000
C	3.34419400	-3.25081600	-1.14022900
H	2.01865900	-1.64351500	-1.69913900
C	4.32540800	-3.69203900	-0.24859500
H	5.51136800	-3.16995100	1.47603200
H	3.00473600	-3.90319400	-1.94035900
H	4.75308600	-4.68495900	-0.34963200
C	3.49106700	1.39975300	-1.02613100
H	4.45394300	1.45322600	-0.51710100
H	3.54813400	0.76890800	-1.91256900
C	2.70660200	2.57785200	-1.13624200
H	1.96284400	2.61460600	-1.93067500
C	2.65542300	3.64836700	-0.20370600
O	1.78602800	4.55150100	-0.23923400
C	3.68806300	3.73701700	0.93043000
H	3.20316800	3.51483900	1.88949000
H	4.55460700	3.07817700	0.81943500
H	4.03846200	4.77151700	0.98824200

TS_D'

Zero-point correction = 0.667118 (Hartree/Particle)

Thermal correction to Energy = 0.704935

Thermal correction to Enthalpy = 0.705879

Thermal correction to Gibbs Free Energy = 0.596509

Sum of electronic and zero-point Energies =-1550.544554

Sum of electronic and thermal Energies =-1550.506737

Sum of electronic and thermal Enthalpies =-1550.505793

Sum of electronic and thermal Free Energies =-1550.615162

Cartesian coordinates

Cu	-0.69894900	-0.75666600	-0.80024100
N	-2.42056500	-0.06945200	-1.37969400
H	-2.47465600	0.12131800	-2.37783900
C	-3.17622800	0.86736500	-0.68192700
C	-3.17927600	0.86618500	0.73071500
C	-4.00896100	1.80388400	-1.33646300
C	-3.97034400	1.76316800	1.44550200
H	-2.54525600	0.15681500	1.25335200
C	-4.78911600	2.70160500	-0.61388100
H	-4.02960800	1.82144800	-2.42495800
C	-4.78029300	2.68987100	0.78457300
H	-3.95041700	1.73960400	2.53250300
H	-5.41122700	3.41628000	-1.14741800
H	-5.39080000	3.39053600	1.34629300
C	-3.53346300	-1.94917200	-1.43382700
H	-2.69750100	-2.31090500	-2.02127300
H	-4.38297800	-1.56730300	-1.99214800
C	-3.70880000	-2.43326900	-0.15397300
H	-4.66762600	-2.34573200	0.34685600
C	-2.58227400	-2.90568500	0.57998500
O	-1.39882200	-2.78770400	0.15563100
C	-2.79331000	-3.54095800	1.94462600
H	-2.34929700	-2.90913900	2.72241000
H	-3.85000100	-3.69543500	2.17772900
H	-2.27299900	-4.50372600	1.97933700
C	1.19350100	-0.95308200	-0.77702100
N	2.09912600	-0.16075500	-0.23063600
C	1.91510900	-2.08786000	-1.50083600
C	3.56460500	-0.54217400	-0.47591900
C	1.73410700	1.00558500	0.56390000
C	3.39418200	-1.62354300	-1.56464900
C	1.73586500	-3.38320600	-0.67085100
C	1.32506600	-2.31165100	-2.90480900
C	4.38905900	0.65187400	-0.97012600
C	4.22462100	-1.08516200	0.80158300
C	1.56365500	2.25471400	-0.08185100

C	1.52994700	0.86304300	1.95694500
H	4.09626200	-2.45010600	-1.42170600
H	3.60318300	-1.18676200	-2.54733500
H	0.67692700	-3.60089300	-0.51514100
H	2.20642400	-3.30530300	0.31384000
H	2.20520300	-4.22031700	-1.20051300
H	0.28280600	-2.63750300	-2.84019100
H	1.89307000	-3.08764400	-3.43101500
H	1.36140500	-1.39737000	-3.50671500
H	4.41559700	1.45869000	-0.23248700
H	4.00838300	1.04872700	-1.91217400
H	5.41830200	0.32038900	-1.14048900
H	4.24256900	-0.32891400	1.58995500
H	5.26149700	-1.35304000	0.57525800
H	3.72628800	-1.97781500	1.18322500
C	1.59407500	2.44521600	-1.59853200
C	1.26573900	3.36809400	0.71365700
C	1.23318200	2.01480600	2.69764300
C	1.52186200	-0.48086300	2.68486600
H	1.91010400	1.50515200	-2.05686200
C	0.17897300	2.74947300	-2.13433200
C	2.57710900	3.54648700	-2.04233300
H	1.12787300	4.33419900	0.23858200
C	1.11878200	3.25974300	2.09150300
H	1.07149600	1.92709500	3.76738000
C	0.08312100	-0.87719300	3.07573800
H	1.87914900	-1.24842800	1.99785700
C	2.43639100	-0.49564600	3.92504900
H	-0.52512400	1.95890900	-1.86254500
H	0.20131200	2.83587100	-3.22700600
H	-0.20157600	3.69438700	-1.73223100
H	3.58942800	3.37589500	-1.66543700
H	2.25644700	4.53341500	-1.69333700
H	2.62391100	3.59026900	-3.13590100
H	0.88878200	4.13856900	2.68696500
H	-0.54433800	-0.99543400	2.18895900
H	-0.37292100	-0.12550500	3.72900700
H	0.08868400	-1.83302700	3.61141300
H	3.46055200	-0.19202200	3.68793100
H	2.47249300	-1.50336200	4.35231800
H	2.06703500	0.17462000	4.70809300

TS_E

Zero-point correction = 0.673114 (Hartree/Particle)

Thermal correction to Energy = 0.711906

Thermal correction to Enthalpy = 0.712851

Thermal correction to Gibbs Free Energy = 0.600684

Sum of electronic and zero-point Energies =-1625.756043

Sum of electronic and thermal Energies =-1625.717251

Sum of electronic and thermal Enthalpies =-1625.716307

Sum of electronic and thermal Free Energies =-1625.828473

Cartesian coordinates

Cu	-0.85507400	-0.37908600	0.14235200
N	1.98827600	-0.77049000	0.25211100
C	3.16858200	-1.71716300	0.51286900
C	2.42134800	-2.92401700	1.11639900
H	2.50291200	-2.89298900	2.20848100
H	2.85580300	-3.87105400	0.78484100
C	0.78897600	-1.30625100	0.35786800
C	0.93074300	-2.78368100	0.70242100
C	2.28016100	0.99621600	-1.46777700
C	2.18741400	0.62938000	-0.10398800
C	2.01941200	0.03569000	-2.62790500
H	1.95047400	-0.97683400	-2.22867000
C	3.89915900	-2.06325000	-0.79403600
H	4.32926000	-1.17163800	-1.25663000
H	3.24860800	-2.55746900	-1.51751600

H	4.72211800	-2.74724400	-0.56472000
C	4.18231400	-1.10791900	1.48750400
H	4.62476700	-0.18939700	1.09185400
H	4.99151900	-1.82812300	1.64368500
H	3.73770800	-0.89443500	2.46054500
C	-0.02119700	-3.18916200	1.84378900
H	-1.06228200	-3.14799500	1.51341800
H	0.10426000	-2.54696300	2.72265100
H	0.18957600	-4.22110000	2.14652600
C	2.53181900	2.34218000	-1.76648000
H	2.60893600	2.64644500	-2.80550200
C	2.50502200	2.92476000	0.56529200
H	2.55864600	3.68293300	1.33997700
C	0.65932700	0.34528000	-3.28840500
H	-0.15830300	0.27503600	-2.56477000
H	0.45761000	-0.36740700	-4.09529700
H	0.64600300	1.35288200	-3.71768000
C	2.25432300	1.59573900	0.92862300
C	2.66372900	3.29690900	-0.76485800
H	2.86313000	4.33335800	-1.02144700
C	0.59819900	1.86999000	2.81064800
H	-0.20454500	1.48611600	2.17428500
H	0.59143800	2.96218900	2.73291700
H	0.37142900	1.60456300	3.84927100
C	0.57768200	-3.62586300	-0.55148700
H	-0.48886300	-3.56139300	-0.78590700
H	0.80602900	-4.67710300	-0.34284100
H	1.15733200	-3.32715800	-1.43082600
C	1.96766500	1.28918600	2.39854600
H	1.89944600	0.20548400	2.51745700
C	3.07195700	1.79834500	3.34469700
H	4.05911900	1.41647100	3.06891600
H	2.86018700	1.48380700	4.37214000
H	3.12814900	2.89164000	3.34709200
C	3.14035500	0.04791300	-3.68469400
H	4.12303900	-0.15099400	-3.24687000
H	3.19803600	1.01101900	-4.20214600
H	2.94733400	-0.71677100	-4.44422100
H	-3.15586500	0.18087100	0.76239600
N	-2.53586900	0.60536100	0.07300000
C	-2.70791500	2.00836400	0.09121700
C	-3.83593800	2.60547700	0.68516800
C	-1.77950700	2.84006000	-0.56181500
C	-4.01997100	3.98629800	0.63779500
H	-4.56602500	1.97657500	1.19018200
C	-1.97273400	4.21896100	-0.61156100
H	-0.90138200	2.39155400	-1.01844600
C	-3.09179500	4.80329100	-0.01211500
H	-4.89477000	4.42530500	1.11030700
H	-1.23943400	4.84231700	-1.11669800
H	-3.23733600	5.87874500	-0.04950300
C	-3.28331700	-0.26836900	-1.40873700
H	-4.31886000	-0.11259700	-1.11421800
H	-2.95695900	0.42123900	-2.18491700
C	-2.79731800	-1.59240800	-1.47549700
H	-1.96351500	-1.83719800	-2.12493800
C	-3.24268400	-2.63269900	-0.61392700
O	-2.81048800	-3.78839800	-0.53846700
O	-4.26336100	-2.21860500	0.24621200
C	-4.80942100	-3.24841500	1.06484300
H	-4.05641700	-3.67220400	1.73730200
H	-5.60677000	-2.77991700	1.64669900
H	-5.21880200	-4.06420400	0.46050100

TS_E'

Zero-point correction = 0.673178 (Hartree/Particle)

Thermal correction to Energy = 0.711697

Thermal correction to Enthalpy = 0.712642

Thermal correction to Gibbs Free Energy = 0.602091

Sum of electronic and zero-point Energies =-1625.762026

Sum of electronic and thermal Energies =-1625.723506

Sum of electronic and thermal Enthalpies =-1625.722562

Sum of electronic and thermal Free Energies =-1625.833112

Cartesian coordinates

Cu	-0.71253800	-0.52032100	-0.88409600
N	-2.33267900	0.44542000	-1.42127600
H	-2.24566300	0.79705400	-2.37383200
C	-2.92287800	1.43776000	-0.62376500
C	-3.07616800	1.22847700	0.76194800
C	-3.44319200	2.62754000	-1.17431700
C	-3.71609400	2.17708800	1.55783800
H	-2.69139400	0.31381200	1.20007500
C	-4.06944100	3.57615800	-0.36967900
H	-3.34395900	2.80423200	-2.24397200
C	-4.21343600	3.35882700	1.00360700
H	-3.82368600	1.99100000	2.62353300
H	-4.45046000	4.48974600	-0.81930700
H	-4.70384600	4.09820400	1.62980700
C	-3.63263100	-1.03960200	-1.75180900
H	-2.92612700	-1.47798800	-2.45172400
H	-4.42145800	-0.45039300	-2.21339600
C	-3.93973900	-1.75394700	-0.59566600
H	-4.87005900	-1.60866600	-0.06107000
C	-2.92768000	-2.55131700	-0.01317200
O	-1.72884400	-2.59552600	-0.38620000
C	1.14376100	-0.94619800	-0.81893800
N	2.11995000	-0.28866800	-0.21875100
C	1.74633300	-2.13091000	-1.57101300
C	3.53601500	-0.83875800	-0.43790100
C	1.87867400	0.88176000	0.61604400
C	3.27097900	-1.84433700	-1.57847300
C	1.39220300	-3.42825400	-0.80235400
C	1.17222200	-2.22764300	-2.99615800
C	4.51977000	0.26096100	-0.85283200
C	4.07607300	-1.50984600	0.83512100
C	1.89825700	2.16800700	0.02355000
C	1.60947300	0.71034100	1.99465500
H	3.86613200	-2.75401400	-1.45719600
H	3.55815800	-1.39353500	-2.53473000
H	0.30986300	-3.53207900	-0.70000000
H	1.83031500	-3.44149700	0.20039800
H	1.78869200	-4.29081500	-1.35039900
H	0.09753700	-2.42854700	-2.96682000
H	1.65838500	-3.04522300	-3.54101100
H	1.33514900	-1.30198400	-3.55869000
H	4.62075600	1.02773500	-0.07982600
H	4.22662900	0.73984800	-1.78798000
H	5.50483400	-0.19121000	-1.00582200
H	4.16032400	-0.79213500	1.65469600
H	5.07855900	-1.89847900	0.63021900
H	3.45606700	-2.34562900	1.16346000
C	1.99995900	2.41339200	-1.48198700
C	1.72529300	3.27749000	0.86030500
C	1.44513400	1.85979800	2.77881100
C	1.39085400	-0.64924600	2.65759500
H	2.21069900	1.46020800	-1.97242300
C	0.64923200	2.91152100	-2.03781700
C	3.12362800	3.40019100	-1.85468300
H	1.73364000	4.27231900	0.42635800
C	1.51957200	3.13283000	2.22729600
H	1.23641900	1.75072800	3.83835700
C	-0.10275000	-0.85465100	2.98392000
H	1.66532700	-1.42882700	1.94603000

C	2.24643700	-0.84549300	3.92392500
H	-0.15341600	2.20603700	-1.80876100
H	0.71002100	3.03150600	-3.12577900
H	0.37794700	3.88150100	-1.60810600
H	4.09545300	3.09020200	-1.46058800
H	2.91721600	4.40516500	-1.47262900
H	3.20791100	3.47995000	-2.94392700
H	1.38965400	4.00911500	2.85574500
H	-0.71156300	-0.82085800	2.07659900
H	-0.47018600	-0.08421800	3.67001300
H	-0.25637900	-1.82964100	3.45967900
H	3.31133500	-0.68249200	3.73292200
H	2.12341700	-1.86455500	4.30575300
H	1.94655600	-0.16186300	4.72477600
O	-3.33753200	-3.28611200	1.06736700
C	-2.35411100	-4.12477500	1.66576700
H	-1.48407200	-3.55138900	1.99910500
H	-2.84360200	-4.59251000	2.52231200
H	-2.01191800	-4.89763100	0.96885100

TS_F

Zero-point correction = 0.721684 (Hartree/Particle)

Thermal correction to Energy = 0.763906

Thermal correction to Enthalpy = 0.764850

Thermal correction to Gibbs Free Energy = 0.643803

Sum of electronic and zero-point Energies =-2177.455955

Sum of electronic and thermal Energies =-2177.413733

Sum of electronic and thermal Enthalpies =-2177.412789

Sum of electronic and thermal Free Energies =-2177.533836

Cartesian coordinates

Cu	-0.10894400	0.08743900	0.02891800
N	-2.51143000	-1.47587500	-0.14790200
C	-3.15850200	-2.84303600	-0.41310000
C	-1.94476900	-3.77066100	-0.20145100
H	-1.93362200	-4.58433200	-0.93177800
H	-2.00252300	-4.22772200	0.79205500
C	-1.19562400	-1.46533700	-0.10752900
C	-0.67202900	-2.88249700	-0.29332700
C	-3.70536700	0.07494200	1.35550100
C	-3.30733600	-0.26839200	0.04046300
C	-3.22177000	-0.66119300	2.60562500
H	-2.72655000	-1.58322900	2.29388600
C	-4.30555600	-3.13694500	0.55952100
H	-5.10962700	-2.40072800	0.47354600
H	-3.96722900	-3.16991300	1.59615000
H	-4.72437000	-4.11857900	0.31716100
C	-3.70371600	-2.91192100	-1.84794300
H	-4.49814500	-2.17968700	-2.00870000
H	-4.13015100	-3.90616300	-2.01327300
H	-2.92315800	-2.75566100	-2.59522300
C	0.03682400	-2.98093100	-1.66667000
H	0.93506300	-2.35840900	-1.68545200
H	-0.61750100	-2.68891900	-2.49463700
H	0.34990400	-4.01727700	-1.83343000
C	-4.51414900	1.20582500	1.52019600
H	-4.83128900	1.48891300	2.51885200
C	-4.45199300	1.66105100	-0.83912800
H	-4.71828800	2.30004300	-1.67494700
C	-2.16261300	0.17881600	3.34981400
H	-1.30773100	0.39900300	2.70279500
H	-1.79388300	-0.36241500	4.22807800
H	-2.58163600	1.13098400	3.69261000
C	-3.63808900	0.54355600	-1.06964100
C	-4.90335300	1.98323700	0.43485100
H	-5.53491400	2.85388200	0.58576600
C	-2.05991200	1.44157100	-2.82249900
H	-1.24623200	1.47683400	-2.09228500

H	-2.53335400	2.42873800	-2.84133300
H	-1.62371500	1.25792600	-3.81040600
C	0.34387900	-3.23770400	0.81122500
H	1.26058300	-2.65302000	0.70483400
H	0.61261700	-4.29687400	0.72663200
H	-0.07789900	-3.07726600	1.80998500
C	-3.08136600	0.33665400	-2.47780300
H	-2.54117900	-0.61106200	-2.49926500
C	-4.18164800	0.27743300	-3.55504700
H	-4.93700200	-0.48325800	-3.33646400
H	-3.73988900	0.04523800	-4.52964000
H	-4.69937800	1.23702100	-3.65405000
C	-4.36897400	-1.04647300	3.55882200
H	-5.14490500	-1.62714300	3.05159500
H	-4.84725100	-0.16359800	3.99482800
H	-3.98191900	-1.64695200	4.38881600
H	1.65200000	1.47061100	-0.81767700
N	1.05991200	1.61479700	0.00494700
C	0.61560900	2.95835700	0.03639600
C	1.19926000	3.93891400	-0.78806500
C	-0.36542700	3.36059100	0.96085400
C	0.79872500	5.27159400	-0.70107700
H	1.96543700	3.64305100	-1.50080500
C	-0.75740800	4.69493400	1.04641900
H	-0.82032700	2.61220100	1.60404100
C	-0.18084100	5.65977300	0.21573100
H	1.25708200	6.01045500	-1.35317400
H	-1.52049100	4.98292500	1.76492200
H	-0.49042100	6.69849500	0.28272600
C	2.48886900	1.30617100	1.18230900
H	3.10752400	2.09053500	0.74957200
H	2.02250300	1.60897300	2.11756600
C	2.94513900	-0.02061100	1.12041800
H	2.59146900	-0.80563800	1.77687900
S	3.70949100	-0.57442600	-0.30745100
C	5.49926200	-0.67224600	-0.04860500
C	6.30422400	0.42458200	-0.36423100
C	6.05331400	-1.83338900	0.49583300
C	7.67680100	0.35925300	-0.12107900
H	5.85352800	1.30203200	-0.81492500
C	7.42622300	-1.88952000	0.73646300
H	5.41229500	-2.68345000	0.70363900
C	8.23836900	-0.79374800	0.43262900
H	8.30911700	1.20677600	-0.37089700
H	7.86376900	-2.79202100	1.15432100
H	9.30761400	-0.84182000	0.61899700
O	3.53375400	0.46318000	-1.36657600
O	3.29073400	-1.97602400	-0.58165600

TS_F'

Zero-point correction = 0.721175 (Hartree/Particle)

Thermal correction to Energy = 0.763394

Thermal correction to Enthalpy = 0.764339

Thermal correction to Gibbs Free Energy = 0.643674

Sum of electronic and zero-point Energies =-2177.455753

Sum of electronic and thermal Energies =-2177.413534

Sum of electronic and thermal Enthalpies =-2177.412589

Sum of electronic and thermal Free Energies =-2177.533254

Cartesian coordinates

Cu	0.00106000	0.18953500	-0.91064400
N	-0.61534500	1.96478800	-1.48614600
H	-0.35459500	2.10054000	-2.46373700
C	-0.23015900	3.11748000	-0.76503700
C	-0.38889100	3.15622200	0.63396900
C	0.24093500	4.27360700	-1.41670900
C	-0.07373200	4.31246500	1.34701300
H	-0.77023100	2.28225300	1.15081800

C	0.56691900	5.41963700	-0.69411400
H	0.36006800	4.26301800	-2.49881500
C	0.41069300	5.44816600	0.69397500
H	-0.20633100	4.32175200	2.42570900
H	0.94152300	6.29456800	-1.21928500
H	0.66286600	6.34183500	1.25721500
C	-2.53050400	1.90804200	-1.63871300
H	-2.50452800	1.05469600	-2.31124100
H	-2.64695800	2.86659600	-2.14146600
C	-3.21624200	1.77163400	-0.43007800
H	-3.50965600	2.60445600	0.19558100
O	-2.28491700	-0.65246600	-0.39910800
C	1.03446300	-1.40896500	-0.78443800
N	2.18505900	-1.58378800	-0.16385400
C	0.66140500	-2.70512500	-1.49967400
C	2.83718700	-2.96363000	-0.33571000
C	2.80371900	-0.54254000	0.64953900
C	1.96599800	-3.54400800	-1.46974800
C	-0.49302500	-3.38193900	-0.71940900
C	0.19216300	-2.42546300	-2.93885800
C	4.31182600	-2.85065800	-0.73795300
C	2.75445000	-3.78634800	0.95957600
C	3.70346300	0.36424600	0.03758900
C	2.47652100	-0.44606200	2.02300900
H	1.77143600	-4.60982900	-1.32015000
H	2.49440900	-3.44088400	-2.42390800
H	-1.35765700	-2.71881000	-0.64875800
H	-0.19624000	-3.65277100	0.29797500
H	-0.78584100	-4.30189900	-1.23844200
H	-0.72642800	-1.83151800	-2.93875700
H	-0.01231200	-3.37007500	-3.45591800
H	0.95220500	-1.88351000	-3.51203500
H	4.90280800	-2.34045900	0.02754500
H	4.43810700	-2.32843300	-1.68728500
H	4.71886200	-3.85972400	-0.85726800
H	3.30082600	-3.30113300	1.77152800
H	3.21721600	-4.76270500	0.78477300
H	1.72664800	-3.95784900	1.28287600
C	3.96410400	0.42557100	-1.46781800
C	4.32606700	1.31803100	0.85183900
C	3.13466800	0.53000200	2.78340400
C	1.38743200	-1.27359800	2.70495100
H	3.47281700	-0.42959800	-1.93789300
C	3.32801700	1.69376300	-2.07449900
C	5.46349100	0.36458400	-1.81925700
H	5.01610900	2.02576900	0.40349100
C	4.06245800	1.39343600	2.21464800
H	2.89712300	0.62358400	3.83821300
C	0.15726100	-0.39934100	3.02126900
H	1.05348700	-2.04473000	2.00956500
C	1.88405400	-1.97636100	3.98368100
H	2.25675700	1.73737200	-1.86236700
H	3.46952300	1.70490700	-3.16153700
H	3.78618100	2.60082500	-1.66685600
H	5.95378000	-0.51379500	-1.39047700
H	5.99599600	1.24995700	-1.45727000
H	5.59431700	0.33073100	-2.90634100
H	4.55910900	2.14139500	2.82595000
H	-0.27324000	0.03926100	2.11936100
H	0.41572200	0.41487900	3.70707300
H	-0.62819000	-0.99963300	3.49074500
H	2.77382900	-2.58811500	3.80562100
H	1.09840800	-2.62782600	4.38029700
H	2.13192200	-1.25489800	4.76910600
S	-3.20162500	0.26001900	0.36792800
C	-4.83011600	-0.52171000	0.23080700

C	-5.74832100	-0.36972500	1.27139200
C	-5.16533300	-1.23522500	-0.92291900
C	-7.01964400	-0.93341800	1.14968300
H	-5.45280100	0.16745900	2.16604500
C	-6.43654700	-1.79741800	-1.03445600
H	-4.42903000	-1.35921800	-1.70977800
C	-7.36568700	-1.64408200	-0.00145800
H	-7.73743300	-0.82242400	1.95758500
H	-6.70151300	-2.35928600	-1.92582100
H	-8.35519900	-2.08319700	-0.09206300
O	-2.98022700	0.42809500	1.82401200

Aniline

Zero-point correction = 0.117231 (Hartree/Particle)

Thermal correction to Energy = 0.123020

Thermal correction to Enthalpy = 0.123965

Thermal correction to Gibbs Free Energy = 0.088088

Sum of electronic and zero-point Energies =-287.499264

Sum of electronic and thermal Energies = -287.493475

Sum of electronic and thermal Enthalpies = -287.492531

Sum of electronic and thermal Free Energies = -287.528408

Cartesian coordinates

C	-1.17146100	1.20239700	-0.00329000
C	0.22127100	1.20820700	0.00520000
C	0.93906800	-0.00001000	0.00990600
C	0.22129200	-1.20813000	0.00514700
C	-1.17152600	-1.20235900	-0.00317100
C	-1.88124400	-0.00004000	-0.00829700
H	-1.70511400	2.14891600	-0.00882800
H	0.76283500	2.15119300	0.01323000
H	0.76290000	-2.15110600	0.01199700
H	-1.70525000	-2.14883800	-0.00835900
H	-2.96649500	-0.00013800	-0.01656600
N	2.33585800	0.00006300	0.07705200
H	2.77768000	-0.83595500	-0.28104100
H	2.77804200	0.83509700	-0.28277400

4F

Zero-point correction = 0.173106 (Hartree/Particle)

Thermal correction to Energy = 0.183263

Thermal correction to Enthalpy = 0.184207

Thermal correction to Gibbs Free Energy = 0.136314

Sum of electronic and zero-point Energies =-458.305094

Sum of electronic and thermal Energies = -458.294938

Sum of electronic and thermal Enthalpies = -458.293994

Sum of electronic and thermal Free Energies = -458.341886

Cartesian coordinates

C	-3.31842100	0.81158600	-0.08675900
C	-1.99705300	1.24014000	-0.04332900
C	-0.94214100	0.31174000	0.04448100
C	-1.25522400	-1.05720200	0.08128900
C	-2.58724500	-1.47394000	0.04422500
C	-3.62748400	-0.55103600	-0.04078200
H	-4.11345100	1.54874200	-0.15582800
H	-1.76833100	2.30321700	-0.06900600
H	-0.46910200	-1.80183800	0.13503300
H	-2.80577100	-2.53772200	0.07470200
H	-4.65986500	-0.88375300	-0.07371700
N	0.37254400	0.79031500	0.12970100
H	0.48310800	1.69976100	-0.30171800
C	1.50648500	-0.08864400	-0.08146900
H	1.52502900	-0.54463800	-1.08494000
H	1.46318500	-0.90852000	0.64200000
C	2.80737300	0.70049800	0.15311800
H	2.87535700	1.54114200	-0.54934500
H	2.80189000	1.12377800	1.16351500
C	3.99907900	-0.13265400	-0.01356600

N	4.93541700	-0.80504300	-0.14740800

Phenol

Zero-point correction = 0.103778 (Hartree/Particle)

Thermal correction to Energy = 0.108933

Thermal correction to Enthalpy = 0.109877

Thermal correction to Gibbs Free Energy = 0.074980

Sum of electronic and zero-point Energies =-307.368334

Sum of electronic and thermal Energies = -307.363178

Sum of electronic and thermal Enthalpies = -307.362234

Sum of electronic and thermal Free Energies = -307.397131

Cartesian coordinates

C	1.15569900	-1.20762400	0.00499500
C	-0.23983000	-1.21147200	-0.01272500
C	-0.93485400	0.00007300	-0.01675900
C	-0.23967700	1.21154700	-0.01262700
C	1.15583000	1.20754400	0.00503800
C	1.85671900	-0.00009300	0.01670700
H	1.69538600	-2.15036000	0.00760200
H	-0.80140300	-2.14022400	-0.03209300
H	-0.80121600	2.14032100	-0.03187100
H	1.69566400	2.15019400	0.00770500
H	2.94240000	-0.00013800	0.02923100
O	-2.32177200	0.00027600	-0.08730100
H	-2.67997300	-0.00184500	0.81005500

6D

Zero-point correction = 0.160637 (Hartree/Particle)

Thermal correction to Energy = 0.170507

Thermal correction to Enthalpy = 0.171451

Thermal correction to Gibbs Free Energy = 0.124085

Sum of electronic and zero-point Energies =-478.178880

Sum of electronic and thermal Energies = -478.169010

Sum of electronic and thermal Enthalpies = -478.168066

Sum of electronic and thermal Free Energies = -478.215432

Cartesian coordinates

C	3.25346300	-0.85100000	-0.00006700
C	1.92252100	-1.25239100	-0.00012300
C	0.90420500	-0.28984900	-0.00005100
C	1.22383600	1.07139800	0.00002900
C	2.56816000	1.45793000	0.00009600
C	3.58596100	0.50787200	0.00005400
H	4.03662900	-1.60348500	-0.00011300
H	1.64566000	-2.30144800	-0.00024500
H	0.45014400	1.83003900	-0.00005100
H	2.81112700	2.51653800	0.00017400
H	4.62594500	0.81805600	0.00010700
C	-1.45688400	0.13066000	-0.00005300
H	-1.42982500	0.77358500	-0.88957200
H	-1.42942400	0.77405400	0.88911500
C	-2.72949500	-0.72499400	0.00040400
H	-2.73249700	-1.37482200	-0.88114800
H	-2.73235300	-1.37383500	0.88265700
C	-3.94015100	0.09693700	0.00003100
N	-4.88970000	0.76403200	-0.00028000
O	-0.37590000	-0.78578500	-0.00011100

Vinyl cyanide

Zero-point correction = 0.050863 (Hartree/Particle)

Thermal correction to Energy = 0.055012

Thermal correction to Enthalpy = 0.055956

Thermal correction to Gibbs Free Energy = 0.024978

Sum of electronic and zero-point Energies =-170.785381

Sum of electronic and thermal Energies = -170.781232

Sum of electronic and thermal Enthalpies = -170.780288

Sum of electronic and thermal Free Energies = -170.811266

Cartesian coordinates

C	1.32122600	-0.98591500	0.00000000
H	2.03142400	-0.16598600	0.00000000

H	1.71941100	-1.99470200	0.00000000
C	0.00000000	-0.77424900	0.00000000
H	-0.70360800	-1.60272200	0.00000000
C	-0.57874300	0.53440800	0.00000000
N	-1.07173200	1.58827700	0.00000000

Methyl vinyl ketone

Zero-point correction = 0.089690 (Hartree/Particle)

Thermal correction to Energy = 0.095473

Thermal correction to Enthalpy = 0.096417

Thermal correction to Gibbs Free Energy = 0.060865

Sum of electronic and zero-point Energies =-231.154109

Sum of electronic and thermal Energies = -231.148326

Sum of electronic and thermal Enthalpies = -231.147382

Sum of electronic and thermal Free Energies = -231.182934

Cartesian coordinates

C	1.94219300	0.17212700	-0.00020600
H	1.85007500	1.25421800	-0.00062700
H	2.95266400	-0.22504600	-0.00009600
C	0.87656600	-0.63492800	0.00030100
H	0.99286000	-1.71615200	0.00062500
C	-0.54447200	-0.18875300	0.00007600
O	-1.43574500	-1.02446900	-0.00023000
C	-0.85805200	1.29809300	0.00012600
H	-0.43323700	1.78817000	0.88277000
H	-0.43322800	1.78800800	-0.88262800
H	-1.94058600	1.42732100	0.00001300

Methyl acrylate

Zero-point correction = 0.095493 (Hartree/Particle)

Thermal correction to Energy = 0.102160

Thermal correction to Enthalpy = 0.103104

Thermal correction to Gibbs Free Energy = 0.064943

Sum of electronic and zero-point Energies =-306.379831

Sum of electronic and thermal Energies = -306.373164

Sum of electronic and thermal Enthalpies = -306.372220

Sum of electronic and thermal Free Energies = -306.410381

Cartesian coordinates

C	2.17358500	-0.76436300	0.00081400
H	1.66654000	-1.72316800	0.00227300
H	3.25912900	-0.77192100	0.00081300
C	1.49089200	0.38250800	-0.00087000
H	1.98914000	1.34696800	-0.00216700
C	0.01091600	0.48506000	-0.00033500
O	-0.58862700	1.54223000	0.00082600
O	-0.60466000	-0.72085400	-0.00107800
C	-2.03927100	-0.67143800	0.00027500
H	-2.40848300	-0.15096300	-0.88693700
H	-2.36985700	-1.70994200	-0.00037500
H	-2.40689400	-0.15258900	0.88909800

Vinyl sulphone

Zero-point correction = 0.143623 (Hartree/Particle)

Thermal correction to Energy = 0.153626

Thermal correction to Enthalpy = 0.154570

Thermal correction to Gibbs Free Energy = 0.107265

Sum of electronic and zero-point Energies =-858.078343

Sum of electronic and thermal Energies = -858.068340

Sum of electronic and thermal Enthalpies = -858.067396

Sum of electronic and thermal Free Energies = -858.114701

Cartesian coordinates

C	-2.77826400	1.18947900	1.21739200
H	-3.00413200	1.75690100	0.31979600
H	-3.26324100	1.47837000	2.14486700
C	-1.93847600	0.16104100	1.17458000
H	-1.67314000	-0.46495800	2.02096300
S	-1.21251900	-0.35569100	-0.38057200
O	-1.43341500	-1.80647000	-0.49525100
O	-1.66651700	0.57777400	-1.42433700

C	0.55088100	-0.09359900	-0.13337200
C	1.33079000	-1.14285900	0.35602500
C	1.10660500	1.14967900	-0.44246900
C	2.69634200	-0.93399500	0.55090400
H	0.87233500	-2.10529300	0.55575800
C	2.47257400	1.34532500	-0.24394700
H	0.47744200	1.93487300	-0.84730800
C	3.26373400	0.30722700	0.25498000
H	3.31717500	-1.74182400	0.92585500
H	2.92068400	2.30434000	-0.48498300
H	4.32752000	0.46442800	0.40635700

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