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Supporting Information of

Hematin supported on Colour Catcher®: Biodegradable Heterogeneous Catalyst for Halogen-free CO_2 Cycloadditions

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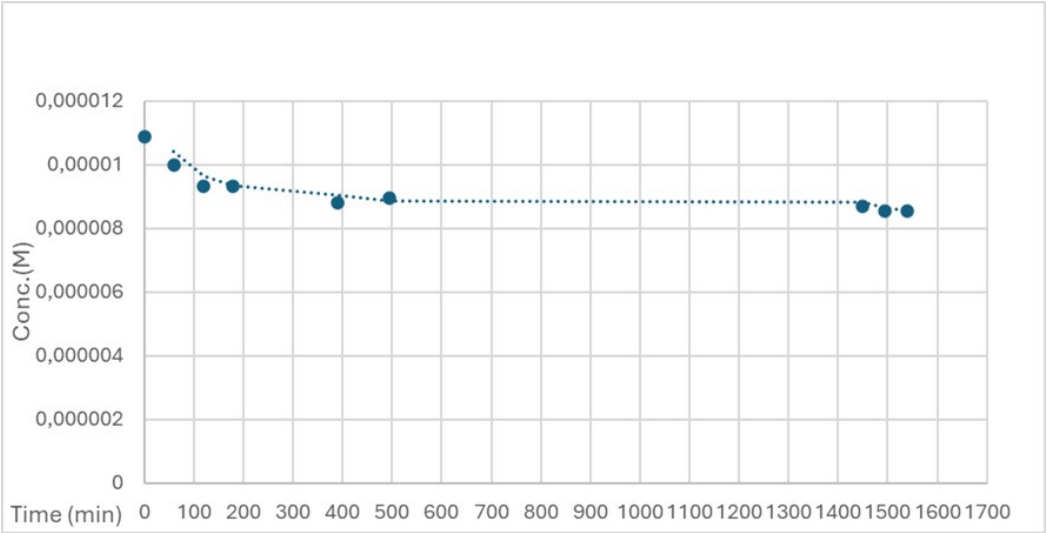
1. General methods

All air- and moisture-sensitive manipulations were carried out with standard Schlenk techniques under nitrogen atmosphere. Unless otherwise specified, DCE was distilled over calcium hydride and kept under nitrogen. *N*-alkyl aziridines were synthesized by following already reported procedures.[1] All the other starting materials were commercial products and used as received. NMR spectra were recorded at room temperature either on a Bruker Avance 300-DRX, operating at 300 MHz for ^{1}H and at 75 MHz for ^{13}C or on a Bruker Avance 400-DRX spectrometers, operating at 400 MHz for ^{1}H and at 101 MHz for ^{13}C. Chemical shifts (ppm) are reported relative to TMS. ^{1}H NMR signals of the compounds described in the following were attributed by 2D NMR techniques. Assignments of the resonances in ^{13}C NMR were made by using the APT pulse sequence, HSQC and HMBC techniques. Infrared spectra were recorded on a Varian Scimitar FTS 1000 spectrophotometer. UV-Visible spectra were recorded on an Agilent 8453E instrument. UV-Visible spectra of CC strips were recorded on a Cary 100 spectrophotometer. Morphology and chemical compositions were studied using a Scanning Electron Microscope (SEM) equipped with energy-dispersive X-ray microanalysis (EDX) by using a Hitachi TM 1000 SEM/EDX. TGA analyses were recorded by using a Perkin Elmer TGA 7 Thermogravimetric Analyzer. ICP analyses were performed by using a PerkinElmer Optima 8000 ICP-OES instrument. Mass spectra were recorded in the analytical laboratories of Milan University.

2. Optimization of the loading of 3 onto CC sheet

1 (65.0 mg, 1.00 x 10^{-4} mol) was dissolved in 100.0 mL of NaOH 0.1 M and the mixture was stirred at room temperature until the complete dissolution of the starting hemin. The obtained solution ([**3**] = 1.00 x 10^{-3} M) was then placed in a coded test tube and 25 cm^2 of Colour Catcher® were immersed into the **3**-containing solution. The decrease in the concentration of **3** was monitored using UV-visible spectroscopy. The absorption spectrum of the **3**-containing solution, appropriately diluted by a factor of 100, was acquired at various immersion times and the resulting absorbance values were plotted as a function of time, as shown below.



ENTRY	abs	Concentration (M)	TIME (min)
0	0,59013	1,08668E-05	0
1	0,54188	9,97827E-06	60
2	0,5064	9,32494E-06	120
3	0,50619	9,32107E-06	180
4	0,47695	8,78264E-06	390
5	0,48674	8,96291E-06	495
6	0,47216	8,69444E-06	1450
7	0,46433	8,55025E-06	1495
8	0,46362	8,53718E-06	1540

Figure S1: Variation of concentration of **3** in function of time.

3. Characterization of 3@CC

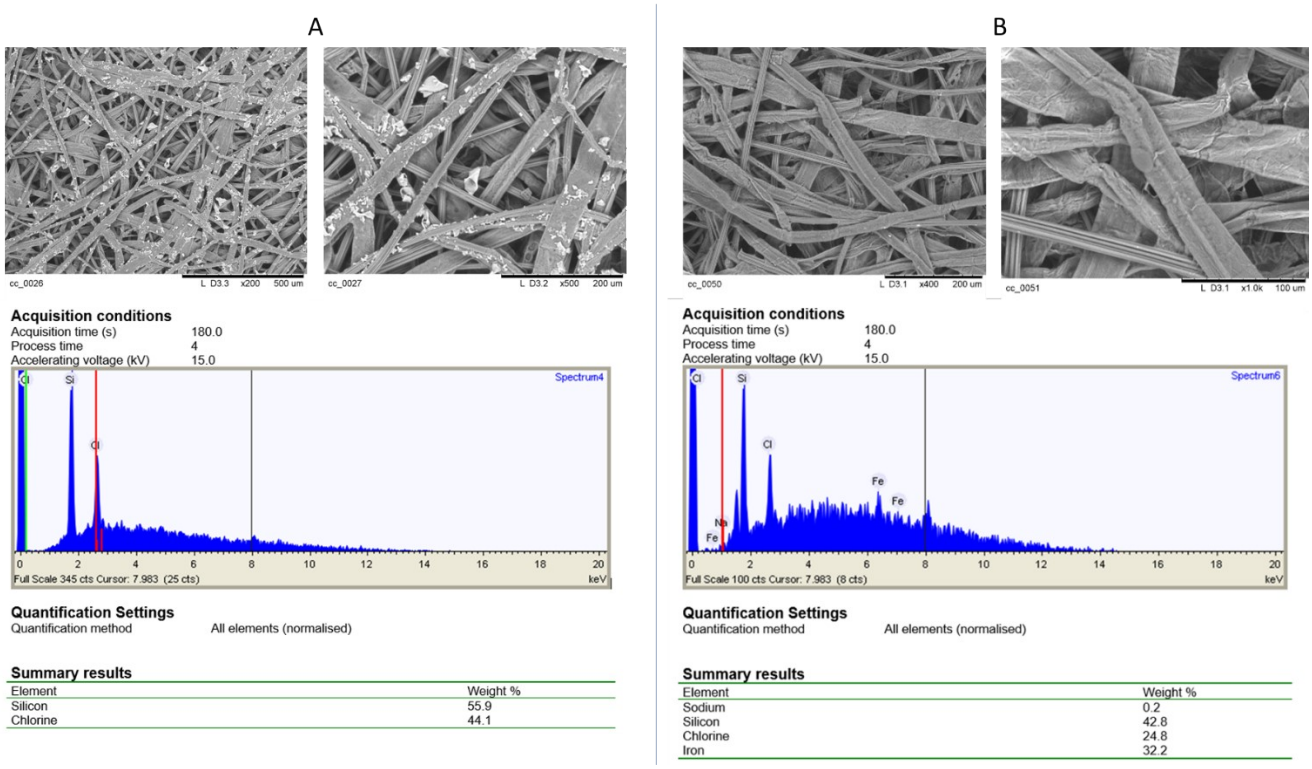


Figure S2: SEM images and EDX analysis of CC (A) and **3@CC** 0.054 mg/cm^2 (B).

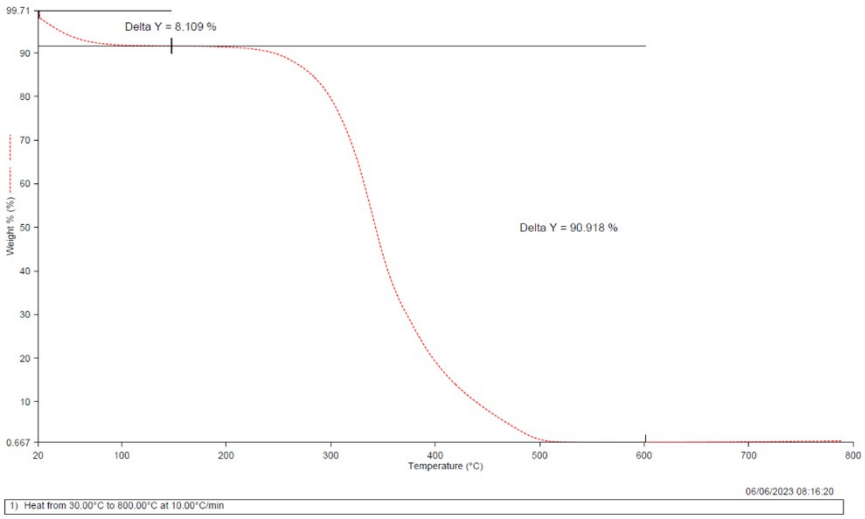
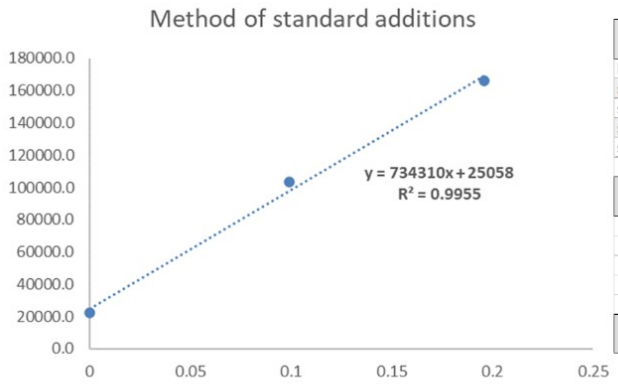


Figure S3: TGA analysis of **3@CC** 0.054 mg/cm^2.



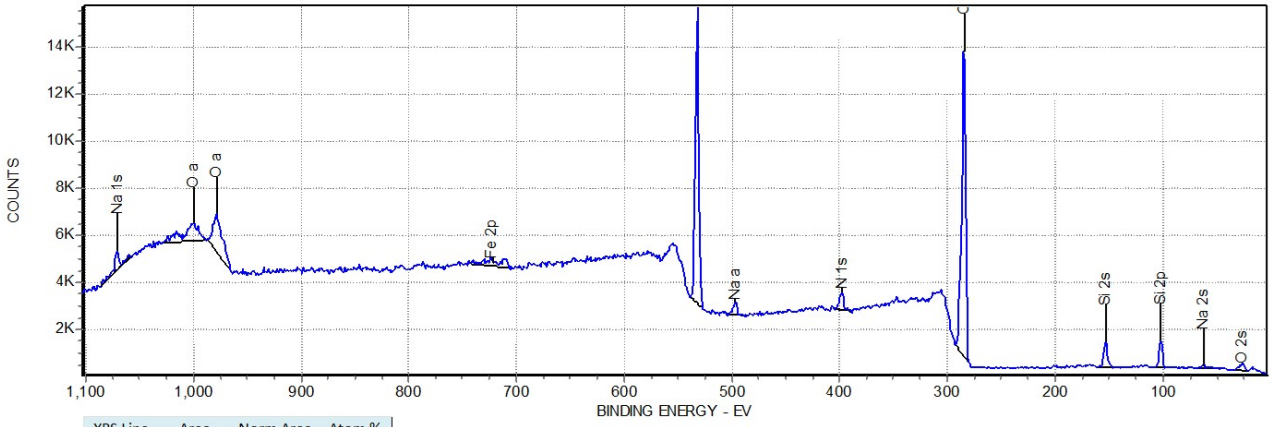
Sample Id	R	Fe 238.204 (cps)	Fe 238.204 (mg/L)
blank		5024.2	
std 1		21950.9	0.05
std 2		46866.0	0.1
std 3		97498.8	0.2
std 4		383117.7	1

y = mx+C			
m-->	734310.496	25057.63047	<--C
Sm-->	49597.7578	6287.969491	<--Sc
R^2-->	0.99545862	6874.02021	<--t
	219.197394	1	

with y=0 -->> x=-C/m (mg/L)

x	sample V(L)	final V(L)	mg Fe	sample weight	% Fe
0.034124	0.002	0.05	0.042655033	37.6	0.113444235

Figure S4: ICP-OES analysis of **3@CC** 0.054 mg/cm^2.



XPS Line	Area	Norm Area	Atom %
Na 1s	4437	16,497	1,328
O 1s	46787	282,582	22,748
C 1s	55845	840,94	67,697
Si 2p	3800	63,429	5,106
N 1s	3505	31,43	2,53
Fe 2p	5827	7,333	0,59

Figure S5: XPS analysis of **3@CC** 0.054 mg/cm^2.

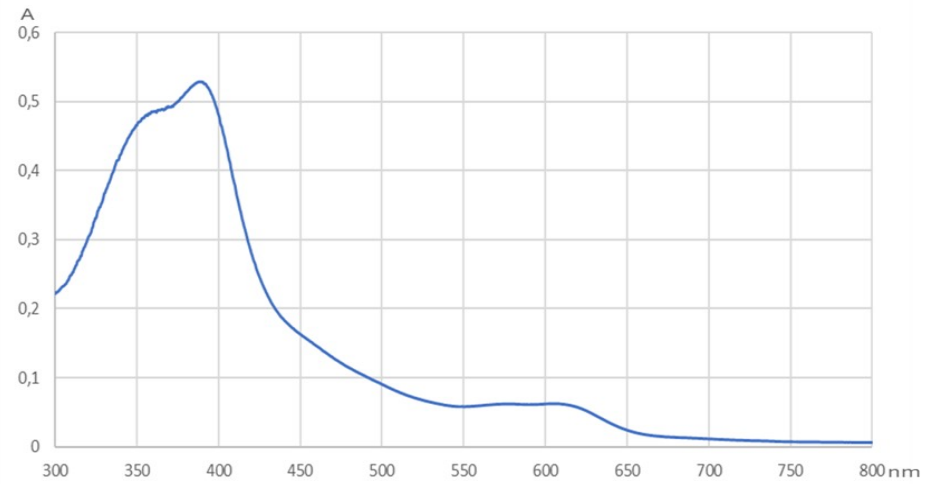


Figure S6: UV/visible spectrum of **3@CC** (catalytic loading = 0.054 mg/cm^2).

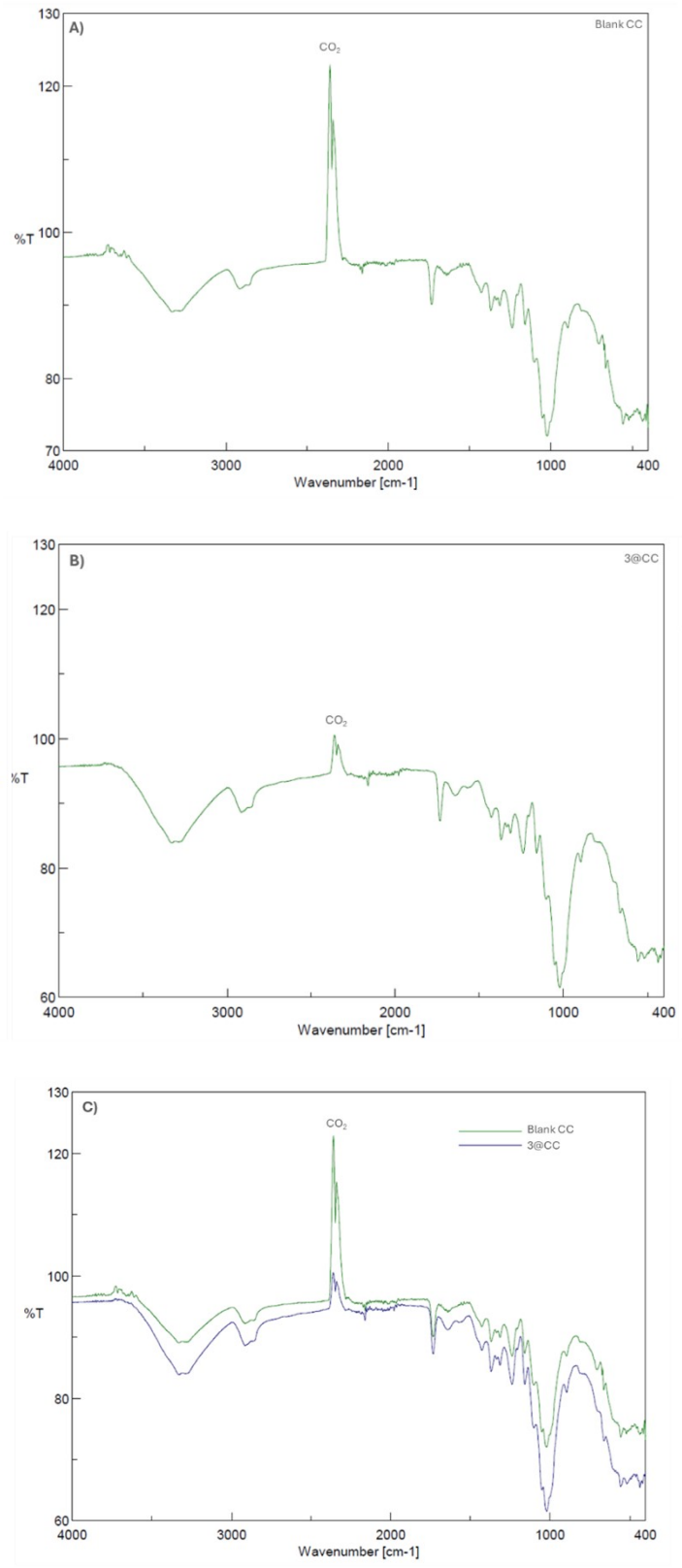


Figure S7: ATR spectra of porphyrin-free Colour Catcher® (A), **3@CC** (catalytic loading = 0.054 mg/cm^2) (B) and superimposed spectrum of A and B (C).

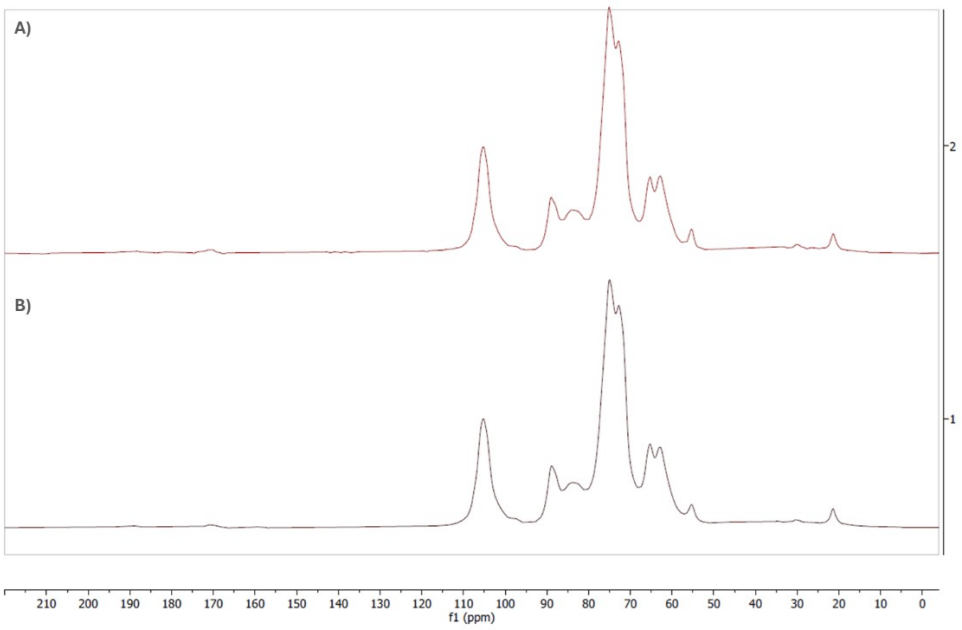
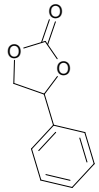


Figure S8: CPMAS spectra of porphyrin-free Colour Catcher® (A) and **3@CC** (catalytic loading = 0.054 mg/cm^2) (B).

4. Synthesis of cyclic carbonates

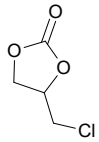
Synthesis of 4-phenyl-1,3-dioxolan-2-one (4)



The general catalytic procedure was followed by using styrene oxide as the reagent (0.318 mL) to obtain a yellowish oil as the product (*Method A*: 96% yield; *Method B*: 94% yield; *Method C*: 40% yield). Collected data are in accordance with those reported in literature. [2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.30 (m, 5H), 4.79 (dd, *J* = 8.4, 3.4 Hz, 1H), 3.71 (dd, *J* = 11.5, 3.5 Hz, 1H), 3.63 ppm (dd, *J* = 11.5, 8.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.51, 128.51, 127.93, 126.11, 74.73, 68.03 ppm. LR-MS (ESI) m/z calcd. for ($C_9H_8O_3$): 164.05, found 165.39 $[M+H]^+$.

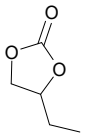
Synthesis of 4-(chloromethyl)-1,3-dioxolan-2-one (5)



Method B of the general catalytic procedure was followed by using epichlorohydrin as the reagent (0.144 mL) to obtain a yellowish oil as the product (100% yield). Collected data are in accordance with those reported in literature. [3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.02 – 4.97 (m, 1H), 4.57 (t, *J* = 8.6 Hz, 1H), 4.38 – 4.35 (m, 1H), 3.81 (dd, *J* = 12.4, 4.6 Hz, 1H), 3.71 ppm (dd, *J* = 12.3, 3.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.57, 74.57, 67.00, 44.21 ppm. LR-MS (ESI) m/z calcd. for ($C_4H_5ClO_3$): 135.99, found 156.08 $[M+Na]^+$.

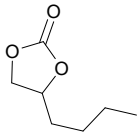
Synthesis of 4-ethyl-1,3-dioxolan-2-one (6)



Method B of the general catalytic procedure was followed by using 1,2-epoxybutane as the reagent (0.160 mL) to obtain a yellowish oil as the product (75% yield). Collected data are in accordance with those reported in literature.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.68 – 4.62 (m, 1H), 4.50 (t, *J* = 8.2 Hz, 1H), 4.05 (dd, *J* = 8.5, 6.9 Hz, 1H), 1.83 – 1.66 (m, 2H), 0.98 ppm (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.21, 78.10, 69.06, 26.83, 8.40 ppm. LR-MS (ESI) m/z calcd. for ($C_5H_8O_3$): 116.05, found 117.47 $[M+H]^+$.

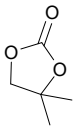
Synthesis of 4-butyl-1,3-dioxolan-2-one (7)



Method B of the general catalytic procedure was followed by using 1,2-epoxyhexane as the reagent (0.333 mL) to obtain a yellowish oil as the product (75% yield). Collected data are in accordance with those reported in literature.[2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.69 – 4.62 (m, 1H), 4.50 – 4.46 (pst, *J* = 8.4 Hz, 1H), 4.01 (dd, *J* = 8.5, 7.1 Hz, 1H), 1.79 – 1.53 (m, 2H), 1.49 – 1.24 (m, 4H), 0.85 ppm (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.18, 77.16, 69.34, 33.36, 26.40, 22.22, 13.69 ppm. LR-MS (ESI) m/z calcd. for ($C_7H_{12}O_3$): 144.08 found 145.62 $[M+H]^+$.

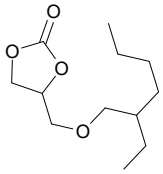
Synthesis of 4,4-dimethyl-1,3-dioxolan-2-one (8)



Method B of the general catalytic procedure was followed by using 2,2-dimethyloxirane as the reagent (0.245 mL) to obtain a yellowish oil as the product (100% yield). Collected data are in accordance with those reported in literature.[2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.14 (s, 2H), 1.50 ppm (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.65, 81.80, 75.32, 25.91 ppm. LR-MS (ESI) m/z calcd. for ($C_5H_8O_3$): 116.05, found 139.48 $[M+Na]^+$.

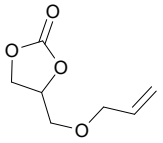
Synthesis of 4-(((2-ethylhexyl)oxy)methyl)-1,3-dioxolan-2-one (9)



Method B of the general catalytic procedure was followed by using 2-ethylhexyl-glycidylether as the reagent (0.577 mL) to obtain a yellowish oil as the product (35% yield). Collected data are in accordance with those reported in literature.[4]

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.81 – 4.76 (m, 1H), 4.46 (t, *J* = 8.4 Hz, 1H), 4.35 (dd, *J* = 8.3, 5.9 Hz, 1H), 3.63 (ddd, *J* = 11.1, 3.5, 2.2 Hz, 1H), 3.54 (ddd, *J* = 11.2, 3.5, 2.2 Hz, 2H), 3.36 (dd, *J* = 5.8, 2.0 Hz, 1H), 1.50 – 1.44 (m, 1H), 1.36 – 1.20 (m, 8H), 0.87 – 0.81 ppm (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.11, 75.27, 74.65, 70.08, 66.08, 39.54, 30.39, 29.00, 23.72, 22.95, 13.98, 10.98 ppm. LR-MS (ESI) m/z calcd. for ($C_{12}H_{22}O_4$): 230.15, found 253.22 $[M+Na]^+$.

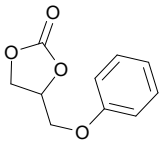
Synthesis of 4-((allyloxy)methyl)-1,3-dioxolan-2-one (10)



Method B of the general catalytic procedure was followed by using allyl-glycidylether as the reagent (0.211 mL) to obtain a yellowish oil as the product (98% yield). Collected data are in accordance with those reported in literature.[2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.85 – 5.78 (m, 1H), 5.29 – 5.17 (m, 1H), 4.82 (dq, *J* = 7.9, 3.7 Hz, 1H), 4.52 – 4.47 (m, 1H), 4.39 – 4.35 (m, 1H), 4.03 (dd, *J* = 5.6, 1.4 Hz, 2H), 3.71 – 3.66 (m, 1H), 3.62 – 3.57 ppm (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.07, 133.75, 117.78, 75.20, 72.49, 68.88, 66.26 ppm. LR-MS (ESI) m/z calcd. for ($C_7H_{10}O_4$): 158.06 found 173.29 $[M+Na]^+$.

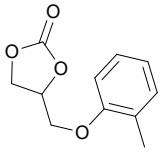
Synthesis of 4-(phenoxymethyl)-1,3-dioxolan-2-one (11)



Method B of the general catalytic procedure was followed by using glycidyl-phenylether as the reagent (0.374 mL) to obtain a white solid as the product (74% yield). Collected data are in accordance with those reported in literature.[4]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.31 (m, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.93 (d, *J* = 7.7 Hz, 2H), 5.08 – 5.02 (m, 1H), 4.64 (t, *J* = 8.4 Hz, 1H), 4.57 – 4.54 (m, 1H), 4.26 (dd, *J* = 10.6, 4.3 Hz, 1H), 4.17 ppm (dd, *J* = 10.6, 3.6 Hz,1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.77, 154.66, 129.75, 122.03, 114.60, 74.12, 66.92, 66.27 ppm. LR-MS (ESI) m/z calcd. for ($C_{10}H_{10}O_4$): 194.06, found 217.26 $[M+Na]^+$.

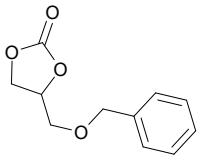
Synthesis of 4-((o-tolyloxy)methyl)-1,3-dioxolan-2-one (12)



Method B of the general catalytic procedure was followed by using glycidyl-2-methylphenylether as the reagent (0.420 mL) to obtain a white solid as the product (45% yield). Collected data are in accordance with those reported in literature.[4]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 7.17 (m, 2H), 6.97 – 6.93 (m, 1H), 6.81 (d, *J* = 8.3 Hz, 1H), 5.10 – 5.04 (d, *J* = 20.5 Hz, 1H), 4.67 – 4.58 (d, *J* = 36.5 Hz, 2H), 4.28 (dd, *J* = 10.6, 3.6 Hz, 1H), 4.16 (dd, *J* = 10.7, 3.1 Hz, 1H), 2.24 ppm (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.78, 154.77, 131.11, 126.90, 121.66, 110.88, 74.22, 67.05, 66.25, 15.96 ppm. LR-MS (ESI) m/z calcd. for ($C_{11}H_{12}O_4$): 208.07, found 209.58 $[M+H]^+$.

Synthesis of 4-((benzyloxy)methyl)-1,3-dioxolan-2-one (13)

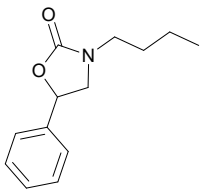


Method B of the general catalytic procedure was followed by using 2-(benzyloxy)methyloxirane as the reagent (0.424 mL) to obtain a white solid as the product (72% yield). Collected data are in accordance with those reported in literature.[4]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.32 (d, *J* = 9.8 Hz, 1H), 4.86 – 4.80 (m, 1H), 4.66 – 4.57 (m, 2H), 4.49 (t, *J* = 8.4 Hz, 1H), 4.40 (dd, *J* = 8.4, 6.0 Hz, 1H), 3.73 (dd, *J* = 10.9, 4.0 Hz, 1H), 3.64 ppm (dd, *J* = 11.0, 3.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.97, 137.11, 128.60, 128.10, 127.77, 75.04, 73.72, 68.87, 66.32 ppm. LR-MS (ESI) m/z calcd. for ($C_{11}H_{12}O_4$): 208.07, found 231.37 $[M+Na]^+$.

5. Synthesis of *N*-alkyl oxazolidin-2-ones

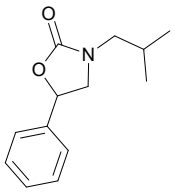
Synthesis of 3-butyl-5-phenyloxazolidin-2-onen (14)



The general catalytic procedure was followed by using 1-butyl-2-phenyl aziridine as the reagent (0.194 mL) to obtain a yellowish oil as the product (*Method A*: 95% yield, A/B = 99:1; *Method B*: 80% yield, A/B = 99:1; *Method C*: 68% yield, A/B = 96:4; *Method D*: 70% yield, A/B = 96:4;). Collected data are in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 5H), 5.39 (pt, *J* = 8.0 Hz, 1H), 3.83 (pt, *J* = 8.8 Hz, 1H), 3.34 (pt, *J* = 8.0 Hz, 1H), 3.29 – 3.13 (m, 2H), 1.51 – 1.41 (m, 2H), 1.33 –1.23 (m, 2H), 0.86 ppm (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.42, 129.40, 129.26, 126.00, 74.81, 66.81, 52.67, 44.42, 29.92, 20.34, 14.20 ppm. LR-MS (ESI) m/z calcd. for ($C_{13}H_{17}NO_2$): 219.13, found 220.19 $[M+H]^+$.

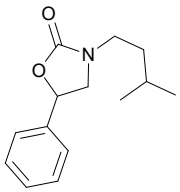
Synthesis of 3-isobutyl-5-phenyloxazolidin-2-one (15)



Method D of the general catalytic procedure was followed by using 1-isobutyl-2-phenyl aziridine as the reagent (0.195 mL) to obtain a yellowish oil as the product (56% yield, A/B = 98:2). Collected data are in accordance with those reported in literature.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 5H), 5.40 (pt, *J* = 8.4 Hz, 1H), 3.84 (pt, *J* = 8.8 Hz, 1H), 3.34 (dd, *J* = 8.7, 7.4 Hz, 1H), 3.09 – 2.94 (m, 2H) 1.83 – 1.75 (m, 1H), 0.87 – 0.83 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.53, 139.28, 129.17, 129.02, 125.77, 74.58, 53.07, 52.05, 27.10, 20.21, 20.17. LR MS (ESI) m/z calcd. for ($C_{13}H_{17}NO_2$): 219.13, found 242.16 $[M+Na]^+$.

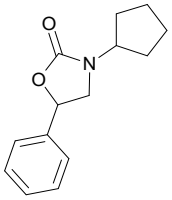
Synthesis of 3-isopentyl-5-phenyloxazolidin-2-one (16)



Method D of the general catalytic procedure was followed by using 1-isopentyl-2-phenyl aziridine as the reagent (0.211 mL) to obtain a yellowish oil as the product (91% yield, A/B = 99:1). Collected data are in accordance with those reported in literature.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.28 (m, 5H), 5.51 – 5.45 (m, 1H), 3.91 (pt, *J* = 8.7 Hz, 1H), 3.45 (pt, *J* = 8.0, 1H), 3.42 – 3.23 (m, 2H), 1.68 – 1.57 (m, 1H), 1.55 – 1.43 (m, 2H), 0.95 – 0.92 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 129.44, 129.31, 126.04, 74.86, 52.68, 43.16, 36.65, 26.29, 23.01, 22.94 ppm. LR MS (ESI) m/z calcd. for ($C_{14}H_{19}NO_2$): 233.14, found 256.22 $[M+Na]^+$.

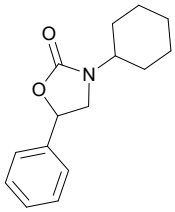
Synthesis of 3-cyclopentyl-5-phenyloxazolidin-2-one (17)



Method D of the general catalytic procedure was followed by using 1-cyclopentyl-2-phenyl aziridine as the reagent (0.193 mL) to obtain a yellowish oil as the product (31% yield, A/B = 94:6). Collected data are in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.31 (m, 5H), 5.47 (pt, *J* = 8.0 Hz, 1H), 4.33 – 4.27 (m, 1H), 3.91 – 3.86 (m, 1H), 3.40 (pt, *J* = 8.2 Hz, 1H), 2.00 – 1.88 (m, 2H), 1.70 – 1.54 ppm (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 129.37, 129.22, 125.96, 74.93, 55.13, 49.06, 29.63, 29.10, 24.39, 24.37 ppm. LR MS (ESI) m/z calcd. for ($C_{14}H_{17}NO_2$): 231.29, found 232.21 $[M+H]^+$.

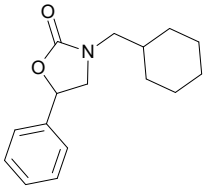
Synthesis of 3-cyclohexyl-5-phenyloxazolidin-2-one (18)



Method D of the general catalytic procedure was followed by using 1-cyclohexyl-2-phenyl aziridine as the reagent (0.219 mL) to obtain a yellowish oil as the product (20% yield, A/B = 95:5). Collected data are in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.32 (m, 5H), 5.49 – 5.44 (m, 1H), 3.91 – 3.80 (m, 1H), 3.79 – 3.69 (m, 1H), 3.42 – 3.37 (m, 1H), 1.90 – 1.04 ppm (m, 10H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 129.33, 129.17, 125.93, 75.03, 53.02, 48.78, 31.03, 30.56, 25.83, 25.78, 25.73 ppm. LR MS (ESI) m/z calcd. for ($C_{15}H_{19}NO_2$): 245.32, found 268.41 $[M+Na]^+$.

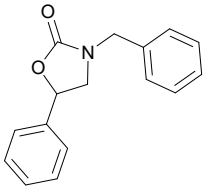
Synthesis of 3-(cyclohexylmethyl)-5-phenyloxazolidin-2-one (19)



Method D of the general catalytic procedure was followed by using 1-cyclohexylmethyl-2-phenyl aziridine as the reagent (0.219 mL) to obtain a yellowish oil as the product (85% yield, A/B = 99:1). Collected data are in accordance with those reported in literature.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.31 (m, 5H), 5.46 (pt, *J* = 8.2 Hz, 1H), 3.89 (pt, *J* = 8.8 Hz, 1H), 3.40 (dd, *J* = 8.7, 7.6 Hz, 1H), 3.19 - 3.03 (m, 2H), 1.72 - 1.63 (m, 6H), 1.24 - 1.01 (m, 3H), 0.97 - 0.88 ppm (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.57, 139.29, 129.22, 129.07, 125.83, 74.67, 53.36, 50.91, 36.41, 30.96, 26.66, 26.01 ppm. LR MS (ESI) m/z calcd. for ($C_{16}H_{21}NO_2$): 259.16, found 282.28 $[M+Na]^+$.

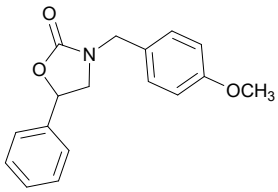
Synthesis of 3-benzyl-5-phenyloxazolidin-2-one (20)



Method D of the general catalytic procedure was followed by using 1-benzyl-2-phenyl aziridine as the reagent (0.197 mL) to obtain a yellowish oil as the product (75% yield, A/B = 96:4). Collected data are in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.32 (m, 10H), 5.52 – 5.47 (m, 1H), 4.58 (d, *J* = 15.0 Hz, 1H), 4.43 (d, *J* = 15.0 Hz, 1H), 3.79 (pt, *J* = 8.7 Hz, 1H), 3.36 – 3.30 ppm (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.03, 136.08, 129.33, 129.25, 128.63, 128.50, 125.96, 74.97, 52.00, 48.87 ppm. LR MS (ESI) m/z calcd. for ($C_{16}H_{15}NO_2$): 253.11, found 276.27 $[M+Na]^+$.

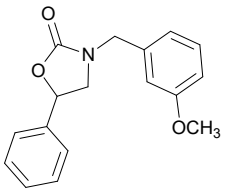
Synthesis of 3-(4-methoxybenzyl)-5-phenyloxazolidin-2-one (21)



Method D of the general catalytic procedure was followed by using 1-(4-methoxybenzyl)-2-phenyl aziridine as the reagent (0.182 mL) to obtain a yellowish oil as the product (42% yield, A/B = 98:2). Collected data are in accordance with those reported in literature.[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.35 (m, 3H), 7.32 – 7.30 (m, 2H), 7.23 (d, *J* = 8.6 Hz, 2H), 6.89 (d, *J* = 8.6 Hz, 2H), 5.47 (pt, *J* = 8.2 Hz, 1H), 4.49 (d, *J* = 14.7 Hz, 1H), 4.37 (d, *J* = 14.7 Hz, 1H), 3.82 (s, 3H), 3.76 (pt, *J* = 8.8 Hz, 1H), 3.30 ppm (dd, *J* = 8.7, 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.79, 129.94, 129.23, 129.15, 128.03, 125.89, 114.60, 74.87, 55.66, 51.79, 48.20 ppm. LR MS (ESI) *m/z* calcd. for ($C_{17}H_{17}NO_3$): 283.12, found 306.39 $[M+Na]^+$.

Synthesis of 3-(3-methoxybenzyl)-5-phenyloxazolidin-2-one (22)



Method D of the general catalytic procedure was followed by using 1-(3-methoxybenzyl)-2-phenyl aziridine as the reagent (0.182 mL) to obtain a yellowish oil as the product (55% yield, A/B = 93:7). Collected data are in accordance with those reported in literature.[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 7H), 7.00 – 6.85 (m, 2H), 5.48 – 5.41 (m, 1H), 4.51 (d, *J* = 14.7 Hz, 2H), 3.84 – 3.80 (m, 4H), 3.37 – 3.31 (m, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.07, 157.95,

138.66, 137.23, 130.20, 129.43, 128.82, 125.60, 120.80, 113.64, 110.48, 74.50, 55.36, 51.98, 43.11 ppm. LR MS (ESI) *m/z* calcd. for ($C_{17}H_{17}NO_3$): 283.12, found 306.39 $[M+Na]^+$.

6. Recycling test

In a 2.0 mL glass liner equipped with a screw cap and glass wool, 3.0 cm^2 of **3@CC** (0.1% mol of anchored hematin, 1.0 x 10^{-6} mol) and 1-butyl-2-phenyl aziridine (0.194 mL**,** 1.0 x 10^{-3} mol) were suspended in 0.6 mL of DCE. The vessel was transferred into a stainless-steel autoclave and 1.2 MPa of CO_2 were charged at room temperature. The autoclave was placed in a preheated oil bath at 125°C, stirred for 12 hours and then quenched in an ice bath and slowly vented. At the end of the reaction **3@CC** was collected in a filter and washed three times with DCE (3 x 1.0 mL). The recovered heterogenous catalyst was reused by repeating the above-described procedure for three consecutive times. All the organic phases were combined and dried under vacuum. The resulting crude was analysed by ^1H NMR spectroscopy by using mesitylene as the internal standard. The desired product (**14**) was obtained in 70% of global yield and A/B = 94:6.

7. Characterization of 3@CC after the catalytic synthesis of 14a

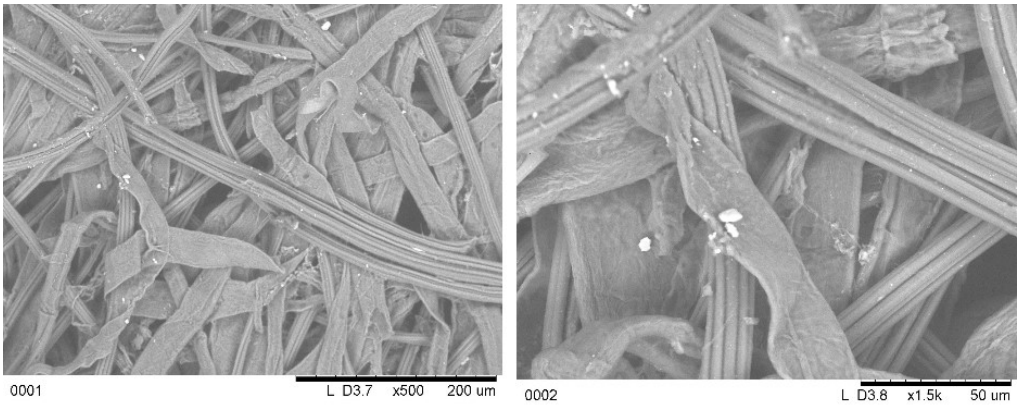


Figure S9: SEM images of **3@CC** after the catalytic synthesis of **14a**.

entry	sample V (L)	mg Fe	sample weight	% Fe
1	0,012	0,0132598	12	0,1104962
2	0,012	0,0193589	15,6	0,1240958

Figure S10: ICP-OES analyses of **3@CC** (entry 1) and **3@CC** after the catalytic synthesis of **14a** (entry 2).

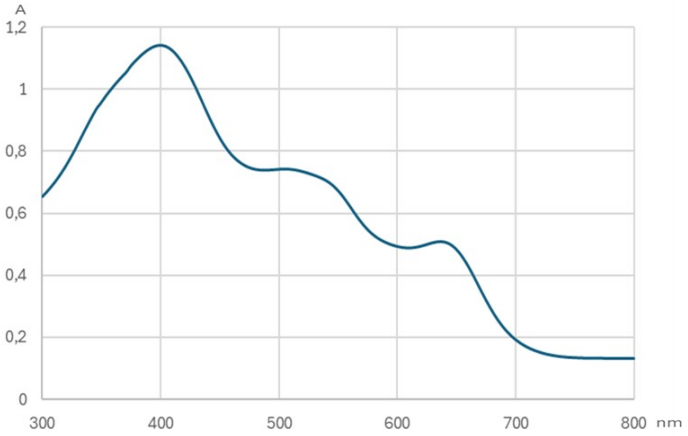


Figure S11: UV/visible spectrum of **3@CC** after the catalytic synthesis of **14a**.

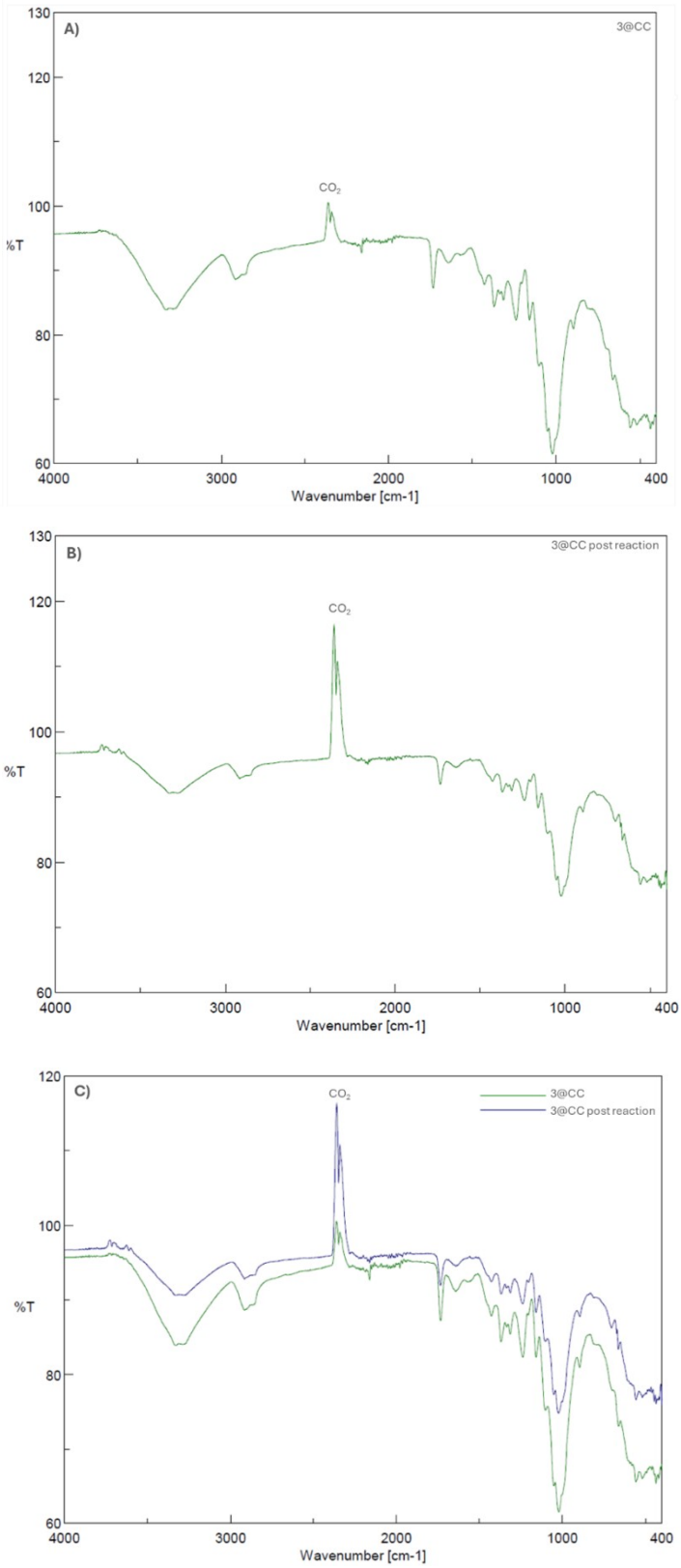


Figure S12: ATR spectra of **3@CC** (catalytic loading = 0.054 mg/cm^2) (A), **3@CC** after the catalytic synthesis of **14a** (B) and superimposed spectrum of **3@CC** before and after the synthesis of **14a** (C).

8. UV-Visible studies on the aziridine/epoxide coordination

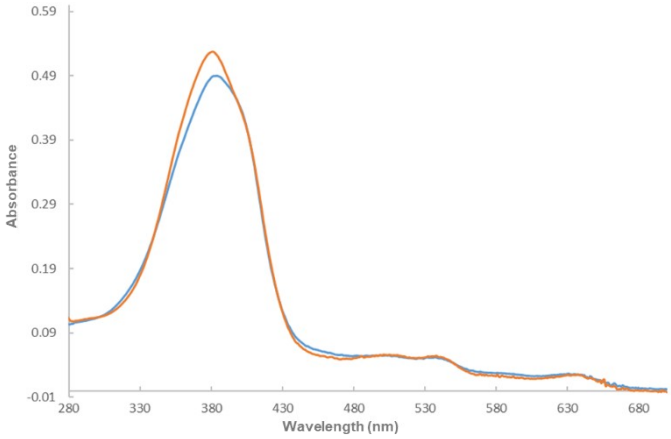


Figure S13: UV-Visible spectra (Sorét region) of **2** (blue line) and **2** + 1-butyl-2-phenyl aziridine (ratio = 1:100; orange line).

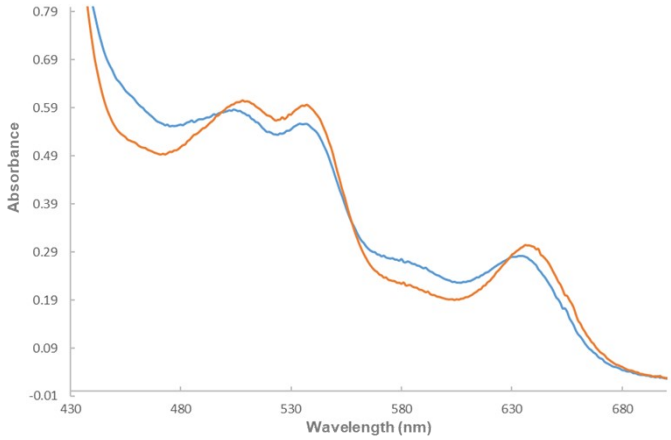


Figure S14: UV-Visible spectra (Q-bands region) of **2** (blue line) and **2** + 1-butyl-2-phenyl aziridine (ratio = 1:100; orange line).

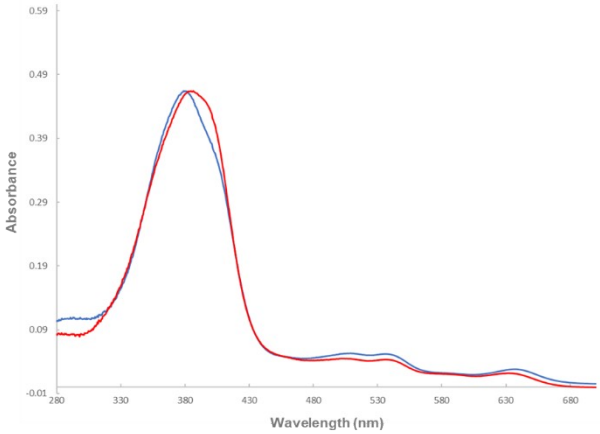


Figure S15: UV-Visible spectra (Sorét region) of **2** (blue line) and **2** + styrene oxide (ratio = 1:100; red line).

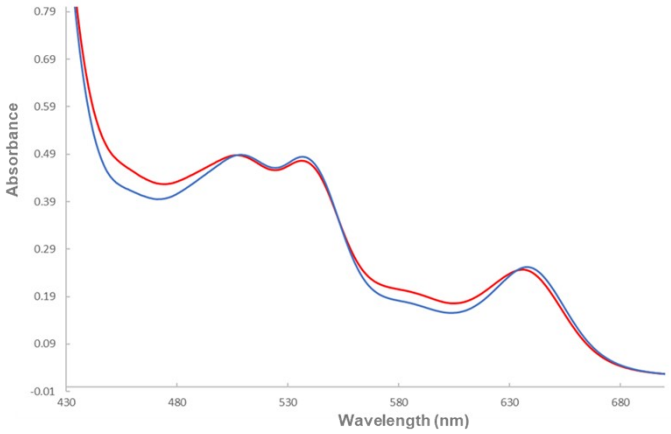
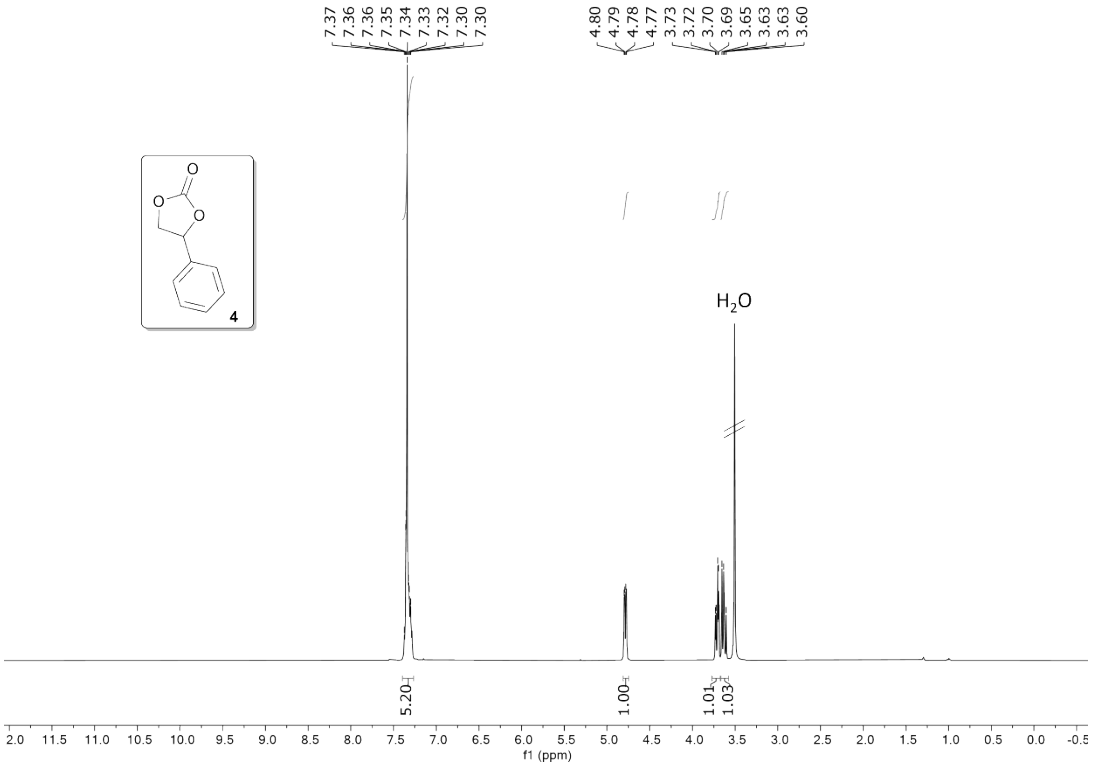


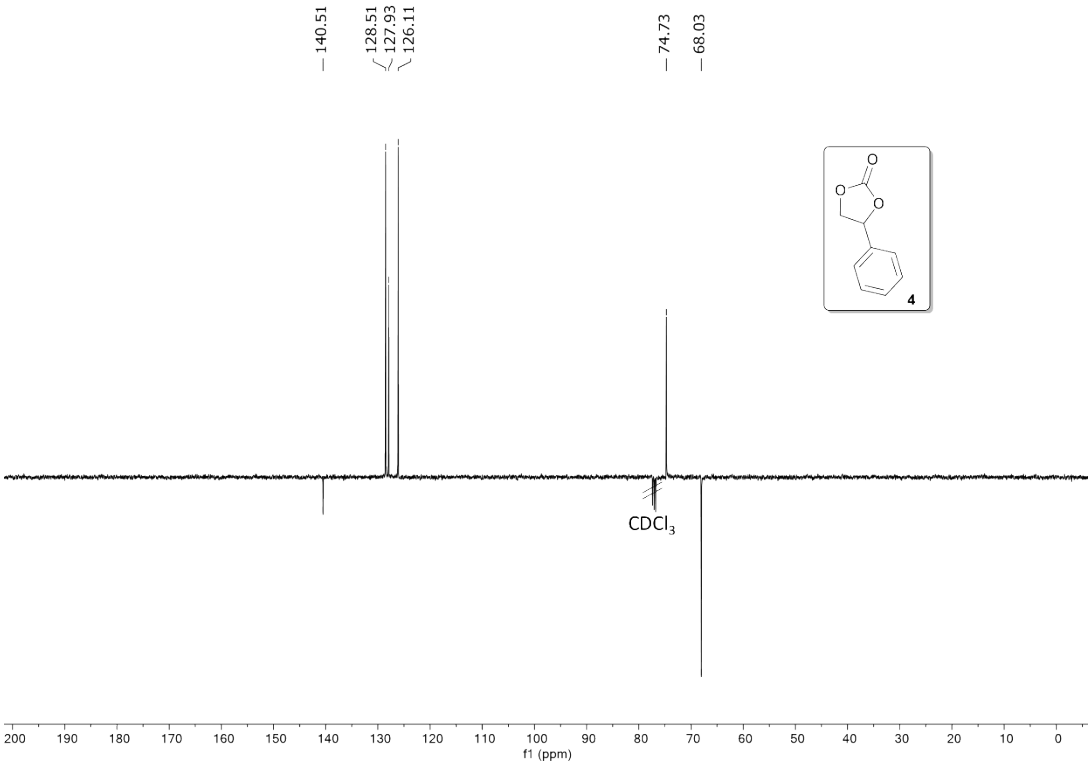
Figure S16: UV-Visible spectra (Q-bands region) of **2** (blue line) and **2** + styrene oxide (red line).

9. ^{1}H and ^{13}C NMR spectra

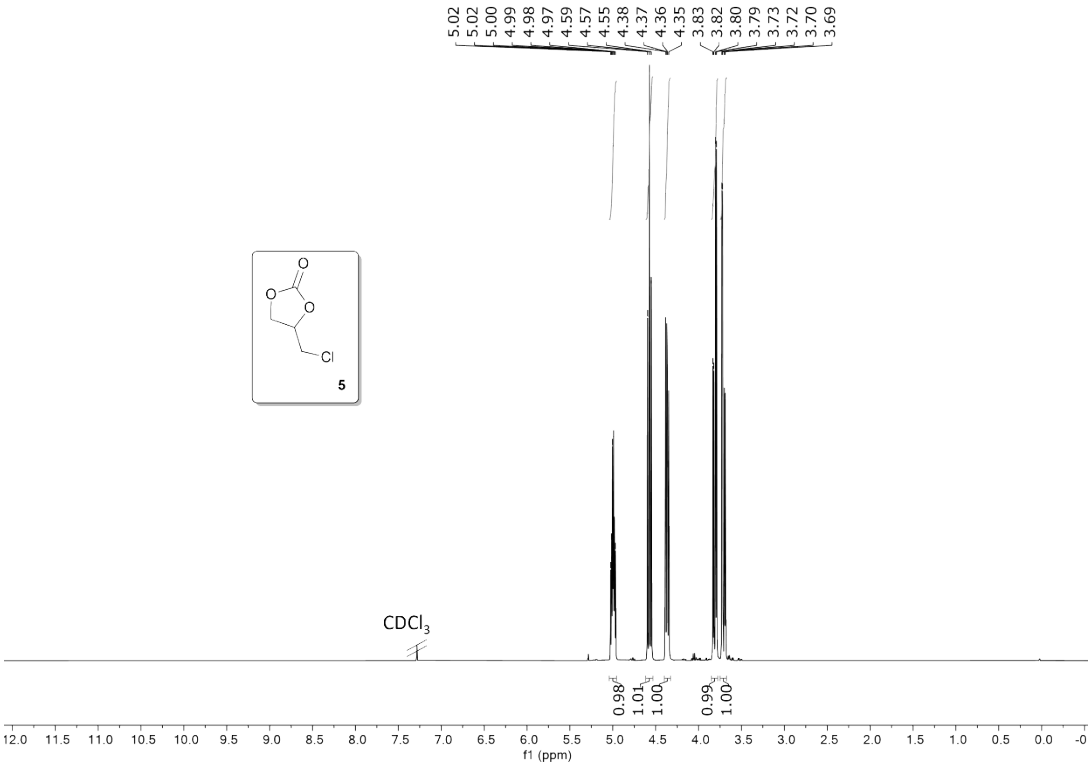
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 4



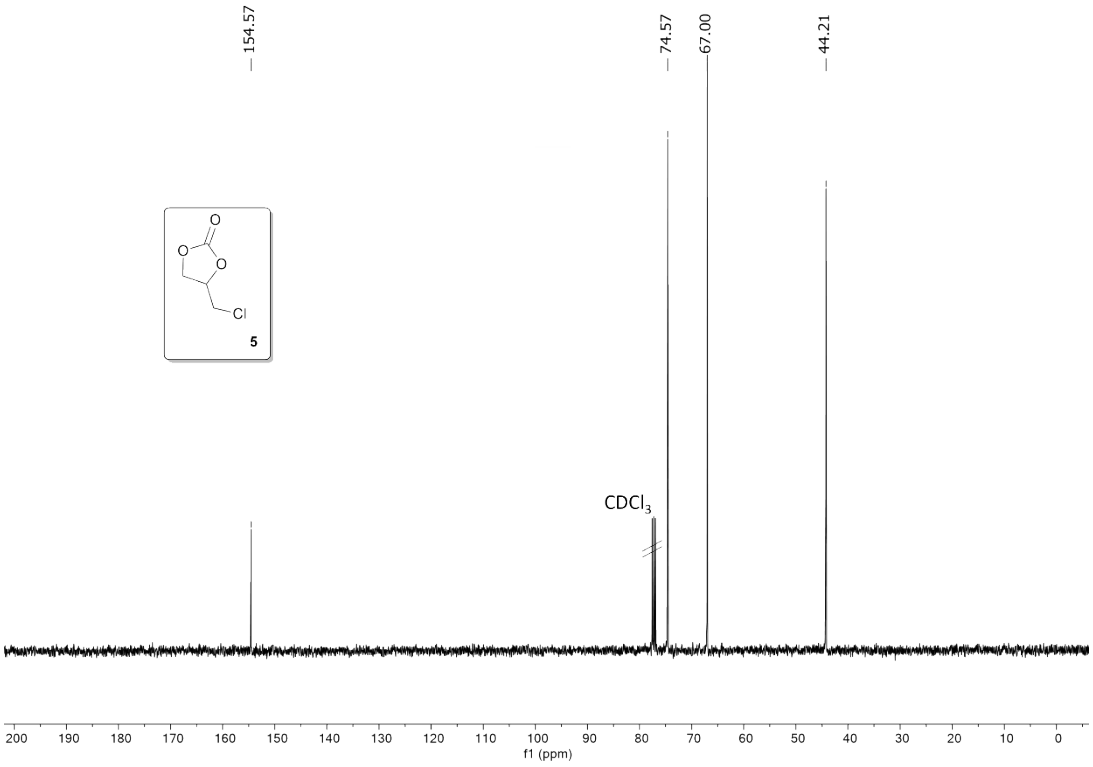
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 4



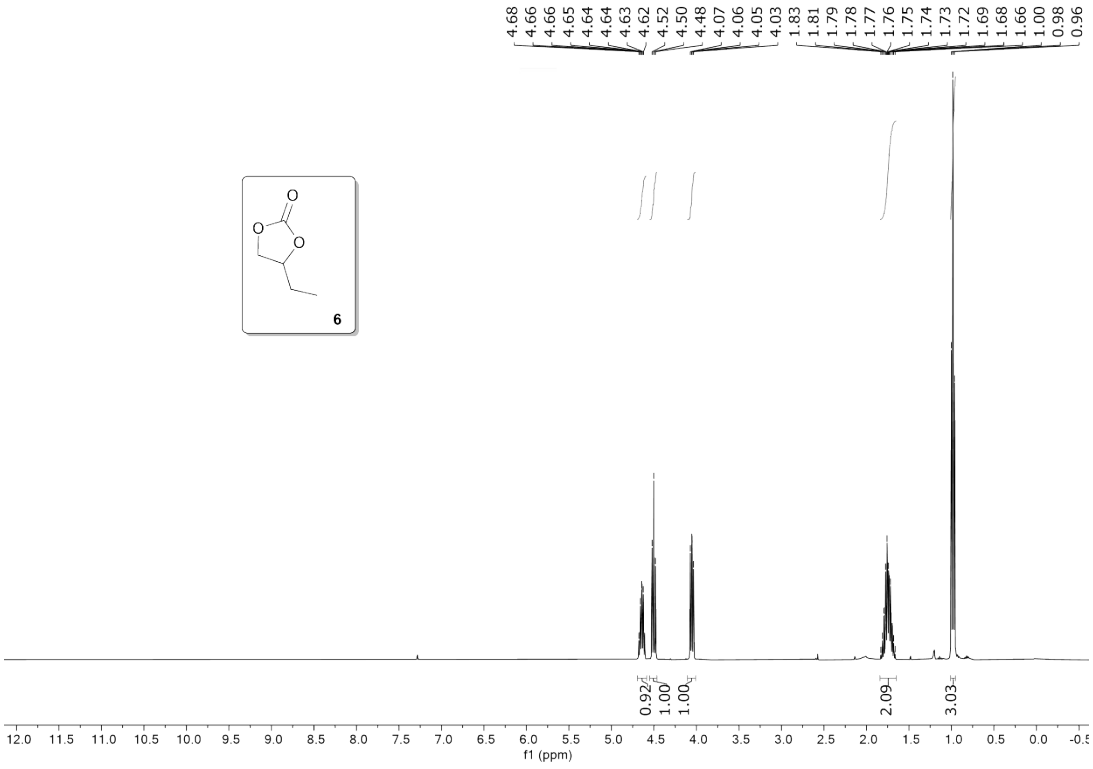
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 5



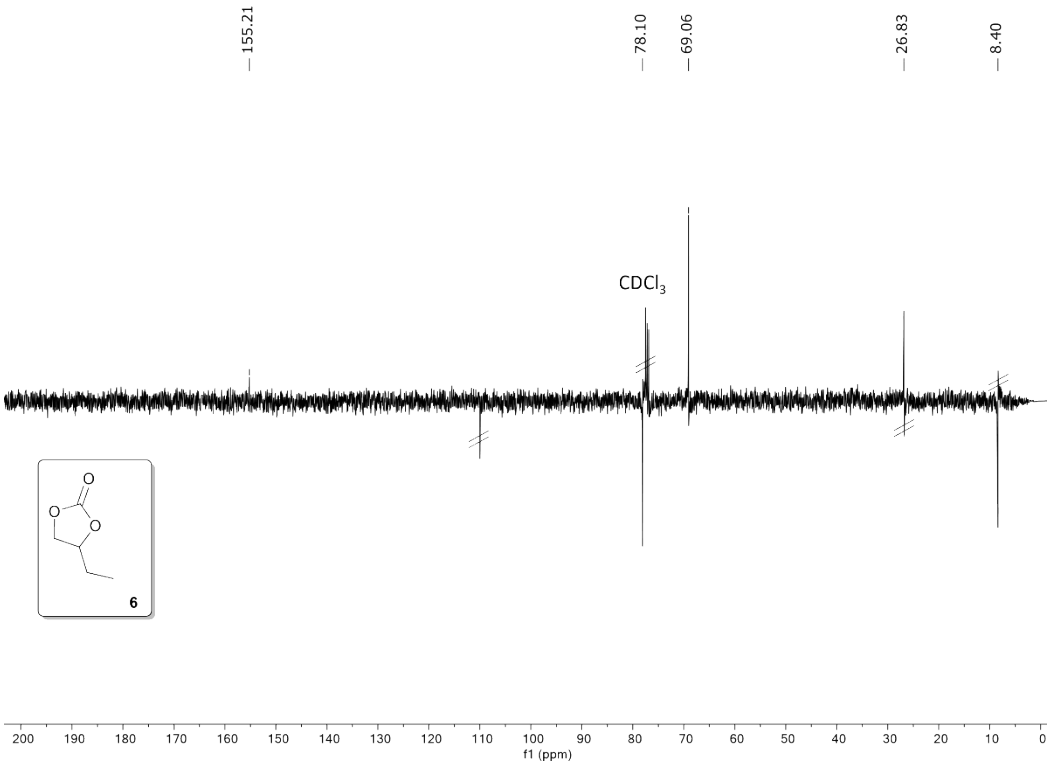
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 5



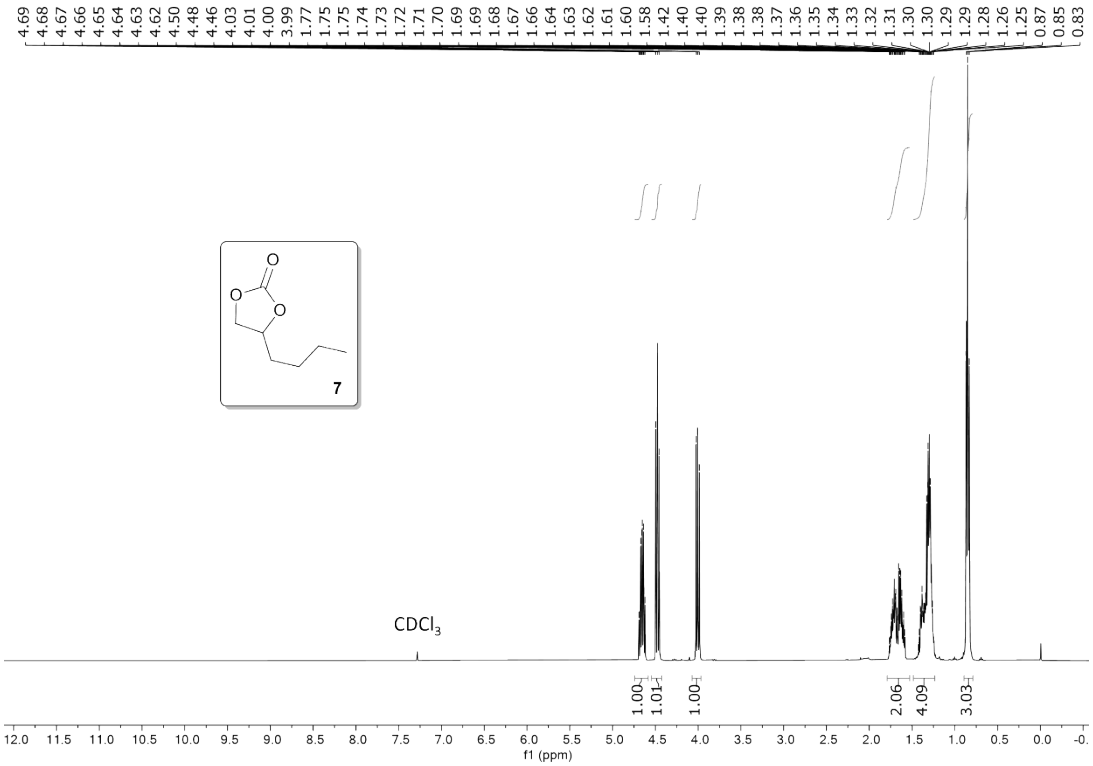
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 6



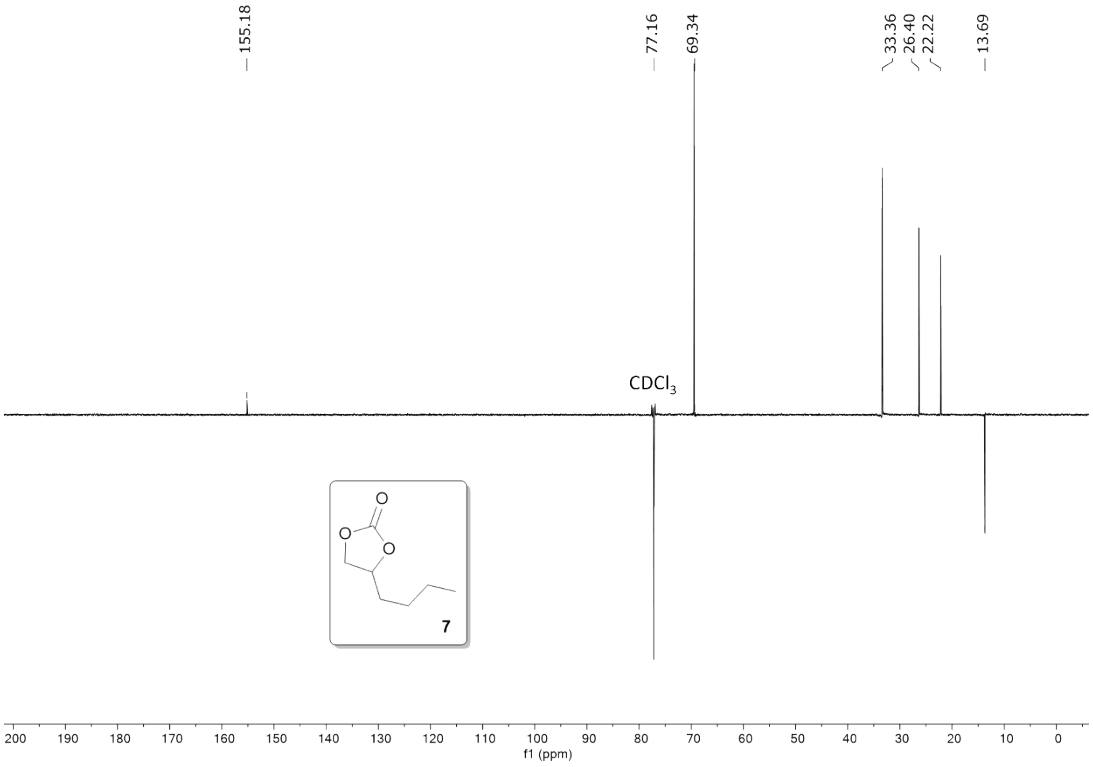
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 6



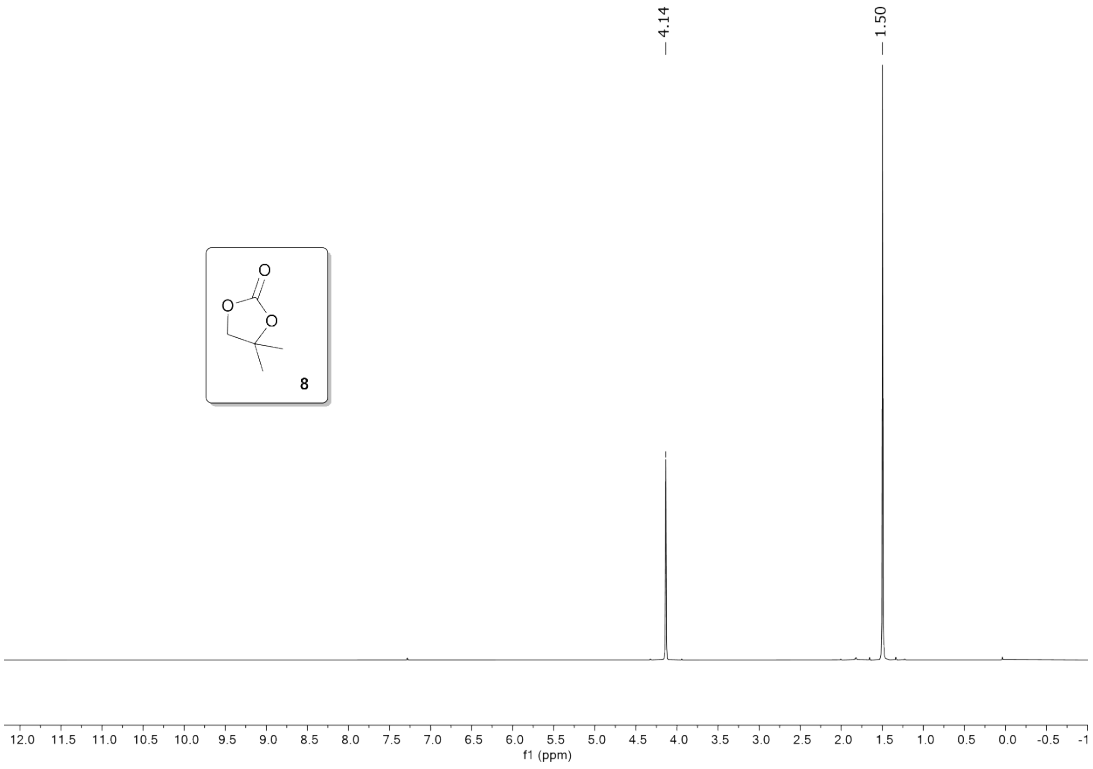
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 7



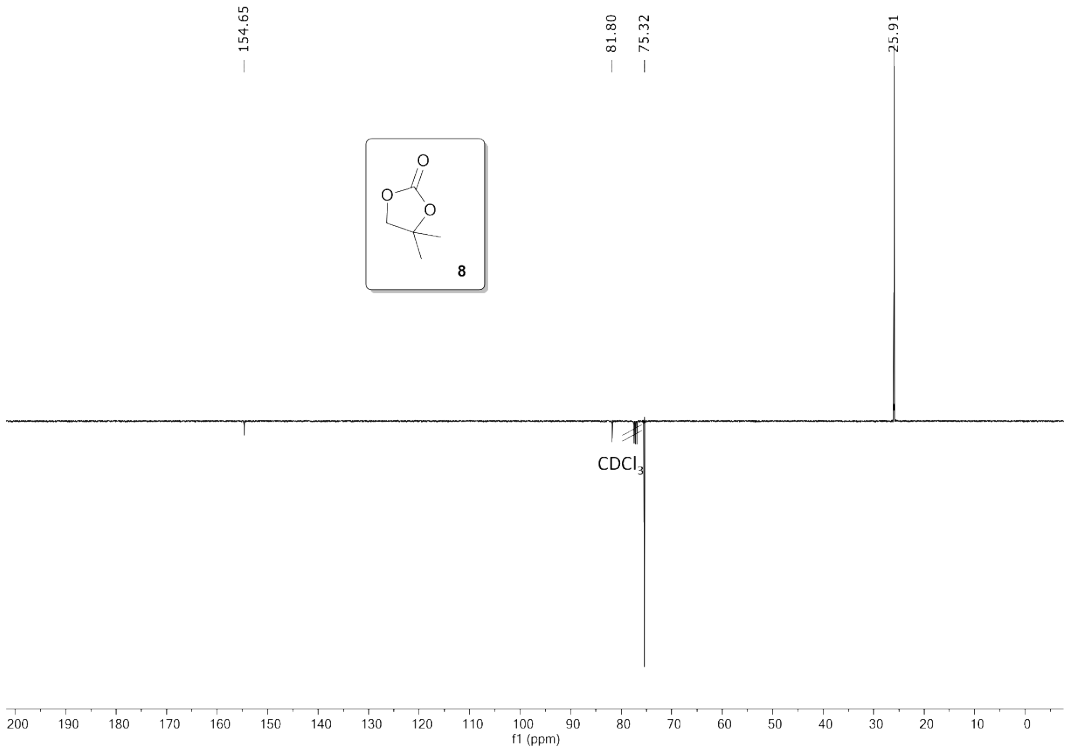
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 7



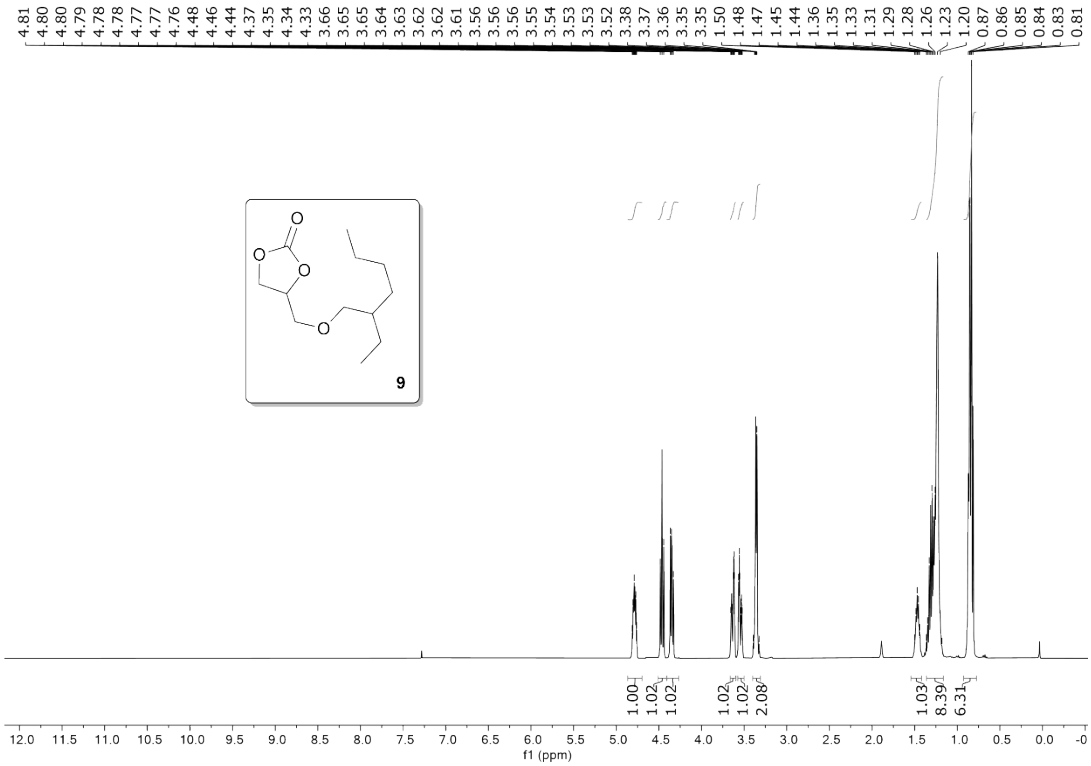
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 8



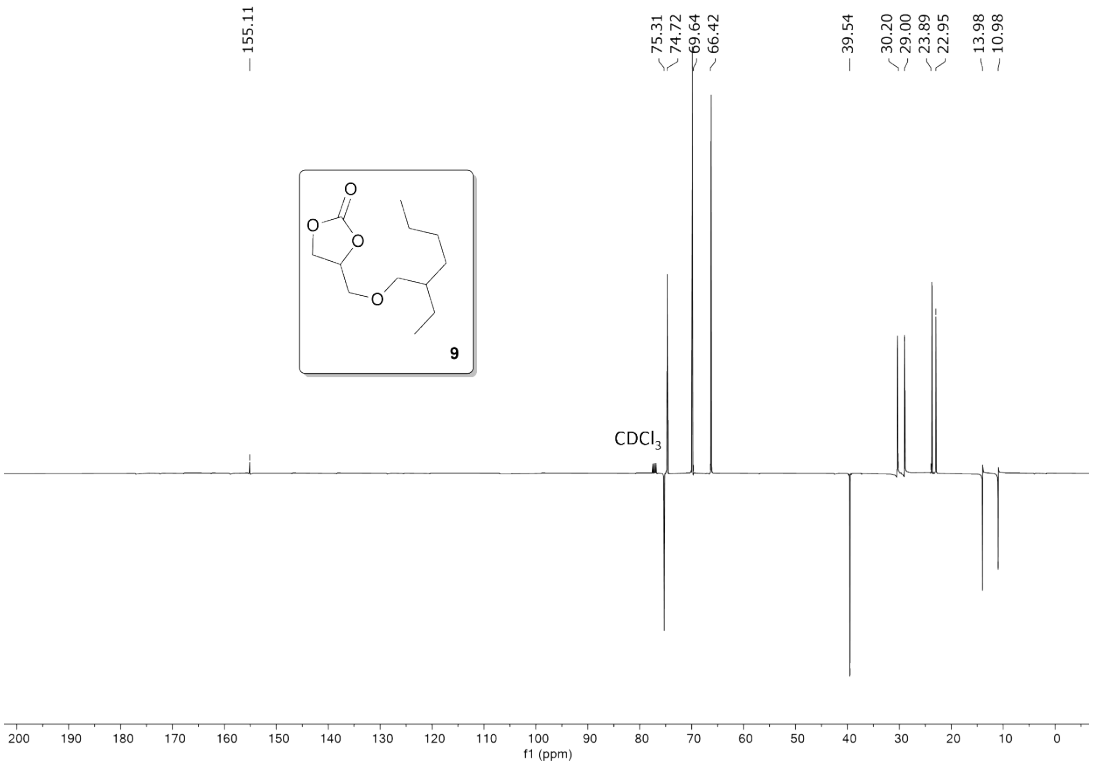
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 8



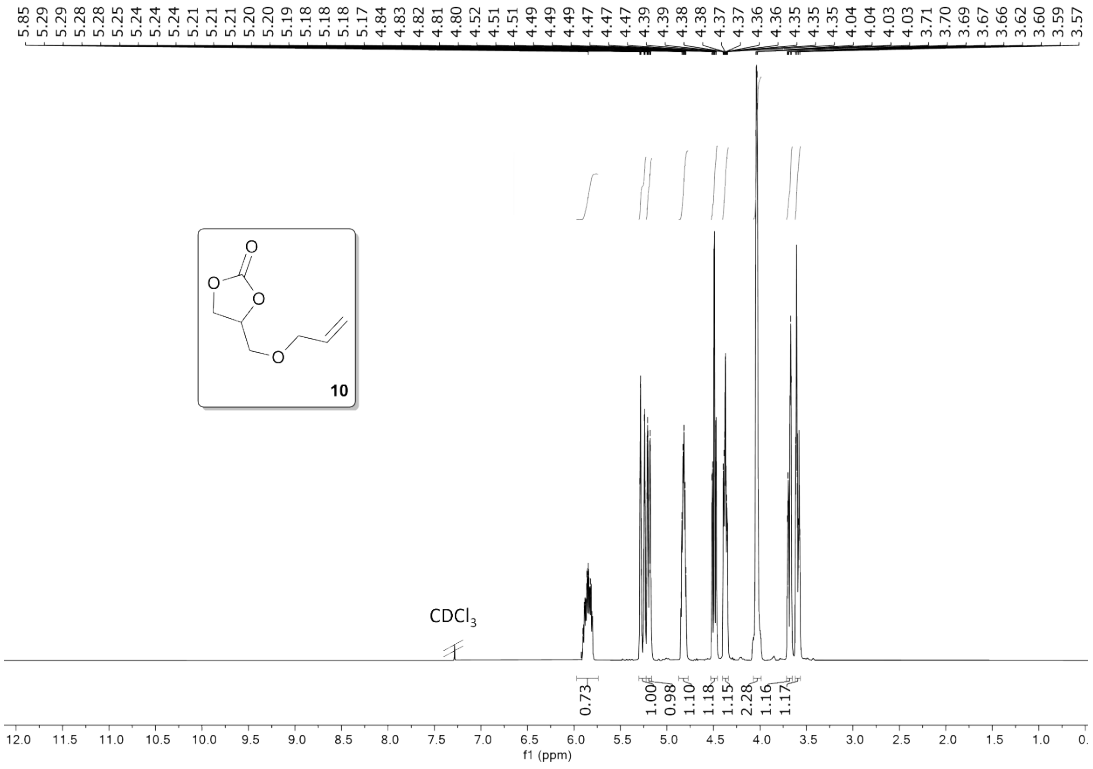
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 9



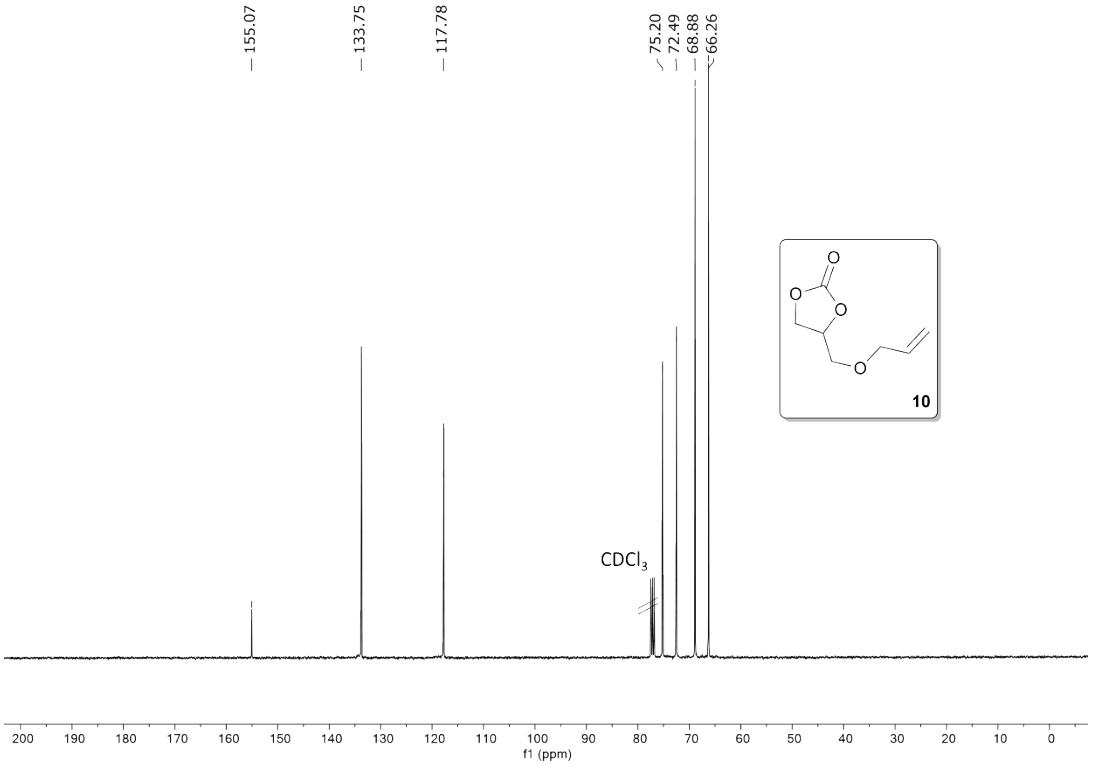
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 9



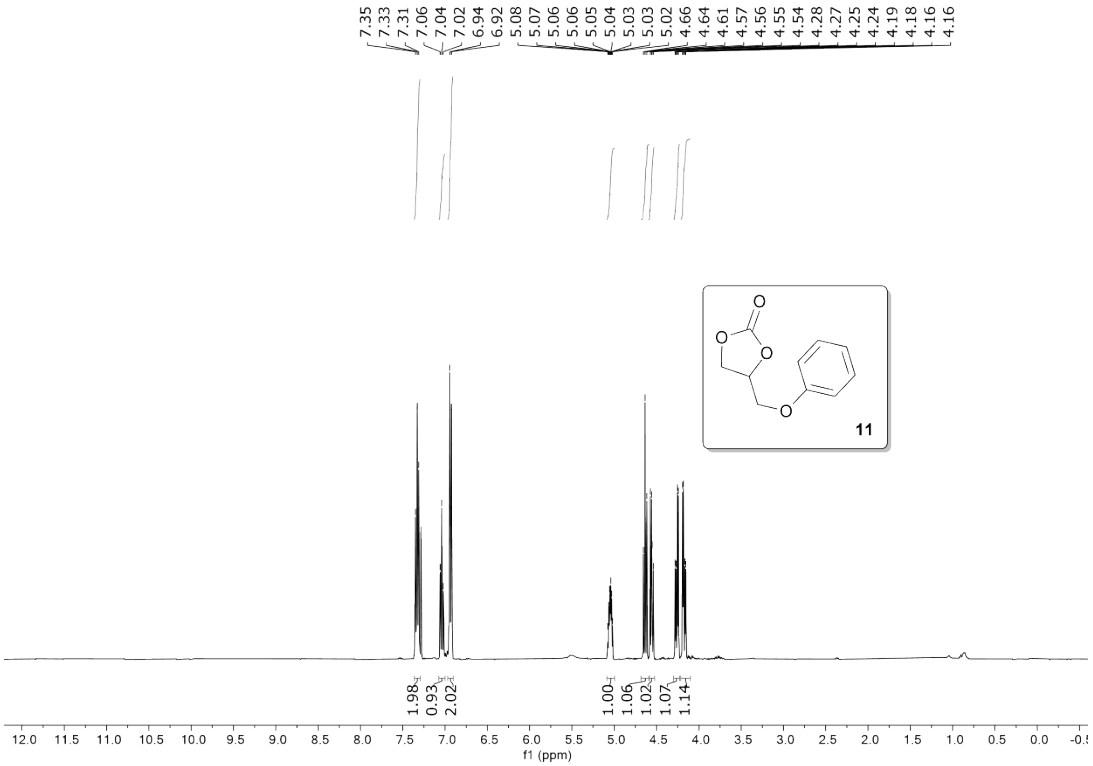
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 10



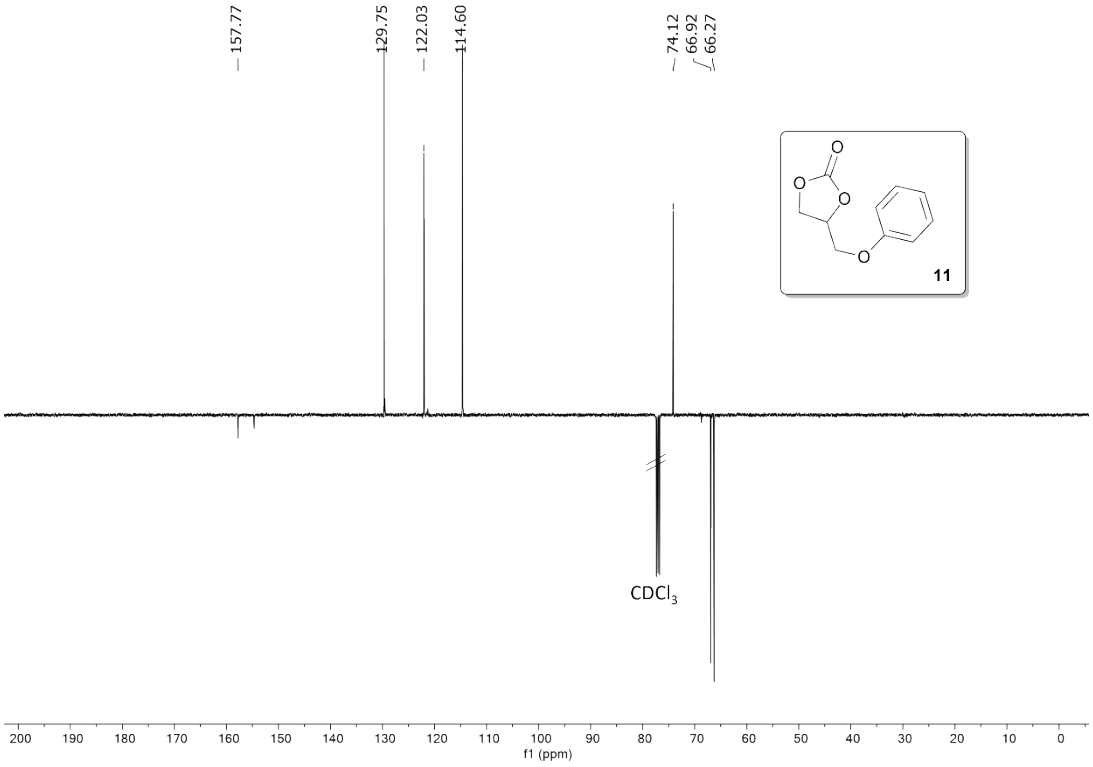
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 10



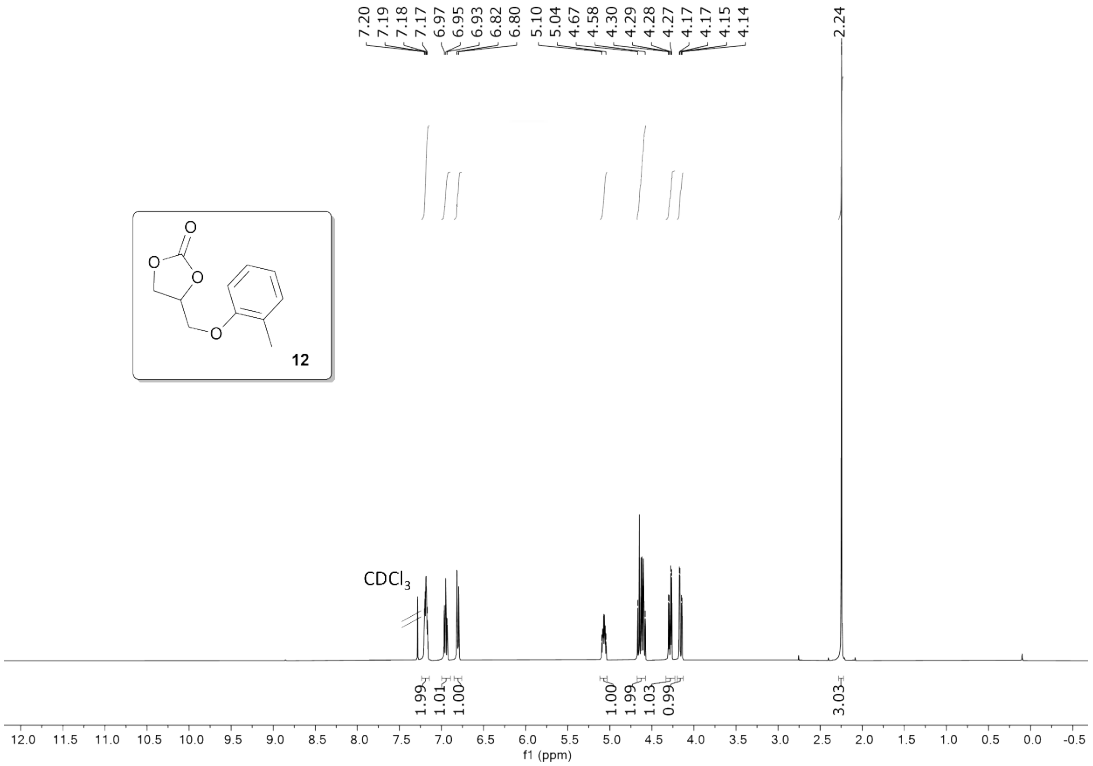
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 11



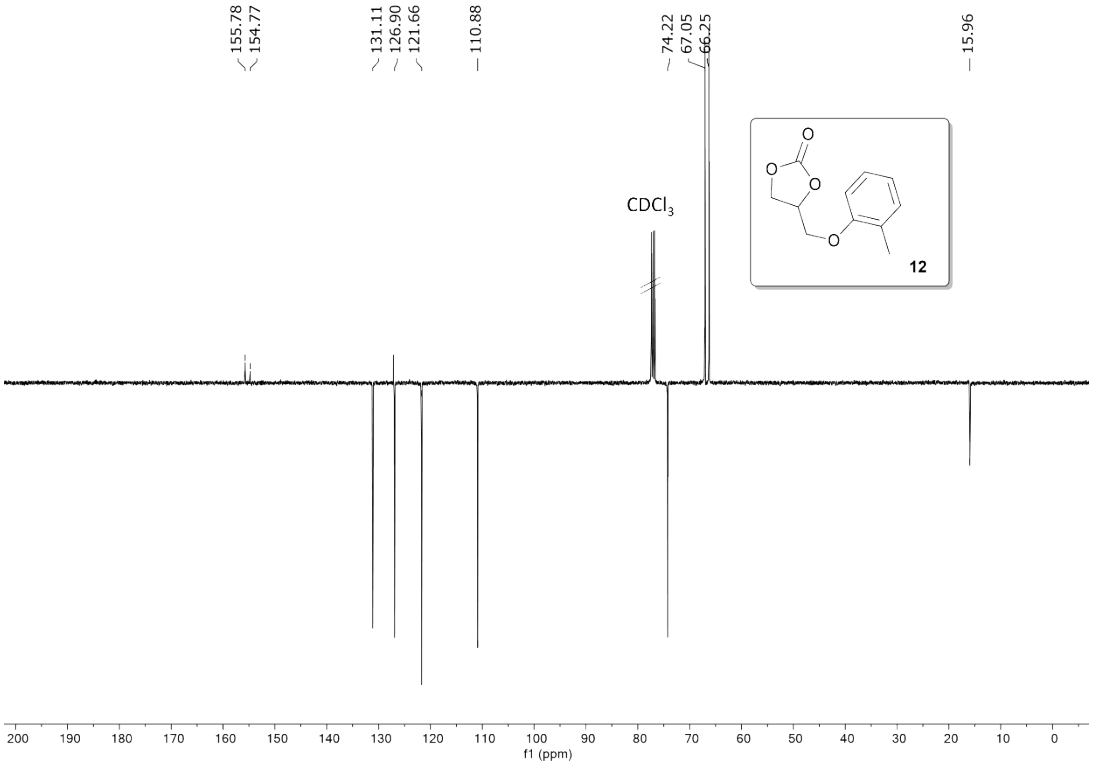
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 11



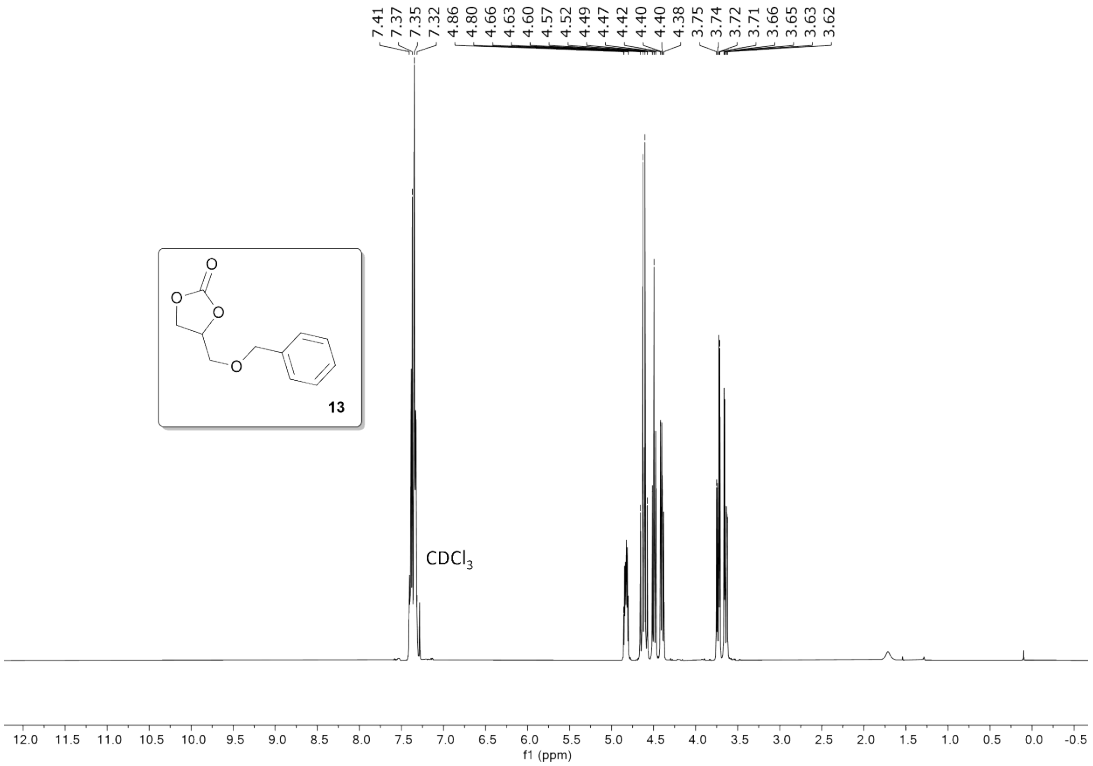
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 12



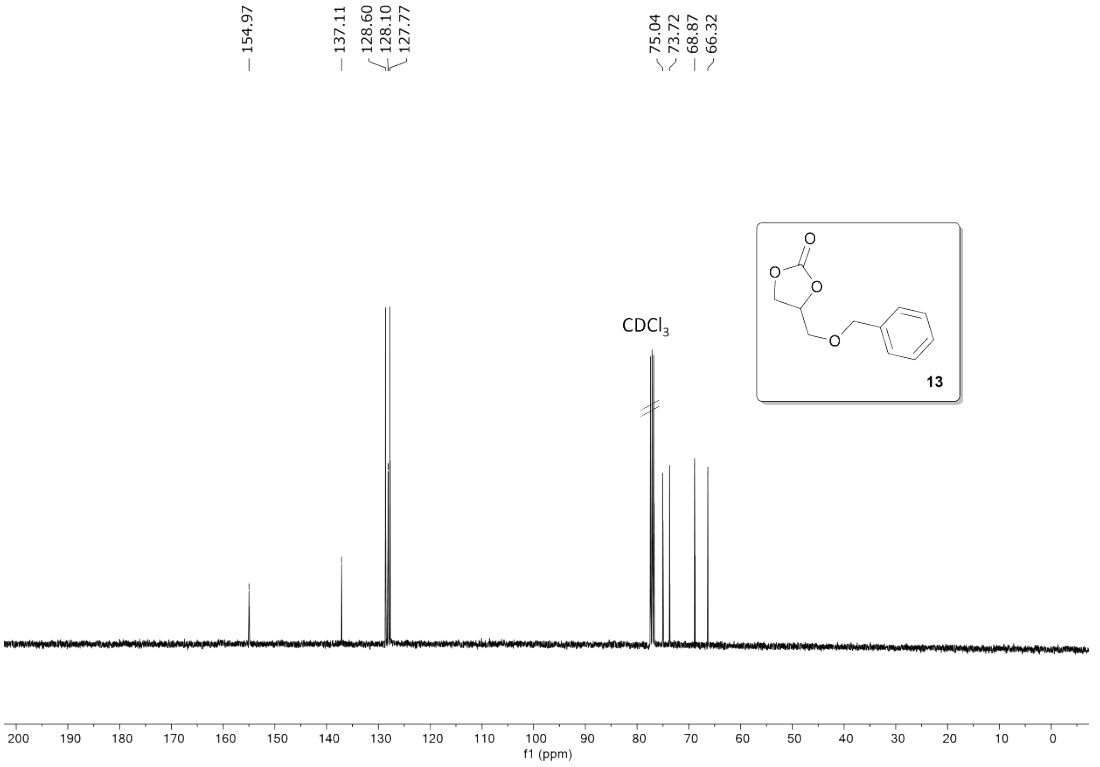
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 12



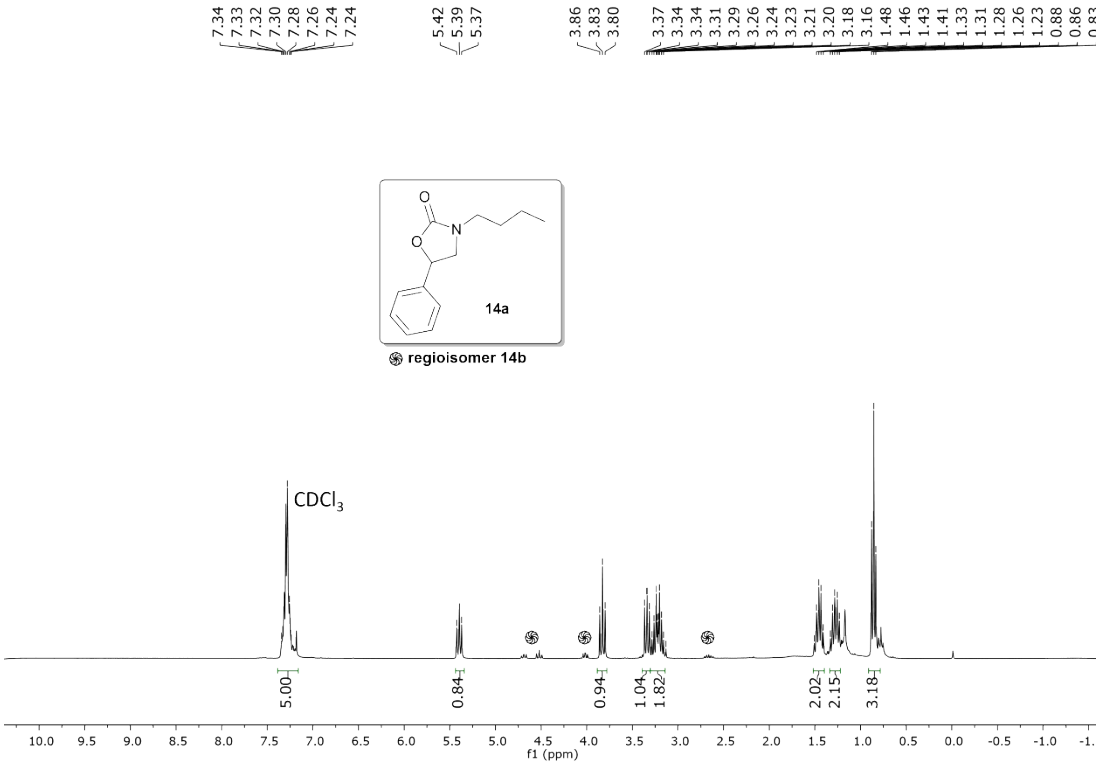
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 13



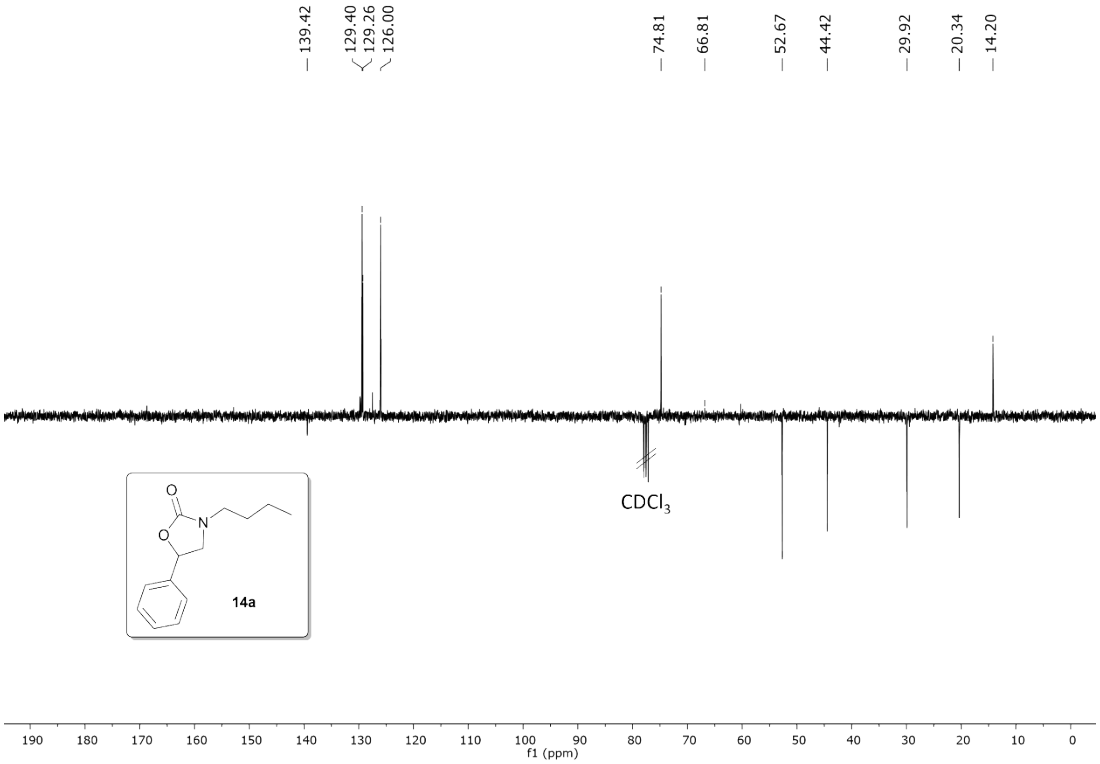
^{13}C NMR spectrum (300 MHz, $CDCl_3$, 298K) of 13



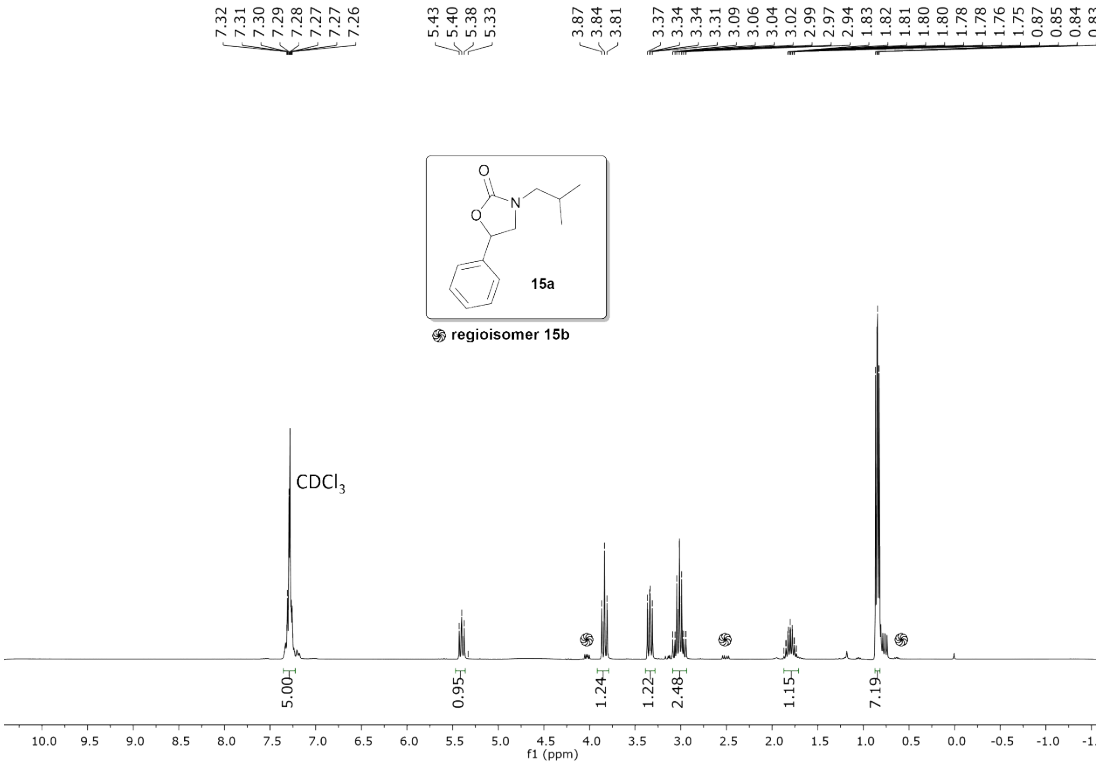
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 14



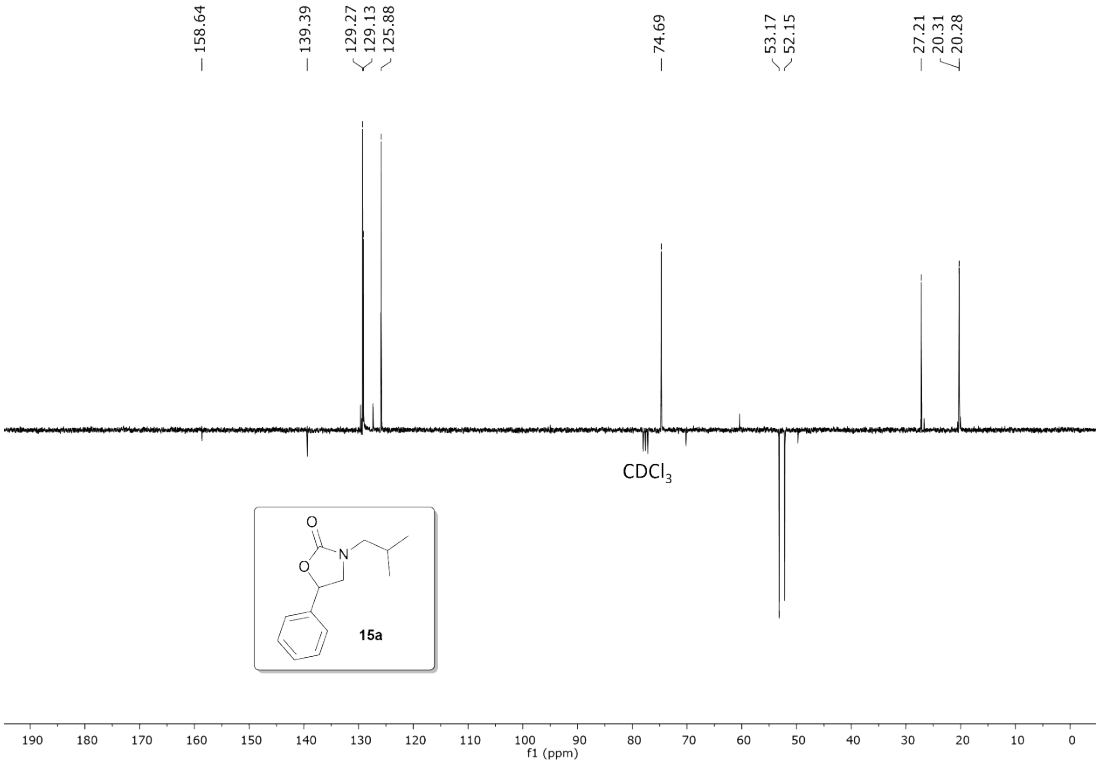
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 14



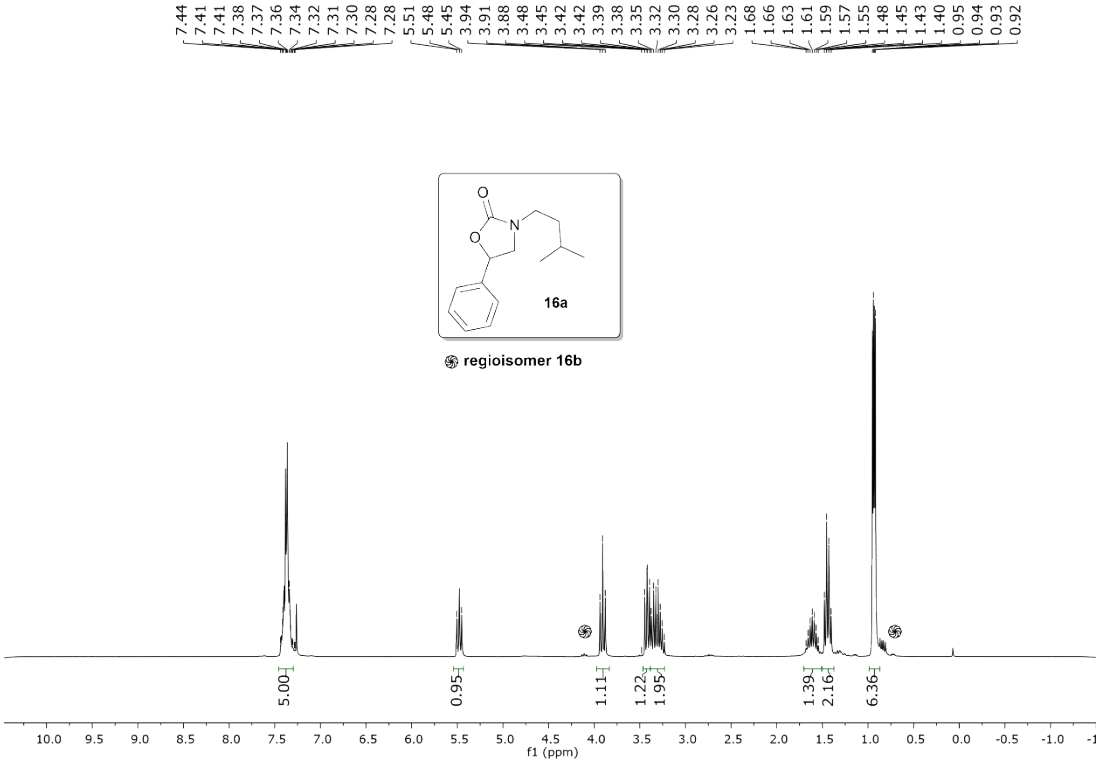
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 15



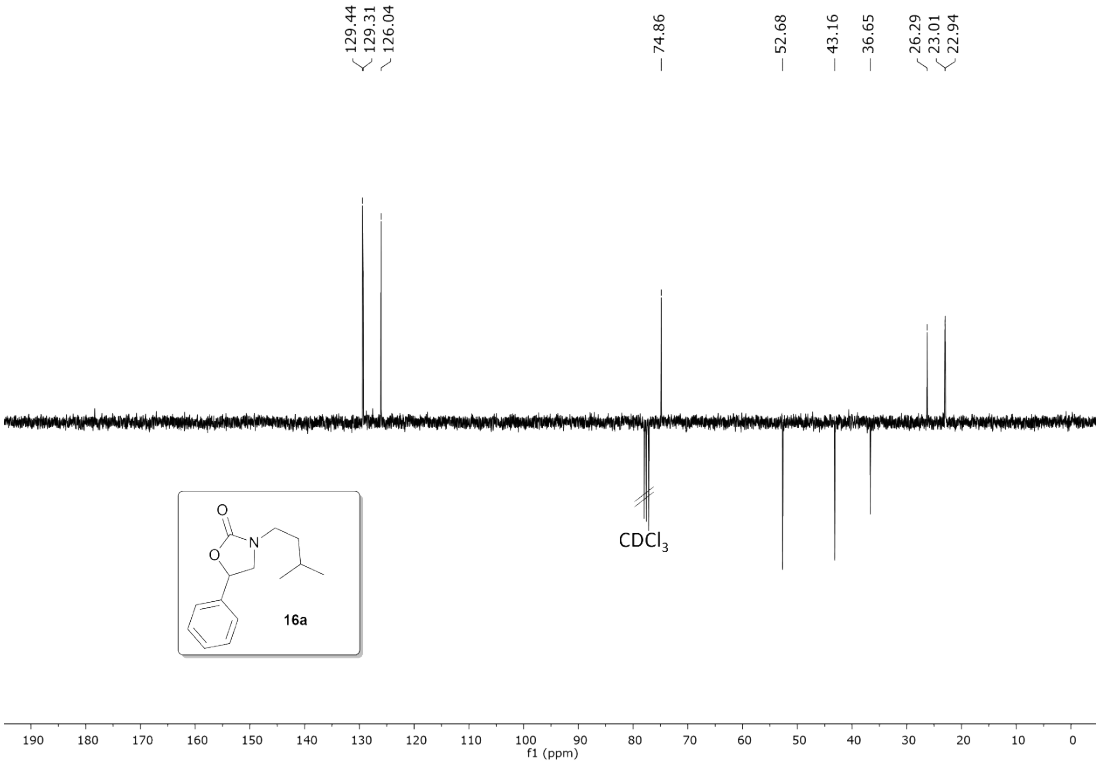
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 15



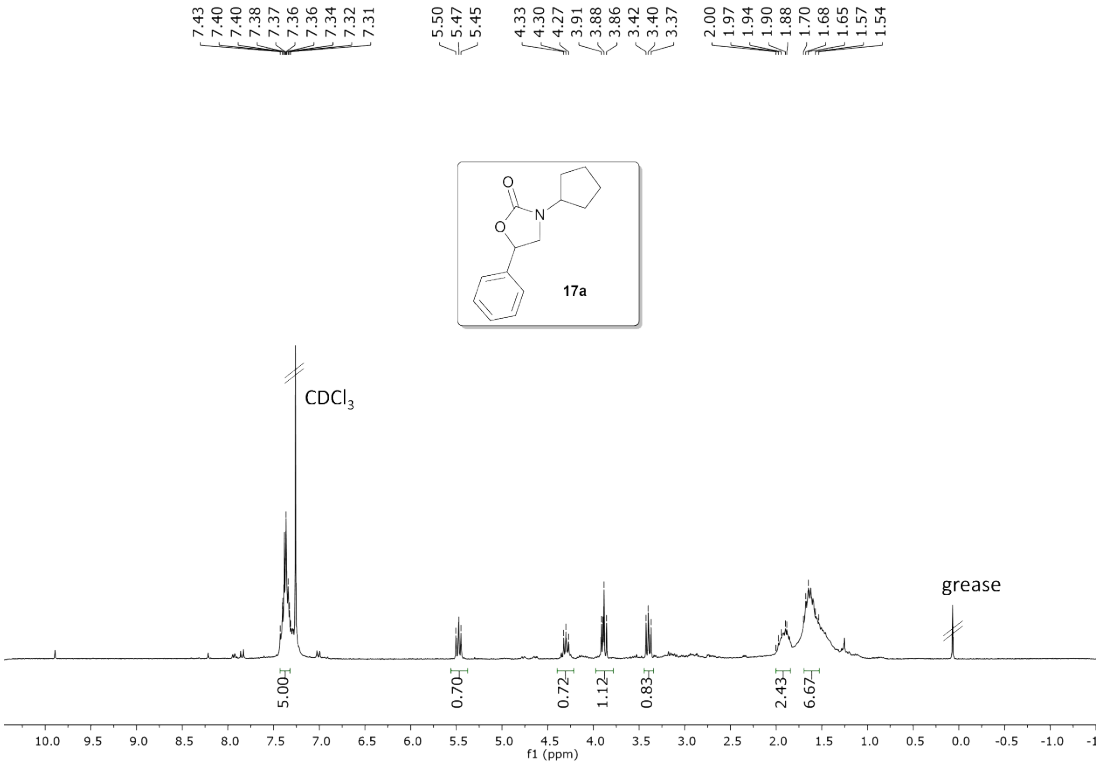
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 16



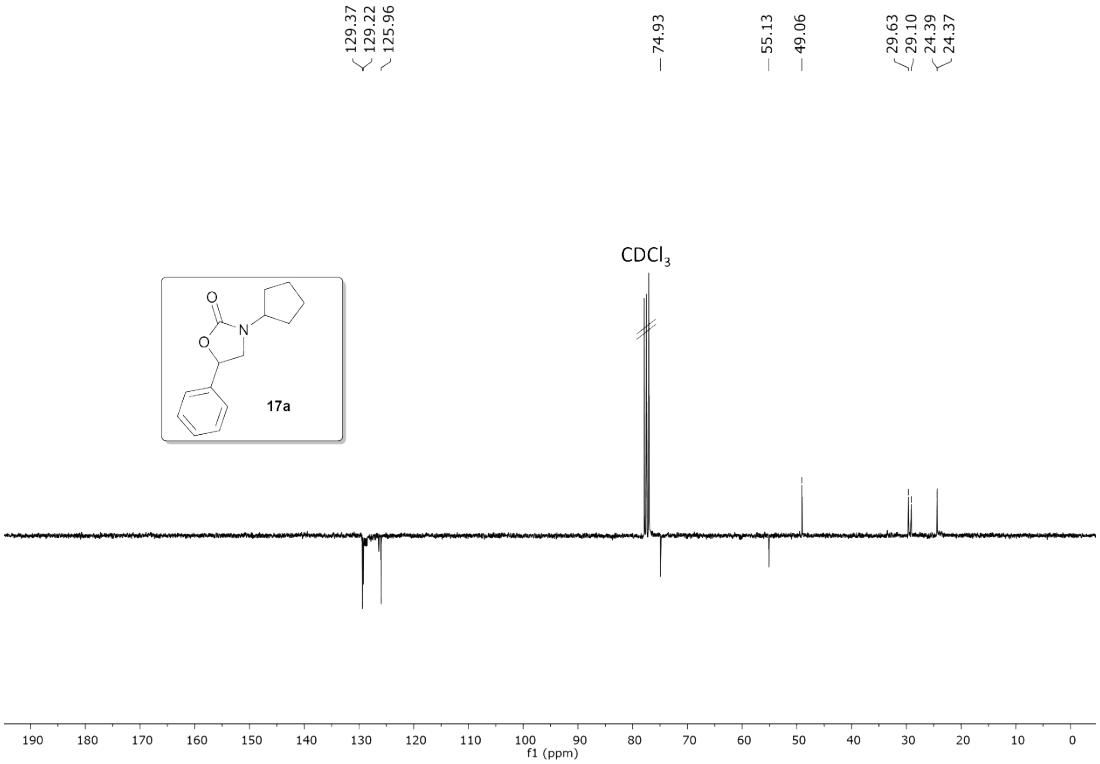
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 16



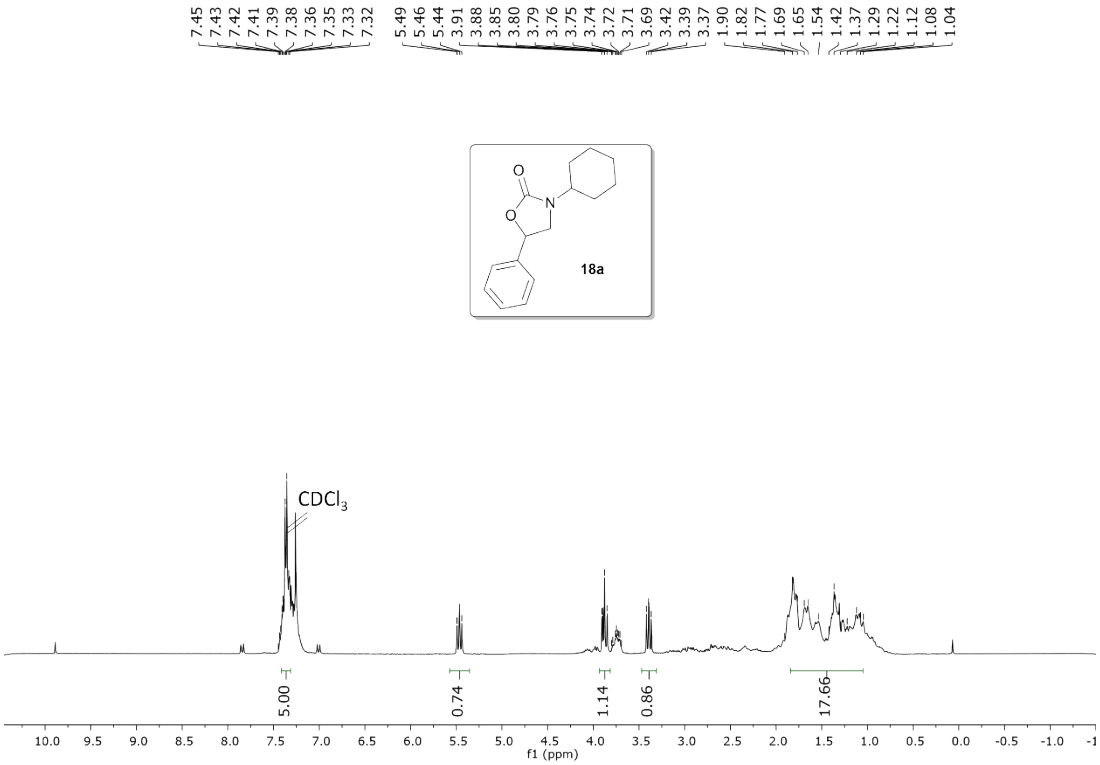
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 17



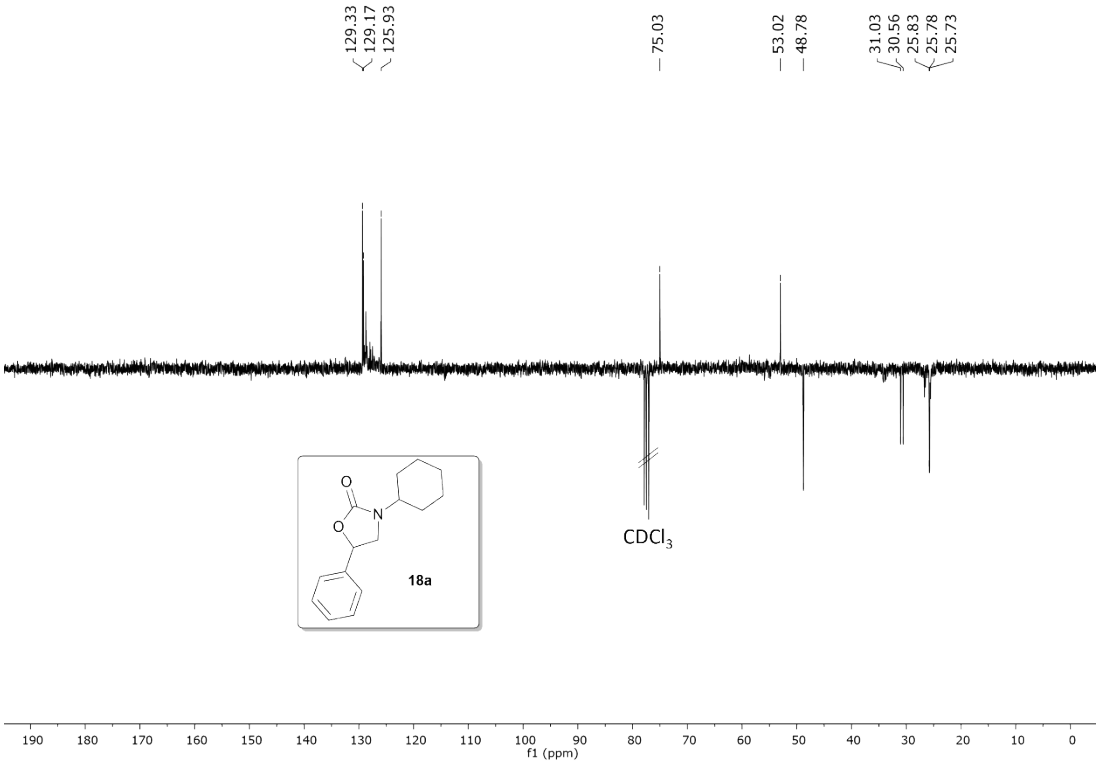
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 17



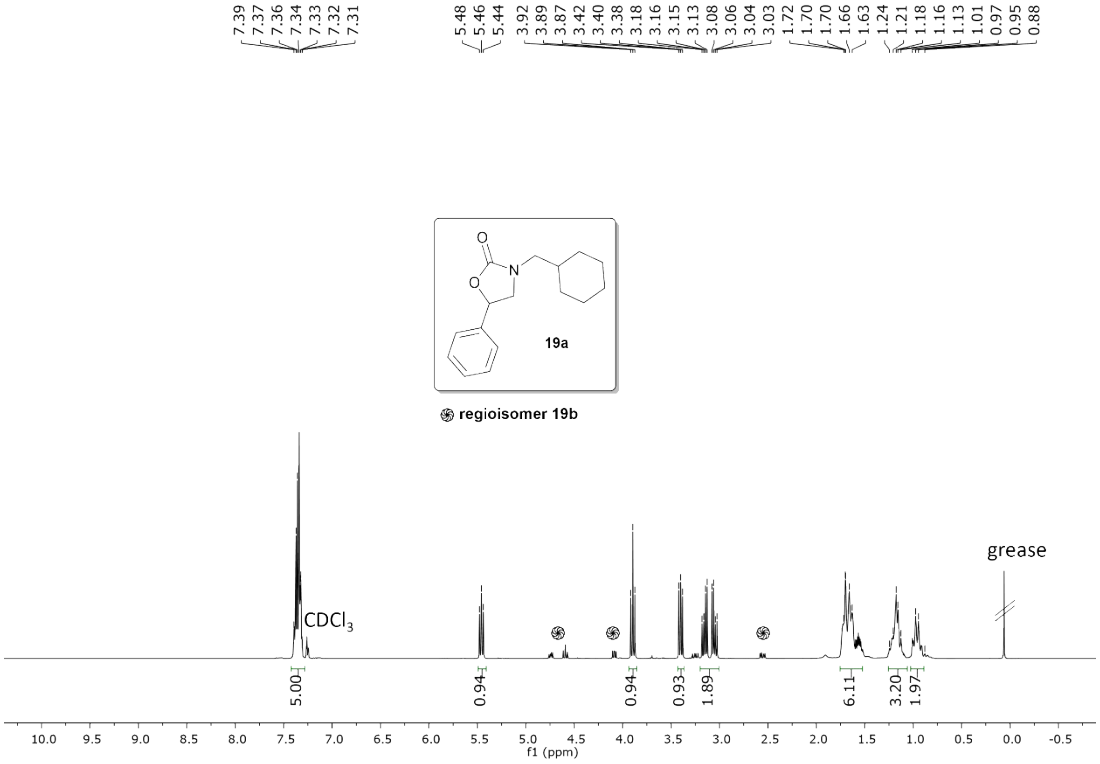
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 18



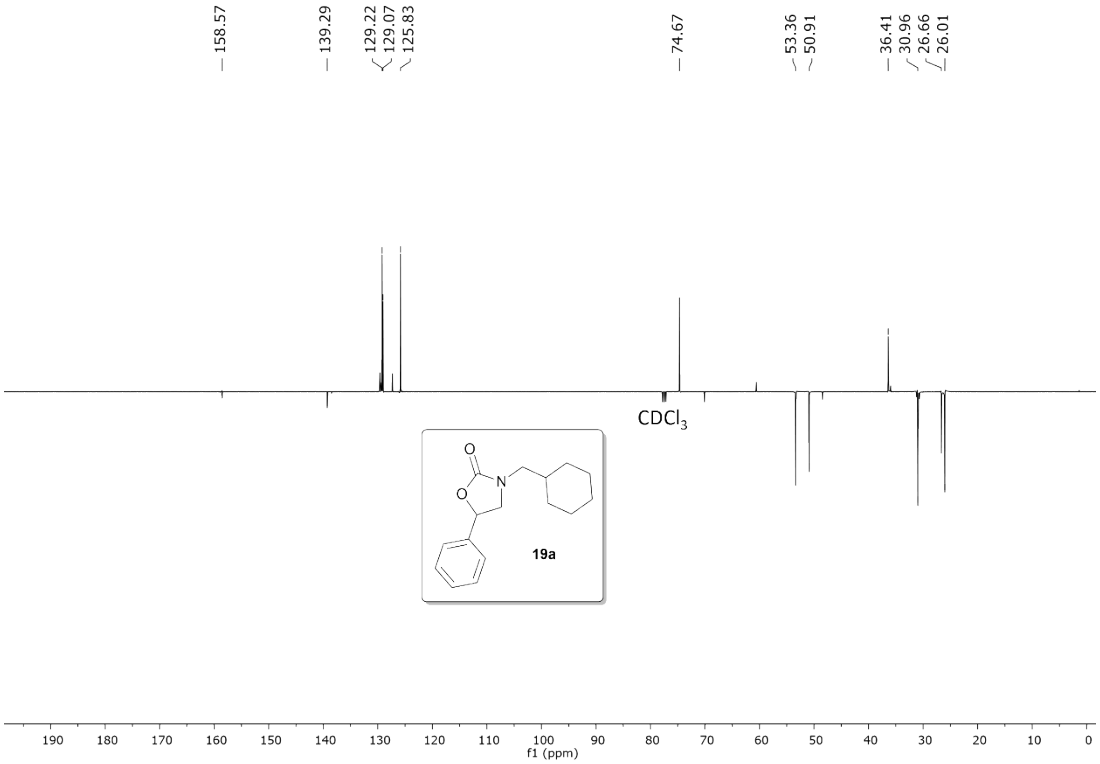
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 18



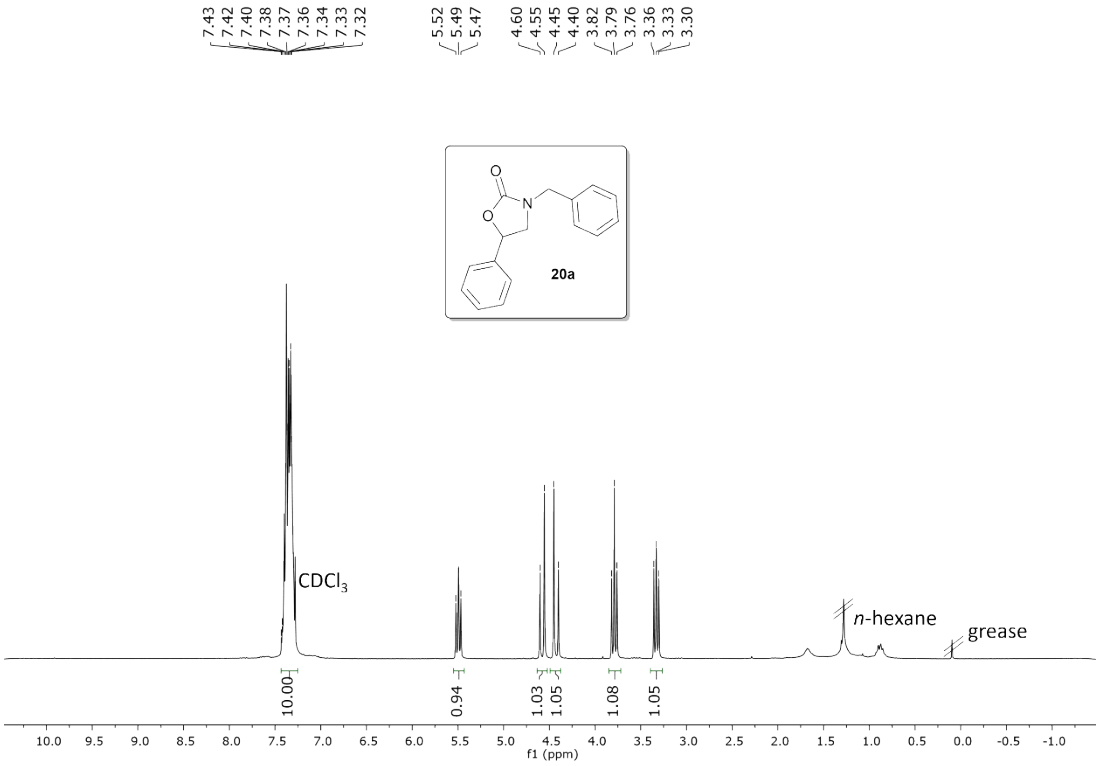
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 19



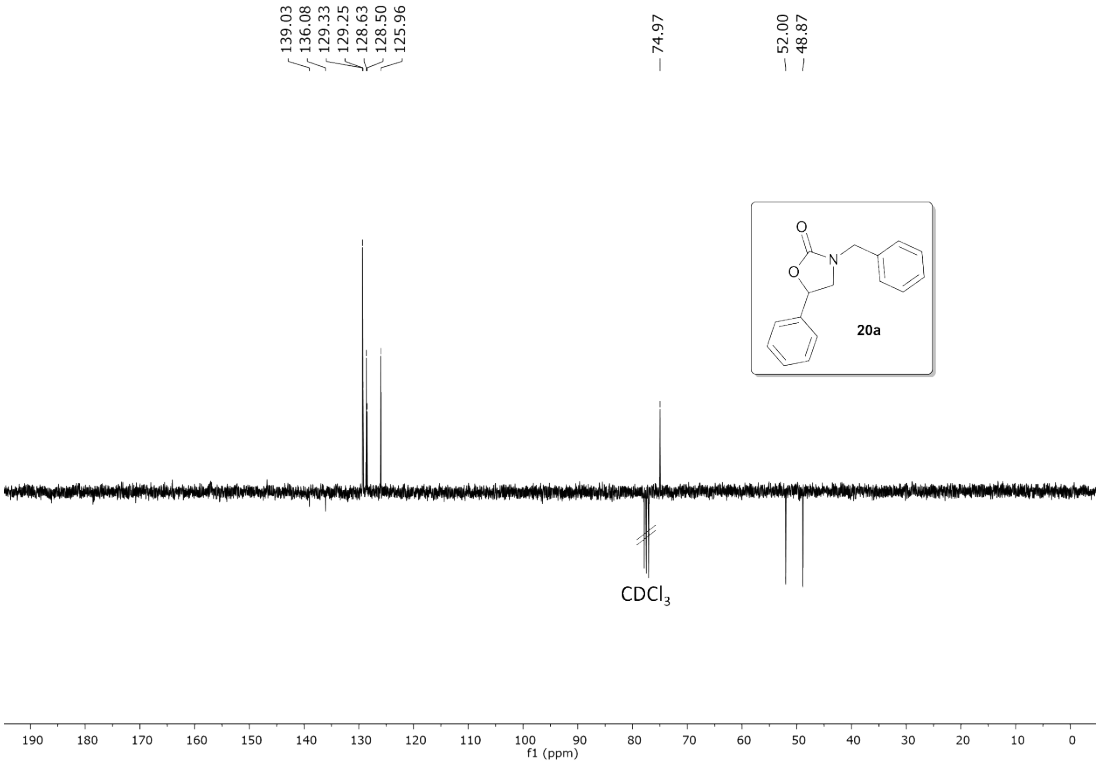
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 19



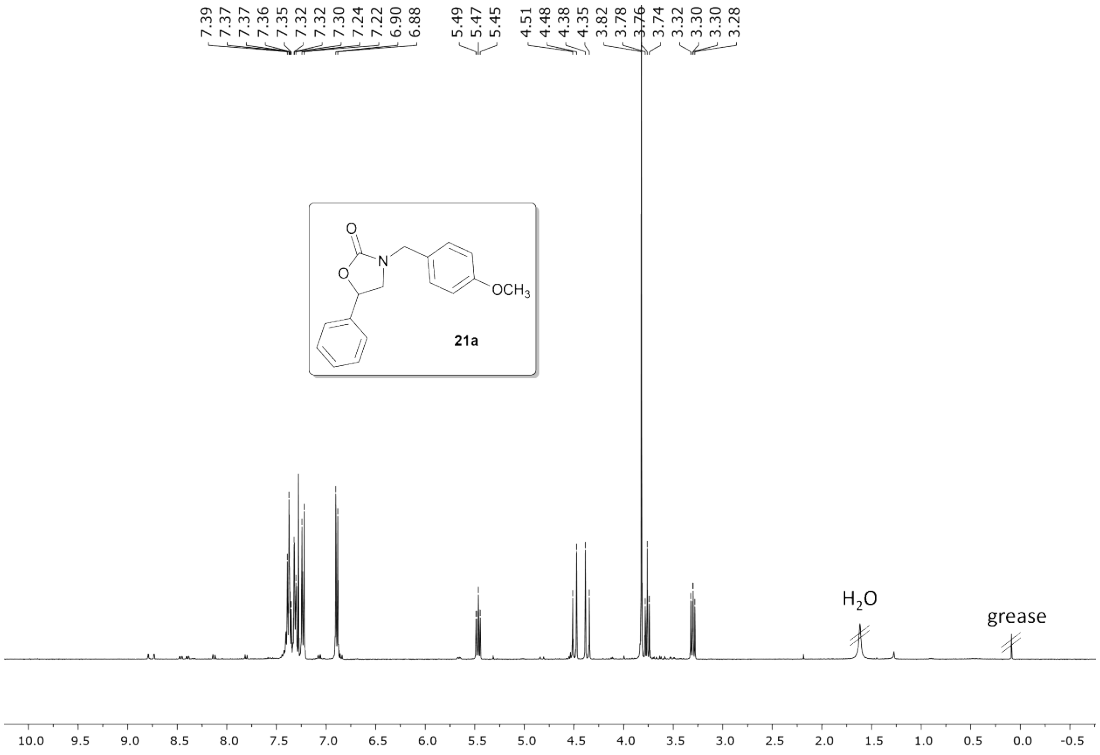
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 20



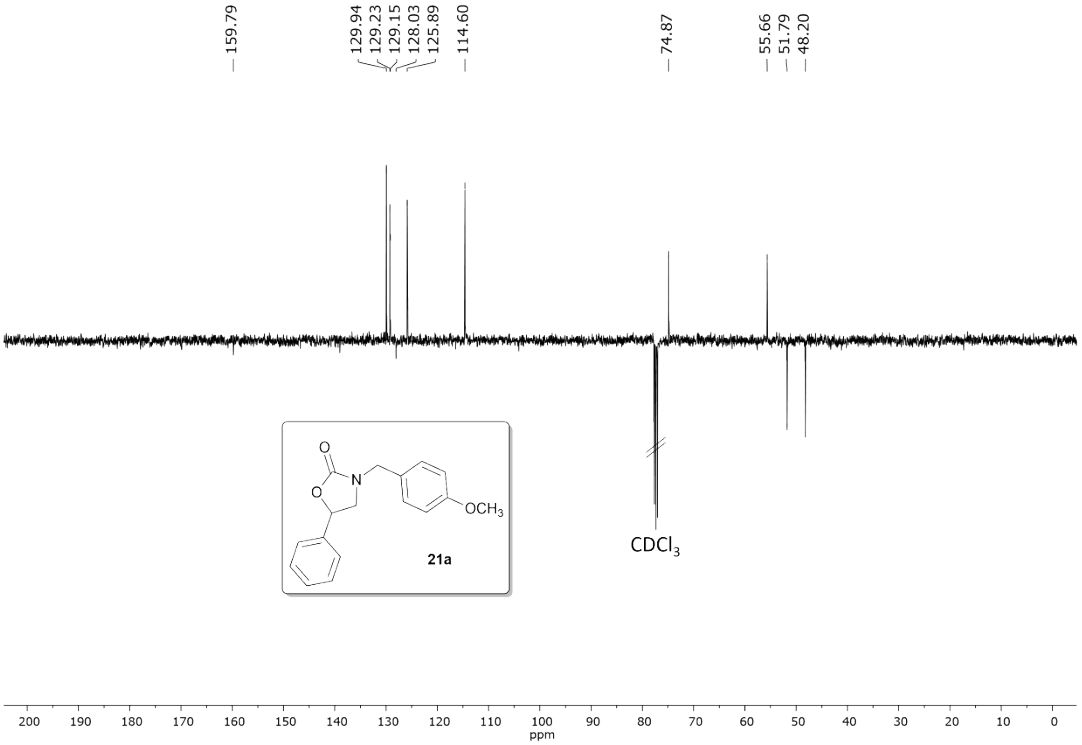
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 20



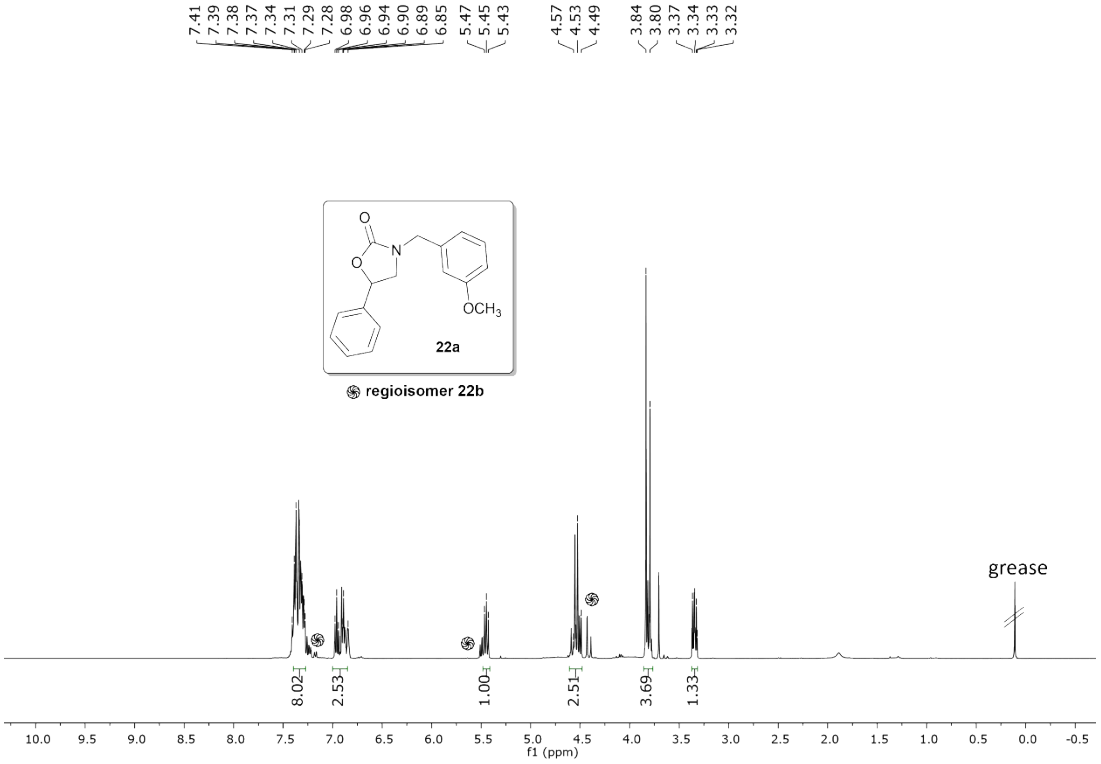
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 21



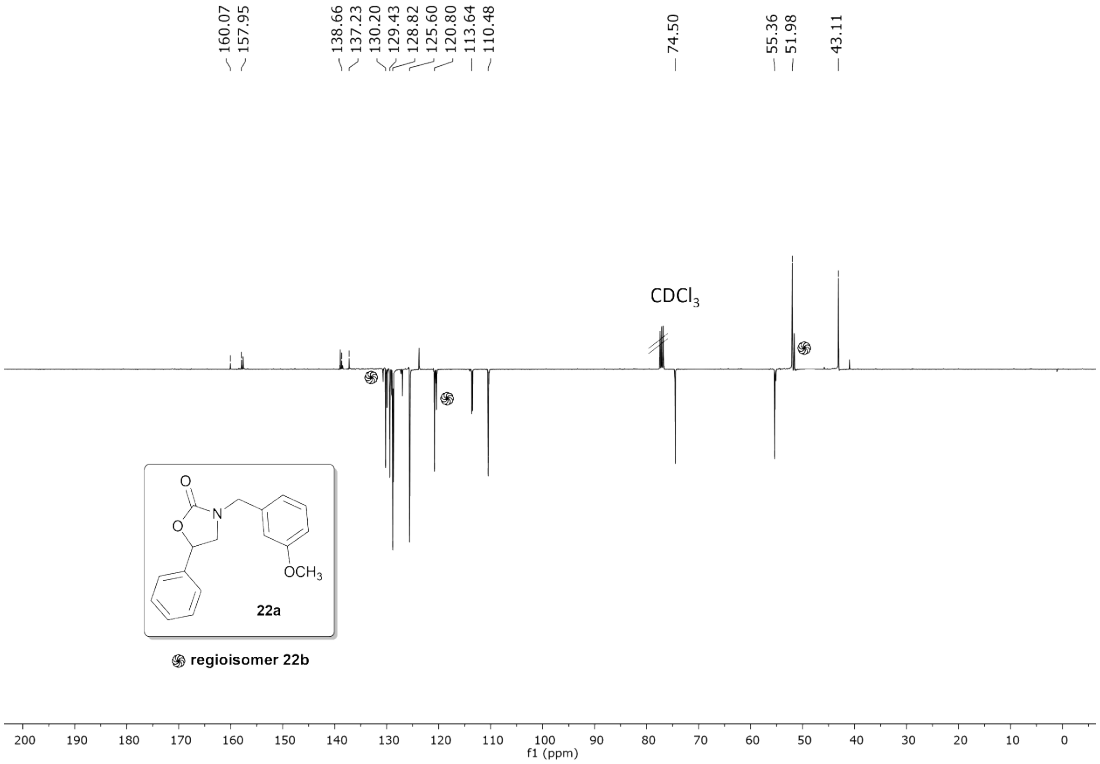
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 21



^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298K) of 22



^{13}C NMR spectrum (101 MHz, $CDCl_3$, 298K) of 22



10. Computational data

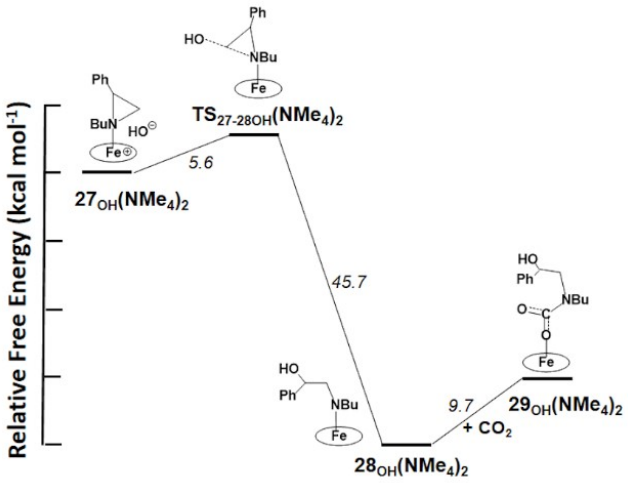


Figure S17: Free Energy (kcal mol^{-1}) reaction pathway for CO_2 activation catalyzed by **$27_{OH}(NMe_4)_2$**.

Table S1. Relative stability in kcal mol^{-1} of the spin-isomers of the different starting compounds.

Spin-isomer	2	$3(NMe_4)_2$
sextet	0	0
quartet	+10.3	+13.7
doublet	+21.7	+18.9

Cartesian coordinates and free energies of all the structures optimized in the computational analysis (B97D level of theory) in DCE solution

Compound $\mathbf{2}_{sext}$

Cartesian Coordinates

Fe	1.0600	-0.0729	0.1484	H	-0.9955	-5.5275	-1.3274
N	-0.3009	1.3783	-0.4999	H	-1.4040	-5.4780	0.3928
N	-0.3465	-1.5193	-0.4330	H	-2.6844	-5.2947	-0.8230
C	1.0580	-3.5249	-0.2502	C	-3.8728	-2.7092	-0.8847
C	1.1572	3.3499	-0.3691	H	-4.2479	-1.9827	-1.6160
C	-0.1687	-2.8832	-0.4049	H	-4.1219	-3.7043	-1.2685
C	-2.3207	2.4764	-0.7797	C	-4.6038	-2.4868	0.4525
C	-2.3901	-2.5693	-0.7227	H	-4.3125	-1.5218	0.8905
C	-1.6878	-1.3022	-0.6271	H	-4.3065	-3.2544	1.1812
C	-1.6525	1.1930	-0.6673	C	-6.1203	-2.5116	0.3248
C	-1.3478	3.4410	-0.6718	C	-3.8020	2.6525	-0.9161
C	-2.2877	-0.0466	-0.7340	H	-4.2085	1.9285	-1.6332
C	-1.4456	-3.5571	-0.5801	H	-4.0333	3.6499	-1.3051
C	-0.0874	2.7371	-0.5019	C	-4.5134	2.4602	0.4363
C	2.3924	2.7150	-0.2085	H	-4.2342	1.4941	0.8795
N	2.5671	1.3560	-0.1548	H	-4.1876	3.2293	1.1513
C	2.3129	-2.9214	-0.1106	C	-6.0310	2.5170	0.3344
N	2.5279	-1.5616	-0.0807	C	3.8514	4.8320	-0.1065
C	3.8807	-1.3745	0.0529	C	4.9862	5.5171	-0.3497
C	4.5599	-2.6655	0.1035	C	5.9962	-2.8293	0.2551
C	3.5676	-3.6309	0.0064	C	6.7250	-3.9267	-0.0292
C	4.5122	-0.1299	0.0963	H	2.9526	5.4137	0.1024
C	3.9189	1.1314	0.0016	H	5.9224	5.0281	-0.6039
C	4.6336	2.3882	0.0409	H	4.9861	6.6048	-0.3157
C	3.6816	3.3887	-0.0979	H	6.5329	-1.9600	0.6375
H	-3.3610	-0.0336	-0.9005	H	6.2871	-4.8283	-0.4478
H	1.1599	4.4349	-0.4044	H	7.8001	-3.9279	0.1402
H	5.5927	-0.1403	0.1941	O	-6.7049	2.2928	1.5031
H	1.0351	-4.6105	-0.2593	O	-6.6628	2.7380	-0.6753
C	6.1086	2.5471	0.2323	O	-6.8090	-2.2765	1.4827
H	6.3181	3.4163	0.8693	O	-6.7395	-2.7161	-0.6962
H	6.5548	1.6616	0.6978	C	-1.5071	4.9293	-0.7016
H	6.6233	2.7181	-0.7251	H	-2.5406	5.2080	-0.9349
C	3.7266	-5.1179	0.0430	H	-1.2471	5.3751	0.2694
H	2.7957	-5.6175	0.3324	H	-0.8494	5.3858	-1.4540
H	4.0290	-5.5147	-0.9378	H	-6.0819	2.1280	2.2302
H	4.5098	-5.4000	0.7588	H	-6.1953	-2.1281	2.2211
C	-1.6452	-5.0409	-0.5868	O	0.8333	0.0617	1.9954

C	0.7185	1.2759	2.7090	H	0.6045	1.0676	3.7856
H	-0.1578	1.8548	2.3680	H	1.6133	1.9066	2.5659

Free Energy: -2073.074253 hartrees

Compound $\mathbf{2}_{\mathbf{quart}}$

Cartesian Coordinates

Fe	1.0771	-0.0755	-0.0359	H	-2.6613	-5.2741	-0.7652
N	-0.2853	1.3533	-0.4853	C	-3.8527	-2.6914	-0.8620
N	-0.3204	-1.4881	-0.4476	H	-4.2362	-1.9661	-1.5899
C	1.0592	-3.5072	-0.2397	H	-4.1008	-3.6870	-1.2453
C	1.1423	3.3430	-0.3202	C	-4.5736	-2.4739	0.4814
C	-0.1519	-2.8554	-0.4012	H	-4.2776	-1.5117	0.9221
C	-2.3098	2.4574	-0.7597	H	-4.2727	-3.2454	1.2045
C	-2.3690	-2.5494	-0.7120	C	-6.0910	-2.4956	0.3633
C	-1.6681	-1.2848	-0.6333	C	-3.7905	2.6313	-0.9043
C	-1.6398	1.1783	-0.6590	H	-4.1927	1.9092	-1.6254
C	-1.3409	3.4204	-0.6330	H	-4.0187	3.6292	-1.2934
C	-2.2845	-0.0464	-0.7372	C	-4.5097	2.4376	0.4438
C	-1.4244	-3.5325	-0.5611	H	-4.2310	1.4725	0.8891
C	-0.0846	2.7163	-0.4660	H	-4.1900	3.2076	1.1604
C	2.3639	2.6982	-0.1691	C	-6.0267	2.4910	0.3318
N	2.5356	1.3351	-0.1432	C	3.8078	4.8214	-0.0292
C	2.2988	-2.8898	-0.1101	C	4.9344	5.5101	-0.2963
N	2.5045	-1.5255	-0.1063	C	5.9723	-2.7967	0.2928
C	3.8593	-1.3476	0.0479	C	6.7020	-3.8890	-0.0056
C	4.5374	-2.6338	0.1217	H	2.9162	5.3973	0.2217
C	3.5480	-3.5983	0.0295	H	5.8597	5.0240	-0.5927
C	4.5012	-0.1186	0.1045	H	4.9384	6.5968	-0.2393
C	3.8913	1.1260	0.0186	H	6.5032	-1.9370	0.7036
C	4.6000	2.3815	0.0803	H	6.2665	-4.7782	-0.4529
C	3.6450	3.3767	-0.0448	H	7.7741	-3.8991	0.1810
H	-3.3574	-0.0354	-0.8997	O	-6.7078	2.2651	1.4958
H	1.1410	4.4276	-0.3367	O	-6.6519	2.7107	-0.6823
H	5.5796	-0.1274	0.2132	O	-6.7718	-2.2657	1.5267
H	1.0354	-4.5919	-0.2296	O	-6.7167	-2.6931	-0.6549
C	6.0738	2.5416	0.2800	C	-1.4995	4.9088	-0.6445
H	6.2777	3.4267	0.8960	H	-2.5359	5.1880	-0.8631
H	6.5143	1.6681	0.7728	H	-1.2288	5.3439	0.3282
H	6.5973	2.6861	-0.6770	H	-0.8513	5.3739	-1.3999
C	3.7023	-5.0847	0.0945	H	-6.0897	2.1014	2.2273
H	2.7809	-5.5738	0.4288	H	-6.1532	-2.1227	2.2622
H	3.9679	-5.5057	-0.8868	O	0.8512	-0.0029	1.8663
H	4.5091	-5.3515	0.7890	C	0.7429	1.2040	2.5785
C	-1.6193	-5.0167	-0.5464	H	-0.1306	1.7969	2.2460
H	-0.9795	-5.5112	-1.2902	H	0.6291	1.0021	3.6591
H	-1.3640	-5.4407	0.4352	H	1.6372	1.8411	2.4406

Free Energy: -2073.057781 hartrees

Compound $\mathbf{2}_{\mathbf{dou}}$

Cartesian Coordinates

Fe	1.0787	-0.0648	-0.1212	C	-0.1492	-2.8398	-0.5143
N	-0.2692	1.3587	-0.5232	C	-2.3004	2.4775	-0.7398
N	-0.3109	-1.4672	-0.5161	C	-2.3707	-2.5255	-0.7589
C	1.0566	-3.4994	-0.3545	C	-1.6674	-1.2648	-0.6466
C	1.1648	3.3448	-0.4418	C	-1.6328	1.1954	-0.6335

C	-1.3226	3.4351	-0.6903
C	-2.2849	-0.0250	-0.6882
C	-1.4230	-3.5122	-0.6762
C	-0.0661	2.7246	-0.5522
C	2.3752	2.6943	-0.2428
N	2.5239	1.3259	-0.1626
C	2.2862	-2.8877	-0.1480
N	2.4813	-1.5214	-0.0898
C	3.8239	-1.3539	0.1607
C	4.5016	-2.6427	0.2406
C	3.5262	-3.6026	0.0473
C	4.4603	-0.1279	0.2640
C	3.8655	1.1166	0.1044
C	4.5825	2.3662	0.1648
C	3.6524	3.3651	-0.0675
H	-3.3638	-0.0090	-0.8068
H	1.1730	4.4284	-0.4926
H	5.5286	-0.1378	0.4489
H	1.0312	-4.5840	-0.3800
C	6.0411	2.5207	0.4601
H	6.2130	3.4295	1.0507
H	6.4356	1.6651	1.0190
H	6.6318	2.6188	-0.4631
C	3.6791	-5.0909	0.0656
H	2.7403	-5.5918	0.3272
H	4.0021	-5.4769	-0.9130
H	4.4438	-5.3844	0.7961
C	-1.6140	-4.9967	-0.7250
H	-0.9968	-5.4538	-1.5110
H	-1.3273	-5.4667	0.2267
H	-2.6617	-5.2478	-0.9233
C	-3.8575	-2.6619	-0.8814
H	-4.2545	-1.9167	-1.5818
H	-4.1152	-3.6465	-1.2861
C	-4.5529	-2.4798	0.4805
H	-4.2546	-1.5258	0.9374
H	-4.2331	-3.2656	1.1798
C	-6.0721	-2.5087	0.3915
C	-3.7853	2.6538	-0.8272
H	-4.2164	1.9332	-1.5333
H	-4.0270	3.6527	-1.2056
C	-4.4543	2.4592	0.5464
H	-4.1598	1.4938	0.9813
H	-4.1083	3.2287	1.2512
C	-5.9745	2.5090	0.4902
C	3.8338	4.8072	-0.1059
C	4.9848	5.4737	-0.3217
C	5.9225	-2.8073	0.5011
C	6.6774	-3.8858	0.2139
H	2.9347	5.4039	0.0538
H	5.9234	4.9671	-0.5287
H	4.9974	6.5618	-0.3127
H	6.4199	-1.9608	0.9767
H	6.2775	-4.7592	-0.2939
H	7.7345	-3.8997	0.4721
O	-6.6109	2.3174	1.6854
O	-6.6383	2.6965	-0.5057
O	-6.7314	-2.3155	1.5740
O	-6.7168	-2.6827	-0.6192
C	-1.4663	4.9243	-0.7517
H	-2.5100	5.2080	-0.9256
H	-1.1390	5.3952	0.1865
H	-0.8557	5.3520	-1.5590
H	-5.9649	2.1796	2.3977
H	-6.0990	-2.1885	2.3006
O	0.8441	-0.0784	1.6672
C	0.5753	1.1370	2.3450
H	-0.4271	1.5268	2.1043
H	0.6248	0.9202	3.4252
H	1.3157	1.9163	2.1074

Free Energy: -2073.039577 hartrees

Compound **3(NMe$_4$)$_{2sext}$**

Cartesian Coordinates

Fe	-2.7493	-0.0354	0.7180
N	-1.2384	1.4101	0.5760
N	-1.2234	-1.4684	0.5830
C	-2.6183	-3.4652	0.2477
C	-2.6524	3.3918	0.2259
C	-1.4070	-2.8332	0.5145
C	0.7787	2.5062	0.9134
C	0.8022	-2.5435	0.9359
C	0.1133	-1.2681	0.8356
C	0.1019	1.2238	0.8264
C	-0.1800	3.4702	0.7047
C	0.7210	-0.0184	0.9604
C	-0.1467	-3.5180	0.7328
C	-1.4343	2.7719	0.4956
C	-3.8707	2.7676	-0.0555
N	-4.0631	1.4098	-0.0781
C	-3.8460	-2.8558	-0.0314
N	-4.0535	-1.4938	-0.0667
C	-5.3708	-1.3016	-0.4008
C	-6.0343	-2.5890	-0.5756
C	-5.0679	-3.5592	-0.3481
C	-5.9818	-0.0554	-0.5441
C	-5.3852	1.1999	-0.4070
C	-6.0617	2.4635	-0.5992
C	-5.1173	3.4550	-0.3723
H	1.7883	-0.0127	1.1609
H	-2.6395	4.4773	0.2136
H	-7.0377	-0.0585	-0.7924
H	-2.5978	-4.5508	0.2387
C	-7.4921	2.6349	-1.0023
H	-7.5947	3.4808	-1.6945
H	-7.8860	1.7371	-1.4910
H	-8.1318	2.8511	-0.1333
C	-5.2188	-5.0446	-0.4442
H	-4.2558	-5.5395	-0.6107
H	-5.6566	-5.4648	0.4737
H	-5.8924	-5.3071	-1.2705
C	0.0489	-5.0023	0.6978

H	-0.6878	-5.5190	1.3281
H	-0.0654	-5.3950	-0.3233
H	1.0517	-5.2694	1.0495
C	2.2765	-2.7167	1.1263
H	2.6648	-1.9621	1.8214
H	2.4866	-3.6937	1.5767
C	3.0345	-2.6042	-0.2119
H	2.8162	-1.6288	-0.6690
H	2.6552	-3.3571	-0.9171
C	4.5783	-2.7585	-0.1273
C	2.2520	2.6955	1.0957
H	2.6514	1.9484	1.7924
H	2.4545	3.6768	1.5400
C	3.0040	2.5841	-0.2461
H	2.7930	1.6046	-0.6979
H	2.6136	3.3302	-0.9526
C	4.5467	2.7545	-0.1705
C	-5.2575	4.8996	-0.4503
C	-6.4006	5.6104	-0.3859
C	-7.4298	-2.7467	-0.9494
C	-8.1949	-3.8449	-0.7912
H	-4.3278	5.4588	-0.5650
H	-7.3708	5.1456	-0.2344
H	-6.3755	6.6955	-0.4655
H	-7.9007	-1.8713	-1.3989
H	-7.8264	-4.7518	-0.3199
H	-9.2318	-3.8415	-1.1215
O	5.1619	2.6415	-1.2755
O	5.0747	2.9712	0.9570
O	5.1982	-2.6489	-1.2301
O	5.1029	-2.9594	1.0048
C	0.0020	4.9558	0.6559
H	1.0016	5.2354	1.0068
H	-0.1140	5.3378	-0.3691
H	-0.7406	5.4716	1.2800
O	-3.1834	-0.0345	2.5476
H	-2.4402	0.0287	3.1661
C	5.1597	0.0184	2.5102
H	5.0475	0.0264	3.5976
H	4.7306	0.9209	2.0679
H	4.7402	-0.8954	2.0822
C	6.8261	0.0134	0.7016
H	6.3537	0.9124	0.2998
H	7.9009	0.0192	0.5005
H	6.3658	-0.8980	0.3138
C	7.2654	1.2681	2.7713
H	7.1078	1.2622	3.8529
H	8.3335	1.2453	2.5403
H	6.7767	2.1257	2.3023
C	7.2785	-1.2043	2.7910
H	7.1199	-1.1832	3.8722
H	6.7995	-2.0744	2.3351
H	8.3466	-1.1737	2.5606
C	6.5799	-0.0055	-2.6775
H	6.5046	-0.9013	-2.0565
H	7.4983	-0.0087	-3.2706
H	6.4948	0.9057	-2.0806
C	5.4619	1.2012	-4.5044
H	6.4053	1.1946	-5.0561
H	4.6141	1.1676	-5.1932
H	5.3954	2.0702	-3.8452
C	4.1243	-0.0226	-2.8437
H	3.2940	-0.0373	-3.5550
H	4.1342	-0.9212	-2.2218
H	4.1229	0.8918	-2.2451
C	5.4769	-1.2739	-4.4713
H	5.4189	-2.1255	-3.7889
H	4.6299	-1.2678	-5.1619
H	6.4212	-1.2712	-5.0217
N	5.4116	-0.0252	-3.6343
N	6.6377	0.0239	2.1992

Free Energy: -2460.981823 hartrees

Compound **3(NMe$_4$)$_{2quart}$**

Cartesian Coordinates

Fe	-2.9650	-0.2715	0.3843
N	-1.9679	1.4822	0.3856
N	-1.1767	-1.2323	0.2540
C	-1.9822	-3.5407	0.0150
C	-3.8690	3.0330	0.2048
C	-0.9839	-2.5966	0.1876
C	-0.3129	3.0826	0.7210
C	1.0801	-1.7305	0.5122
C	0.0719	-0.6897	0.4637
C	-0.6140	1.6732	0.5812
C	-1.5082	3.7502	0.5976
C	0.3356	0.6634	0.6233
C	0.4188	-2.9203	0.3335
C	-2.5262	2.7457	0.3925
C	-4.8680	2.1000	-0.0408
N	-4.6758	0.7416	-0.0954
C	-3.3370	-3.2694	-0.1388
N	-3.8957	-2.0063	-0.1304
C	-5.2436	-2.1874	-0.3387
C	-5.5522	-3.6026	-0.4714
C	-4.3467	-4.2755	-0.3520
C	-6.1840	-1.1697	-0.4164
C	-5.9211	0.1900	-0.3179
C	-6.9260	1.2205	-0.4301
C	-6.2710	2.4270	-0.2496
H	1.3678	0.9562	0.7857
H	-4.1525	4.0793	0.2456
H	-7.2176	-1.4592	-0.5671
H	-1.6741	-4.5808	-0.0042
C	-8.3755	0.9964	-0.7246
H	-8.7593	1.7972	-1.3697
H	-8.5448	0.0370	-1.2255
H	-8.9795	1.0056	0.1952
C	-4.1004	-5.7470	-0.4630
H	-3.0703	-5.9639	-0.7660
H	-4.2825	-6.2586	0.4940

H	-4.7810	-6.1912	-1.2005
C	1.0029	-4.2977	0.2728
H	0.4467	-4.9992	0.9092
H	0.9779	-4.6970	-0.7519
H	2.0479	-4.2865	0.6025
C	2.5556	-1.5263	0.6608
H	2.7683	-0.6279	1.2521
H	2.9888	-2.3695	1.2120
C	3.2628	-1.4178	-0.7048
H	2.8944	-0.5364	-1.2494
H	3.0014	-2.2856	-1.3267
C	4.8104	-1.3304	-0.6447
C	1.0485	3.6829	0.8781
H	1.7177	3.0008	1.4156
H	0.9829	4.5941	1.4846
C	1.6754	4.0435	-0.4840
H	1.8104	3.1312	-1.0837
H	0.9815	4.6780	-1.0533
C	3.0467	4.7777	-0.4143
C	-6.7986	3.7812	-0.2860
C	-8.0809	4.1555	-0.1100
C	-6.8829	-4.1336	-0.7198
C	-7.3093	-5.3877	-0.4745
H	-6.0679	4.5697	-0.4711
H	-8.8712	3.4453	0.1167
H	-8.3579	5.2060	-0.1723
H	-7.6042	-3.4331	-1.1426
H	-6.6733	-6.1416	-0.0186
H	-8.3314	-5.6755	-0.7128
O	3.5642	5.0613	-1.5363
O	3.5506	5.0088	0.7221
O	5.4018	-1.2315	-1.7600
O	5.3731	-1.3445	0.4917
H	5.8848	2.2222	1.5380
H	4.4265	2.7924	0.6707
C	7.2736	1.4295	-0.5872
H	7.8564	1.5871	0.3238
C	-1.7410	5.2289	0.6271
H	-0.8479	5.7509	0.9880
H	-1.9733	5.6155	-0.3761
H	-2.5839	5.4910	1.2806
O	-3.2360	-0.4097	2.2932
H	-2.7573	0.2910	2.7615
C	8.4614	-2.3583	-1.0824
H	7.4685	-1.9021	-1.1753
H	9.2556	-1.6224	-1.2319
H	8.5747	-3.1873	-1.7857
C	9.9371	-3.5895	0.4661
H	10.0134	-3.9763	1.4850
H	9.9949	-4.4042	-0.2596
H	10.7190	-2.8503	0.2767
C	8.4842	-1.7840	1.3104
H	7.4976	-1.3333	1.1692
H	8.5887	-2.2054	2.3134
H	9.2892	-1.0731	1.1089
C	7.4928	-3.9074	0.5650
H	7.6221	-4.3121	1.5718
H	6.5468	-3.3674	0.4774
H	7.5744	-4.7016	-0.1810
N	8.6014	-2.9135	0.3150
C	6.5880	3.8022	-0.4965
H	7.2070	3.9849	-1.3786
H	5.7112	4.4569	-0.4866
H	7.1787	3.9153	0.4162
C	5.2796	2.1846	-1.8126
H	5.9260	2.4006	-2.6675
H	4.9507	1.1437	-1.8436
H	4.4488	2.8934	-1.7820
C	5.2556	2.0825	0.6549
H	4.9216	1.0452	0.5934
H	6.8801	0.4107	-0.6369
H	7.8756	1.6603	-1.4697
N	6.1023	2.3758	-0.5603

Free Energy: -2460.960015 hartrees

Compound **3(NMe$_4$)$_{2dou}$**

Cartesian Coordinates

Fe	-2.9865	-0.3115	0.3724
N	-1.9679	1.4822	0.3856
N	-1.3094	-1.1610	0.2637
C	-1.9822	-3.5407	0.0150
C	-3.8690	3.0330	0.2048
C	-0.9839	-2.5966	0.1876
C	-0.3129	3.0826	0.7210
C	1.0801	-1.7305	0.5122
C	0.0719	-0.6897	0.4637
C	-0.6140	1.6732	0.5812
C	-1.5082	3.7502	0.5976
C	0.3356	0.6634	0.6233
C	0.4188	-2.9203	0.3335
C	-2.5262	2.7457	0.3925
C	-4.8680	2.1000	-0.0408
N	-4.6758	0.7416	-0.0954
C	-3.3370	-3.2694	-0.1388
N	-3.8957	-2.0063	-0.1304
C	-5.2436	-2.1874	-0.3387
C	-5.5522	-3.6026	-0.4714
C	-4.3467	-4.2755	-0.3520
C	-6.1840	-1.1697	-0.4164
C	-5.9211	0.1900	-0.3179
C	-6.9260	1.2205	-0.4301
C	-6.2710	2.4270	-0.2496
H	1.3678	0.9562	0.7857
H	-4.1525	4.0793	0.2456
H	-7.2176	-1.4592	-0.5671
H	-1.6741	-4.5808	-0.0042
C	-8.3755	0.9964	-0.7246

H	-8.7593	1.7972	-1.3697
H	-8.5448	0.0370	-1.2255
H	-8.9795	1.0056	0.1952
C	-4.1004	-5.7470	-0.4630
H	-3.0703	-5.9639	-0.7660
H	-4.2825	-6.2586	0.4940
H	-4.7810	-6.1912	-1.2005
C	1.0029	-4.2977	0.2728
H	0.4467	-4.9992	0.9092
H	0.9779	-4.6970	-0.7519
H	2.0479	-4.2865	0.6025
C	2.5556	-1.5263	0.6608
H	2.7683	-0.6279	1.2521
H	2.9888	-2.3695	1.2120
C	3.2628	-1.4178	-0.7048
H	2.8944	-0.5364	-1.2494
H	3.0014	-2.2856	-1.3267
C	4.8104	-1.3304	-0.6447
C	1.0485	3.6829	0.8781
H	1.7177	3.0008	1.4156
H	0.9829	4.5941	1.4846
C	1.6754	4.0435	-0.4840
H	1.8104	3.1312	-1.0837
H	0.9815	4.6780	-1.0533
C	3.0467	4.7777	-0.4143
C	-6.7986	3.7812	-0.2860
C	-8.0809	4.1555	-0.1100
C	-6.8829	-4.1336	-0.7198
C	-7.3093	-5.3877	-0.4745
H	-6.0679	4.5697	-0.4711
H	-8.8712	3.4453	0.1167
H	-8.3579	5.2060	-0.1723
H	-7.6042	-3.4331	-1.1426
H	-6.6733	-6.1416	-0.0186
H	-8.3314	-5.6755	-0.7128
O	3.5642	5.0613	-1.5363
O	3.5506	5.0088	0.7221
O	5.4018	-1.2315	-1.7600
O	5.3731	-1.3445	0.4917
C	-1.7410	5.2289	0.6271
H	-0.8479	5.7509	0.9880
H	-1.9733	5.6155	-0.3761
H	-2.5839	5.4910	1.2806
O	-3.2273	-0.4053	2.2322
H	-2.7486	0.2954	2.7005
C	8.4850	-2.3990	-1.0827
H	7.4921	-1.9428	-1.1756
H	9.2792	-1.6631	-1.2322
H	8.5983	-3.2280	-1.7860
C	9.9607	-3.6302	0.4658
H	10.0370	-4.0170	1.4847
H	10.0185	-4.4449	-0.2599
H	10.7426	-2.8910	0.2764
C	8.5078	-1.8247	1.3101
H	7.5212	-1.3740	1.1689
H	8.6123	-2.2461	2.3131
H	9.3128	-1.1138	1.1086
C	7.5164	-3.9481	0.5647
H	7.6457	-4.3528	1.5715
H	6.5704	-3.4081	0.4771
H	7.5980	-4.7423	-0.1813
N	8.6250	-2.9542	0.3147
C	6.5880	3.8022	-0.4965
H	7.2070	3.9849	-1.3786
H	5.7112	4.4569	-0.4866
H	7.1787	3.9153	0.4162
C	5.2796	2.1846	-1.8126
H	5.9260	2.4006	-2.6675
H	4.9507	1.1437	-1.8436
H	4.4488	2.8934	-1.7820
C	5.2556	2.0825	0.6549
H	4.9216	1.0452	0.5934
H	5.8848	2.2222	1.5380
H	4.4265	2.7924	0.6707
C	7.2736	1.4295	-0.5872
H	7.8564	1.5871	0.3238
H	6.8801	0.4107	-0.6369
H	7.8756	1.6603	-1.4697
N	6.1023	2.3758	-0.5603

Free Energy: -2460.952180 hartrees

Compound ***N*-butyl-2-phenyl aziridine**

Cartesian Coordinates

C	0.764614	0.757065	2.782264
C	-0.205786	-0.314871	2.411974
H	0.561315	1.790299	2.496297
H	1.316853	0.643260	3.717799
H	-1.042106	-0.030089	1.770663
N	1.098846	-0.168231	1.693006
C	-0.521370	-1.491706	3.278108
C	0.022187	-1.689108	4.559039
C	-1.398331	-2.466699	2.767035
C	-0.289807	-2.834513	5.299795
H	0.685559	-0.943502	4.988927
C	-1.715768	-3.609421	3.506367
H	-1.833023	-2.321581	1.778772
C	-1.158234	-3.799458	4.777007
H	0.140820	-2.968060	6.290535
H	-2.397219	-4.350356	3.092210
H	-1.403028	-4.687693	5.356213
C	2.165860	-1.137543	1.992926

C	3.533164	-0.534707	1.666289
H	1.990602	-2.029723	1.374922
H	2.159666	-1.462261	3.047668
C	4.681043	-1.513549	1.947215
H	3.555277	-0.231366	0.609481
H	3.674741	0.376739	2.266690
C	6.055704	-0.911607	1.624592
H	4.647844	-1.815566	3.004893
H	4.528832	-2.428063	1.354278
H	6.864314	-1.625619	1.830712
H	6.115021	-0.625526	0.564996
H	6.235310	-0.009647	2.226625

Free Energy: -521.800802 hartrees

Compound **Styrene Epoxide**

Cartesian Coordinates

C	2.381146	1.087867	1.656255
H	2.835502	1.067822	0.661970
C	0.920407	1.302629	1.730846
H	0.508258	1.756895	2.635719
H	0.348243	1.453129	0.811575
C	3.302127	1.494568	2.756720
C	4.523088	2.109015	2.438307
C	2.967049	1.292092	4.105896
C	5.392124	2.527704	3.452099
H	4.792532	2.255718	1.393122
C	3.836796	1.705971	5.117804
H	2.030461	0.797161	4.353783
C	5.050508	2.328365	4.794616
H	6.336324	3.003202	3.193485
H	3.569891	1.541941	6.160191
H	5.726944	2.649395	5.584323
O	1.472601	-0.017775	1.908190

Free Energy: -384.599147 hartrees

Compound **25**$_{\mathbf{OMesext}}$

Cartesian Coordinates

Fe	0.5940	0.6629	-0.8623
N	-0.6659	-0.9961	-0.8984
N	-0.8466	1.6908	0.2492
C	0.4516	3.7203	0.7227
C	0.8901	-2.6254	-1.8769
C	-0.7287	2.9721	0.7214
C	-2.5377	-2.3399	-0.7528
C	-2.9032	2.3958	1.0200
C	-2.1506	1.3130	0.4068
C	-1.9802	-1.0181	-0.5126
C	-1.5279	-3.1058	-1.2851
C	-2.6669	0.0562	0.0649
C	-2.0198	3.4313	1.2166
C	-0.3575	-2.2422	-1.3753
C	2.0391	-1.8319	-2.0098
N	2.1183	-0.5176	-1.6527
C	1.7052	3.3566	0.2034
N	1.9763	2.1662	-0.4194
C	3.2747	2.1971	-0.8379
C	3.8856	3.4663	-0.4395
C	2.8923	4.1894	0.2083
C	3.9213	1.1545	-1.5167
C	3.4093	-0.1005	-1.8746
C	4.1881	-1.1889	-2.4277
C	3.3383	-2.2853	-2.5027
H	-3.7110	-0.1167	0.3110
H	0.9715	-3.6608	-2.1943
H	4.9676	1.3177	-1.7544
H	0.3814	4.7093	1.1664
C	5.6251	-1.1120	-2.8356
H	5.7928	-1.6858	-3.7566
H	5.9409	-0.0775	-3.0100
H	6.2859	-1.5392	-2.0661
C	2.9870	5.5700	0.7761
H	1.9989	6.0280	0.8946
H	3.4747	5.5675	1.7627
H	3.5919	6.2125	0.1223
C	-2.2910	4.7860	1.7934
H	-1.5838	5.0252	2.5996
H	-2.1881	5.5705	1.0296
H	-3.3068	4.8432	2.2003
C	-4.3764	2.3577	1.2870
H	-4.6625	1.3908	1.7196
H	-4.6541	3.1277	2.0150
C	-5.1786	2.5752	-0.0096
H	-4.8637	1.8533	-0.7764
H	-4.9671	3.5714	-0.4236
C	-6.6831	2.4413	0.1757
C	-3.9610	-2.7214	-0.4850
H	-4.2797	-2.3401	0.4935
H	-4.0649	-3.8111	-0.4512
C	-4.9036	-2.1571	-1.5644
H	-4.7675	-1.0708	-1.6588
H	-4.6535	-2.5825	-2.5472
C	-6.3747	-2.4328	-1.2887
C	3.6053	-3.6332	-2.9741
C	4.8077	-4.2228	-3.1288
C	5.2596	3.8382	-0.7292
C	5.9856	4.8108	-0.1422
H	2.7240	-4.2285	-3.2176
H	5.7405	-3.7258	-2.8784
H	4.8721	-5.2440	-3.4996

H	5.7511	3.2518	-1.5071
H	5.5980	5.4249	0.6656
H	7.0103	4.9950	-0.4594
O	-7.2517	-1.8714	-2.1756
O	-6.8093	-3.0931	-0.3706
O	-7.4300	2.6086	-0.9581
O	-7.2473	2.2011	1.2204
C	-1.5700	-4.5429	-1.7017
H	-2.5472	-4.9873	-1.4830
H	-1.3814	-4.6513	-2.7793
H	-0.8016	-5.1293	-1.1781
H	-6.7738	-1.3682	-2.8557
H	-6.8576	2.7962	-1.7205
C	0.9865	0.5277	2.5931
C	0.1938	-0.6657	2.1929
H	0.5702	1.5223	2.4543
H	1.6748	0.4166	3.4292
H	-0.7584	-0.4731	1.7081
N	1.3197	-0.1928	1.3521
C	2.5804	-0.9721	1.2840
C	3.3743	-1.2703	2.5614
H	3.2353	-0.4058	0.6177
H	2.3364	-1.9119	0.7749
C	4.6150	-2.1076	2.2169
H	3.6958	-0.3287	3.0295
H	2.7671	-1.8103	3.2951
C	5.4729	-2.4152	3.4513
H	4.2917	-3.0477	1.7454
H	5.2170	-1.5717	1.4673
H	6.3530	-3.0171	3.1881
H	5.8233	-1.4857	3.9218
H	4.8899	-2.9713	4.1989
C	0.2381	-1.9769	2.9068
C	0.1293	-3.1575	2.1540
C	0.3595	-2.0640	4.3008
C	0.1651	-4.4051	2.7836
H	0.0209	-3.0919	1.0737
C	0.3884	-3.3114	4.9339
H	0.4441	-1.1507	4.8865
C	0.2971	-4.4854	4.1761
H	0.0883	-5.3141	2.1894
H	0.4848	-3.3674	6.0167
H	0.3248	-5.4561	4.6675
O	0.0421	1.4717	-2.5029
C	-0.2826	2.8244	-2.6950
H	-0.5321	3.0146	-3.7539
H	-1.1494	3.1209	-2.0751
H	0.5596	3.4831	-2.4121

Free Energy: -2594.874843 hartrees

Compound **25**$_{\mathbf{OMequart}}$

Cartesian Coordinates

Fe	0.6052	0.6409	-0.7994
N	-0.6379	-0.9538	-0.8872
N	-0.8147	1.6706	0.2186
C	0.4620	3.6966	0.7488
C	0.8849	-2.6040	-1.8755
C	-0.7023	2.9433	0.7250
C	-2.5205	-2.3012	-0.7636
C	-2.8698	2.3747	1.0243
C	-2.1258	1.3066	0.3867
C	-1.9608	-0.9866	-0.5190
C	-1.5101	-3.0676	-1.2859
C	-2.6624	0.0699	0.0474
C	-1.9818	3.3981	1.2391
C	-0.3431	-2.2069	-1.3654
C	2.0075	-1.7927	-2.0135
N	2.0794	-0.4829	-1.6241
C	1.6924	3.3216	0.2129
N	1.9406	2.1338	-0.4331
C	3.2387	2.1877	-0.8629
C	3.8560	3.4439	-0.4520
C	2.8757	4.1524	0.2226
C	3.8907	1.1771	-1.5618
C	3.3618	-0.0633	-1.9023
C	4.1251	-1.1298	-2.5073
C	3.2842	-2.2287	-2.5646
H	-3.7071	-0.0998	0.2874
H	0.9643	-3.6353	-2.2027
H	4.9279	1.3500	-1.8261
H	0.3985	4.6741	1.2156
C	5.5404	-1.0260	-2.9801
H	5.6807	-1.6213	-3.8915
H	5.8193	0.0110	-3.1971
H	6.2461	-1.4134	-2.2297
C	2.9749	5.5224	0.8149
H	1.9926	5.9992	0.9030
H	3.4246	5.4958	1.8189
H	3.6160	6.1601	0.1924
C	-2.2365	4.7404	1.8511
H	-1.5335	4.9460	2.6699
H	-2.1158	5.5439	1.1103
H	-3.2548	4.7998	2.2506
C	-4.3409	2.3337	1.3021
H	-4.6270	1.3594	1.7174
H	-4.6080	3.0888	2.0493
C	-5.1541	2.5830	0.0182
H	-4.8490	1.8782	-0.7682
H	-4.9434	3.5879	-0.3747
C	-6.6571	2.4496	0.2161

C	-3.9491	-2.6751	-0.5133
H	-4.2822	-2.2858	0.4569
H	-4.0545	-3.7643	-0.4718
C	-4.8729	-2.1191	-1.6128
H	-4.7329	-1.0341	-1.7161
H	-4.6086	-2.5545	-2.5873
C	-6.3488	-2.3879	-1.3567
C	3.5411	-3.5653	-3.0746
C	4.7435	-4.1477	-3.2506
C	5.2271	3.8208	-0.7533
C	5.9695	4.7508	-0.1210
H	2.6586	-4.1527	-3.3316
H	5.6753	-3.6551	-2.9871
H	4.8097	-5.1569	-3.6522
H	5.6965	3.2831	-1.5783
H	5.6010	5.3097	0.7346
H	6.9872	4.9546	-0.4484
O	-7.2090	-1.8473	-2.2721
O	-6.7999	-3.0255	-0.4306
O	-7.4152	2.6430	-0.9057
O	-7.2108	2.1891	1.2616
C	-1.5475	-4.5043	-1.7041
H	-2.5296	-4.9447	-1.5007
H	-1.3425	-4.6125	-2.7786
H	-0.7897	-5.0930	-1.1682
H	-6.7183	-1.3616	-2.9558
H	-6.8506	2.8451	-1.6701
C	0.9931	0.4990	2.6473
C	0.1941	-0.6851	2.2303
H	0.5871	1.4994	2.5123
H	1.6701	0.3752	3.4913
H	-0.7534	-0.4851	1.7368
N	1.3300	-0.2129	1.4043
C	2.5808	-1.0036	1.3234
C	3.3863	-1.2922	2.5950
H	3.2297	-0.4533	0.6361
H	2.3196	-1.9480	0.8304
C	4.6198	-2.1408	2.2540
H	3.7146	-0.3462	3.0497
H	2.7796	-1.8192	3.3390
C	5.4837	-2.4376	3.4869
H	4.2882	-3.0851	1.7966
H	5.2202	-1.6179	1.4940
H	6.3589	-3.0478	3.2260
H	5.8422	-1.5041	3.9433
H	4.9023	-2.9809	4.2451
C	0.2285	-2.0022	2.9339
C	0.0960	-3.1742	2.1711
C	0.3674	-2.1054	4.3252
C	0.1244	-4.4286	2.7875
H	-0.0260	-3.0964	1.0930
C	0.3898	-3.3596	4.9453
H	0.4694	-1.1995	4.9194
C	0.2738	-4.5246	4.1771
H	0.0285	-5.3304	2.1851
H	0.4993	-3.4277	6.0262
H	0.2957	-5.5006	4.6584
O	0.0409	1.4326	-2.5061
C	-0.2415	2.7918	-2.6804
H	-0.5150	3.0075	-3.7314
H	-1.0820	3.1244	-2.0379
H	0.6263	3.4303	-2.4190

Free Energy: -2594.860918 hartrees

Compound **$25_{OHsext}(NMe_4)_2$**

Cartesian Coordinates

Fe	2.1913	0.9090	-1.2564
N	0.6707	2.1430	-0.5462
N	0.7474	-0.4226	-1.9453
C	2.2063	-2.3473	-2.4098
C	2.0721	3.8317	0.5586
C	0.9663	-1.7050	-2.3830
C	-1.3944	3.1252	-0.2073
C	-1.2772	-1.3822	-2.5114
C	-0.6062	-0.2060	-1.9827
C	-0.6692	2.0002	-0.7855
C	-0.4528	3.9382	0.3785
C	-1.2504	0.9273	-1.4710
C	-0.2966	-2.3185	-2.7523
C	0.8409	3.3106	0.1491
C	3.3434	3.2662	0.3855
N	3.5834	2.0623	-0.2189
C	3.4460	-1.8449	-1.9889
N	3.6441	-0.5953	-1.4598
C	4.9786	-0.4618	-1.1990
C	5.6765	-1.6916	-1.5722
C	4.7049	-2.5590	-2.0531
C	5.5741	0.6797	-0.6470
C	4.9419	1.8417	-0.1837
C	5.6033	2.9555	0.4599
C	4.6059	3.8559	0.8192
H	-2.3320	0.9509	-1.5713
H	2.0290	4.7883	1.0709
H	6.6525	0.6503	-0.5326
H	2.2023	-3.3627	-2.7955
C	7.0725	3.0703	0.7158
H	7.2555	3.5012	1.7091
H	7.5712	2.0965	0.6637
H	7.5572	3.7341	-0.0159
C	4.8805	-3.9741	-2.5049
H	3.9357	-4.5278	-2.4718
H	5.2645	-4.0273	-3.5348

H	5.6081	-4.4906	-1.8646
C	-0.4694	-3.7227	-3.2425
H	0.2338	-3.9547	-4.0540
H	-0.2869	-4.4498	-2.4371
H	-1.4886	-3.8823	-3.6122
C	-2.7581	-1.5628	-2.6278
H	-3.2423	-0.6165	-2.8980
H	-2.9901	-2.2738	-3.4294
C	-3.3614	-2.0821	-1.3071
H	-3.1473	-1.3607	-0.5061
H	-2.8579	-3.0130	-1.0116
C	-4.8918	-2.3472	-1.3199
C	-2.8830	3.2771	-0.1866
H	-3.3199	2.9205	-1.1276
H	-3.1537	4.3356	-0.0965
C	-3.5075	2.4948	0.9861
H	-3.2354	1.4336	0.8939
H	-3.0685	2.8353	1.9343
C	-5.0534	2.5795	1.1104
C	4.7160	5.1267	1.5144
C	5.8199	5.8863	1.6626
C	7.1018	-1.9082	-1.3962
C	7.8615	-2.8603	-1.9743
H	3.7916	5.5019	1.9558
H	6.7791	5.6181	1.2293
H	5.7690	6.8211	2.2176
H	7.6038	-1.2130	-0.7218
H	7.4617	-3.5765	-2.6864
H	8.9246	-2.9224	-1.7498
O	-5.5547	1.9655	2.1027
O	-5.6957	3.2169	0.2279
O	-5.3819	-2.7623	-0.2241
O	-5.5345	-2.1225	-2.3844
C	-0.6750	5.2099	1.1373
H	-1.7138	5.5448	1.0390
H	-0.4642	5.0771	2.2089
H	-0.0177	6.0128	0.7757
O	2.4673	1.7570	-2.9642
H	1.9253	1.3568	-3.6607
C	-5.8489	1.2067	-2.4361
H	-5.8541	1.6828	-3.4202
H	-5.4034	1.8659	-1.6870
H	-5.3568	0.2321	-2.4788
C	-7.3076	0.3140	-0.6694
H	-6.8274	0.9942	0.0373
H	-8.3533	0.1480	-0.3964
H	-6.7740	-0.6358	-0.7466
C	-8.0107	2.2866	-1.9611
H	-7.9683	2.7496	-2.9503
H	-9.0473	2.0879	-1.6772
H	-7.5049	2.9001	-1.2114
C	-7.9462	0.0587	-3.0308
H	-7.9125	0.5463	-4.0083
H	-7.3906	-0.8825	-3.0352
H	-8.9817	-0.0940	-2.7157
C	-6.6924	-1.1263	2.3426
H	-6.6608	-1.6528	1.3859
H	-7.5372	-1.4584	2.9519
H	-6.7023	-0.0425	2.2039
C	-5.4118	-0.7647	4.4107
H	-6.2815	-1.0939	4.9847
H	-4.4867	-1.0259	4.9305
H	-5.4560	0.3082	4.2079
C	-4.2350	-1.0155	2.2693
H	-3.3302	-1.2735	2.8242
H	-4.2826	-1.5478	1.3162
H	-4.3344	0.0653	2.1430
C	-5.3488	-2.9629	3.2740
H	-5.3416	-3.4167	2.2799
H	-4.4277	-3.1935	3.8133
H	-6.2219	-3.2813	3.8491
N	-5.4226	-1.4720	3.0832
N	-7.2840	0.9686	-2.0292
C	3.0549	-0.4889	1.7032
H	3.9039	-0.0857	1.1600
C	2.0656	0.4976	2.2173
H	1.4883	0.2172	3.0972
H	2.2509	1.5624	2.0957
N	1.7919	-0.2378	0.9717
C	0.7204	-1.2617	0.9517
C	0.1353	-1.7937	2.2665
H	1.1054	-2.0993	0.3583
H	-0.1000	-0.8167	0.3831
C	-0.9210	-2.8688	1.9723
H	0.9136	-2.2221	2.9057
H	-0.3343	-0.9728	2.8277
C	-1.4948	-3.4845	3.2547
H	-1.7276	-2.4333	1.3664
H	-0.4663	-3.6606	1.3587
H	-2.2720	-4.2269	3.0309
H	-0.7030	-3.9811	3.8322
H	-1.9339	-2.7100	3.9001
C	3.3484	-1.7991	2.3578
C	3.6316	-2.9092	1.5453
C	3.3746	-1.9483	3.7516
C	3.9110	-4.1535	2.1179
H	3.6281	-2.7924	0.4641
C	3.6608	-3.1911	4.3272
H	3.1560	-1.0895	4.3834
C	3.9237	-4.2985	3.5113
H	4.1208	-5.0090	1.4781
H	3.6764	-3.2960	5.4106
H	4.1413	-5.2668	3.9583

Free Energy: -2982.780508 hartrees

Compound **$25_{OHquart}(NMe_4)_2$**

Cartesian Coordinates

Fe	2.2271	-0.3916	-1.3082
N	1.3173	1.3991	-1.4696
N	0.4161	-1.2867	-1.2271
C	1.1543	-3.6242	-1.1500
C	3.3104	2.8293	-1.6140
C	0.1806	-2.6409	-1.2446
C	-0.2790	3.0696	-1.6752
C	-1.8689	-1.6820	-1.2817
C	-0.8151	-0.6819	-1.2710
C	-0.0343	1.6530	-1.4852
C	0.9540	3.6650	-1.7989
C	-1.0285	0.6886	-1.3684
C	-1.2441	-2.9045	-1.2805
C	1.9386	2.6139	-1.6573
C	4.2706	1.8782	-1.2788
N	4.0078	0.5572	-1.0350
C	2.5120	-3.4036	-0.9286
N	3.1082	-2.1631	-0.8808
C	4.4234	-2.3749	-0.5522
C	4.6745	-3.7981	-0.3775
C	3.4694	-4.4382	-0.6253
C	5.3893	-1.3813	-0.4404
C	5.2033	-0.0246	-0.6881
C	6.2623	0.9589	-0.6817
C	5.6882	2.1552	-1.0802
H	-2.0578	1.0321	-1.3949
H	3.6459	3.8460	-1.7890
H	6.3954	-1.6962	-0.1874
H	0.8116	-4.6530	-1.1771
C	7.6787	0.7084	-0.2728
H	8.0713	1.5730	0.2784
H	7.7631	-0.1773	0.3665
H	8.3328	0.5576	-1.1447
C	3.1713	-5.8999	-0.5212
H	2.1015	-6.0877	-0.3848
H	3.4972	-6.4439	-1.4202
H	3.7091	-6.3356	0.3312
C	-1.8719	-4.2636	-1.2594
H	-1.4093	-4.9319	-1.9982
H	-1.7579	-4.7392	-0.2740
H	-2.9439	-4.1970	-1.4770
C	-3.3391	-1.4096	-1.2215
H	-3.5866	-0.4820	-1.7520
H	-3.8878	-2.2133	-1.7263
C	-3.8355	-1.3115	0.2351
H	-3.3495	-0.4636	0.7393
H	-3.5259	-2.2077	0.7914
C	-5.3686	-1.1575	0.4100
C	-1.6162	3.7376	-1.6261
H	-2.3925	3.0887	-2.0495
H	-1.6038	4.6491	-2.2352
C	-1.9985	4.1097	-0.1783
H	-2.0517	3.1983	0.4351
H	-1.2014	4.7234	0.2653
C	-3.3418	4.8775	-0.0102
C	6.2935	3.4682	-1.2222
C	7.6040	3.7456	-1.3702
C	5.9514	-4.3595	0.0282
C	6.3557	-5.6388	-0.1006
H	5.6025	4.3120	-1.2104
H	8.3623	2.9701	-1.4311
H	7.9388	4.7776	-1.4553
H	6.6517	-3.6593	0.4856
H	5.7441	-6.4010	-0.5748
H	7.3377	-5.9406	0.2583
O	-3.6682	5.1355	1.1875
O	-4.0107	5.1607	-1.0451
O	-5.7792	-1.0566	1.6041
O	-6.0970	-1.1262	-0.6272
C	1.2610	5.1196	-1.9771
H	0.3547	5.6749	-2.2432
H	1.6632	5.5575	-1.0515
H	2.0097	5.2790	-2.7647
O	2.4441	-0.5927	-3.2644
H	1.9545	0.1114	-3.7156
C	-8.9372	-1.9946	1.5610
H	-7.9211	-1.5877	1.4833
H	-9.6585	-1.2220	1.8396
H	-8.9698	-2.8206	2.2763
C	-10.7083	-3.1507	0.2882
H	-10.9712	-3.5339	-0.7007
H	-10.6814	-3.9617	1.0196
H	-11.4133	-2.3763	0.5994
C	-9.3362	-1.4110	-0.7966
H	-8.3170	-1.0144	-0.8341
H	-9.6364	-1.8215	-1.7640
H	-10.0553	-0.6595	-0.4614
C	-8.3321	-3.5799	-0.2189
H	-8.6496	-3.9797	-1.1852
H	-7.3624	-3.0828	-0.3004
H	-8.3189	-4.3689	0.5369
N	-9.3367	-2.5372	0.2093
C	-6.8770	4.0550	0.5883
H	-7.3474	4.2465	1.5563
H	-5.9806	4.6688	0.4559
H	-7.5919	4.2159	-0.2227
C	-5.4728	2.3470	1.6714
H	-5.9761	2.5749	2.6149
H	-5.1969	1.2906	1.6389
H	-4.6198	3.0149	1.5301
C	-5.8130	2.3035	-0.7753
H	-5.5259	1.2504	-0.7818
H	-6.5562	2.4946	-1.5541
H	-4.9607	2.9739	-0.9003
C	-7.6583	1.7149	0.7373
H	-8.3573	1.9193	-0.0775
H	-7.3124	0.6782	0.7132
H	-8.1154	1.9525	1.7010
N	-6.4582	2.6064	0.5560
C	2.3124	1.4024	1.6272

H	2.4852	2.0235	0.7540
N	2.0047	-0.0027	1.2248
C	0.9433	0.8409	1.7926
H	0.6094	0.5897	2.8004
H	0.1571	1.1384	1.1013
C	3.2355	1.7120	2.7592
C	4.5813	1.9826	2.4537
C	2.8328	1.7271	4.1036
C	5.5046	2.2509	3.4672
H	4.9021	1.9744	1.4148
C	3.7559	1.9962	5.1211
H	1.7936	1.5341	4.3583
C	5.0946	2.2568	4.8071
H	6.5429	2.4560	3.2120
H	3.4272	2.0066	6.1588
H	5.8114	2.4668	5.5988
C	2.4794	-1.0970	2.0921
C	1.4603	-2.2353	2.1228
H	2.6764	-0.7501	3.1185
H	3.4274	-1.4486	1.6712
C	2.0624	-3.5488	2.6334
H	0.6058	-1.9446	2.7520
H	1.0742	-2.3906	1.1134
C	1.0448	-4.6967	2.5960
H	2.9259	-3.8052	2.0039
H	2.4414	-3.4150	3.6583
H	1.4884	-5.6412	2.9388
H	0.1789	-4.4729	3.2353
H	0.6768	-4.8430	1.5714

Free Energy: -2982.768609 hartrees

Compound **26_{OMe}**

Cartesian Coordinates

Fe	1.2042	0.3289	-0.6921
N	-0.3163	-1.0905	-0.4799
N	-0.1023	1.7282	0.1518
C	1.4804	3.5699	0.5146
C	0.9815	-3.1312	-0.8970
C	0.1962	3.0329	0.4693
C	-2.4226	-2.0470	-0.4125
C	-2.0604	2.8766	0.6034
C	-1.4681	1.6076	0.2247
C	-1.6492	-0.8248	-0.2985
C	-1.5290	-3.0580	-0.6577
C	-2.1791	0.4263	0.0121
C	-1.0253	3.7685	0.7530
C	-0.2118	-2.4428	-0.6928
C	2.2722	-2.5925	-0.9108
N	2.5635	-1.2675	-0.7301
C	2.6835	2.9031	0.2553
N	2.7810	1.5770	-0.0989
C	4.1153	1.3014	-0.2585
C	4.9054	2.4989	0.0099
C	3.9984	3.5007	0.3271
C	4.6373	0.0460	-0.5772
C	3.9344	-1.1461	-0.7747
C	4.5439	-2.4380	-1.0055
C	3.5052	-3.3556	-1.0806
H	-3.2555	0.4774	0.1469
H	0.8925	-4.2041	-1.0366
H	5.7181	-0.0241	-0.6388
H	1.5510	4.6179	0.7901
C	6.0100	-2.6978	-1.1495
H	6.1887	-3.4548	-1.9243
H	6.5581	-1.7891	-1.4213
H	6.4448	-3.0846	-0.2155
C	4.2876	4.9321	0.6514
H	3.4125	5.5695	0.4841
H	4.5950	5.0537	1.7010
H	5.1127	5.3049	0.0304
C	-1.0933	5.2185	1.1197
H	-0.4433	5.4443	1.9763
H	-0.7624	5.8542	0.2857
H	-2.1169	5.5095	1.3799
C	-3.5332	3.1167	0.7325
H	-4.0081	2.2890	1.2743
H	-3.7230	4.0267	1.3115
C	-4.2003	3.2480	-0.6496
H	-3.9560	2.3773	-1.2739
H	-3.8041	4.1254	-1.1807
C	-5.7156	3.3745	-0.5802
C	-3.9112	-2.1188	-0.2848
H	-4.2434	-1.5131	0.5665
H	-4.2258	-3.1471	-0.0795
C	-4.6133	-1.6140	-1.5584
H	-4.2332	-0.6203	-1.8349
H	-4.3857	-2.2737	-2.4081
C	-6.1258	-1.5202	-1.4168
C	3.5518	-4.7906	-1.3051
C	4.6112	-5.6084	-1.1451
C	6.3546	2.5608	-0.0837
C	7.1676	3.4874	0.4611
H	2.6164	-5.2461	-1.6333
H	5.5747	-5.2563	-0.7877
H	4.5178	-6.6716	-1.3575
H	6.8250	1.7602	-0.6564
H	6.7974	4.3015	1.0777
H	8.2435	3.4285	0.3082
O	-6.7884	-1.0328	-2.5097
O	-6.7635	-1.8325	-0.4351
O	-6.3551	3.4302	-1.7878
O	-6.3733	3.4258	0.4358
C	-1.8010	-4.5176	-0.8365
H	-2.8695	-4.7324	-0.7259
H	-1.4837	-4.8646	-1.8303
H	-1.2554	-5.1107	-0.0903
H	-6.1627	-0.8231	-3.2227

H	-5.7149	3.3777	-2.5167
C	1.1334	-0.2480	3.6625
C	0.0087	-0.4992	2.7352
H	1.3853	0.7798	3.9379
H	1.3978	-1.0219	4.3879
H	-0.5173	0.3724	2.3433
C	-0.8006	-1.7500	2.7803
C	-2.1916	-1.6549	2.9326
C	-0.2067	-3.0151	2.6724
C	-2.9779	-2.8084	2.9926
H	-2.6581	-0.6725	2.9869
C	-0.9938	-4.1684	2.7252
H	0.8683	-3.0836	2.5257
C	-2.3809	-4.0696	2.8867
H	-4.0571	-2.7225	3.1026
H	-0.5255	-5.1462	2.6272
H	-2.9932	-4.9688	2.9180
O	1.0721	0.8343	-2.4894
C	1.0891	2.1705	-2.9466
H	1.0044	2.1915	-4.0459
H	0.2501	2.7471	-2.5183
H	2.0259	2.6783	-2.6567
O	1.3787	-0.5971	2.2850

Free Energy: -2457.671314 hartrees

Compound **27**$_{\mathbf{OMe}}$

Cartesian Coordinates

Fe	-0.9131	0.4308	-0.5634
N	0.7032	1.7361	-0.4105
N	0.4467	-1.0882	-0.9609
C	-1.1315	-2.8154	-1.7141
C	-0.4975	3.8798	-0.3993
C	0.1388	-2.3745	-1.3416
C	2.8030	2.5277	0.1581
C	2.3394	-2.4085	-0.8013
C	1.7794	-1.0806	-0.6362
C	2.0037	1.3614	-0.1628
C	1.9667	3.6169	0.0796
C	2.4883	0.0536	-0.2340
C	1.3201	-3.2151	-1.2527
C	0.6548	3.1040	-0.2699
C	-1.7952	3.4224	-0.6504
N	-2.1308	2.1050	-0.8324
C	-2.3192	-2.0750	-1.7162
N	-2.4092	-0.7367	-1.3947
C	-3.7349	-0.3926	-1.4867
C	-4.5271	-1.5612	-1.8439
C	-3.6291	-2.6100	-2.0023
C	-4.2305	0.8980	-1.2790
C	-3.4995	2.0596	-1.0057
C	-4.0595	3.3899	-0.9071
C	-2.9932	4.2527	-0.6883
H	3.5355	-0.0906	0.0167
H	-0.3716	4.9470	-0.2463
H	-5.3049	1.0198	-1.3705
H	-1.2113	-3.8611	-1.9938
C	-5.5048	3.7435	-1.0590
H	-5.6113	4.6846	-1.6145
H	-6.0607	2.9632	-1.5897
H	-5.9865	3.8914	-0.0808
C	-3.9190	-4.0248	-2.3800
H	-3.0604	-4.4911	-2.8765
H	-4.1506	-4.6084	-1.4768
H	-4.7854	-4.0767	-3.0510
C	1.3595	-4.6773	-1.5671
H	0.6260	-5.2280	-0.9612
H	1.1143	-4.8651	-2.6221
H	2.3526	-5.0951	-1.3693
C	3.7739	-2.7601	-0.5546
H	4.1304	-2.2737	0.3620
H	3.8825	-3.8396	-0.4054
C	4.6679	-2.3172	-1.7283
H	4.4993	-1.2554	-1.9545
H	4.4000	-2.8700	-2.6402
C	6.1532	-2.5244	-1.4682
C	4.2721	2.4996	0.4478
H	4.5220	1.6321	1.0706
H	4.5662	3.3915	1.0118
C	5.0958	2.4287	-0.8517
H	4.7584	1.5845	-1.4697
H	4.9345	3.3326	-1.4559
C	6.5904	2.2659	-0.6130
C	-2.9871	5.6981	-0.5396
C	-4.0296	6.4887	-0.2164
C	-5.9729	-1.5575	-1.9954
C	-6.7926	-2.6207	-1.8859
H	-2.0235	6.1835	-0.7013
H	-5.0186	6.0945	-0.0009
H	-3.8965	7.5662	-0.1424
H	-6.4268	-0.5870	-2.2019
H	-6.4251	-3.6127	-1.6375
H	-7.8659	-2.5045	-2.0236
O	7.3627	2.2259	-1.7408
O	7.1245	2.1612	0.4692
O	6.9906	-2.0444	-2.4369
O	6.6289	-3.0776	-0.5013
C	2.2940	5.0574	0.3200
H	3.3521	5.1814	0.5746
H	2.0834	5.6679	-0.5693
H	1.6930	5.4660	1.1445
H	6.8130	2.3249	-2.5360
H	6.4828	-1.6270	-3.1525
C	-2.5698	-0.5544	1.9728
C	-1.5507	-1.5968	1.6910
H	-3.3985	-0.4235	1.2805
H	-2.7696	-0.2864	3.0093
N	-1.2405	-0.1354	1.4641
C	-0.3671	0.5668	2.4406
C	-0.8353	2.0076	2.6323
H	0.6467	0.5394	2.0273
H	-0.3596	0.0307	3.3985

C	0.2516	2.8896	3.2572
H	-1.1147	2.4253	1.6611
H	-1.7383	2.0192	3.2591
C	-0.2150	4.3426	3.4145
H	0.5473	2.4815	4.2354
H	1.1415	2.8566	2.6132
H	0.5777	4.9749	3.8357
H	-0.5038	4.7573	2.4392
H	-1.0896	4.4028	4.0774
C	-0.8104	-2.3602	2.7330
C	0.4381	-2.9073	2.3928
C	-1.3211	-2.5583	4.0218
C	1.1700	-3.6333	3.3347
H	0.8324	-2.7602	1.3897
C	-0.5916	-3.2927	4.9642
H	-2.2922	-2.1452	4.2848
C	0.6557	-3.8284	4.6237
H	2.1382	-4.0500	3.0632
H	-0.9979	-3.4472	5.9618
H	1.2231	-4.3978	5.3574
H	-1.6622	-2.1274	0.7509
O	-3.5807	-4.2545	1.0486
C	-2.4282	-4.9417	0.7788
H	-1.5185	-4.5028	1.2519
H	-2.4764	-5.9860	1.1812
H	-2.2093	-5.0567	-0.3097

Free Energy: -2594.836212 hartrees

Transition State **$TS_{27\text{-}28OMe}$**
Imaginary Frequency at -356 cm^{-1}
Cartesian Coordinates

Fe	-0.9878	0.2720	-0.5778
N	0.5118	1.7186	-0.5156
N	0.5110	-1.1284	-0.9929
C	-0.9145	-3.0183	-1.6471
C	-0.8851	3.7434	-0.5076
C	0.3178	-2.4469	-1.3317
C	2.5235	2.7040	0.0678
C	2.5212	-2.2643	-0.8374
C	1.8404	-0.9903	-0.6915
C	1.8404	1.4683	-0.2593
C	1.5864	3.7086	-0.0065
C	2.4450	0.2112	-0.3174
C	1.5751	-3.1732	-1.2475
C	0.3312	3.0754	-0.3665
C	-2.1333	3.1701	-0.7665
N	-2.3484	1.8259	-0.9219
C	-2.1653	-2.3887	-1.6487
N	-2.3698	-1.0518	-1.3754
C	-3.7221	-0.8272	-1.4677
C	-4.4112	-2.0729	-1.7748
C	-3.4247	-3.0450	-1.9001
C	-4.3303	0.4216	-1.3091
C	-3.7063	1.6528	-1.0859
C	-4.3847	2.9305	-1.0206
C	-3.4015	3.8895	-0.8221
H	3.5019	0.1689	-0.0696
H	-0.8574	4.8180	-0.3565
H	-5.4115	0.4444	-1.3961
H	-0.9035	-4.0785	-1.8779
C	-5.8564	3.1466	-1.1778
H	-6.0492	4.0675	-1.7435
H	-6.3357	2.3118	-1.7006
H	-6.3518	3.2590	-0.2017
C	-3.5962	-4.4916	-2.2346
H	-2.6824	-4.9182	-2.6624
H	-3.8502	-5.0761	-1.3379
H	-4.4143	-4.6259	-2.9537
C	1.7415	-4.6343	-1.5226
H	1.0758	-5.2313	-0.8827
H	1.4912	-4.8756	-2.5653
H	2.7728	-4.9538	-1.3375
C	3.9845	-2.4744	-0.6002
H	4.2961	-1.9574	0.3162
H	4.1977	-3.5385	-0.4532
C	4.8279	-1.9468	-1.7758
H	4.5637	-0.9035	-1.9969
H	4.6072	-2.5173	-2.6895
C	6.3271	-2.0158	-1.5212
C	3.9895	2.8116	0.3548
H	4.3142	1.9850	0.9986
H	4.2059	3.7398	0.8947
C	4.8139	2.7783	-0.9459
H	4.5391	1.9003	-1.5473
H	4.5836	3.6563	-1.5660
C	6.3170	2.7360	-0.7100
C	-3.5236	5.3323	-0.7023
C	-4.6318	6.0322	-0.3886
C	-5.8511	-2.1969	-1.9264
C	-6.5812	-3.3252	-1.8303
H	-2.6075	5.8980	-0.8784
H	-5.5802	5.5542	-0.1602
H	-4.5964	7.1186	-0.3359
H	-6.3880	-1.2685	-2.1261
H	-6.1393	-4.2890	-1.5936
H	-7.6601	-3.2924	-1.9689
O	7.0865	2.6964	-1.8397
O	6.8609	2.7292	0.3723
O	7.1136	-1.4854	-2.5060
O	6.8544	-2.4908	-0.5396
C	1.7736	5.1733	0.2377
H	2.8080	5.3938	0.5224
H	1.5346	5.7603	-0.6603
H	1.1134	5.5271	1.0418
H	6.5290	2.7109	-2.6354
H	6.5671	-1.1382	-3.2303
C	-2.3820	-0.8697	1.9697
C	-1.2901	-1.8408	1.7897
H	-3.2356	-0.9590	1.2974
H	-2.6664	-0.6006	2.9891
N	-1.2531	-0.0913	1.4244

C	-0.5458	0.7739	2.3847
C	-1.3190	2.0797	2.6095
H	0.4412	0.9905	1.9634
H	-0.3954	0.2533	3.3398
C	-0.4391	3.1630	3.2449
H	-1.6863	2.4445	1.6455
H	-2.1988	1.8863	3.2399
C	-1.1850	4.4967	3.3823
H	-0.0829	2.8257	4.2298
H	0.4509	3.3020	2.6142
H	-0.5424	5.2724	3.8199
H	-1.5238	4.8470	2.3975
H	-2.0712	4.3851	4.0227
C	-0.3479	-2.2876	2.8122
C	0.8537	-2.8917	2.3932
C	-0.5876	-2.1333	4.1902
C	1.7999	-3.3151	3.3284
H	1.0468	-3.0079	1.3299
C	0.3569	-2.5625	5.1251
H	-1.5201	-1.6887	4.5289
C	1.5550	-3.1513	4.6976
H	2.7275	-3.7728	2.9895
H	0.1582	-2.4414	6.1881
H	2.2907	-3.4820	5.4281
H	-1.2160	-2.3097	0.8204
O	-2.6491	-4.0542	1.8565
C	-1.7461	-4.9607	1.3608
H	-0.7647	-4.9536	1.8941
H	-2.1284	-6.0069	1.4587
H	-1.5218	-4.8282	0.2743

Free Energy: -2594.826728 hartrees

Compound **28**$_{\mathbf{OMe}}$

Cartesian Coordinates

Fe	0.9674	0.1923	-0.6339
N	-0.3599	-1.4171	-0.8759
N	-0.6838	1.4786	-0.7872
C	0.5160	3.6182	-0.8678
C	1.2862	-3.2216	-1.0975
C	-0.6384	2.8508	-0.7172
C	-2.2523	-2.7156	-0.5683
C	-2.8058	2.2967	-0.3574
C	-1.9899	1.1158	-0.5714
C	-1.7139	-1.3693	-0.6628
C	-1.1938	-3.5762	-0.7302
C	-2.4607	-0.1985	-0.5225
C	-1.9659	3.3809	-0.4510
C	-0.0128	-2.7445	-0.9175
C	2.4425	-2.4587	-1.3001
N	2.4701	-1.0913	-1.3488
C	1.8123	3.1524	-1.1228
N	2.1532	1.8251	-1.2313
C	3.5019	1.7746	-1.4708
C	4.0494	3.1289	-1.5204
C	2.9812	3.9876	-1.3040
C	4.2434	0.5980	-1.6072
C	3.7837	-0.7214	-1.5403
C	4.6268	-1.8948	-1.6189
C	3.7924	-2.9909	-1.4551
H	-3.5208	-0.3235	-0.3205
H	1.4054	-4.3006	-1.0722
H	5.3113	0.7179	-1.7584
H	0.3910	4.6934	-0.7782
C	6.1051	-1.8924	-1.8477
H	6.3989	-2.7532	-2.4620
H	6.4344	-0.9768	-2.3516
H	6.6589	-1.9688	-0.8997
C	2.9927	5.4833	-1.2884
H	1.9944	5.8970	-1.4681
H	3.3480	5.8726	-0.3224
H	3.6735	5.8693	-2.0588
C	-2.3027	4.8328	-0.3130
H	-1.6611	5.3192	0.4345
H	-2.1568	5.3672	-1.2629
H	-3.3463	4.9661	-0.0075
C	-4.2852	2.2720	-0.1256
H	-4.5430	1.4832	0.5924
H	-4.6195	3.2195	0.3101
C	-5.0536	2.0171	-1.4359
H	-4.6599	1.1242	-1.9405
H	-4.9019	2.8534	-2.1337
C	-6.5509	1.8338	-1.2342
C	-3.7030	-3.0338	-0.3744
H	-4.1281	-2.3980	0.4129
H	-3.8256	-4.0713	-0.0456
C	-4.5053	-2.8152	-1.6708
H	-4.3209	-1.8068	-2.0664
H	-4.1681	-3.5147	-2.4493
C	-6.0065	-2.9899	-1.4914
C	4.1185	-4.4066	-1.4380
C	5.3220	-4.9589	-1.1885
C	5.4451	3.4382	-1.7814
C	6.0876	4.5937	-1.5186
H	3.2873	-5.0853	-1.6354
H	6.1971	-4.3646	-0.9413
H	5.4438	-6.0402	-1.2080
H	6.0290	2.6356	-2.2345
H	5.6016	5.4372	-1.0365
H	7.1402	4.7041	-1.7720
O	-6.7644	-2.7248	-2.5988
O	-6.5596	-3.3347	-0.4702
O	-7.2552	1.4833	-2.3531
O	-7.1435	1.9731	-0.1868
C	-1.2017	-5.0732	-0.7301
H	-2.1946	-5.4604	-0.4759
H	-0.9246	-5.4724	-1.7165

H	-0.4803	-5.4745	-0.0047
H	-6.2004	-2.4583	-3.3437
H	-6.6625	1.3996	-3.1185
C	1.2545	1.3385	2.0930
C	-0.1865	1.6009	2.6064
H	1.5481	2.2197	1.5055
H	1.9253	1.2628	2.9644
N	1.3271	0.1549	1.2623
C	1.7628	-1.0745	1.9095
C	3.2974	-1.1941	1.9914
H	1.3813	-1.9228	1.3259
H	1.3332	-1.1521	2.9209
C	3.7453	-2.5867	2.4501
H	3.7136	-0.9909	0.9984
H	3.6920	-0.4264	2.6737
C	5.2719	-2.7414	2.4236
H	3.3645	-2.7851	3.4636
H	3.2903	-3.3374	1.7869
H	5.5815	-3.7460	2.7422
H	5.6531	-2.5732	1.4071
H	5.7506	-2.0089	3.0889
C	-0.6708	0.4740	3.4980
C	-1.4704	-0.5420	2.9605
C	-0.2483	0.3788	4.8317
C	-1.8306	-1.6502	3.7346
H	-1.7912	-0.4707	1.9245
C	-0.6170	-0.7202	5.6136
H	0.3688	1.1716	5.2502
C	-1.4030	-1.7429	5.0644
H	-2.4441	-2.4380	3.3003
H	-0.2860	-0.7852	6.6488
H	-1.6830	-2.6020	5.6713
H	-0.8446	1.6646	1.7294
O	-0.1552	2.8757	3.2680
C	-1.4714	3.3835	3.5109
H	-2.0310	2.7314	4.2008
H	-1.3537	4.3752	3.9613
H	-2.0340	3.4689	2.5660

Free Energy: -2594.890174 hartrees

Compound **CO_2**
Cartesian Coordinates

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.168139
O	0.000000	0.000000	-1.168139

Free Energy: -188.561534 hartrees

Compound **14**
Cartesian Coordinates

C	-0.144510	3.390337	-1.095617
C	1.372072	3.137716	-1.255932
H	-0.451336	3.362261	-0.044428
H	-0.443405	4.353416	-1.533226
H	1.743863	2.537160	-0.417428
N	-0.701875	2.272229	-1.846691
C	2.213009	4.373539	-1.425422
C	3.245360	4.648336	-0.519227
C	1.968845	5.265064	-2.482679
C	4.021812	5.805017	-0.658367
H	3.439504	3.953703	0.296668
C	2.749580	6.413605	-2.629748
H	1.174189	5.052260	-3.195247
C	3.775778	6.688159	-1.714788
H	4.819148	6.011411	0.052750
H	2.557853	7.097060	-3.454526
H	4.381010	7.585375	-1.828387
C	0.210966	1.760907	-2.723831
C	-2.140915	2.123343	-2.052729
C	-2.735761	3.195493	-2.976791
H	-2.624476	2.157278	-1.067849
H	-2.306349	1.127363	-2.478203
C	-4.245354	3.004956	-3.170852
H	-2.544948	4.193350	-2.556830
H	-2.226013	3.147382	-3.949576
C	-4.853415	4.069786	-4.093959
H	-4.431387	2.003205	-3.586116
H	-4.742097	3.037107	-2.189510
H	-5.933203	3.917204	-4.222202
H	-4.697259	5.076237	-3.680969
H	-4.383357	4.036302	-5.086734
O	0.030086	0.952878	-3.620184
O	1.456084	2.287060	-2.454869

Free Energy: -710.369852 hartrees

Compound **29_{OMe}**

Cartesian Coordinates

Fe	-0.1042	1.1465	0.4259
N	-1.9317	1.6907	-0.4429
N	-1.0815	-0.5202	1.2079
C	0.6572	-1.2958	2.7577
C	-1.3301	3.9430	-1.2136
C	-0.5247	-1.4640	2.0445
C	-3.9983	1.5294	-1.4759
C	-2.4451	-2.3904	1.2821
C	-2.2560	-1.0601	0.7397
C	-3.0145	0.8690	-0.6389
C	-3.4872	2.7659	-1.7881
C	-3.1477	-0.4142	-0.1132
C	-1.3666	-2.6446	2.0965
C	-2.1885	2.8491	-1.1403
C	-0.1021	4.0901	-0.5627
N	0.4612	3.1476	0.2630
C	1.4824	-0.1686	2.7567
N	1.2671	0.9613	1.9973
C	2.3138	1.8144	2.2521
C	3.2259	1.2091	3.2132
C	2.6914	-0.0301	3.5319
C	2.4907	3.0594	1.6505
C	1.6412	3.6866	0.7363
C	1.8490	5.0028	0.1808
C	0.7591	5.2617	-0.6416
H	-4.0379	-0.9677	-0.3966
H	-1.6642	4.7706	-1.8315
H	3.3856	3.6059	1.9282
H	0.9657	-2.1272	3.3843
C	3.0034	5.9051	0.4805
H	2.6641	6.9467	0.5520
H	3.4979	5.6361	1.4199
H	3.7586	5.8667	-0.3188
C	3.2152	-1.0385	4.5025
H	2.4076	-1.6529	4.9162
H	3.9371	-1.7168	4.0261
H	3.7363	-0.5401	5.3289
C	-1.0785	-3.8714	2.9036
H	-0.0826	-4.2728	2.6711
H	-1.0971	-3.6518	3.9807
H	-1.8190	-4.6536	2.7050
C	-3.6394	-3.2531	1.0128
H	-3.8951	-3.2244	-0.0538
H	-3.4192	-4.2966	1.2602
C	-4.8627	-2.7895	1.8279
H	-5.0598	-1.7240	1.6504
H	-4.6596	-2.8883	2.9043
C	-6.1241	-3.5835	1.5180
C	-5.3348	0.9496	-1.8235
H	-5.2363	-0.1128	-2.0776
H	-5.7510	1.4506	-2.7042
C	-6.3196	1.0883	-0.6469
H	-5.8605	0.7126	0.2785
H	-6.5480	2.1477	-0.4642
C	-7.6280	0.3386	-0.8550
C	0.4547	6.4494	-1.4222
C	1.3224	7.3969	-1.8283
C	4.4407	1.8401	3.7017
C	5.5200	1.2112	4.2046
H	-0.5899	6.5706	-1.7112
H	2.3873	7.3422	-1.6211
H	0.9705	8.2498	-2.4053
H	4.4741	2.9282	3.6313
H	5.5838	0.1286	4.2687
H	6.3798	1.7829	4.5480
O	-8.5330	0.4501	0.1643
O	-7.9107	-0.3348	-1.8213
O	-7.2832	-3.0757	2.0356
O	-6.1680	-4.6077	0.8725
C	-4.1154	3.8519	-2.6044
H	-5.0324	3.4965	-3.0871
H	-4.3754	4.7182	-1.9790
H	-3.4311	4.2095	-3.3858
H	-8.1845	1.0193	0.8704
H	-7.1114	-2.2482	2.5147
C	1.8992	-3.1414	-1.2979
C	2.3617	-3.3108	-2.7638
H	0.8994	-3.5764	-1.2081
H	2.5746	-3.7012	-0.6480
N	1.8470	-1.7483	-0.8527
C	3.0579	-1.1000	-0.2933
C	3.9021	-1.9810	0.6281
H	2.7235	-0.2277	0.2699
H	3.6936	-0.7440	-1.1157
C	5.1182	-1.1974	1.1396
H	3.2935	-2.3364	1.4713
H	4.2723	-2.8615	0.0900
C	6.0868	-2.0778	1.9394
H	5.6480	-0.7701	0.2753
H	4.7797	-0.3541	1.7535
H	6.9351	-1.4939	2.3203
H	5.5830	-2.5418	2.7990
H	6.4827	-2.8882	1.3115
C	3.6892	-2.6246	-3.0246
C	3.7240	-1.4083	-3.7178
C	4.8809	-3.1513	-2.5068
C	4.9273	-0.7097	-3.8699
H	2.7992	-1.0015	-4.1244
C	6.0855	-2.4607	-2.6600
H	4.8553	-4.1026	-1.9793
C	6.1101	-1.2323	-3.3345
H	4.9410	0.2395	-4.4023
H	7.0043	-2.8734	-2.2470
H	7.0473	-0.6907	-3.4474
H	1.5963	-2.8597	-3.4146
O	2.4042	-4.7284	-2.9825
C	2.5628	-5.0636	-4.3648
H	3.5231	-4.6945	-4.7587
H	2.5365	-6.1565	-4.4318
H	1.7431	-4.6367	-4.9676
C	0.7918	-0.9906	-1.3206
O	-0.1321	-1.4769	-1.9854
O	0.8408	0.3096	-1.0058

Free energy: 2783.436513 hartrees

Compound **$27_{OH}(NMe_4)_2$**

Cartesian Coordinates

Fe	2.0278	0.6441	-0.9393
N	0.5800	2.1041	-0.7431
C	1.9870	3.8841	0.2032
C	0.8667	-1.7878	-2.4477
C	-1.4831	3.1207	-0.4585
C	-1.3812	-1.4980	-2.5010
C	-0.7119	-0.3111	-2.0017
C	-0.7718	1.9531	-0.9456
C	-0.5302	3.9788	0.0455
C	-1.3623	0.8326	-1.5334
C	-0.3956	-2.4195	-2.7741
C	0.7537	3.3335	-0.1460
C	3.2515	3.3153	0.0199
N	3.4766	2.0725	-0.5219
C	3.3529	-1.8606	-2.1956
N	3.5328	-0.5893	-1.6935
C	4.8818	-0.4330	-1.4835
C	5.5890	-1.6499	-1.8614
C	4.6203	-2.5446	-2.2986
C	5.4804	0.7252	-0.9858
C	4.8446	1.8893	-0.5468
C	5.5156	3.0491	-0.0084
C	4.5198	3.9517	0.3470
H	-2.4453	0.8418	-1.6152
H	1.9541	4.8735	0.6493
H	6.5623	0.7179	-0.9134
H	2.1126	-3.4233	-2.9198
C	6.9924	3.1996	0.1648
H	7.2107	3.7359	1.0968
H	7.4934	2.2270	0.2034
H	7.4372	3.7798	-0.6578
C	4.8122	-3.9613	-2.7376
H	3.8875	-4.5412	-2.6447
H	5.1409	-4.0191	-3.7859
H	5.5886	-4.4443	-2.1301
C	-0.5596	-3.8235	-3.2673
H	0.0938	-4.0254	-4.1271
H	-0.3000	-4.5512	-2.4844
H	-1.5960	-4.0106	-3.5692
C	-2.8625	-1.6950	-2.5668
H	-3.3630	-0.7634	-2.8573
H	-3.1124	-2.4373	-3.3335
C	-3.4204	-2.1664	-1.2080
H	-3.1793	-1.4185	-0.4398
H	-2.9089	-3.0884	-0.8979
C	-4.9516	-2.4274	-1.1625
C	-2.9702	3.2786	-0.4335
H	-3.4188	2.8465	-1.3362
H	-3.2383	4.3413	-0.4267
C	-3.5777	2.5941	0.8075
H	-3.2889	1.5335	0.8084
H	-3.1416	3.0243	1.7199
C	-5.1248	2.6667	0.9296
C	4.6408	5.2648	0.9578
N	0.6526	-0.5045	-1.9893
C	2.1117	-2.4054	-2.5418
C	5.7285	6.0598	0.9635
C	7.0232	-1.8383	-1.7255
C	7.7810	-2.7655	-2.3434
H	3.7448	5.6382	1.4554
H	6.6534	5.7890	0.4623
H	5.6983	7.0243	1.4664
H	7.5282	-1.1473	-1.0494
H	7.3718	-3.4728	-3.0591
H	8.8508	-2.8149	-2.1501
O	-5.6146	2.1188	1.9650
O	-5.7766	3.2317	0.0062
O	-5.4091	-2.7851	-0.0335
O	-5.6235	-2.2558	-2.2187
C	-0.7420	5.3103	0.6960
H	-1.7810	5.6380	0.5808
H	-0.5199	5.2658	1.7723
H	-0.0866	6.0775	0.2614
C	-5.9672	1.0568	-2.5220
H	-5.9957	1.4697	-3.5339
H	-5.5127	1.7649	-1.8247
H	-5.4685	0.0847	-2.5125
C	-7.3851	0.2694	-0.6740
H	-6.8986	0.9982	-0.0221
H	-8.4240	0.1131	-0.3713
H	-6.8442	-0.6788	-0.7010
C	-8.1294	2.1491	-2.0751
H	-8.1101	2.5486	-3.0923
H	-9.1582	1.9605	-1.7582
H	-7.6147	2.8131	-1.3761
C	-8.0648	-0.1418	-3.0021
H	-8.0463	0.2794	-4.0105
H	-7.5053	-1.0791	-2.9513
H	-9.0952	-0.2765	-2.6632
C	-6.7244	-0.9661	2.4041
H	-6.6902	-1.5699	1.4942
H	-7.5641	-1.2544	3.0418
H	-6.7457	0.1025	2.1769
C	-5.4399	-0.4143	4.4273
H	-6.3054	-0.6975	5.0315
H	-4.5116	-0.6219	4.9653
H	-5.4918	0.6359	4.1298
C	-4.2681	-0.8440	2.3118
H	-3.3593	-1.0469	2.8828
H	-4.3159	-1.4549	1.4069
H	-4.3755	0.2214	2.0956
C	-5.3644	-2.7045	3.4864
H	-5.3564	-3.2431	2.5355
H	-4.4409	-2.8820	4.0414
H	-6.2344	-2.9781	4.0887
N	-5.4495	-1.2364	3.1670
N	-7.3923	0.8352	-2.0732

C	3.1630	-0.4727	1.6562
H	3.9847	-0.0843	1.0611
C	2.2202	0.5310	2.1948
H	1.6712	0.2932	3.1023
H	2.4208	1.5866	2.0263
N	1.8281	-0.2316	0.9824
C	0.7404	-1.2573	1.0544
C	0.1598	-1.6137	2.4231
H	1.1344	-2.1568	0.5676
H	-0.0687	-0.8719	0.4283
C	-0.9033	-2.7115	2.2691
H	0.9436	-1.9643	3.1019
H	-0.2992	-0.7236	2.8760
C	-1.4769	-3.1499	3.6224
H	-1.7088	-2.3516	1.6139
H	-0.4537	-3.5785	1.7637
H	-2.2521	-3.9167	3.4970
H	-0.6853	-3.5646	4.2611
H	-1.9182	-2.2969	4.1576
C	3.4370	-1.8034	2.2666
C	3.6962	-2.8864	1.4116
C	3.4559	-2.0009	3.6533
C	3.9505	-4.1563	1.9380
H	3.6985	-2.7308	0.3346
C	3.7162	-3.2693	4.1812
H	3.2686	-1.1581	4.3148
C	3.9582	-4.3509	3.3248
H	4.1456	-4.9911	1.2673
H	3.7313	-3.4139	5.2599
H	4.1577	-5.3383	3.7366
O	5.7474	1.0430	2.7804
H	5.3430	1.6398	2.1335

Free Energy: -2982.738596 hartrees

Transition State $\mathbf{TS_{27\text{-}28OH}(NMe_4)_2}$
Imaginary Frequency at -227 cm^{-1}
Cartesian Coordinates

Fe	1.9850	0.5299	-0.7339
N	0.4621	1.9735	-0.7736
N	0.6491	-0.7698	-1.6484
C	2.2081	-2.6200	-2.0916
C	1.7845	3.8732	0.0369
C	0.9283	-2.0835	-1.9629
C	-1.6351	2.9594	-0.6933
C	-1.3318	-1.9080	-2.0355
C	-0.7205	-0.6390	-1.6863
C	-0.8738	1.7560	-0.9980
C	-0.7290	3.8897	-0.2430
C	-1.4184	0.5401	-1.4137
C	-0.3038	-2.8111	-2.1918
C	0.5796	3.2585	-0.3037
C	3.0723	3.3480	-0.1149
N	3.3527	2.1068	-0.6354
C	3.4249	-1.9408	-1.9652
N	3.5432	-0.6189	-1.6027
C	4.8805	-0.3195	-1.6213
C	5.6498	-1.4911	-2.0327
C	4.7284	-2.5107	-2.2246
C	5.4208	0.9029	-1.2179
C	4.7272	2.0096	-0.7194
C	5.3453	3.2076	-0.2031
C	4.3109	4.0565	0.1735
H	-2.4988	0.5000	-1.5176
H	1.7107	4.8875	0.4176
H	6.5005	0.9959	-1.2543
H	2.2596	-3.6694	-2.3664
C	6.8174	3.4350	-0.0678
H	7.0315	3.9953	0.8513
H	7.3671	2.4884	-0.0294
H	7.2161	4.0249	-0.9068
C	4.9983	-3.9383	-2.5784
H	4.1644	-4.5886	-2.2926
H	5.1681	-4.0643	-3.6582
H	5.9038	-4.2907	-2.0671
C	-0.3995	-4.2676	-2.5247
H	0.2617	-4.5317	-3.3613
H	-0.1032	-4.8905	-1.6680
H	-1.4257	-4.5375	-2.7975
C	-2.8029	-2.1628	-2.1286
H	-3.3091	-1.2964	-2.5706
H	-2.9960	-3.0103	-2.7962
C	-3.4256	-2.4587	-0.7494
H	-3.2406	-1.6094	-0.0766
H	-2.9192	-3.3196	-0.2904
C	-4.9541	-2.7451	-0.7538
C	-3.1206	3.0988	-0.8194
H	-3.4803	2.5433	-1.6943
H	-3.3844	4.1496	-0.9878
C	-3.8606	2.5879	0.4319
H	-3.5738	1.5433	0.6167
H	-3.5320	3.1496	1.3176
C	-5.4132	2.6518	0.3630
C	4.3727	5.3810	0.7688
C	5.4156	6.2337	0.7455
C	7.0983	-1.5248	-2.1370
C	7.8470	-2.4394	-2.7850
H	3.4678	5.7093	1.2820
H	6.3434	6.0086	0.2272
H	5.3439	7.1999	1.2413
H	7.6277	-0.7145	-1.6344
H	7.4118	-3.2618	-3.3454
H	8.9324	-2.3607	-2.7785
O	-6.0253	2.2462	1.3994
O	-5.9511	3.0692	-0.7015
O	-5.4679	-2.9757	0.3838
O	-5.5693	-2.7161	-1.8576
C	-0.9955	5.2871	0.2243
H	-2.0493	5.5496	0.0793
H	-0.7632	5.3999	1.2934

H	-0.3797	6.0173	-0.3193
C	-5.9010	0.4770	-2.7907
H	-5.8318	0.7070	-3.8572
H	-5.5262	1.3079	-2.1880
H	-5.3961	-0.4645	-2.5620
C	-7.4859	-0.0335	-0.9823
H	-7.0732	0.8034	-0.4148
H	-8.5478	-0.1660	-0.7579
H	-6.9340	-0.9591	-0.8045
C	-8.1069	1.5717	-2.7415
H	-7.9988	1.7925	-3.8066
H	-9.1588	1.4143	-2.4896
H	-7.6642	2.3572	-2.1236
C	-7.9286	-0.8372	-3.2648
H	-7.8149	-0.5848	-4.3221
H	-7.3676	-1.7388	-3.0072
H	-8.9861	-0.9426	-3.0091
C	-7.1021	-0.8163	2.2969
H	-6.9524	-1.5688	1.5187
H	-7.9722	-1.0505	2.9160
H	-7.1740	0.1898	1.8768
C	-6.0278	0.2055	4.2564
H	-6.9328	-0.0122	4.8292
H	-5.1464	0.1621	4.9008
H	-6.0991	1.1746	3.7563
C	-4.6615	-0.5273	2.3506
H	-3.7988	-0.5015	3.0184
H	-4.5729	-1.3194	1.6034
H	-4.8349	0.4519	1.8994
C	-5.7299	-2.2083	3.7917
H	-5.6176	-2.9184	2.9688
H	-4.8407	-2.2030	4.4265
H	-6.6230	-2.4253	4.3832
N	-5.8812	-0.8403	3.1841
N	-7.3613	0.2956	-2.4501
C	4.0308	-0.3863	1.7781
H	4.5195	-0.1290	0.8510
C	2.8707	0.4700	2.1317
H	2.5292	0.3447	3.1640
H	3.0842	1.5267	1.9536
N	1.9024	-0.0364	1.1426
C	0.9911	-1.0745	1.6125
C	0.0406	-0.6267	2.7377
H	1.5559	-1.9526	1.9715
H	0.3989	-1.4078	0.7533
C	-0.9412	-1.7476	3.1115
H	0.6191	-0.3495	3.6297
H	-0.5092	0.2698	2.4181
C	-1.6563	-1.4745	4.4416
H	-1.6727	-1.8746	2.3008
H	-0.3918	-2.6980	3.1881
H	-2.4070	-2.2452	4.6612
H	-0.9323	-1.4598	5.2678
H	-2.1556	-0.4960	4.4301
C	4.2147	-1.7388	2.2321
C	5.0081	-2.6145	1.4523
C	3.6189	-2.2320	3.4153
C	5.1922	-3.9386	1.8394
H	5.4547	-2.2422	0.5331
C	3.8119	-3.5568	3.8037
H	3.0136	-1.5710	4.0297
C	4.5957	-4.4131	3.0177
H	5.7951	-4.6054	1.2265
H	3.3507	-3.9263	4.7170
H	4.7401	-5.4480	3.3212
O	5.7938	0.8620	2.8237
H	5.5403	1.6191	2.2714

Free Energy: --2982.729987 hartrees

Compound **$28_{OH}(NMe_4)_2$**

Cartesian Coordinates

Fe	2.2696	0.3342	-0.8178
N	0.9374	1.8810	-1.2781
N	0.9379	-0.9456	-1.8207
C	2.3822	-2.9288	-1.9637
C	2.3658	3.7835	-0.6472
C	1.1534	-2.2798	-2.0744
C	-1.0925	2.9974	-1.3258
C	-1.0792	-1.9735	-2.3210
C	-0.4094	-0.7301	-1.9654
C	-0.4100	1.7240	-1.4900
C	-0.1250	3.9243	-1.0163
C	-1.0315	0.5113	-1.8019
C	-0.1012	-2.9355	-2.3978
C	1.1386	3.2102	-0.9834
C	3.5946	3.1337	-0.4881
N	3.7902	1.7896	-0.6603
C	3.6018	-2.3827	-1.5455
N	3.7947	-1.0603	-1.2080
C	5.1057	-0.9312	-0.8285
C	5.7804	-2.2212	-0.9229
C	4.8282	-3.1271	-1.3722
C	5.7068	0.2706	-0.4441
C	5.1128	1.5353	-0.3830
C	5.7964	2.7628	-0.0298
C	4.8511	3.7755	-0.1055
H	-2.1093	0.5398	-1.9353
H	2.3491	4.8539	-0.4646
H	6.7608	0.2250	-0.1908
H	2.3801	-3.9890	-2.1992
C	7.2349	2.8771	0.3646
H	7.3525	3.6122	1.1717
H	7.6380	1.9180	0.7084
H	7.8583	3.2199	-0.4752
C	4.9966	-4.5966	-1.5977
H	4.0354	-5.1217	-1.5803
H	5.4750	-4.8052	-2.5665

H	5.6419	-5.0297	-0.8220
C	-0.2717	-4.3952	-2.6844
H	0.4546	-4.7478	-3.4294
H	-0.1239	-4.9984	-1.7760
H	-1.2802	-4.5999	-3.0617
C	-2.5596	-2.1738	-2.4157
H	-3.0590	-1.2457	-2.7179
H	-2.8006	-2.9248	-3.1776
C	-3.1157	-2.6308	-1.0506
H	-2.7430	-1.9549	-0.2715
H	-2.7026	-3.6201	-0.8056
C	-4.6610	-2.7268	-0.9339
C	-2.5781	3.1780	-1.3315
H	-3.0428	2.5695	-2.1176
H	-2.8401	4.2215	-1.5405
C	-3.1538	2.7619	0.0368
H	-2.8203	1.7397	0.2557
H	-2.7167	3.3884	0.8257
C	-4.6955	2.8041	0.1897
C	4.9969	5.1976	0.1553
C	6.1407	5.9104	0.1880
C	7.1701	-2.4446	-0.5624
C	7.9485	-3.4870	-0.9152
H	4.0683	5.7406	0.3379
H	7.1121	5.4694	-0.0169
H	6.1146	6.9762	0.4072
H	7.6242	-1.6730	0.0611
H	7.5988	-4.2869	-1.5617
H	8.9782	-3.5430	-0.5669
O	-5.1406	2.3709	1.2988
O	-5.3891	3.2370	-0.7729
O	-5.1162	-2.8375	0.2468
O	-5.3451	-2.6888	-1.9960
C	-0.3068	5.3767	-0.7002
H	-1.3330	5.6955	-0.9142
H	-0.1058	5.5794	0.3622
H	0.3790	6.0052	-1.2851
C	-5.7581	0.5366	-2.7230
H	-5.8806	0.7609	-3.7860
H	-5.2575	1.3609	-2.2095
H	-5.2430	-0.4170	-2.5847
C	-7.0022	0.0818	-0.6493
H	-6.4684	0.9077	-0.1729
H	-8.0103	-0.0123	-0.2363
H	-6.4591	-0.8616	-0.5553
C	-7.8878	1.6925	-2.2857
H	-7.9635	1.9055	-3.3553
H	-8.8824	1.5640	-1.8509
H	-7.3216	2.4690	-1.7640
C	-7.8730	-0.7236	-2.8041
H	-7.9542	-0.4782	-3.8661
H	-7.2945	-1.6381	-2.6483
H	-8.8661	-0.7993	-2.3535
C	-6.0089	-0.5506	2.6510
H	-6.1392	-1.3779	1.9486
H	-6.6830	-0.6416	3.5065
H	-6.1283	0.4146	2.1532
C	-4.3362	0.5467	4.0892
H	-5.0350	0.4784	4.9269
H	-3.3043	0.4803	4.4423
H	-4.4938	1.4606	3.5107
C	-3.6493	-0.5325	1.9875
H	-2.6262	-0.5982	2.3634
H	-3.8963	-1.3702	1.3304
H	-3.8361	0.4280	1.5041
C	-4.3705	-1.9167	3.8819
H	-4.5543	-2.7234	3.1683
H	-3.3367	-1.9422	4.2339
H	-5.0664	-1.9710	4.7226
N	-4.5899	-0.6139	3.1641
N	-7.1358	0.3977	-2.1194
C	2.9916	-1.9409	2.0682
H	3.2947	-2.2893	1.0721
C	2.8493	-0.3950	1.9994
H	2.6141	-0.0337	3.0146
H	3.8326	0.0036	1.7130
N	1.8493	0.0301	1.0420
C	0.5253	0.2916	1.5906
C	0.4029	1.6957	2.2136
H	0.2728	-0.4594	2.3556
H	-0.2141	0.1976	0.7854
C	-0.9513	1.8974	2.9024
H	1.2146	1.8428	2.9415
H	0.5346	2.4444	1.4231
C	-1.1528	3.3326	3.4028
H	-1.7513	1.6485	2.1948
H	-1.0384	1.1910	3.7421
H	-2.1296	3.4551	3.8901
H	-0.3717	3.6093	4.1250
H	-1.1005	4.0399	2.5635
C	1.6806	-2.6019	2.4401
C	0.8325	-3.0645	1.4244
C	1.2401	-2.6487	3.7714
C	-0.4430	-3.5504	1.7271
H	1.1679	-3.0171	0.3922
C	-0.0303	-3.1468	4.0796
H	1.8962	-2.2879	4.5608
C	-0.8789	-3.5913	3.0567
H	-1.0970	-3.8888	0.9264
H	-0.3633	-3.1793	5.1158
H	-1.8696	-3.9735	3.2948
O	4.0476	-2.1931	3.0214
H	4.1480	-3.1535	3.0840

Free Energy: -2982.802932 hartrees

Compound **$29_{OH}(NMe_4)_2$**

Cartesian Coordinates

Fe	-2.0915	1.2123	-0.6109
N	-0.8118	0.1585	-1.8599
N	-0.6065	2.6687	-0.4718
C	-1.9154	4.4540	0.5970

C	-2.3974	-1.4625	-2.8115
C	-0.7246	3.9015	0.1332
C	1.1511	-0.8594	-2.5586
C	1.4894	3.6417	-0.2826
C	0.7331	2.4824	-0.7238
C	0.5632	0.2674	-1.8591
C	0.1045	-1.6325	-3.0084
C	1.2702	1.3476	-1.3332
C	0.5775	4.5265	0.2449
C	-1.1119	-0.9866	-2.5665
C	-3.5933	-0.9282	-2.3307
N	-3.6810	0.1889	-1.5350
C	-3.1910	3.8864	0.5321
N	-3.4772	2.6663	-0.0460
C	-4.8325	2.4768	0.0766
C	-5.4336	3.6105	0.7665
C	-4.3960	4.4909	1.0481
C	-5.5324	1.3911	-0.4509
C	-5.0144	0.3438	-1.2147
C	-5.8007	-0.7072	-1.8177
C	-4.9165	-1.5011	-2.5353
H	2.3491	1.3180	-1.4424
H	-2.4630	-2.3638	-3.4126
H	-6.6057	1.3834	-0.2943
H	-1.8381	5.4315	1.0633
C	-7.2742	-0.8978	-1.6481
H	-7.5123	-1.9669	-1.5762
H	-7.6450	-0.3988	-0.7462
H	-7.8346	-0.4993	-2.5071
C	-4.4740	5.7976	1.7714
H	-3.5003	6.0973	2.1734
H	-4.8261	6.6026	1.1092
H	-5.1876	5.7306	2.6031
C	0.8568	5.8687	0.8464
H	0.1114	6.6121	0.5351
H	0.8376	5.8251	1.9456
H	1.8487	6.2246	0.5448
C	2.9770	3.8036	-0.3396
H	3.4148	3.0660	-1.0206
H	3.2332	4.7877	-0.7526
C	3.6287	3.6561	1.0571
H	3.1192	2.8703	1.6251
H	3.4828	4.5851	1.6269
C	5.1527	3.3524	1.0184
C	2.6124	-1.1665	-2.6511
H	3.2048	-0.2508	-2.5469
H	2.8572	-1.5860	-3.6340
C	3.0238	-2.1712	-1.5500
H	2.5343	-1.9051	-0.6077
H	2.6426	-3.1670	-1.8118
C	4.5537	-2.2932	-1.3110
C	-5.1763	-2.7010	-3.3131
C	-6.3584	-3.0966	-3.8243
C	-6.8478	3.7168	1.0834
C	-7.5293	4.8353	1.4004
H	-4.3120	-3.3387	-3.5021
H	-7.2665	-2.5094	-3.7211
H	-6.4283	-4.0272	-4.3840
H	-7.4094	2.7822	1.0530
H	-7.0665	5.8177	1.4218
H	-8.5920	4.7810	1.6288
O	4.9112	-2.5977	-0.1309
O	5.3195	-2.0772	-2.2930
O	5.6092	2.6530	1.9757
O	5.8169	3.8090	0.0453
C	0.1807	-2.9153	-3.7751
H	1.2046	-3.0976	-4.1199
H	-0.1218	-3.7693	-3.1517
H	-0.4832	-2.8999	-4.6500
C	6.0137	1.2489	-2.2054
H	6.2269	1.6631	-3.1942
H	5.4102	0.3418	-2.2884
H	5.5512	2.0039	-1.5650
C	7.0591	0.2885	-0.2020
H	6.4175	-0.5889	-0.3224
H	8.0190	0.0028	0.2367
H	6.5838	1.0681	0.4000
C	8.0081	-0.1802	-2.4237
H	8.1810	0.2519	-3.4128
H	8.9587	-0.4364	-1.9487
H	7.3417	-1.0461	-2.4778
C	8.2013	2.0815	-1.4406
H	8.3880	2.4727	-2.4441
H	7.6605	2.8084	-0.8255
H	9.1394	1.7761	-0.9701
C	5.3644	-0.6372	2.6986
H	5.8428	0.3273	2.5140
H	5.6086	-1.0116	3.6962
H	5.6203	-1.3703	1.9291
C	3.1618	-1.7194	2.8927
H	3.4645	-2.0833	3.8780
H	2.0888	-1.5202	2.8594
H	3.4613	-2.4184	2.1066
C	3.5137	0.0736	1.2526
H	2.4325	0.2192	1.2177
H	4.0523	1.0064	1.0976
H	3.8396	-0.6910	0.5500
C	3.4607	0.6134	3.6465
H	4.0077	1.5320	3.4128
H	2.3810	0.7544	3.5535
H	3.7184	0.2392	4.6409
N	3.8742	-0.4197	2.6318
N	7.3279	0.8604	-1.5719
C	-3.0900	-2.6880	1.7620
H	-3.2580	-1.7514	2.3152
C	-2.2258	-2.3611	0.5278
H	-2.1093	-3.2641	-0.0746
H	-2.7584	-1.6256	-0.0701
N	-0.9064	-1.8382	0.8782
C	0.2156	-2.7669	1.1077
C	0.3515	-3.8772	0.0670
H	0.1520	-3.2081	2.1125
H	1.1232	-2.1624	1.0722
C	1.6088	-4.7125	0.3419
H	-0.5178	-4.5460	0.0848
H	0.4079	-3.4276	-0.9326
C	1.8103	-5.8119	-0.7083
H	2.4890	-4.0559	0.3594

H	1.5246	-5.1634	1.3420
H	2.7067	-6.4090	-0.4951
H	0.9450	-6.4892	-0.7357
H	1.9247	-5.3742	-1.7100
C	-2.4114	-3.6839	2.6790
C	-2.2323	-5.0165	2.2778
C	-1.8661	-3.2576	3.8971
C	-1.5046	-5.9035	3.0746
H	-2.6596	-5.3494	1.3342
C	-1.1326	-4.1416	4.6966
H	-2.0026	-2.2226	4.2075
C	-0.9453	-5.4655	4.2831
H	-1.3632	-6.9331	2.7511
H	-0.7065	-3.7977	5.6372
H	-0.3718	-6.1546	4.9001
O	-4.3399	-3.1760	1.2264
H	-4.8947	-3.4229	1.9799
C	-0.7757	-0.5367	1.3153
O	0.2331	-0.1311	1.9165
O	-1.8090	0.2620	1.0441

Free Energy: -3171.350597 hartrees

Transition State **$TS_{29\text{-}30OMe}$**
Imaginary Frequency at -534 cm^{-1}
Cartesian Coordinates

Fe	-1.5546	0.5843	-0.4903
N	-0.0113	1.9501	-0.7722
N	-0.2785	-0.8671	-1.2691
C	-1.8988	-2.6839	-1.5982
C	-1.2553	4.0139	-0.2862
C	-0.6040	-2.1798	-1.5388
C	2.1279	2.8351	-0.7036
C	1.6595	-2.1098	-1.5258
C	1.0964	-0.7999	-1.2775
C	1.3240	1.6435	-0.8818
C	1.2550	3.8744	-0.4848
C	1.8343	0.3669	-1.0983
C	0.6005	-2.9691	-1.7077
C	-0.0800	3.3023	-0.5140
C	-2.5566	3.5041	-0.2628
N	-2.8786	2.1805	-0.4429
C	-3.0845	-1.9897	-1.3461
N	-3.1539	-0.6527	-1.0139
C	-4.4838	-0.3592	-0.8294
C	-5.2907	-1.5560	-1.0334
C	-4.4049	-2.5717	-1.3691
C	-4.9803	0.9040	-0.5059
C	-4.2527	2.0856	-0.3456
C	-4.8253	3.3845	-0.0822
C	-3.7642	4.2812	-0.0249
H	2.9156	0.2696	-1.1146
H	-1.1388	5.0760	-0.0947
H	-6.0545	0.9843	-0.3798
H	-1.9903	-3.7404	-1.8282
C	-6.2839	3.6825	0.0576
H	-6.5235	4.6429	-0.4170
H	-6.9032	2.9047	-0.4015
H	-6.5762	3.7638	1.1151
C	-4.7230	-3.9897	-1.7222
H	-3.9218	-4.4494	-2.3106
H	-4.8698	-4.6044	-0.8221
H	-5.6535	-4.0387	-2.3021
C	0.6347	-4.4375	-1.9914
C	2.1254	-1.0524	2.4257
H	1.4116	-2.9034	1.6046
H	1.1814	-2.7673	3.3550
N	-0.2158	-1.7047	2.1825
C	-1.3827	-2.5830	2.2464
H	0.1803	-5.0101	-1.1704
H	0.0738	-4.6785	-2.9047
H	1.6642	-4.7879	-2.1196
C	3.1258	-2.4079	-1.5744
H	3.6359	-1.9200	-0.7339
H	3.2970	-3.4832	-1.4631
C	3.7659	-1.9272	-2.8902
H	3.5329	-0.8687	-3.0671
H	3.3434	-2.4797	-3.7420
C	5.2778	-2.1084	-2.9169
C	3.6220	2.8648	-0.7982
H	4.0524	2.0153	-0.2531
H	4.0159	3.7741	-0.3323
C	4.0903	2.8009	-2.2641
H	3.6176	1.9527	-2.7785
H	3.7697	3.7020	-2.8062
C	5.5986	2.6609	-2.4131
C	-3.7800	5.7182	0.1909
C	-4.7674	6.4434	0.7517
C	-6.7389	-1.5964	-0.9202
C	-7.5056	-2.6894	-0.7385
H	-2.8868	6.2540	-0.1325
H	-5.6777	5.9938	1.1379
H	-4.6638	7.5219	0.8523
H	-7.2468	-0.6332	-0.9817
H	-7.0870	-3.6855	-0.6272
H	-8.5878	-2.5942	-0.6761
O	6.0523	2.5611	-3.6995
O	6.3972	2.6267	-1.5033
O	5.9215	-1.5323	-3.9765
O	5.9270	-2.7149	-2.0937
C	1.5688	5.3194	-0.2547
H	2.6505	5.4797	-0.1939
H	1.1777	5.9442	-1.0705
H	1.1143	5.6814	0.6778
H	5.3126	2.6018	-4.3282
H	5.2899	-1.0703	-4.5522
C	1.1406	-2.2161	2.4107
C	-1.1749	-3.9225	1.5307
H	-2.2159	-2.0417	1.7877
H	-1.6369	-2.7659	3.3022
C	-2.5019	-4.6753	1.3796

H	-0.7461	-3.7351	0.5413
H	-0.4563	-4.5415	2.0851
C	-2.3330	-6.0147	0.6517
H	-2.9422	-4.8444	2.3734
H	-3.2059	-4.0380	0.8262
H	-3.2928	-6.5378	0.5499
H	-1.9232	-5.8610	-0.3560
H	-1.6411	-6.6707	1.1976
C	2.5062	-0.3375	3.6621
C	3.4553	0.6982	3.5867
C	1.9082	-0.6165	4.9034
C	3.8210	1.4160	4.7287
H	3.8988	0.9411	2.6237
C	2.2715	0.1030	6.0444
H	1.1565	-1.3983	4.9821
C	3.2322	1.1206	5.9643
H	4.5616	2.2104	4.6529
H	1.8016	-0.1283	6.9988
H	3.5138	1.6799	6.8544
H	2.6795	-0.8303	1.5256
O	3.5735	-2.4668	2.7420
C	4.7863	-1.9912	2.2673
H	5.1895	-1.1426	2.8674
H	5.5559	-2.7895	2.2814
H	4.7340	-1.6226	1.2128
C	-0.2411	-0.4079	1.8204
O	0.8724	0.2080	1.8770
O	-1.3424	0.1619	1.4263

Free Energy: -2783.389741 hartrees

Compound **30**$_{\mathbf{OMe}}$

Cartesian Coordinates

Fe	-0.7511	0.6538	-0.7656
N	0.6442	2.0401	-0.1231
N	0.8067	-0.6403	-1.2229
C	-0.5024	-2.4742	-2.2109
C	-0.8548	3.9533	0.2248
C	0.6805	-1.9186	-1.7256
C	2.5869	2.9745	0.7212
C	2.8496	-1.7239	-1.0972
C	2.1208	-0.4997	-0.8325
C	1.9800	1.8085	0.1123
C	1.5961	3.9224	0.8363
C	2.6526	0.6291	-0.2076
C	1.9541	-2.6094	-1.6525
C	0.3862	3.3224	0.3012
C	-2.0334	3.4311	-0.3159
N	-2.1501	2.1734	-0.8560
C	-1.7566	-1.8614	-2.2793
N	-2.0217	-0.5831	-1.8348
C	-3.3441	-0.3293	-2.1137
C	-3.9546	-1.5039	-2.7264
C	-2.9513	-2.4576	-2.8308
C	-3.9985	0.8722	-1.8365
C	-3.4633	2.0279	-1.2587
C	-4.2098	3.2285	-0.9670
C	-3.3194	4.1138	-0.3697
H	3.7020	0.5803	0.0674
H	-0.9012	4.9604	0.6275
H	-5.0532	0.9121	-2.0870
H	-0.4405	-3.4990	-2.5618
C	-5.6533	3.4565	-1.2847
H	-5.8122	4.4908	-1.6159
H	-6.0066	2.7824	-2.0726
H	-6.2883	3.2997	-0.3999
C	-3.0422	-3.8299	-3.4158
H	-2.0648	-4.1861	-3.7596
H	-3.4194	-4.5514	-2.6761
H	-3.7380	-3.8399	-4.2644
C	2.1911	-4.0207	-2.0896
H	1.5243	-4.7132	-1.5568
H	1.9921	-4.1416	-3.1636
H	3.2262	-4.3235	-1.8990
C	4.3075	-1.9194	-0.8160
H	4.5636	-1.5085	0.1687
H	4.5501	-2.9870	-0.7851
C	5.1760	-1.2307	-1.8852
H	4.8906	-0.1742	-1.9839
H	5.0009	-1.6893	-2.8688
C	6.6683	-1.2914	-1.5912
C	4.0403	3.0952	1.0628
H	4.4123	2.1557	1.4899
H	4.1928	3.8700	1.8217
C	4.8728	3.4379	-0.1876
H	4.6640	2.7188	-0.9918
H	4.5833	4.4253	-0.5754
C	6.3739	3.4523	0.0654
C	-3.5437	5.4665	0.1113
C	-4.7264	6.0337	0.4260
C	-5.3439	-1.5785	-3.1467
C	-6.0690	-2.6969	-3.3431
H	-2.6481	6.0765	0.2368
H	-5.6680	5.4946	0.3712
H	-4.7631	7.0648	0.7718
H	-5.8424	-0.6215	-3.3068
H	-5.6669	-3.6907	-3.1666
H	-7.1050	-2.6286	-3.6691
O	7.1525	3.6204	-1.0476
O	6.9105	3.3309	1.1482
O	7.4668	-0.6492	-2.4975
O	7.1806	-1.8472	-0.6466
C	1.7042	5.3124	1.3803
H	2.7009	5.4926	1.7973
H	1.5241	6.0604	0.5948
H	0.9623	5.4880	2.1715
H	6.6003	3.6980	-1.8433
H	6.9319	-0.2483	-3.2025
C	-1.1381	-1.6662	1.3051

C	0.3142	-1.7374	1.7893
H	-1.2654	-2.0709	0.3016
H	-1.8072	-2.2020	1.9832
H	1.0081	-1.6081	0.9616
N	-1.4139	-0.2075	1.3400
C	0.6796	-2.9692	2.5623
C	1.7231	-3.7788	2.0940
C	-0.0250	-3.3457	3.7154
C	2.0543	-4.9625	2.7616
H	2.2620	-3.4809	1.1960
C	0.3118	-4.5211	4.3901
H	-0.8360	-2.7205	4.0838
C	1.3489	-5.3340	3.9111
H	2.8594	-5.5907	2.3860
H	-0.2374	-4.8090	5.2842
H	1.6039	-6.2538	4.4338
C	-0.5563	0.3453	2.3435
C	-2.8477	0.1931	1.4637
C	-3.5581	-0.3149	2.7201
H	-3.3477	-0.1689	0.5630
H	-2.8607	1.2849	1.4445
C	-4.9645	0.2964	2.8104
H	-3.6415	-1.4092	2.7058
H	-2.9803	-0.0360	3.6122
C	-5.7332	-0.1952	4.0437
H	-4.8750	1.3923	2.8385
H	-5.5259	0.0477	1.8974
H	-6.7308	0.2601	4.0977
H	-5.8564	-1.2868	4.0149
H	-5.1908	0.0590	4.9649
O	-0.6822	1.4335	2.8819
O	0.4492	-0.5172	2.6209
O	-2.3516	-4.4567	0.5617
C	-1.1973	-5.0135	0.0855
H	-0.8631	-5.9060	0.6673
H	-1.2275	-5.2953	-0.9936
H	-0.3397	-4.3029	0.1839

Free Energy: -2783.426423 hartrees

Compound **31**$_{\mathbf{OMe}}$

Cartesian Coordinates

Fe	-0.4818	-0.6305	0.2335
N	0.7938	-0.7325	-1.3856
N	0.5036	1.0750	0.8575
C	-1.0253	1.7234	2.6641
C	-0.1520	-2.7179	-2.4844
C	0.1492	1.8653	1.9251
C	2.7284	-0.5516	-2.6412
C	2.0979	2.7215	1.1501
C	1.6768	1.5798	0.3612
C	1.9426	0.0022	-1.5564
C	2.0333	-1.6353	-3.1234
C	2.3322	1.0833	-0.7663
C	1.1443	2.9027	2.1265
C	0.8241	-1.7349	-2.3262
C	-1.3105	-2.8866	-1.7237
N	-1.6487	-2.1127	-0.6460
C	-2.0564	0.7979	2.4648
N	-2.0501	-0.1936	1.5031
C	-3.2254	-0.8890	1.6379
C	-4.0300	-0.2994	2.6975
C	-3.2851	0.7544	3.2180
C	-3.5897	-1.9883	0.8539
C	-2.8761	-2.5556	-0.2033
C	-3.3321	-3.6622	-1.0158
C	-2.3545	-3.8750	-1.9770
H	3.2520	1.5837	-1.0537
H	0.0072	-3.4145	-3.3013
H	-4.5546	-2.4337	1.0710
H	-1.1713	2.4414	3.4652
C	-4.6055	-4.4198	-0.8175
H	-4.4501	-5.4878	-1.0172
H	-4.9887	-4.3092	0.2028
H	-5.3884	-4.0728	-1.5085
C	-3.6461	1.6731	4.3396
H	-2.7545	2.0975	4.8150
H	-4.2566	2.5039	3.9569
H	-4.2289	1.1411	5.1021
C	1.0831	3.9519	3.1907
H	0.1381	4.5105	3.1358
H	1.1385	3.5054	4.1936
H	1.9086	4.6647	3.0904
C	3.3612	3.4890	0.9141
H	3.4655	3.7264	-0.1525
H	3.3391	4.4413	1.4532
C	4.5938	2.6786	1.3624
H	4.5900	1.6875	0.8906
H	4.5560	2.5018	2.4474
C	5.9134	3.3719	1.0531
C	4.1017	-0.0803	-3.0094
H	4.1546	1.0148	-2.9921
H	4.3613	-0.3986	-4.0250
C	5.1351	-0.6451	-2.0149
H	4.8042	-0.4570	-0.9842
H	5.2016	-1.7374	-2.1147
C	6.5282	-0.0535	-2.1674
C	-2.2979	-4.8662	-3.0373
C	-3.3276	-5.5631	-3.5568
C	-5.3431	-0.7809	3.0914
C	-6.2929	-0.0886	3.7499
H	-1.3076	-5.0530	-3.4548

H	-4.3546	-5.4189	-3.2336
H	-3.1522	-6.2905	-4.3469
H	-5.5774	-1.8066	2.8032
H	-6.1633	0.9513	4.0365
H	-7.2436	-0.5589	3.9937
O	7.4736	-0.5626	-1.3187
O	6.8458	0.8158	-2.9482
O	7.0318	2.5951	1.1784
O	6.0368	4.5318	0.7269
C	2.4221	-2.5701	-4.2260
H	3.3639	-2.2567	-4.6893
H	2.5513	-3.5954	-3.8510
H	1.6501	-2.6056	-5.0072
H	7.0921	-1.2574	-0.7567
H	6.7935	1.6850	1.4213
C	-2.1914	2.4582	-0.8345
C	-0.9410	3.2889	-1.1726
H	-2.1921	2.1302	0.2059
H	-3.1178	3.0120	-1.0346
H	-0.1060	2.9778	-0.5466
N	-2.0381	1.3273	-1.7462
C	-1.1139	4.7772	-1.0852
C	-0.3180	5.5059	-0.1917
C	-2.0851	5.4447	-1.8463
C	-0.4975	6.8856	-0.0453
H	0.4312	4.9810	0.3983
C	-2.2581	6.8243	-1.7107
H	-2.7047	4.8828	-2.5426
C	-1.4677	7.5470	-0.8059
H	0.1198	7.4415	0.6579
H	-3.0125	7.3368	-2.3046
H	-1.6095	8.6205	-0.6964
C	-1.2392	1.6700	-2.8066
C	-3.1169	0.3520	-1.9040
C	-4.3771	0.9071	-2.5763
H	-3.3618	-0.0176	-0.9067
H	-2.7170	-0.4863	-2.4803
C	-5.4547	-0.1812	-2.6762
H	-4.7676	1.7555	-1.9967
H	-4.1254	1.2797	-3.5794
C	-6.7452	0.3266	-3.3327
H	-5.0538	-1.0311	-3.2486
H	-5.6747	-0.5593	-1.6666
H	-7.5005	-0.4681	-3.3970
H	-7.1727	1.1579	-2.7547
H	-6.5456	0.6914	-4.3500
O	-1.0642	1.0584	-3.8467
O	-0.6051	2.8616	-2.5445
O	-4.4991	3.5939	1.6396
C	-3.3486	4.3016	1.8695
H	-3.1788	5.1182	1.1272
H	-3.2727	4.7437	2.8929
H	-2.4453	3.6497	1.7581
C	0.2055	-2.0185	3.0219
C	-0.1587	-3.1040	2.0758
H	-0.5545	-1.3118	3.3450
H	1.0096	-2.2070	3.7279
H	-1.1773	-3.0925	1.6953
N	0.5988	-1.9043	1.5991
C	2.0347	-2.0201	1.2011
C	3.0753	-2.3594	2.2687
H	2.2958	-1.0469	0.7814
H	2.0737	-2.7503	0.3857
C	4.4813	-2.2928	1.6519
H	3.0135	-1.6341	3.0919
H	2.9014	-3.3563	2.6887
C	5.5829	-2.6210	2.6673
H	4.5377	-2.9880	0.8014
H	4.6417	-1.2834	1.2451
H	6.5780	-2.5606	2.2067
H	5.5539	-1.9186	3.5118
H	5.4525	-3.6358	3.0676
C	0.4901	-4.4458	2.0450
C	0.9666	-5.0739	3.2029
C	0.6210	-5.0912	0.8042
C	1.5770	-6.3302	3.1230
H	0.8641	-4.5754	4.1643
C	1.2377	-6.3425	0.7227
H	0.2439	-4.6040	-0.0933
C	1.7186	-6.9638	1.8827
H	1.9433	-6.8125	4.0272
H	1.3418	-6.8336	-0.2428
H	2.1976	-7.9390	1.8204

Free Energy: -3305.216668 hartrees

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