

## Supporting information

### Fe(0)-Catalyzed Alkyne Carboxylation with CO<sub>2</sub>

#### Involving Spin Crossover

Huili Wang, <sup>a,†</sup> Qiqi Zhang, <sup>b,†</sup> Haizhu Yu, <sup>b,\*</sup> Kane Jacob, <sup>c</sup> Azzedine Bousseksou, <sup>c,\*</sup> Philippe Hapiot, <sup>d</sup> Jean-Luc Pozzo, <sup>a,\*</sup> Didier Astruc <sup>a,\*</sup>

<sup>a</sup> Université de Bordeaux, ISM, UMR CNRS N° 5255, 33405 Talence Cedex, France.

<sup>b</sup> Department of Chemistry and Center for Atomic Engineering of Advanced Materials, Anhui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Anhui University, Hefei, Anhui, 230601 People's Republic of China.

<sup>c</sup> Université de Toulouse, LCC, UPR CNRS N° 8241, 31077 Toulouse Cedex, France

<sup>d</sup> Univ. Rennes CNRS, ISCR (Institut des Sciences Chimiques de Rennes), UMR 6226, F-35000 Rennes, France

<sup>†</sup> Both authors (HW and QZ) contributed equally to this work.

#### Table of Contents

General data.	S1
Synthesis of 2,9-Diaryl-1,10-phenanthroline.	S1
Synthesis of Darphen-Fe.	S1
Preparation of the reductant EtMgBr.	S2
Catalysis of the carboxylation reaction of terminal alkynes with CO <sub>2</sub> .	S2-S3
Figure S1. The UV-vis spectra of 4 precursors.	S4
Figure S2. Cyclic voltammogram (cathodic waves) of Fe(II)(TIPP)Cl <sub>2</sub>	S5
Details of the DFT calculations.	S5
Table S1. Spin distribution of the key structures involved in the most feasible catalytic pathway.	S6
Table S2. Gibbs Free Energies and Electronic Energies in Solvent of related compounds and Transition States.	S6-S7
Cartesian Coordinates of Intermediates and Transition States.	S7-S71
<sup>1</sup> H NMR and <sup>13</sup> C NMR data for the various targeted products.	S71-S83
References	S83

## Experimental Section

### General Data

2,9-dichloro-1,10-phenanthroline, Pd(dppf)Cl<sub>2</sub>, Ba(OH)<sub>2</sub>·8H<sub>2</sub>O, ArB(OH)<sub>2</sub>, terminal alkynes and FeCl<sub>2</sub> were purchased from BLD Pharm. All commercial chemicals were used without further purification.

<sup>1</sup>H NMR spectra were recorded at 25 °C using a Bruker AC 300 MHz instrument. All chemical shifts are reported in parts per million (δ, ppm) and calibrated using residual protons in deuterated solvents (CDCl<sub>3</sub> at 7.26 ppm for <sup>1</sup>H NMR and 77.16 ppm for <sup>13</sup>C NMR; CD<sub>3</sub>OD at 3.31 ppm for <sup>1</sup>H NMR and 49.00 ppm for <sup>13</sup>C NMR).

The UV-Vis absorption spectra were recorded using Agilent CARY 5000 Spectrophotometer spectrophotometer. The samples were dissolved in dichloromethane and placed in a standard quartz cuvette with a 1 cm path length. Baseline correction was performed using the pure solvent prior to measurement. The spectra were acquired in the range of 200 to 800 nm at a scanning speed of 200 nm/min. All measurements were conducted at room temperature.

### Synthesis of 2,9-diaryl-1,10-phenanthroline

The preparation of the 2,9-diaryl-1,10-phenanthroline followed the procedure described in reference.<sup>1</sup> In brief, 2,9-dichloro-1,10-phenanthroline (747 mg, 3 mmol), Pd(dppf)Cl<sub>2</sub> (329 mg, 0.45 mmol), Ba(OH)<sub>2</sub>·8H<sub>2</sub>O (4.74 g, 15 mmol), and ArB(OH)<sub>2</sub> (9 mmol) were suspended in a mixture of toluene (100 mL) and water (5 mL) and degassed by nitrogen purging. The mixture was heated to 110 °C, and the reaction progress was monitored by thin-layer chromatography (TLC). After cooling to room temperature, the mixture was neutralized with a saturated aqueous solution of ammonium chloride (50 mL) and extracted with dichloromethane (100 mL×3). The organic layers were combined, dried over anhydrous MgSO<sub>4</sub>, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography and recrystallized in hexane/CH<sub>2</sub>Cl<sub>2</sub> [20:1(v/v)] to give 2,9-diaryl-1,10-phenanthroline.

### Synthesis of Darphen-Fe

The preparation of the Darphen-Fe followed the procedure described in reference.<sup>1</sup>

2,9-Diaryl-1,10-phenanthroline (2 mmol) and FeCl<sub>2</sub> (253.5 mg, 2 mmol) were added into a 50-mL Schlenk flask. The flask was evacuated and connected to argon gas. This process was repeated twice. Dry THF (20 mL) was added to the flask. The reaction mixture was stirred at room temperature for 24 hours. The solvent was partially removed under vacuum (approximately 5 mL remained), and then dry *n*-hexane (15 mL) was added, causing a solid to precipitate. The product was collected by filtration, washed with 20 mL of *n*-hexane, and dried under vacuum. This protocol yields the precursors—iPrPhenFeCl<sub>2</sub>, MePhenFeCl<sub>2</sub>, PhenylPhenFeCl<sub>2</sub> and Cl<sub>2</sub>PhenFeCl<sub>2</sub>. While the complexes were fully characterized in the literature (e.g., by IR, EPR analysis, Mössbauer spectra, Magnetic measurement, XPS, Single crystal structures and NMR spectroscopy),<sup>1-8</sup> the precursors were characterized in this work primarily by <sup>1</sup>H NMR spectroscopy and UV-vis spectra.

#### **Preparation of the reductant EtMgBr**

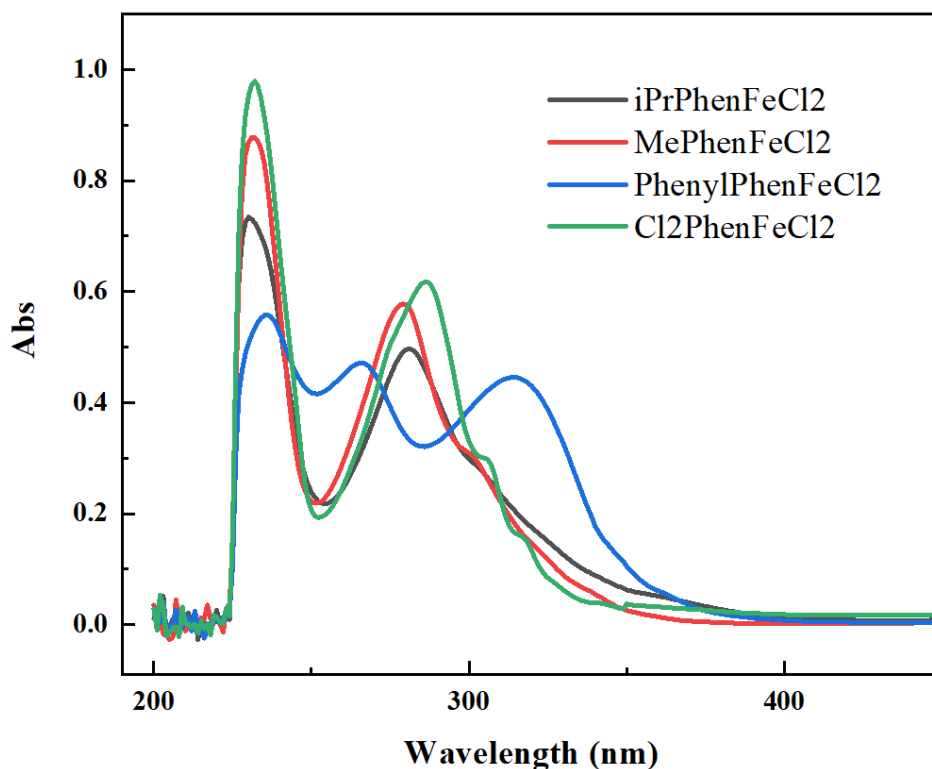
The magnesium chips were lightly rinsed with dilute hydrochloric acid to remove the surface oxide layer, then quickly washed with water followed by ethanol, and dried thoroughly. The treated magnesium chips were transferred to a dry reaction flask, which was subsequently purged with an inert gas to eliminate air and moisture. A small amount of absolutely anhydrous ether was added—just enough to submerge the magnesium chips. Ethyl bromide was then added dropwise to the flask. The reaction mixture became turbid and exhibited gentle boiling (ether reflux). The system was cooled in a cold-water bath to control the reaction temperature. After the addition of ethyl bromide was complete, the magnesium chips had almost completely reacted and disappeared, yielding a gray ethylmagnesium bromide (EtMgBr) solution in ether.

#### **Catalysis of the carboxylation reaction of terminal alkynes with CO<sub>2</sub>**

A terminal alkyne (1.0 mmol) and Cs<sub>2</sub>CO<sub>3</sub> (1.5 mmol) were placed in a 10 mL Schlenk tube **1**. The tube was evacuated and then refilled with CO<sub>2</sub> (99.9%) using a balloon. This process was repeated twice. Another Schlenk tube **2**, containing the ArPhenFeCl<sub>2</sub> catalyst precursor, was evacuated and connected to argon. This process was repeated twice. Then, 1 mL of DMF was injected into tube **2**. Tube **2** was stirred at

room temperature (25-35°C) for 1 minute, after which EtMgBr (0.044 mmol) was added, resulting in a black solution. The black solution was transferred to tube **1** and reacted at room temperature with magnetic stirring (1400 rpm) for 8 h. After removing the CO<sub>2</sub> balloon, deionized water (15 mL) was added to the reaction mixture and stirred for 30 minutes. The solid catalyst was separated from the reaction mixture by centrifugation (8000 rpm, 5 minutes). The resulting liquid phase was washed with dichloromethane (3 × 10 mL) in a 125 mL separatory funnel, and the aqueous phase was retained. The aqueous phase was then acidified to pH = 1 with concentrated aqueous HCl at 0 °C. The product-containing solution was then extracted with ethyl acetate. The aqueous phase was monitored by TLC during the extraction process until the product was free. The organic phase was collected, dried over anhydrous sodium sulfate, and filtered. The solvent was then removed by rotary evaporation to yield propiolic acid. The final product was analyzed by <sup>1</sup>H NMR. In recovery experiments, the catalyst was isolated by centrifugation and washed twice with DMF and twice with methanol. The catalyst was then dried at 60 °C overnight before use.

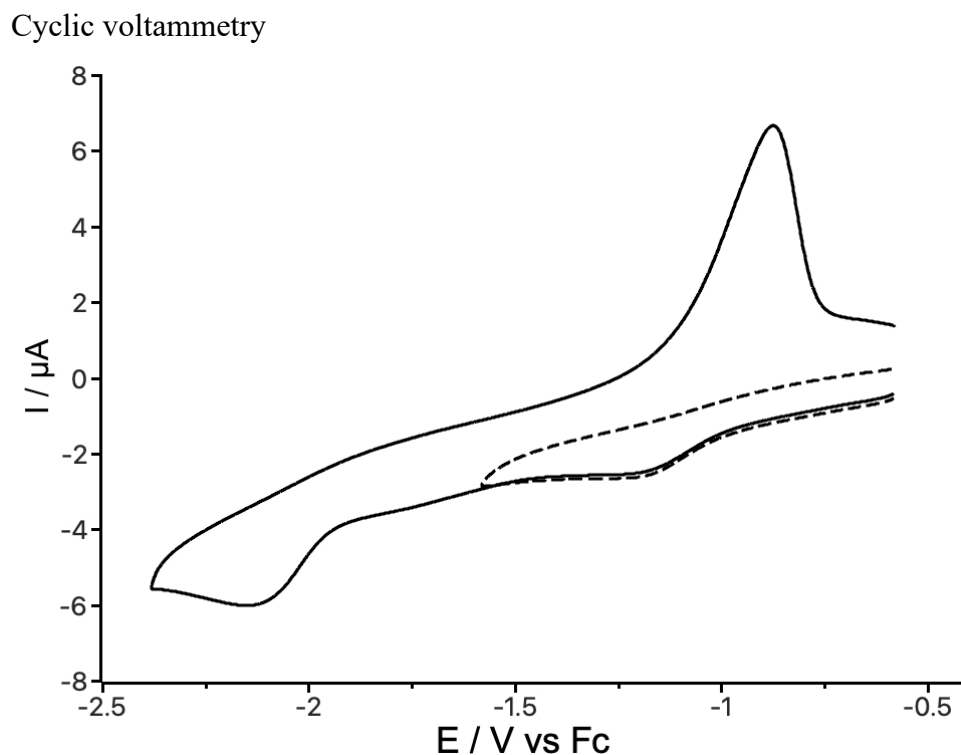
The electronic structures of a series of 2,9-substituted 1,10-phenanthroline iron(II) dichloride complexes (iPrPhenFeCl<sub>2</sub>, MePhenFeCl<sub>2</sub>, PhenylPhenFeCl<sub>2</sub>, and Cl<sub>2</sub>PhenFeCl<sub>2</sub>) were characterized *inter alia* using UV-vis absorption spectroscopy, as shown in Figure S1. All measurements were conducted in spectroscopic-grade solvents (e.g., dichloromethane) at concentrations ranging from 1\*10<sup>-5</sup> to 1\*10<sup>-4</sup> mol/L to ensure absorbance values remained within the optimal linear range according to the Beer-Lambert law.



**Figure S1.** The UV-vis spectra of 4 precursors.

The experimental spectra reveal three primary characteristic absorption regions between 200 and 450 nm. The first is the ligand-internal  $\pi \rightarrow \pi^*$  transition (200–250 nm).<sup>9, 10</sup> Notably,  $\text{Cl}_2\text{PhenFeCl}_2$  displays the highest molar absorptivity, which is attributed to the strong inductive effect of the chloro-substituents on the phenanthroline backbone, thereby enhancing the intensity of the  $n \rightarrow \pi^*$  transitions. In this region, the impact of substituents on the energy levels is most pronounced. Following this are conjugation extension and steric hindrance effects (250–350 nm).  $\text{PhenylPhenFeCl}_2$  shows a significant red-shift, with a prominent absorption peak at 315 nm. This is due to the effective  $\pi$ -conjugation extension between the 2,9-phenyl rings and the phenanthroline core, which reduces the electronic transition energy gap. On contrast,  $i\text{PrPhenFeCl}_2$ , containing bulky 2,4,6-triisopropylphenyl (Tipp) groups, exhibits a much smaller red-shift. The sheer bulk of the Tipp groups induces a large dihedral angle (twisted conformation) between the aryl substituents and the phenanthroline plane, thereby limiting effective  $\pi$ -delocalization. Finally, metal-ligand charge transfer (MLCT) (350–450 nm) was observed.<sup>11, 12</sup> Broad, low-intensity absorption bands are

observed at the edge of the visible region. PhenylPhenFeCl<sub>2</sub> exhibits the most defined MLCT absorption, suggesting a superior energetic match between the iron (II) d-orbitals and the ligand  $\pi^*$  orbitals in this less sterically hindered system.

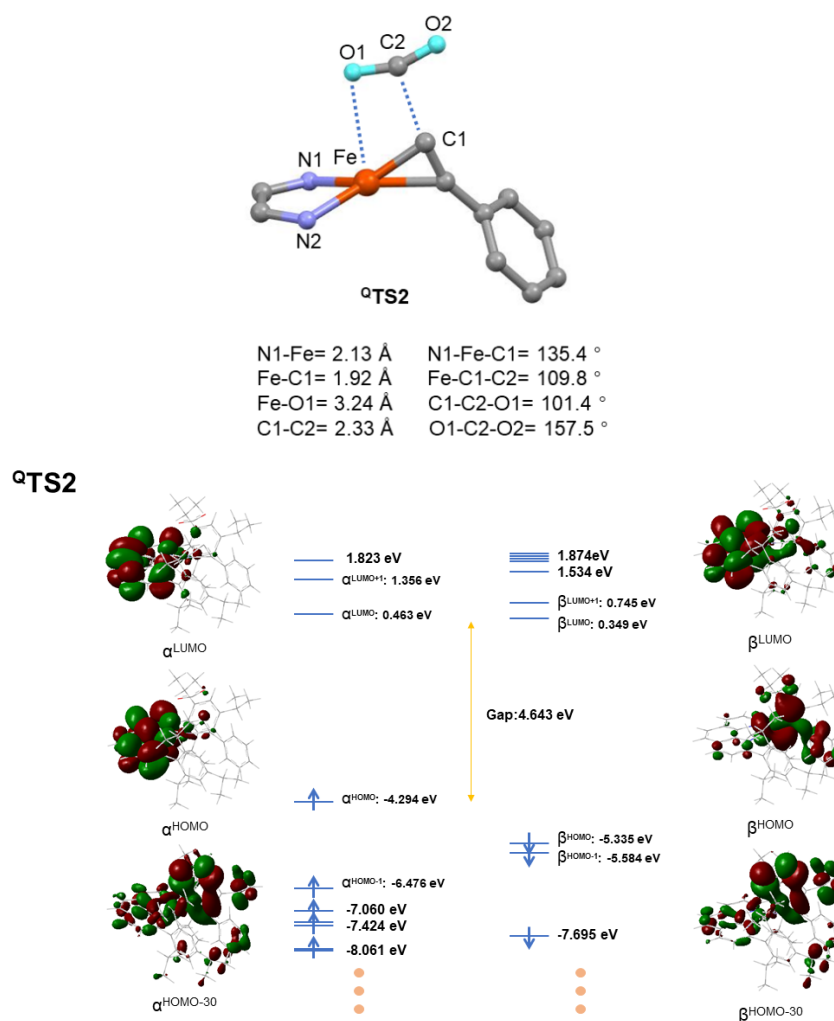


**Figure S2.** Cyclic voltammogram (cathodic waves) of Fe(II)(TIPP)Cl<sub>2</sub>

Cyclic voltammogram recorded at a scan rate of 0.2 V/sec with a Vionic-Methrom potentiostat of a 20% Et<sub>2</sub>O/80% DMF solvent mixture with the background electrolyte *n*-Bu<sub>4</sub>NPF<sub>6</sub> (0.1 mol L<sup>-1</sup>) on a 1 mm-diameter disk gold electrode of a solution (1.1 mg/5mL) of the complex Fe(II)(TIPP)Cl<sub>2</sub>, showing the two successive irreversible cathodic waves at -1.2 V and -2.1 V vs. ferricenium/ferrocene corresponding to the expected successive reductions of the first and second Cl-ligands of the complex Fe(II)(TIPP)Cl<sub>2</sub>.

## Details of the DFT calculations

All calculations were carried out with the Gaussian 09 package at the density-functional-theory (DFT) level. Minimum-energy crossing points (MECPs) were located with the sobMECP code modified by Lu, which is derived from the original program developed by Harvey and co-workers. Geometry optimizations and frequency analyses employed the  $\omega$ B97XD functional (restricted or unrestricted) together with a mixed basis set: def2-TZVP for Fe and 6-31G\* for H, C, N, and Si. Single-point energies were computed with the same functional but with the larger def2-TZVPP basis set. Both optimization and single-point energy calculation steps included the CPCM solvation model with THF as solvent (corresponding to the reaction conditions), and the solute cavity was defined by the UAHF protocol.



**Figure S3.** Optimized structure and the frontier orbitals of TS2.

According to the optimized structure of TS2, CO<sub>2</sub> is bent into a nonlinear structure

via the nucleophilic attack from the catalyst (with the O-C-O bond angle to be 157.5°), which is inherently initiated by the electron-rich Fe(0) center. The highest occupied molecular orbital mainly shows the bonding interaction between the Fe(0) center and the phenanthroline ( $\alpha^{\text{HOMO}}$ ) and alkyne groups ( $\beta^{\text{HOMO}}$ ).

**Table S1. Spin distribution of the key structures involved in the most feasible catalytic pathway.**

Structure	Fe	TIPP	PhC≡C(H/CO <sub>2</sub> ) <sup>1</sup>	PhC≡C(H) <sup>2</sup>	CO <sub>3</sub> <sup>2-</sup>	CO <sub>2</sub>
<sup>T</sup> In1	2.353	0.047	-0.202	-0.198	-	-
<sup>Q</sup> In1	3.268	1.123	-0.171	-0.220	-	-
<sup>Q</sup> In2	3.221	1.044	-0.265	-	-	-
<sup>Q</sup> In3	3.632	0.236	0.029	-	0.104	-
<sup>Q</sup> In4	3.117	0.889	-0.006	-	-	-
<sup>Q</sup> In5	3.216	1.064	-0.280	-	-	-
<sup>Q</sup> TS1	3.642	0.227	0.042	-	0.089	-
<sup>Q</sup> TS2	3.015	1.038	-	-	-	-0.053

The subscript of <sup>1</sup> and <sup>2</sup> denote the first and second phenylacetylene substrate.

**Table S2. Gibbs Free Energies and Electronic Energies in Solvent of related compounds and Transition States**

	Gibbs Free Energies in solvent (Hartree)	Electronic Energy in solvent (Hartree)
<sup>T</sup> Fe(iprphen)(DMF) <sub>2</sub> -1	-3501.3781	-3502.3461
<sup>Q</sup> Fe(iprphen)(DMF) <sub>2</sub> -1	-3501.3764	-3502.3443
<sup>S</sup> Fe(iprphen)(DMF) <sub>2</sub> -1	-3501.3095	-3502.2829
<sup>T</sup> Fe(iprphen)(DMF) <sub>2</sub> -2	-3501.2789	-3502.2496
<sup>Q</sup> Fe(iprphen)(DMF) <sub>2</sub> -2	-3501.3060	-3502.2779
<sup>S</sup> Fe(iprphen)(DMF) <sub>2</sub> -2	-3501.3204	-3502.2893
<sup>S</sup> In1	-3621.0790	-3622.0680
<sup>T</sup> In1	-3621.1269	-3622.1137
<sup>Q</sup> In1	-3621.1100	-3622.0925
<sup>S</sup> In6	-3501.3604	-3502.2556
<sup>T</sup> In6	-3501.3885	-3502.2749
<sup>Q</sup> In6	-3501.3731	-3502.2607
<sup>S</sup> In2	-3312.7521	-3313.6323
<sup>T</sup> In2	-3312.7551	-3313.6336

<sup>Q</sup> In2	-3312.8026	-3313.6723
<sup>T</sup> In3	-3576.8423	-3577.7248
<sup>Q</sup> In3	-3576.8362	-3577.7207
<sup>T</sup> In4	-3312.2937	-3313.1527
<sup>Q</sup> In4	-3312.2881	-3313.1445
<sup>T</sup> In5	-3500.9227	-3501.7992
<sup>Q</sup> In5	-3500.9209	-3501.7968
<sup>T</sup> TS1	-3576.8433	-3577.7228
<sup>Q</sup> TS1	-3576.8430	-3577.7213
<sup>T</sup> TS2	-3500.8909	-3501.7589
<sup>Q</sup> TS2	-3500.8897	-3501.7581
MECP		-3621.2271
<sup>Q</sup> In7	-3500.8984	-3501.7708
<sup>Q</sup> In8	-3500.9114	-3501.7800
<sup>Q</sup> In9	-3500.9088	-3501.7786
CO <sub>2</sub>	-188.6163	-188.6073
CO <sub>3</sub> <sup>2-</sup>	-264.0346	-264.0242
HCO <sub>3</sub> <sup>-</sup>	-264.5760	-264.5772
Phenylacetylene	-308.3145	-308.3950
DMF	-248.4668	-248.5411

---

### Cartesian Coordinates of Intermediates and Transition States

<sup>T</sup>Fe(iprphen)(DMF)<sub>2</sub>-1

ATOM	X	Y	Z
Fe	-0.01289200	0.05161300	-0.27420100
N	1.49383700	1.41359000	0.55558600
N	-1.20220500	1.51330100	0.53447800
C	3.37671500	-0.07021600	0.41370700
C	3.39832000	-1.03681900	1.44197300
C	3.84489300	-2.32025600	1.12875300
H	3.85710400	-3.06941700	1.91793400
C	4.27016200	-2.67729600	-0.15111800
C	4.28006200	-1.69246100	-1.13046600
H	4.63606900	-1.94530100	-2.12712500
C	3.84573400	-0.39007500	-0.87072900
C	2.81258300	1.29126700	0.66955800
C	3.63909500	2.37324500	1.01958500
H	4.71158800	2.22570500	1.07817800
C	3.06411900	3.60968700	1.27721900
H	3.68593500	4.46202900	1.53940100
C	1.67629100	3.75776200	1.22690600
C	0.99069800	4.97735700	1.52875800
H	1.57671900	5.85717900	1.78156200

C	-0.36845900	5.03312100	1.51433600
H	-0.87963100	5.96104300	1.75787300
C	-1.17560300	3.87782100	1.20618400
C	-2.57119200	3.87858300	1.24894900
H	-3.11107600	4.78360800	1.51032200
C	-3.25957200	2.66249500	1.01125300
H	-4.33959900	2.61072200	1.10742100
C	-2.56392300	1.52398500	0.67443800
C	-0.51123300	2.66858400	0.86411700
C	0.90000800	2.61339600	0.87481200
C	-3.24921900	0.20620200	0.50413000
C	-3.96898400	-0.09425000	-0.66215400
C	-4.58106900	-1.34679200	-0.77912800
H	-5.13286900	-1.58539600	-1.68661200
C	-4.49646200	-2.30510700	0.22321900
C	-3.77833500	-1.98357100	1.37697300
H	-3.70632700	-2.72083300	2.17206300
C	-3.14386600	-0.75425600	1.53384900
C	-4.08444400	0.88686100	-1.81642500
H	-3.52507500	1.78446700	-1.54231800
C	-2.39414000	-0.45507100	2.82537400
H	-1.69320500	0.35969900	2.62502800
C	3.07323100	-0.77176100	2.91267600
H	2.98735100	-1.76610200	3.36773900
C	3.94674600	0.64921000	-1.97767900
H	3.50196500	1.57934000	-1.60970900
C	4.71843100	-4.09302200	-0.46377900
H	4.98172400	-4.12351700	-1.52894500
C	-5.14339300	-3.66790600	0.05843200
C	0.56857600	2.20925800	-2.21518400
C	-0.71683500	-1.83642700	-0.78398300
C	4.25524400	-0.07127800	3.60247200
H	4.07201900	0.01341000	4.67984400
H	5.18709800	-0.62725900	3.45414700
H	4.39312000	0.93974500	3.20395100
C	1.75883600	-0.04610700	3.23546700
H	1.83445100	1.03455700	3.08720600
H	0.93187900	-0.41787300	2.62482700
H	1.51261600	-0.21587000	4.29013300
C	5.41771500	0.95984900	-2.29012200
H	5.93386500	0.07233000	-2.67412200
H	5.49026600	1.74733300	-3.04866100
H	5.94656200	1.29695700	-1.39210700
C	3.18742300	0.23630000	-3.24423700

H	3.24108300	1.03456300	-3.99382600
H	3.61766800	-0.66641200	-3.69241000
H	2.13303800	0.04024400	-3.02774500
C	5.96954400	-4.47711600	0.33780600
H	6.31477200	-5.47859300	0.05740200
H	6.78487100	-3.76870700	0.15681700
H	5.76061400	-4.48392900	1.41402400
C	3.58572300	-5.10292200	-0.23573900
H	3.30205700	-5.14471800	0.82236000
H	2.69475700	-4.83136600	-0.81192100
H	3.89973900	-6.10823100	-0.53819400
C	-1.55941200	-1.64297300	3.31754100
H	-0.93761800	-1.33388100	4.16505800
H	-2.18476100	-2.47541500	3.66002100
H	-0.89945800	-2.00761900	2.52270400
C	-3.37490300	0.02698200	3.90354800
H	-3.91519000	0.91815500	3.56576500
H	-4.11135900	-0.75219800	4.13522100
H	-2.84225100	0.27793500	4.82818300
C	-6.20495600	-3.92648800	1.13583000
H	-6.69817000	-4.89020100	0.96631500
H	-5.75353500	-3.95379100	2.13440700
H	-6.96987600	-3.14303100	1.13167700
C	-5.53904800	1.31554900	-2.04806600
H	-6.16479600	0.46518000	-2.34380900
H	-5.96861200	1.75041800	-1.13894700
H	-5.59429400	2.06552900	-2.84537800
C	-3.45831200	0.31767000	-3.09691100
H	-2.40670400	0.05837400	-2.93377000
H	-3.98514100	-0.58257900	-3.43397300
H	-3.51189500	1.05436500	-3.90769400
C	-4.08896700	-4.78321900	0.04437800
H	-3.34051800	-4.60717800	-0.73564900
H	-3.56521500	-4.84092200	1.00575200
H	-4.55852700	-5.75588000	-0.14075200
H	-5.64819000	-3.67445500	-0.91617800
O	0.01366600	1.09514500	-2.19985200
O	0.29005600	-1.80138400	0.06508600
N	-0.05284900	3.37235000	-2.37700600
N	-0.53035100	-2.29221400	-2.10015600
C	0.78571000	-2.72880200	-2.50455700
H	0.97179800	-3.78498600	-2.24190500
H	0.89238700	-2.62555800	-3.59034700
H	1.54941800	-2.12027300	-2.01723400

C	-1.63645500	-2.97799500	-2.72837900
H	-2.58075700	-2.56118400	-2.36679200
H	-1.59715500	-2.84024400	-3.81500600
H	-1.63036700	-4.06262000	-2.52068600
C	0.65637200	4.63020300	-2.21463100
H	0.50566400	5.26297300	-3.09396500
H	0.28289500	5.14852500	-1.32523500
H	1.72406700	4.44144200	-2.08574500
C	-1.49789600	3.43622000	-2.50232500
H	-1.95169300	3.69581900	-1.53878700
H	-1.76180800	4.19503200	-3.24358700
H	-1.86331900	2.46383500	-2.82603400
H	1.65373700	2.30104600	-2.09080800
H	-1.72683600	-2.01376700	-0.40009000

<sup>Q</sup>Fe(iprphen)(DMF)<sub>2</sub>-1

ATOM	X	Y	Z
Fe	-0.04928100	-0.03025800	-0.26834300
N	-1.51532400	-1.38951200	0.57367100
N	1.19397400	-1.50702600	0.56960200
C	-3.39058900	0.09410600	0.42846700
C	-3.40052500	1.07224500	1.44609300
C	-3.81802200	2.36139600	1.11596200
H	-3.82156200	3.11881600	1.89730000
C	-4.22366100	2.71385500	-0.17167400
C	-4.24603700	1.71912400	-1.14097400
H	-4.58778200	1.96920800	-2.14334600
C	-3.84065100	0.41077000	-0.86413300
C	-2.83776100	-1.27039200	0.69319800
C	-3.66317800	-2.34699600	1.03909400
H	-4.73514900	-2.19910000	1.10392600
C	-3.08455000	-3.59547900	1.28121500
H	-3.70744800	-4.44940500	1.53589400
C	-1.70427500	-3.74399000	1.22279500
C	-1.01741000	-4.97444700	1.50549700
H	-1.60842800	-5.85562000	1.74250800
C	0.33777300	-5.03888400	1.49434500
H	0.84410600	-5.97320500	1.72327000
C	1.15197600	-3.87814100	1.20782800
C	2.53834500	-3.87972600	1.26150500
H	3.07274000	-4.79122000	1.51409800
C	3.24179600	-2.67022900	1.03317400
H	4.32174800	-2.62719600	1.12660200
C	2.54426600	-1.52615900	0.70138000

C	0.48673900	-2.65768000	0.87990600
C	-0.91848700	-2.59554000	0.88581400
C	3.24210300	-0.21531200	0.52338600
C	3.96927800	0.06443000	-0.64325000
C	4.59373500	1.30943100	-0.77073700
H	5.15056400	1.53351600	-1.67879000
C	4.51227700	2.27986600	0.22056500
C	3.78555000	1.97812800	1.37395600
H	3.71493000	2.72549500	2.15953600
C	3.14021200	0.75561400	1.54271800
C	4.07212100	-0.92700900	-1.79002500
H	3.49815500	-1.81417200	-1.51216200
C	2.38543600	0.47583600	2.83588800
H	1.67316700	-0.33036400	2.64082200
C	-3.08695600	0.81475700	2.92042200
H	-3.00251900	1.81117400	3.37140600
C	-3.95433200	-0.63978800	-1.95961900
H	-3.51876200	-1.56965800	-1.58093100
C	-4.63821400	4.13577900	-0.50276300
H	-4.88328700	4.16307900	-1.57234600
C	5.16809100	3.63659700	0.04137900
C	-0.59531900	-2.27335900	-2.15771900
C	0.76705600	1.81289400	-0.83655600
C	-4.27322400	0.11856400	3.60695200
H	-4.09610800	0.03933800	4.68579800
H	-5.20359300	0.67499700	3.45077900
H	-4.40923300	-0.89387100	3.21183900
C	-1.77458500	0.08940300	3.25250800
H	-1.84696900	-0.99020300	3.09704100
H	-0.94216600	0.46502300	2.65131100
H	-1.53774600	0.25544300	4.30999400
C	-5.43010500	-0.93669100	-2.26283000
H	-5.93749600	-0.04673600	-2.65307800
H	-5.51554400	-1.73069800	-3.01328700
H	-5.95851700	-1.25865900	-1.35901400
C	-3.19530600	-0.25289000	-3.23433800
H	-3.26570700	-1.05890500	-3.97423200
H	-3.61259100	0.65140300	-3.69153000
H	-2.13663800	-0.07310400	-3.02542300
C	-5.89451900	4.55009200	0.27538100
H	-6.21207900	5.55838200	-0.01333600
H	-6.72222400	3.85965000	0.08162900
H	-5.70410400	4.55499900	1.35502500
C	-3.49008500	5.12540900	-0.26340100

H	-3.22575500	5.17324300	0.79940400
H	-2.59391400	4.83033700	-0.81951300
H	-3.77812300	6.13344000	-0.58222200
C	1.56756600	1.67835200	3.32052800
H	0.93799500	1.38188900	4.16674800
H	2.20474100	2.50198800	3.66244000
H	0.91683700	2.05046000	2.52164000
C	3.35967600	-0.01311400	3.91703900
H	3.88711100	-0.91419900	3.58530700
H	4.10707400	0.75731300	4.14280000
H	2.82382100	-0.24995300	4.84349100
C	6.22094400	3.90719800	1.12420500
H	6.72023800	4.86573000	0.94361800
H	5.76099800	3.95307700	2.11820300
H	6.98216000	3.12028900	1.13948800
C	5.52009400	-1.37979700	-2.01621600
H	6.16002700	-0.54077700	-2.31387600
H	5.94041000	-1.81773000	-1.10427900
H	5.56512400	-2.13384000	-2.81026800
C	3.45626000	-0.35663800	-3.07497600
H	2.41070600	-0.07300400	-2.91278900
H	4.00107400	0.52931800	-3.42112900
H	3.49376200	-1.10133900	-3.87915700
C	4.11848400	4.75581600	-0.00023500
H	3.37619800	4.57013100	-0.78389600
H	3.58668300	4.83077600	0.95552000
H	4.59362300	5.72349600	-0.19668600
H	5.68182800	3.62538700	-0.92850600
O	-0.05239100	-1.15290200	-2.13050800
O	-0.22066100	1.83530600	0.03674900
N	0.03801600	-3.42241700	-2.36460000
N	0.57561200	2.25557600	-2.15428400
C	-0.74541400	2.67843500	-2.55749000
H	-0.94579500	3.72973300	-2.28763700
H	-0.84824000	2.58062300	-3.64398400
H	-1.50391300	2.05787400	-2.07664100
C	1.67375000	2.94954000	-2.78952200
H	2.62306600	2.54445000	-2.42782200
H	1.63274000	2.80523800	-3.87510800
H	1.65699900	4.03479300	-2.58712200
C	-0.64999200	-4.69379800	-2.21626700
H	-0.49532000	-5.30948000	-3.10683600
H	-0.26358000	-5.21998000	-1.33716800
H	-1.71953700	-4.52333600	-2.07820100

C	1.48242500	-3.45961700	-2.50894300
H	1.95295400	-3.71006700	-1.55086400
H	1.75074300	-4.21387400	-3.25298200
H	1.82624900	-2.48078000	-2.83743000
H	-1.67601700	-2.38001200	-2.01013100
H	1.79052600	1.94975500	-0.47662200

<sup>5</sup>Fe(iprphen)(DMF)<sub>2</sub>-1

ATOM	X	Y	Z
Fe	0.08767400	-0.06296500	0.16922500
N	1.46582800	-1.28964000	-0.68461400
N	-1.16780100	-1.43544600	-0.54497700
C	3.37216000	0.19133000	-0.49176300
C	3.38668600	1.24731100	-1.42698400
C	3.86232800	2.48860700	-1.00632200
H	3.85833800	3.30887900	-1.72113800
C	4.33563100	2.71541200	0.28656800
C	4.36510600	1.64009900	1.16498700
H	4.76104900	1.79068300	2.16712300
C	3.89471200	0.37686800	0.79874700
C	2.78515700	-1.13513600	-0.84559100
C	3.59997900	-2.18806100	-1.30271800
H	4.66668000	-2.01572700	-1.39744800
C	3.05243400	-3.41602100	-1.60279000
H	3.67618500	-4.23896300	-1.93833000
C	1.66159100	-3.58866500	-1.48008900
C	0.97976800	-4.81605600	-1.78322600
H	1.56793800	-5.67096600	-2.10319400
C	-0.37082100	-4.90283300	-1.68420600
H	-0.88481900	-5.82874300	-1.92409700
C	-1.15899700	-3.76922500	-1.28457200
C	-2.56393700	-3.78294600	-1.23346200
H	-3.11113800	-4.68759300	-1.48080500
C	-3.22210700	-2.62258600	-0.89726900
H	-4.30552100	-2.57871600	-0.88650200
C	-2.50606000	-1.45538600	-0.56370800
C	-0.51295400	-2.56819200	-0.94271200
C	0.91437000	-2.48354100	-1.03541400
C	-3.28467000	-0.21277200	-0.28691600
C	-3.74439300	0.06511300	1.00841400
C	-4.53428800	1.19527600	1.20614400
H	-4.89443200	1.42524500	2.20621900
C	-4.85819400	2.06106200	0.16289100
C	-4.37171100	1.76930700	-1.10917700

H	-4.58942800	2.44803200	-1.93041100
C	-3.58557400	0.64350700	-1.35686500
C	-3.36403000	-0.82559800	2.17826200
H	-2.47598500	-1.38536300	1.87637700
C	-3.02441500	0.42039500	-2.75374300
H	-2.42184400	-0.49378100	-2.74271200
C	3.02302900	1.12032000	-2.90598100
H	2.93924100	2.15249900	-3.26764400
C	4.01340800	-0.76274200	1.80113100
H	3.57432900	-1.65983500	1.35328200
C	4.78773500	4.09430000	0.73117400
H	5.22243500	3.98650300	1.73331500
C	-5.64963500	3.32741100	0.43737000
C	0.65781600	-2.43474000	1.97105600
C	-0.76977200	1.64611800	0.44444200
C	4.18141600	0.47391800	-3.68306500
H	3.97731700	0.50064100	-4.75976000
H	5.12626800	0.99669200	-3.49938200
H	4.31006400	-0.57521500	-3.39397900
C	1.69020000	0.44138000	-3.25110500
H	1.76287000	-0.65014500	-3.20987300
H	0.90064700	0.76562100	-2.56889400
H	1.41320300	0.70737200	-4.27827600
C	5.48811900	-1.08981900	2.07692400
H	5.99870000	-0.24250600	2.54870900
H	5.56936700	-1.95000800	2.75091300
H	6.01766100	-1.32847900	1.14820100
C	3.25582200	-0.47723800	3.10262600
H	3.33285600	-1.33307900	3.78357100
H	3.66583300	0.39788200	3.61858700
H	2.19704400	-0.28811600	2.90538900
C	5.87186700	4.67593400	-0.18502200
H	6.23136900	5.63295300	0.20917400
H	6.72608100	3.99535900	-0.26617500
H	5.48538600	4.85650700	-1.19453300
C	3.58811400	5.04640100	0.84210500
H	3.11338100	5.18995600	-0.13586200
H	2.83154100	4.64738700	1.52631300
H	3.90609600	6.02777100	1.21235500
C	-2.08511600	1.56909200	-3.14958000
H	-1.61635400	1.35874600	-4.11839700
H	-2.63490300	2.51354500	-3.24401400
H	-1.29639000	1.70048200	-2.39993500
C	-4.13810300	0.21688100	-3.78861700

H	-4.77768600	-0.63087800	-3.51836300
H	-4.77336000	1.10669100	-3.86917800
H	-3.70858200	0.02220200	-4.77779700
C	-6.79589400	3.54305000	-0.55744900
H	-7.38535800	4.42193500	-0.27329200
H	-6.41912100	3.71353200	-1.57234800
H	-7.46459200	2.67614300	-0.58547500
C	-4.47856500	-1.82879700	2.50200800
H	-5.39722000	-1.30772000	2.79755900
H	-4.71187500	-2.45945500	1.63687000
H	-4.18115300	-2.48484800	3.32919000
C	-2.96069200	-0.02073500	3.41953300
H	-2.23538000	0.75640500	3.15633400
H	-3.82510700	0.45753200	3.89549300
H	-2.50658200	-0.68570100	4.16371600
C	-4.70759100	4.54060000	0.46557400
H	-3.91732400	4.40316600	1.21157400
H	-4.22827900	4.67928400	-0.51111700
H	-5.25705300	5.45732200	0.70872000
H	-6.09189400	3.22575400	1.43690900
O	-0.00817800	-1.39319000	1.89556800
O	0.21147200	1.61734600	-0.53361700
N	0.16107400	-3.62068000	2.32166200
N	-0.55249200	2.52322500	1.58955300
C	0.60765700	2.18694400	2.39061500
H	1.57087000	2.33303300	1.86718000
H	0.62748300	2.80450500	3.29897000
H	0.54246400	1.13646700	2.69083100
C	-0.52413200	3.92508000	1.20558100
H	-1.42536300	4.16371800	0.62831800
H	-0.50808800	4.56793300	2.09624600
H	0.35463600	4.18360400	0.58520700
C	0.96960600	-4.82622900	2.24355600
H	0.94915700	-5.35899600	3.19835000
H	0.58796500	-5.48440700	1.45579100
H	2.00280900	-4.56240200	2.00800200
C	-1.26218700	-3.75823300	2.59073800
H	-1.83786500	-3.74701900	1.65771900
H	-1.43309500	-4.70455600	3.10613200
H	-1.59858400	-2.93609800	3.22405200
H	1.72965700	-2.44997100	1.73957200
H	-1.75996500	1.89193600	0.03725100

<sup>T</sup>Fe(iprphen)(DMF)<sub>2</sub>-2

ATOM	X	Y	Z
Fe	0.08279600	0.63147800	-0.35320000
N	-1.12100500	2.15566100	-0.36296300
N	1.46660700	2.03302200	-0.13558100
C	-3.12909200	0.90200100	0.20780000
C	-3.93940700	0.15467900	-0.66472600
C	-4.55966600	-0.99979200	-0.18616400
H	-5.19701100	-1.57143300	-0.85714000
C	-4.40166000	-1.43229200	1.13176400
C	-3.57716200	-0.68579000	1.96808000
H	-3.45424900	-1.00416800	3.00136900
C	-2.94002900	0.47997200	1.53704400
C	-2.47242900	2.17604500	-0.21761600
C	-3.18755400	3.35844300	-0.30705200
H	-4.26378300	3.32913800	-0.17643100
C	-2.52627500	4.58690000	-0.50893700
H	-3.09109400	5.51114300	-0.58806400
C	-1.13845300	4.60816300	-0.52662500
C	-0.32466000	5.80016600	-0.59920900
H	-0.82407500	6.75887800	-0.70970500
C	1.02766400	5.73834800	-0.51382300
H	1.62163700	6.64729700	-0.55935800
C	1.71813200	4.48121200	-0.34407800
C	3.09132800	4.34569500	-0.20901900
H	3.73583600	5.21987600	-0.23021900
C	3.63395200	3.06136000	-0.04294400
H	4.70478400	2.92082200	0.05345300
C	2.81299800	1.94156100	-0.01261100
C	0.92930400	3.30055100	-0.30236700
C	-0.46008400	3.36626900	-0.41898200
C	3.41097500	0.58182200	0.13132000
C	3.60691000	0.03471700	1.40801600
C	4.18325300	-1.23059700	1.51050200
H	4.34782800	-1.66645400	2.49303000
C	4.53031200	-1.97448800	0.38516400
C	4.30881400	-1.41304300	-0.87082600
H	4.56664200	-1.98284500	-1.76129200
C	3.76129500	-0.13958400	-1.01973400
C	3.21347700	0.80560500	2.65941700
H	2.46226800	1.54792300	2.36812700
C	3.54632000	0.42385500	-2.41686300
H	3.14520800	1.43735900	-2.31856200
C	-4.18193300	0.60318100	-2.09754500
H	-3.46420100	1.39860900	-2.32229900

C	-2.14980300	1.29818400	2.55213500
H	-1.67810800	2.13587300	2.03362600
C	-5.13701400	-2.64959700	1.66646600
H	-4.91393000	-2.71602600	2.73903400
C	5.09065900	-3.37776800	0.52955000
H	5.25311100	-3.55609700	1.60041300
C	4.86757900	0.53315000	-3.18860200
H	5.59019100	1.14576600	-2.63853700
H	5.31806500	-0.45229500	-3.35493000
H	4.70186800	0.99524100	-4.16835100
C	2.50726200	-0.39601200	-3.19156100
H	2.33658200	0.03730200	-4.18396000
H	2.83531600	-1.43368100	-3.32815300
H	1.55345100	-0.40630500	-2.65305500
C	6.44052700	-3.54458100	-0.17905500
H	7.16945100	-2.81147200	0.18245600
H	6.84576200	-4.54732100	-0.00284400
H	6.33878500	-3.41300200	-1.26257400
C	4.07081800	-4.41326100	0.03558700
H	3.88324200	-4.29135100	-1.03831900
H	4.43611100	-5.43306100	0.20246500
H	3.11627600	-4.28988500	0.55706600
C	4.42067400	1.56076600	3.23425300
H	5.21190300	0.85727600	3.52006300
H	4.83503900	2.26010600	2.50071700
H	4.13311500	2.13018300	4.12580700
C	2.57147100	-0.08407900	3.72950800
H	3.29970400	-0.76212100	4.18906500
H	2.15135500	0.53551400	4.52946200
H	1.76550600	-0.68630100	3.30062900
C	-5.59248000	1.19084400	-2.24855900
H	-6.35414500	0.42892800	-2.04316000
H	-5.75440800	2.02204500	-1.55416600
H	-5.74961500	1.56125500	-3.26801400
C	-3.94505100	-0.51711200	-3.11566700
H	-4.67513300	-1.32793700	-3.00729600
H	-4.03899600	-0.12489700	-4.13470300
H	-2.94225700	-0.93142200	-2.98958000
C	-4.65447300	-3.95115900	1.01640400
H	-5.17534200	-4.81378500	1.44675400
H	-4.84728300	-3.94631100	-0.06280700
H	-3.57931400	-4.09352200	1.17385600
C	-6.65726600	-2.49732500	1.52000000
H	-6.95171900	-2.46074000	0.46466000

H	-7.17288500	-3.34694500	1.98139400
H	-7.00933800	-1.57871400	2.00073400
C	-3.09389000	1.89485400	3.60610000
H	-3.87091600	2.50502200	3.13258600
H	-3.58822500	1.10871500	4.18879300
H	-2.53524000	2.53072400	4.30223900
C	-1.02262200	0.48972800	3.20431600
H	-0.44243800	1.12641600	3.88203800
H	-1.41035300	-0.35275700	3.78944000
H	-0.34258800	0.09147000	2.44445500
O	-0.90651700	-0.54984400	-1.46869900
C	-1.10088800	-1.78838000	-1.07778500
H	-1.73125100	-1.94791000	-0.19262300
O	0.85010300	-0.94731200	0.39838600
C	0.64794600	-2.10189400	-0.17429800
H	1.19739900	-2.31768700	-1.10366100
N	-1.29608300	-2.75929800	-2.04440300
C	-2.34138600	-3.74514600	-1.91257400
H	-3.22829800	-3.47333400	-2.50545400
H	-1.98838500	-4.72772300	-2.24814100
H	-2.64416100	-3.82491600	-0.86784200
C	-0.72548800	-2.60142100	-3.36118100
H	-0.34046400	-3.56445900	-3.71792000
H	-1.46728800	-2.23886300	-4.08853800
H	0.09142400	-1.88128200	-3.32417600
N	0.56860400	-3.22206700	0.64850800
C	-0.08662900	-3.06937200	1.93038500
H	-1.18562100	-3.03456100	1.83336400
H	0.17555000	-3.91580600	2.57196200
H	0.24586500	-2.14520600	2.40203800
C	0.40458500	-4.51718300	0.02403700
H	0.87685500	-5.28724100	0.64397900
H	-0.65331000	-4.78576400	-0.10584700
H	0.88589900	-4.51887000	-0.95725200

<sup>Q</sup>Fe(iprphen)(DMF)<sub>2</sub>-2

ATOM	X	Y	Z
Fe	0.07933300	0.60287500	-0.37373400
N	-1.13035800	2.15850300	-0.37474800
N	1.48306900	2.03806100	-0.13516200
C	-3.13952100	0.92325900	0.21598300
C	-3.97670900	0.17159100	-0.62814400
C	-4.59075200	-0.97537700	-0.12408200
H	-5.24577600	-1.55039400	-0.77484400

C	-4.40379900	-1.39694000	1.19336500
C	-3.55417600	-0.64833700	2.00181600
H	-3.40976700	-0.95692700	3.03527100
C	-2.91891300	0.50829000	1.54399600
C	-2.48459800	2.18856000	-0.23929300
C	-3.19202500	3.36963300	-0.35032700
H	-4.26767500	3.35310700	-0.21119500
C	-2.51691800	4.59550600	-0.56655100
H	-3.07391400	5.52317300	-0.65994400
C	-1.12943000	4.60788500	-0.56604000
C	-0.31059700	5.79796800	-0.63451100
H	-0.80715900	6.75608800	-0.76335200
C	1.04019300	5.73834600	-0.51952700
H	1.63485200	6.64725200	-0.56028600
C	1.72429200	4.48345200	-0.33238800
C	3.09619300	4.34719400	-0.18510500
H	3.73746100	5.22437800	-0.20450200
C	3.64525400	3.07008000	-0.01572700
H	4.71594700	2.93086400	0.08025700
C	2.81856000	1.94719100	0.00292400
C	0.93214500	3.29940000	-0.29962200
C	-0.45556600	3.36288700	-0.43556700
C	3.41620100	0.58543300	0.13205400
C	3.64747900	0.03871200	1.40232100
C	4.21902500	-1.23042800	1.48819100
H	4.40932000	-1.66692800	2.46587800
C	4.53092800	-1.97505400	0.35335100
C	4.27754100	-1.41151000	-0.89599100
H	4.51311400	-1.98049600	-1.79318800
C	3.72926100	-0.13713800	-1.02938900
C	3.29741200	0.81113000	2.66573400
H	2.56882000	1.58251500	2.39303300
C	3.49310400	0.43427600	-2.42043000
H	3.05634200	1.43189300	-2.31275100
C	-4.25213500	0.60347300	-2.06014800
H	-3.54063900	1.39702300	-2.30927800
C	-2.09869100	1.32675400	2.53568800
H	-1.61249100	2.14233900	1.99648600
C	-5.12741600	-2.60830300	1.75648800
H	-4.89663200	-2.65196200	2.82866200
C	5.09493300	-3.37868000	0.47944300
H	5.26139700	-3.56898800	1.54760900
C	4.81571300	0.59933600	-3.18088700
H	5.51103700	1.23114900	-2.61767900

H	5.30093400	-0.36878600	-3.35135200
H	4.64248800	1.06530700	-4.15748700
C	2.49117200	-0.41070000	-3.21728700
H	2.31735200	0.03162200	-4.20493300
H	2.85642900	-1.43382700	-3.36617000
H	1.52932700	-0.46786800	-2.69592700
C	6.44371000	-3.52927000	-0.23532400
H	7.17035600	-2.79773400	0.13395100
H	6.85440000	-4.53242400	-0.07456800
H	6.33710500	-3.38266200	-1.31650300
C	4.08011900	-4.41407000	-0.02494600
H	3.89376300	-4.28464100	-1.09817500
H	4.45091100	-5.43320100	0.13364600
H	3.12367300	-4.29980100	0.49512100
C	4.53784800	1.51828800	3.23042800
H	5.30852400	0.78572500	3.49863700
H	4.96588200	2.20983100	2.49725500
H	4.28253600	2.08870800	4.13106500
C	2.63882200	-0.06684600	3.73577200
H	3.34606200	-0.78317100	4.16917200
H	2.26213900	0.55751400	4.55350600
H	1.79843400	-0.62666200	3.31564300
C	-5.66597100	1.18852100	-2.18784300
H	-6.42269800	0.43034200	-1.95264100
H	-5.81185100	2.03087100	-1.50345800
H	-5.84666200	1.54232800	-3.20932900
C	-4.03692700	-0.52898000	-3.06982900
H	-4.76746100	-1.33631700	-2.93977400
H	-4.14763800	-0.14796000	-4.09149800
H	-3.03361800	-0.94557700	-2.95649200
C	-4.63580300	-3.91708300	1.12780800
H	-5.14133600	-4.77746500	1.58054200
H	-4.84039900	-3.93532600	0.05093900
H	-3.55704900	-4.04254000	1.27568300
C	-6.64986700	-2.47406700	1.61763600
H	-6.95281900	-2.46319000	0.56413800
H	-7.15365900	-3.31899100	2.10032600
H	-7.00811900	-1.54923900	2.08161500
C	-3.01795000	1.96471900	3.58731600
H	-3.78220600	2.58724500	3.10929500
H	-3.52780800	1.20074100	4.18598300
H	-2.43759800	2.59714800	4.26877300
C	-0.98571100	0.50400800	3.19663800
H	-0.37396300	1.14477600	3.84199500

H	-1.38916700	-0.30375800	3.81874000
H	-0.32822400	0.05183400	2.44647100
O	-0.97275700	-0.57767800	-1.47955900
C	-1.16382100	-1.80686900	-1.08227800
H	-1.74840700	-1.97029400	-0.16708600
O	0.88586100	-0.99416400	0.37051100
C	0.66764100	-2.13760200	-0.20291100
H	1.15496000	-2.34078600	-1.16868300
N	-1.37267200	-2.78771600	-2.03601300
C	-2.40952600	-3.77703800	-1.87097700
H	-3.32144100	-3.50503300	-2.42499500
H	-2.06654100	-4.75564400	-2.22791100
H	-2.66900800	-3.86713200	-0.81521400
C	-0.84138800	-2.62812400	-3.36875000
H	-0.46956700	-3.59161400	-3.73815500
H	-1.60071200	-2.26123700	-4.07583600
H	-0.02067300	-1.91082000	-3.35310700
N	0.61313000	-3.26869300	0.60380100
C	0.02843800	-3.12517800	1.92021400
H	-1.07270600	-3.06005000	1.88022900
H	0.30017400	-3.99112400	2.53111200
H	0.41085900	-2.22000600	2.39140500
C	0.40097300	-4.55164600	-0.03073800
H	0.90910200	-5.33633100	0.54092200
H	-0.66499700	-4.81236600	-0.09563100
H	0.81453600	-4.53552100	-1.04242400

<sup>5</sup>Fe(iprphen)(DMF)<sub>2</sub>-2

ATOM	X	Y	Z
Fe	0.02529600	0.65839400	0.04978100
N	-1.24744000	2.10730600	-0.01784900
N	1.28171100	2.02203900	-0.08609900
C	-3.20330100	0.74766200	0.42299000
C	-3.98398600	0.11706100	-0.56774800
C	-4.55611200	-1.12639700	-0.28806700
H	-5.17434900	-1.60283600	-1.04657100
C	-4.39607200	-1.75233000	0.94929300
C	-3.60390300	-1.11832100	1.90355500
H	-3.49081500	-1.58573000	2.87935500
C	-3.00640600	0.12312100	1.67021600
C	-2.59032500	2.08788900	0.16446000
C	-3.36165400	3.23766500	0.12175600
H	-4.43159100	3.15832900	0.28425300
C	-2.76430400	4.48848900	-0.16239300

H	-3.37324400	5.38730600	-0.21940600
C	-1.39947200	4.55274200	-0.35631900
C	-0.63298300	5.74636200	-0.63134900
H	-1.16266200	6.68981700	-0.74281000
C	0.71983600	5.70716500	-0.74085300
H	1.27155100	6.62247900	-0.94489800
C	1.48111200	4.48171900	-0.57513300
C	2.85313800	4.38476000	-0.63275100
H	3.47747600	5.25356000	-0.81895300
C	3.43105900	3.09230200	-0.43488200
H	4.51008400	2.97010700	-0.47708800
C	2.67121100	1.98137100	-0.18546200
C	0.71940200	3.30192100	-0.32279500
C	-0.65039700	3.34014800	-0.25016000
C	3.34814000	0.66673100	0.02372400
C	3.66832400	0.24649600	1.32575300
C	4.41849400	-0.91729100	1.49641200
H	4.69179300	-1.23332400	2.50119600
C	4.85278800	-1.68191900	0.41499900
C	4.48417400	-1.27347200	-0.86613300
H	4.79548300	-1.86596800	-1.72445200
C	3.72994400	-0.11578900	-1.08014300
C	3.25309400	1.06633500	2.53726000
H	2.48625000	1.77349200	2.20823000
C	3.35070700	0.27716400	-2.50042700
H	2.69263800	1.14923500	-2.43916800
C	-4.28519900	0.78547700	-1.90460000
H	-3.72520400	1.72306300	-1.94545900
C	-2.28920100	0.83119900	2.81347600
H	-1.72674000	1.66816500	2.39254700
C	-5.13546800	-3.03418200	1.29771300
H	-4.90115300	-3.26616900	2.34441400
C	5.68421900	-2.93250800	0.64171300
H	5.94004700	-2.96326300	1.70869100
C	4.58786200	0.68886100	-3.30833600
H	5.10077700	1.52883600	-2.82731600
H	5.30053400	-0.14053400	-3.39209300
H	4.30506600	0.99472500	-4.32221600
C	2.56551700	-0.83695800	-3.20437200
H	2.26405400	-0.51568800	-4.20834500
H	3.16002800	-1.75195200	-3.31276700
H	1.65765500	-1.07916700	-2.64224000
C	6.99752900	-2.90712500	-0.15015000
H	7.57864500	-2.00821500	0.08084000

H	7.60813700	-3.78389300	0.09329400
H	6.81170500	-2.92075000	-1.23035400
C	4.87482700	-4.19644700	0.32576700
H	4.59031200	-4.22177500	-0.73332200
H	5.45751200	-5.09959900	0.53980700
H	3.95966200	-4.22867200	0.92656500
C	4.44131300	1.87799900	3.07057200
H	5.25033400	1.21500300	3.40116000
H	4.83713000	2.54008600	2.29304700
H	4.13750900	2.49477900	3.92461600
C	2.62701800	0.20360000	3.63928400
H	3.36263500	-0.46145100	4.10730800
H	2.21433100	0.84253900	4.42846500
H	1.81792500	-0.41092500	3.23302900
C	-5.77613300	1.14283200	-1.99552300
H	-6.40217400	0.24252600	-1.98419700
H	-6.08079000	1.77492700	-1.15446500
H	-5.98335100	1.68530700	-2.92479400
C	-3.84590100	-0.05244100	-3.11059800
H	-4.29688500	-1.05201700	-3.10542200
H	-4.14530000	0.44270100	-4.04096500
H	-2.75875500	-0.16205300	-3.12566200
C	-4.69044200	-4.23076300	0.45065600
H	-5.24411400	-5.13172200	0.73700600
H	-4.87273800	-4.05095500	-0.61531300
H	-3.62339400	-4.43554800	0.59144900
C	-6.65485300	-2.83444300	1.19880100
H	-6.96017900	-2.63811200	0.16448200
H	-7.18207700	-3.73248700	1.53930900
H	-6.98114900	-1.98928600	1.81365700
C	-3.32428800	1.40987100	3.78982200
H	-4.00829000	2.09071500	3.27160900
H	-3.91975500	0.61138000	4.24898600
H	-2.82697000	1.96718600	4.59187400
C	-1.27955900	-0.06406700	3.53952200
H	-0.74577200	0.51584100	4.30092300
H	-1.76406800	-0.90591300	4.04844000
H	-0.53913700	-0.46181500	2.83818400
O	-0.58617700	-0.50490200	-1.47567700
C	-1.25946800	-1.54659400	-1.37701600
H	-1.72490900	-1.83909200	-0.42779400
O	0.79730900	-1.05317500	0.84912200
C	1.23112500	-2.07597300	0.29144300
H	2.01893600	-2.01386500	-0.46635200

N	-1.47579300	-2.38317200	-2.39004300
C	-2.30246100	-3.56279600	-2.22730600
H	-3.23025300	-3.46112500	-2.80083100
H	-1.76259100	-4.44781600	-2.57701600
H	-2.55238200	-3.69298900	-1.17497200
C	-0.95196500	-2.12008500	-3.71949500
H	-0.21778000	-2.88529000	-3.99091800
H	-1.77169500	-2.13770200	-4.44455500
H	-0.47667900	-1.14061100	-3.73178900
N	0.77888800	-3.30356200	0.54686800
C	-0.26738500	-3.53142300	1.53074400
H	-1.01903200	-4.20605100	1.10958000
H	0.15161300	-3.98993000	2.43221100
H	-0.73435300	-2.58179300	1.79268400
C	1.28769200	-4.46209100	-0.16656900
H	1.70809200	-5.18785500	0.53607700
H	0.47480200	-4.93843500	-0.72426700
H	2.06557900	-4.15278600	-0.86661400

<sup>s</sup>In1

ATOM	X	Y	Z
Fe	0.26310500	-0.18576800	-0.13876800
N	1.88699800	-1.15090600	-0.81801300
N	-0.64772200	-1.73012500	-0.99647500
C	3.39992400	0.65187700	-0.35746200
C	3.47453400	1.62509200	-1.37162200
C	3.48624100	2.96733500	-0.98781900
H	3.51377900	3.72571000	-1.76761800
C	3.44049100	3.36612700	0.34652300
C	3.43645700	2.37695000	1.32566400
H	3.42867800	2.67605300	2.37040100
C	3.41377400	1.02083200	0.99942700
C	3.16489000	-0.77170200	-0.73380300
C	4.20847000	-1.66295600	-1.04555900
H	5.23252800	-1.32921700	-0.92139300
C	3.93074800	-2.92355600	-1.52882800
H	4.73075900	-3.61242600	-1.78197000
C	2.58767200	-3.30065600	-1.71700800
C	2.16357900	-4.56251100	-2.25825800
H	2.92049600	-5.28018700	-2.55913800
C	0.84412700	-4.84958700	-2.39866400
H	0.52805100	-5.79988500	-2.81820700
C	-0.16974200	-3.91283600	-1.99547600
C	-1.55008400	-4.14490000	-2.12492200

H	-1.91358300	-5.07093600	-2.55960600
C	-2.42296900	-3.17171600	-1.70074100
H	-3.49280500	-3.30651500	-1.80807300
C	-1.95574600	-1.97097500	-1.12451100
C	0.21972500	-2.68386100	-1.44185600
C	1.60821900	-2.37305800	-1.32649000
C	-2.95200900	-0.94683600	-0.69195600
C	-3.60975000	-1.08361500	0.54456100
C	-4.57104800	-0.13463600	0.88552400
H	-5.08508100	-0.21814900	1.84033500
C	-4.90887800	0.92150800	0.03941300
C	-4.25214900	1.01924700	-1.18491800
H	-4.50547800	1.82811200	-1.86168200
C	-3.27493800	0.10079600	-1.57130200
C	-3.33369400	-2.25753400	1.47797900
H	-2.32763700	-2.63165600	1.26016000
C	-2.65706900	0.16959100	-2.96357900
H	-1.67283500	-0.30716400	-2.91667900
C	3.62077100	1.35487800	-2.87229600
H	3.29943400	2.28469800	-3.35765100
C	3.46868500	-0.03829500	2.08908700
H	2.97751300	-0.93504700	1.70362100
C	3.35329300	4.83336600	0.72507400
H	3.45381400	4.89558600	1.81630100
C	-6.01680400	1.87573400	0.45781100
C	-0.65617600	-0.20891400	1.58434100
H	-1.43072400	0.36405700	2.07099300
C	0.20614300	-1.14590800	1.64097100
C	-0.40715000	1.63501100	-0.24764800
C	0.28717400	1.35668400	-1.29945500
H	0.68418600	1.85976700	-2.17357100
C	-1.04986700	2.71228300	0.49325900
C	-1.96574200	3.58420900	-0.11379200
C	-0.70352600	2.94891700	1.83364900
C	-2.50173300	4.65980100	0.58835900
H	-2.25359100	3.41745200	-1.14637000
C	-1.24116200	4.02368900	2.53590400
H	0.01683700	2.29119700	2.31133700
C	-2.14506400	4.88479400	1.91697500
H	-3.19622100	5.33210100	0.09168000
H	-0.94954800	4.19110800	3.56899300
C	0.68670000	-2.23599800	2.47529200
C	0.17610200	-2.39585300	3.77651700
C	1.65751800	-3.14825200	2.03731100

C	0.61527400	-3.42488800	4.60057700
H	-0.56937100	-1.69192700	4.13407000
C	2.10042100	-4.17881200	2.86235700
H	2.07671300	-3.04264300	1.04349200
C	1.58104100	-4.32427900	4.14645700
H	0.20401200	-3.52693000	5.60115200
H	2.85454000	-4.87120900	2.49853800
C	5.10855300	1.16846200	-3.21554800
H	5.24402700	1.08570900	-4.30004800
H	5.70711300	2.01190700	-2.85593600
H	5.50106500	0.25344000	-2.75760600
C	2.78881700	0.23404300	-3.51758600
H	3.22644600	-0.75462100	-3.35094900
H	1.76035000	0.21658600	-3.15121400
H	2.76838300	0.39657900	-4.60111100
C	4.92989300	-0.40371400	2.39386700
H	5.47135500	0.46590600	2.78524900
H	4.97488000	-1.20125700	3.14422300
H	5.45268000	-0.75051800	1.49619300
C	2.73549700	0.34878800	3.37527200
H	2.69845900	-0.51443500	4.04845200
H	3.24116900	1.16246800	3.90805200
H	1.70562100	0.64937900	3.16185200
C	4.48215500	5.66772400	0.10684100
H	4.43851500	6.69841500	0.47585100
H	5.46414300	5.25345600	0.35844700
H	4.39928900	5.70408200	-0.98554500
C	1.97579200	5.40059900	0.34927700
H	1.81981400	5.34986000	-0.73501600
H	1.17093900	4.83555800	0.83154700
H	1.89284800	6.45010600	0.65435000
C	-2.42945300	1.58983500	-3.48774700
H	-1.91737000	1.54420900	-4.45539800
H	-3.37069500	2.12899200	-3.64456400
H	-1.80283200	2.16393900	-2.80137000
C	-3.52735000	-0.61989900	-3.95585800
H	-3.66378700	-1.65887000	-3.63980300
H	-4.51935000	-0.16028900	-4.04161600
H	-3.06725400	-0.62554500	-4.95056200
C	-7.38872000	1.22298900	0.22372100
H	-8.19396700	1.87855600	0.57436600
H	-7.54277000	1.03498000	-0.84569200
H	-7.47027500	0.26634800	0.75033300
C	-4.34094200	-3.39298100	1.23093900

H	-5.36253800	-3.04331100	1.42191900
H	-4.29990500	-3.76547400	0.20378300
H	-4.13845500	-4.23457600	1.90322800
C	-3.36076500	-1.88201600	2.96476100
H	-2.73284400	-1.01268800	3.17396400
H	-4.37779400	-1.66246500	3.30930900
H	-2.98768500	-2.72129700	3.56145000
C	-5.95231500	3.24424200	-0.22324600
H	-4.96547000	3.70091000	-0.10310600
H	-6.16798600	3.16978200	-1.29561000
H	-6.69844600	3.91634700	0.21404000
H	-5.90690000	2.03724800	1.53861600
H	-2.56416200	5.72578800	2.46135200
H	1.92628100	-5.12791900	4.79026700

<sup>T</sup>In1

ATOM	X	Y	Z
Fe	-0.23201300	0.01971600	-0.10788500
N	0.87083600	-1.66060200	-1.05385400
N	-1.77965500	-1.20003700	-1.08429200
C	3.09315800	-0.77276800	-0.52758800
C	3.56293600	0.21735900	-1.40674000
C	4.47668700	1.15722200	-0.92860400
H	4.83116100	1.92835300	-1.60372100
C	4.92373100	1.14545500	0.38846000
C	4.43478900	0.15432100	1.23862400
H	4.77095400	0.14667200	2.27298000
C	3.52305000	-0.80768200	0.81003300
C	2.18821100	-1.84071400	-1.05770100
C	2.76880300	-3.01109300	-1.59387800
H	3.84652000	-3.12480500	-1.55595700
C	1.97522900	-3.97980800	-2.15743400
H	2.40814500	-4.88502200	-2.57275100
C	0.58301800	-3.78055100	-2.20732900
C	-0.31989400	-4.72599400	-2.80110800
H	0.09186000	-5.63378500	-3.23182500
C	-1.65411400	-4.48893500	-2.82547700
H	-2.33773500	-5.20253200	-3.27553500
C	-2.19707900	-3.28856500	-2.25436500
C	-3.57288800	-2.99421200	-2.26004100
H	-4.27372900	-3.68668900	-2.71679200
C	-4.00887600	-1.82643000	-1.68322200
H	-5.06151600	-1.56705800	-1.67818500
C	-3.08494600	-0.94234000	-1.08676100

C	-1.33925500	-2.34550900	-1.65625400
C	0.08248500	-2.59461200	-1.63681900
C	-3.57855800	0.31587500	-0.44541900
C	-4.02167300	0.28761400	0.88751300
C	-4.49139500	1.47383900	1.45491500
H	-4.83107500	1.47327100	2.48710000
C	-4.52573700	2.67001700	0.74535300
C	-4.09053400	2.66458100	-0.57974900
H	-4.11610000	3.59140500	-1.14569800
C	-3.61659400	1.50758900	-1.19391400
C	-4.02480000	-0.99969800	1.70244100
H	-3.23487000	-1.64894800	1.30774200
C	-3.19867100	1.53354400	-2.65784700
H	-2.44324500	0.75360300	-2.79907600
C	3.12257800	0.26000400	-2.86426400
H	2.13529600	-0.21017300	-2.92659400
C	3.03343600	-1.88318200	1.76859100
H	2.09054000	-2.27807300	1.37674400
C	5.92517700	2.15444700	0.92715700
H	5.56568400	2.45275100	1.92148300
C	-5.01104900	3.94938700	1.40268100
H	-5.30580000	3.69754900	2.42956400
C	-0.64548700	0.45424300	1.71794900
H	-0.84104900	1.30617000	2.35566400
C	-0.47438700	-0.81883600	1.65976700
C	0.61757000	1.70679400	-0.51966700
C	0.04974800	1.27092000	-1.58463300
H	-0.09339300	1.45167600	-2.64088400
C	1.37034000	2.77419400	0.12251100
C	1.53710500	4.01443800	-0.51285500
C	1.95324800	2.58435800	1.38107200
C	2.26654400	5.03224300	0.09367400
H	1.08232500	4.17209600	-1.48746400
C	2.68571200	3.59951300	1.98702100
H	1.83392600	1.62224900	1.86795200
C	2.84352400	4.82805800	1.34743800
H	2.38455700	5.98743300	-0.41028300
H	3.13861500	3.43118700	2.96016100
C	-0.50716400	-2.04711700	2.44226800
C	-0.59931500	-1.99931500	3.84289300
C	-0.43798800	-3.30368800	1.82746700
C	-0.61851600	-3.16510500	4.59923400
H	-0.64820100	-1.03067900	4.33171700
C	-0.45744700	-4.47364000	2.58221600

H	-0.36116300	-3.35757600	0.74749200
C	-0.54646300	-4.40909700	3.97099100
H	-0.68903000	-3.10481800	5.68168700
H	-0.39959000	-5.43727400	2.08412300
C	-5.36876600	-1.73155100	1.55681200
H	-6.18592500	-1.10456800	1.93315900
H	-5.58859800	-1.98099200	0.51490900
H	-5.36119300	-2.66357000	2.13355500
C	-3.72077900	-0.77634100	3.18761600
H	-2.82315700	-0.16620500	3.31848400
H	-4.55546500	-0.28714800	3.70309200
H	-3.55034100	-1.73986600	3.67846100
C	-2.56462500	2.86208200	-3.08724000
H	-2.10452300	2.75016200	-4.07530000
H	-3.31085000	3.66112600	-3.16527600
H	-1.79068500	3.18094400	-2.38239800
C	-4.39720800	1.20805000	-3.56348300
H	-4.82528100	0.22716200	-3.33471800
H	-5.18578500	1.95942800	-3.43640600
H	-4.09402300	1.20784400	-4.61684000
C	-6.24463800	4.52244700	0.69242600
H	-6.00881700	4.81196100	-0.33835800
H	-7.05541100	3.78708500	0.65891600
H	-6.60964900	5.41366700	1.21491300
C	-3.88733200	4.99194800	1.48584200
H	-4.22952500	5.88549000	2.01989700
H	-3.01525000	4.58835300	2.01111500
H	-3.56367600	5.30200300	0.48527600
C	4.03599200	-3.04461500	1.84128400
H	5.00141400	-2.69608600	2.22785000
H	3.66375400	-3.82930700	2.50997400
H	4.20830200	-3.49146200	0.85662100
C	2.73893100	-1.34647600	3.17266900
H	2.28091800	-2.13344100	3.78048000
H	3.65101600	-1.02015400	3.68517200
H	2.03959700	-0.50524900	3.13297000
C	4.09224300	-0.53999900	-3.74854400
H	3.76538200	-0.51894300	-4.79467500
H	5.09806500	-0.10606800	-3.69766000
H	4.16005200	-1.58651100	-3.43572900
C	2.97086400	1.68439200	-3.41149700
H	2.47317400	1.65330200	-4.38716100
H	2.37331600	2.30485900	-2.73839500
H	3.94270400	2.16956500	-3.55869900

C	7.30198400	1.49512700	1.10589100
H	8.01783500	2.20330200	1.53884100
H	7.24490200	0.62136800	1.76368600
H	7.69479900	1.16332700	0.13708200
C	6.04602100	3.42514500	0.08387500
H	6.50779900	3.21926300	-0.88929600
H	5.06801000	3.88578000	-0.08738700
H	6.68162800	4.15365600	0.59893300
H	-0.55920200	-5.32104200	4.56085100
H	3.41405000	5.62184800	1.82095200

<sup>Q</sup>In1

ATOM	X	Y	Z
Fe	-0.20303300	-0.17176900	-0.15006300
N	0.96253100	-1.71008300	-0.98112400
N	-1.73200200	-1.34561800	-0.99616900
C	3.13025300	-0.70313400	-0.51990600
C	3.49577400	0.33436800	-1.39898700
C	4.32257400	1.35580000	-0.92931900
H	4.60633600	2.15219200	-1.60918200
C	4.78461200	1.38423500	0.38339700
C	4.39034100	0.35707900	1.23950800
H	4.74275000	0.37793800	2.26804100
C	3.56675900	-0.68743500	0.81745400
C	2.30174000	-1.84125900	-1.03673500
C	2.91155000	-2.95794400	-1.58831100
H	3.99369800	-3.02092400	-1.60334200
C	2.11682200	-3.98843800	-2.13642700
H	2.58130000	-4.87263500	-2.56423000
C	0.74140800	-3.85614200	-2.14736600
C	-0.15767300	-4.83944000	-2.71076400
H	0.27545600	-5.73773500	-3.14333400
C	-1.49872800	-4.65845200	-2.71052300
H	-2.15623600	-5.40975000	-3.14052300
C	-2.09753000	-3.47249900	-2.14470300
C	-3.45880100	-3.22949000	-2.12248700
H	-4.14510100	-3.95535500	-2.55061200
C	-3.95085600	-2.04249300	-1.54828900
H	-5.01338800	-1.83078500	-1.53050200
C	-3.05719500	-1.13186600	-0.99606000
C	-1.22314400	-2.49324400	-1.57232000
C	0.16548700	-2.68037800	-1.56866400
C	-3.49237600	0.16266500	-0.37807400
C	-3.74033000	0.23466700	1.00490500

C	-4.00586200	1.48367700	1.57051100
H	-4.18371100	1.55938100	2.63947600
C	-4.02691700	2.64951800	0.81050500
C	-3.82013500	2.54496600	-0.56470500
H	-3.85074100	3.44576200	-1.17104600
C	-3.55856500	1.32142300	-1.17806400
C	-3.76840800	-1.02128500	1.86667900
H	-3.02658700	-1.72028400	1.46341600
C	-3.41378000	1.24089000	-2.69213400
H	-2.75986300	0.39215000	-2.92157200
C	3.05260500	0.33264500	-2.85653800
H	2.11781000	-0.23473600	-2.91765200
C	3.19867200	-1.80837100	1.77865200
H	2.26949200	-2.26341000	1.41952600
C	5.72703600	2.46224200	0.89267800
H	5.50050100	2.60989400	1.95726200
C	-4.24609800	4.00065600	1.46720500
H	-4.43403400	3.81956600	2.53330400
C	-0.31490400	0.38907900	1.74181100
H	-0.38457900	1.34967900	2.22558400
C	-0.29541300	-0.87652800	1.74345000
C	0.22829800	1.70568700	-0.77545800
C	-0.16432800	1.02192400	-1.75466600
H	-0.37598500	0.84124800	-2.79327600
C	0.68475600	2.90894200	-0.10936400
C	0.14504200	4.15081200	-0.46878300
C	1.65868400	2.84485200	0.89416300
C	0.57282000	5.30975500	0.17093000
H	-0.61803200	4.19884600	-1.23971200
C	2.09163800	4.00767400	1.52128300
H	2.07811900	1.88143700	1.16722400
C	1.54814400	5.24150600	1.16455600
H	0.14127400	6.26683000	-0.10586700
H	2.85429300	3.94916500	2.29221700
C	-0.33626900	-2.13716300	2.46160900
C	-0.29367000	-2.12941800	3.86431900
C	-0.42702400	-3.36154900	1.79107000
C	-0.33653900	-3.32098600	4.57719700
H	-0.22018300	-1.18008300	4.38568000
C	-0.47182800	-4.55366400	2.50746800
H	-0.46457600	-3.37376200	0.70813500
C	-0.42495800	-4.53724200	3.89967500
H	-0.29961500	-3.30200400	5.66229400
H	-0.54314900	-5.49768800	1.97583700

C	-5.14796200	-1.69530000	1.77942600
H	-5.92544000	-1.01984500	2.15620500
H	-5.39931900	-1.96512500	0.75046100
H	-5.16599600	-2.60834000	2.38579900
C	-3.41553300	-0.77347900	3.33676800
H	-2.49411600	-0.19295200	3.43809800
H	-4.21894600	-0.24211800	3.86052300
H	-3.26885000	-1.73171100	3.84556900
C	-2.79559300	2.49232500	-3.32672300
H	-2.55983000	2.29617100	-4.37831200
H	-3.48888200	3.34071500	-3.30380700
H	-1.87430300	2.79217400	-2.81865600
C	-4.78146000	0.95879100	-3.33571800
H	-5.21654800	0.02945300	-2.95741200
H	-5.48029200	1.77550000	-3.11891100
H	-4.68280100	0.87198300	-4.42380800
C	-5.47005300	4.72775900	0.89545800
H	-5.33156300	4.96017500	-0.16679100
H	-6.37376800	4.11693400	0.99244200
H	-5.63591100	5.67329300	1.42368700
C	-2.98644500	4.87155900	1.35728800
H	-3.12469500	5.82124100	1.88649200
H	-2.11362600	4.36316200	1.78032900
H	-2.76055300	5.09991900	0.30905000
C	4.28281600	-2.89660500	1.77868600
H	5.24193100	-2.48369300	2.11419900
H	4.00610600	-3.71156600	2.45752400
H	4.42231300	-3.31778100	0.77844400
C	2.94178900	-1.31578300	3.20634700
H	2.53949300	-2.13342900	3.81271600
H	3.86188400	-0.96912300	3.69038700
H	2.21547600	-0.49633600	3.21788800
C	4.09502400	-0.37693100	-3.73505100
H	3.77089000	-0.38871100	-4.78224000
H	5.05764300	0.14600100	-3.68267300
H	4.24923900	-1.41098100	-3.41362000
C	2.77304800	1.73572300	-3.41109300
H	2.27170600	1.65461800	-4.38190800
H	2.13200800	2.31599800	-2.74101700
H	3.69942100	2.29914900	-3.57214300
C	7.18128900	1.97466100	0.79079500
H	7.87245800	2.72008600	1.20053900
H	7.32371000	1.03563700	1.33600400
H	7.44933400	1.80042700	-0.25826600

C	5.56362400	3.81433000	0.19217400
H	5.90750300	3.77204400	-0.84788400
H	4.51934300	4.14326700	0.19388400
H	6.16490700	4.57433600	0.70268300
H	-0.45778800	-5.46902600	4.45637400
H	1.88241000	6.14726900	1.66128900

<sup>s</sup>In6

ATOM	X	Y	Z
Fe	0.26395400	-0.40699800	0.48891500
N	1.88047000	-1.58447800	0.06994900
N	-0.68991500	-2.01894000	-0.14693200
C	3.61520600	0.11905800	0.09056500
C	3.94679800	0.71633000	-1.14284200
C	4.26218700	2.07575900	-1.14319600
H	4.49029000	2.55091300	-2.09511400
C	4.27553900	2.84500100	0.02042800
C	3.98846500	2.21184700	1.22410900
H	4.01346300	2.79281800	2.14288000
C	3.65320300	0.85825100	1.28198200
C	3.18423200	-1.30767400	0.11869700
C	4.14986600	-2.33567100	0.13429400
H	5.19320900	-2.06042500	0.23768200
C	3.77638500	-3.65152900	-0.00180300
H	4.51691400	-4.44522000	-0.00472300
C	2.41141000	-3.95421200	-0.16473600
C	1.90040000	-5.27777700	-0.39173400
H	2.60477300	-6.10275300	-0.43290800
C	0.57151000	-5.49286100	-0.56768200
H	0.19184500	-6.49230000	-0.75545900
C	-0.36490500	-4.40494300	-0.51258600
C	-1.75112200	-4.54059200	-0.72018500
H	-2.17879900	-5.51655100	-0.92784200
C	-2.54327200	-3.41890100	-0.68089300
H	-3.60733600	-3.48467000	-0.87566700
C	-1.99459800	-2.14925000	-0.39066700
C	0.10991400	-3.11426700	-0.24546300
C	1.51118900	-2.88012800	-0.09342900
C	-2.88495500	-0.95209100	-0.42348800
C	-3.85018200	-0.76697800	0.57623700
C	-4.75175500	0.29416200	0.45009600
H	-5.49943300	0.43337900	1.22485100
C	-4.70473200	1.17545000	-0.62193000
C	-3.72467400	0.97178700	-1.59610900

H	-3.67741400	1.66581800	-2.43093400
C	-2.81606200	-0.07767400	-1.53075400
C	-3.96954600	-1.69426500	1.77879500
H	-3.10961400	-2.37178200	1.77767700
C	-1.83436900	-0.31807600	-2.67255200
H	-0.92112500	-0.74461500	-2.24825100
C	4.01769100	0.01017900	-2.50049200
H	3.94136100	0.81836500	-3.23806500
C	3.38375700	0.20356000	2.62693000
H	2.89909000	-0.76039100	2.45323800
C	4.55272100	4.33616300	-0.02777900
H	4.59130000	4.69458300	1.00873300
C	-5.68449900	2.32489900	-0.79839100
H	-5.08849400	3.20324200	-1.08148200
C	-0.25626600	1.37992600	0.03121500
C	0.74945200	1.03377500	-0.68481300
H	1.47682200	1.34944400	-1.41566000
C	-1.22059500	2.41883100	0.35728600
C	-1.27487300	3.58623100	-0.42003900
C	-2.10663300	2.27452500	1.42885900
C	-2.20634600	4.57920500	-0.13947900
H	-0.58094700	3.70323500	-1.24807900
C	-3.02886900	3.27537700	1.71627300
H	-2.06308500	1.36666400	2.01759100
C	-3.08791500	4.42492900	0.93129400
H	-2.24357600	5.47562900	-0.75186700
H	-3.71234300	3.15179900	2.55169600
C	5.39828000	-0.63431200	-2.70564400
H	5.48947000	-1.02009900	-3.72742200
H	6.20011300	0.09255900	-2.53916500
H	5.54851600	-1.47265600	-2.01756300
C	2.90082100	-0.98504500	-2.85600400
H	3.05283900	-1.96507300	-2.39409900
H	1.91175000	-0.62111000	-2.56328300
H	2.90152300	-1.13979900	-3.94060300
C	4.70965200	-0.06641700	3.35353600
H	5.24008200	0.87137200	3.55833700
H	4.52827600	-0.57075400	4.30928700
H	5.36783900	-0.70196900	2.75045700
C	2.42860600	1.01790900	3.50674500
H	2.16063400	0.43690700	4.39533500
H	2.88121300	1.95662600	3.84612800
H	1.50478000	1.25700800	2.96912500
C	5.90227400	4.65821700	-0.68168000

H	6.10052900	5.73462500	-0.63329000
H	6.72135000	4.13567300	-0.17636400
H	5.91423800	4.36591700	-1.73807300
C	3.40527800	5.07362800	-0.73398200
H	3.32753000	4.76151400	-1.78226900
H	2.44592300	4.86506600	-0.24818900
H	3.57297200	6.15634200	-0.71561100
C	-1.41655400	0.95887800	-3.40772100
H	-0.58401800	0.73591200	-4.08406900
H	-2.23147900	1.36583700	-4.01752300
H	-1.09085100	1.73050300	-2.70471900
C	-2.41718400	-1.33326500	-3.66952200
H	-2.65652700	-2.28601900	-3.18599700
H	-3.33703800	-0.94125500	-4.11958200
H	-1.70064700	-1.53316500	-4.47443700
C	-6.65457600	2.02102000	-1.95190800
H	-7.33432200	2.86424900	-2.11933000
H	-6.11976700	1.82394100	-2.88676200
H	-7.25963900	1.13708500	-1.71630300
C	-6.46593700	2.68722000	0.46515900
H	-7.16152800	1.88899900	0.75071600
H	-5.79638300	2.87778100	1.30933200
H	-7.05817500	3.59153500	0.28943000
C	-5.24466000	-2.54580100	1.68584500
H	-6.13911400	-1.91289800	1.72755800
H	-5.28464400	-3.11540800	0.75119900
H	-5.29379100	-3.25524700	2.51942800
C	-3.92626700	-0.93390800	3.11065800
H	-2.98454000	-0.38899300	3.20672200
H	-4.75777500	-0.22608500	3.20314200
H	-4.00001400	-1.64190800	3.94428800
C	0.25662300	-1.17324900	2.20633000
O	0.82080800	-1.93978300	2.96700700
O	-0.81778200	-0.51224700	2.19721900
H	-3.81779900	5.19853600	1.15217000

<sup>T</sup>In6

ATOM	X	Y	Z
Fe	0.07057900	0.36718100	0.03080800
N	1.47289800	-1.10600300	-0.79972100
N	-1.18126300	-0.92052000	-1.25130100
C	3.42070400	0.06094000	-0.00228700
C	3.95960800	1.02718100	-0.87573300
C	4.40986300	2.22746300	-0.31865300

H	4.80677000	2.98667900	-0.98971000
C	4.36956800	2.48247700	1.04862100
C	3.89727400	1.47732000	1.88878700
H	3.89259800	1.65569900	2.96001400
C	3.42193000	0.26490400	1.39135900
C	2.78466000	-1.16192000	-0.57481400
C	3.54363500	-2.29381200	-0.93276100
H	4.59976600	-2.31908300	-0.69042300
C	2.95045800	-3.32626800	-1.61865200
H	3.52362800	-4.19907400	-1.91646600
C	1.59039500	-3.22722700	-1.96998200
C	0.90945700	-4.21961900	-2.75315800
H	1.47165500	-5.08097400	-3.10025600
C	-0.40321900	-4.07857000	-3.06029200
H	-0.91604400	-4.82336500	-3.66109200
C	-1.15398900	-2.95140000	-2.58277200
C	-2.52572100	-2.77630900	-2.84653200
H	-3.05383100	-3.49299200	-3.46822300
C	-3.18267800	-1.70364000	-2.29532400
H	-4.24110800	-1.54843500	-2.46999500
C	-2.48810500	-0.79477900	-1.46911500
C	-0.52240100	-1.97171900	-1.79502000
C	0.88803200	-2.09644600	-1.51168800
C	-3.23764400	0.30696000	-0.78863800
C	-3.83970500	0.05244300	0.46022800
C	-4.54636300	1.08181700	1.07684200
H	-5.00418800	0.90032700	2.04493200
C	-4.67320500	2.34361700	0.49615100
C	-4.08469800	2.55897400	-0.74560300
H	-4.18786900	3.53667000	-1.20805200
C	-3.36672100	1.56064400	-1.40804700
C	-3.76158000	-1.31800400	1.12211500
H	-2.83300200	-1.79851200	0.79466300
C	-2.79387900	1.82520900	-2.79350600
H	-1.93684100	1.16032100	-2.93967200
C	4.23235600	0.86011100	-2.37550800
H	4.26259100	1.88282300	-2.77063800
C	2.99108300	-0.84436000	2.34107700
H	2.18822800	-1.40924400	1.85637900
C	4.82300400	3.81598000	1.61412200
H	4.71811200	3.75780400	2.70502300
C	-5.41441700	3.46041800	1.20851000
H	-5.40184500	4.33507600	0.54562000
C	-0.71513000	0.61542700	1.80026500

H	-1.12652500	1.43013200	2.37713100
C	-0.39867200	-0.61619000	1.71159900
C	-0.38626900	-1.91623300	2.36581300
C	-0.55645200	-1.99725200	3.75718600
C	-0.21421400	-3.10288200	1.64460900
C	-0.55107300	-3.22735100	4.40324900
H	-0.69083300	-1.08024500	4.32285000
C	-0.21673300	-4.33615000	2.28961200
H	-0.08351100	-3.05663700	0.57086400
C	-0.38240400	-4.40297500	3.67079600
H	-0.68280900	-3.27159800	5.48041800
H	-0.08556200	-5.24616200	1.71163400
C	5.64305300	0.27237000	-2.56024600
H	5.90867800	0.24788300	-3.62325700
H	6.39478200	0.86593100	-2.02963300
H	5.69039400	-0.75377700	-2.17799700
C	3.23081800	0.10289800	-3.25850800
H	3.30423100	-0.98113700	-3.14142700
H	2.20166300	0.41333400	-3.07485500
H	3.46527000	0.32403100	-4.30632600
C	4.16002300	-1.81155100	2.59173000
H	4.99498100	-1.28783100	3.07232500
H	3.84256200	-2.62667800	3.25174400
H	4.53140000	-2.25420700	1.66257900
C	2.44546300	-0.33795000	3.67822400
H	2.03309500	-1.17814300	4.24505300
H	3.23138000	0.11679200	4.29198800
H	1.64739900	0.39603800	3.52995700
C	6.29773300	4.10128900	1.30194700
H	6.61521800	5.03557400	1.77817200
H	6.94244700	3.29433300	1.66576900
H	6.46086600	4.20512000	0.22293500
C	3.92352600	4.95746900	1.11946400
H	4.01710000	5.08766700	0.03496400
H	2.87102700	4.75578200	1.34468000
H	4.20420300	5.90290300	1.59691100
C	-2.28158200	3.25856700	-2.97458900
H	-1.72087900	3.33274800	-3.91126500
H	-3.10521700	3.98004900	-3.02522900
H	-1.61483600	3.55258300	-2.15897100
C	-3.83873400	1.49947900	-3.87285500
H	-4.16833800	0.45718500	-3.81688000
H	-4.72161800	2.13922400	-3.75676400
H	-3.42159800	1.67008700	-4.87172600

C	-6.88167700	3.09769300	1.47287500
H	-7.40686800	3.94174700	1.93360000
H	-7.39741800	2.83829200	0.54235800
H	-6.96170200	2.24278700	2.15444400
C	-4.69956900	3.85066500	2.50977200
H	-4.70717300	3.02009600	3.22545000
H	-3.65573900	4.12119700	2.31854200
H	-5.19651600	4.70554300	2.98197200
C	-4.93921600	-2.20371200	0.68317500
H	-5.89007400	-1.74528600	0.97951500
H	-4.96078100	-2.35406600	-0.39982100
H	-4.87179500	-3.18810400	1.16001600
C	-3.71900500	-1.25159700	2.65292100
H	-2.97524800	-0.52913700	2.99975000
H	-4.69334300	-0.97640600	3.07298900
H	-3.45249400	-2.23313600	3.05786700
C	0.44063800	1.68947800	-1.46813700
O	0.50144500	2.31987800	-0.38374800
O	0.56104700	1.91035700	-2.65318400
H	-0.38024000	-5.36444100	4.17542000

<sup>Q</sup>In6

ATOM	X	Y	Z
Fe	0.12365200	0.23695200	0.05087700
N	1.52498700	-1.16822200	-0.82877700
N	-1.13362400	-1.04107500	-1.25172600
C	3.40291400	0.08885800	-0.05886200
C	3.80262400	1.12264700	-0.92982400
C	4.12121200	2.35929000	-0.36457900
H	4.40990700	3.16936300	-1.03115800
C	4.06999700	2.59249800	1.00697000
C	3.74505900	1.52725500	1.84270500
H	3.73460600	1.69250000	2.91593200
C	3.41214200	0.27081100	1.33766100
C	2.84184000	-1.16726200	-0.63665000
C	3.63732000	-2.26201900	-1.02835300
H	4.70238400	-2.24144700	-0.82942700
C	3.06124400	-3.32170800	-1.68844200
H	3.66112800	-4.16929500	-2.00590100
C	1.68365000	-3.28882100	-1.98584700
C	1.01102800	-4.31686800	-2.72961800
H	1.58960600	-5.16512200	-3.08175200
C	-0.31602300	-4.22540000	-2.99451700
H	-0.82175200	-4.99915000	-3.56383800

C	-1.08789700	-3.11007400	-2.52166600
C	-2.47015200	-2.97053300	-2.75802100
H	-2.99715300	-3.71845300	-3.34278000
C	-3.13663500	-1.88943000	-2.23534400
H	-4.20003300	-1.75842900	-2.39868200
C	-2.44215600	-0.93515100	-1.46024700
C	-0.46436700	-2.09804600	-1.77255400
C	0.95425100	-2.18216000	-1.51690200
C	-3.17624600	0.20003500	-0.82048700
C	-3.76526900	0.00340900	0.44415000
C	-4.44560800	1.06844200	1.02983300
H	-4.89475900	0.93249400	2.00929000
C	-4.55191900	2.31002100	0.40500600
C	-3.96810200	2.47069700	-0.84784900
H	-4.04676700	3.43710200	-1.33704000
C	-3.27662400	1.43681100	-1.48180700
C	-3.69534900	-1.34005600	1.16078000
H	-2.77571400	-1.84528800	0.84380100
C	-2.68423800	1.64434100	-2.87042600
H	-1.77537800	1.03722900	-2.93886600
C	4.03701800	0.99433900	-2.43770300
H	4.00998200	2.02375900	-2.81442900
C	3.13598300	-0.89462400	2.27885200
H	2.36865400	-1.52775200	1.81934200
C	4.35025600	3.96991000	1.57883400
H	4.21414500	3.90400300	2.66575600
C	-5.25818000	3.46847300	1.08581800
H	-5.24149300	4.31574000	0.38860400
C	-0.52561800	0.61698400	1.83573900
H	-0.86808700	1.48703600	2.37447000
C	-0.28499500	-0.63426700	1.78883100
C	0.31380800	2.17072100	-0.99608500
C	-0.30794600	-1.92431100	2.45808700
C	-0.46906300	-1.98924500	3.85086700
C	-0.18611100	-3.11889900	1.73966600
C	-0.50795500	-3.21594400	4.50214700
H	-0.56437000	-1.06499700	4.41260400
C	-0.23368000	-4.34791200	2.39042100
H	-0.06083600	-3.07952000	0.66419000
C	-0.39321000	-4.40025900	3.77318700
H	-0.63364300	-3.25074300	5.58029600
H	-0.14332200	-5.26549800	1.81679600
C	5.46200600	0.46835000	-2.68179400
H	5.69404700	0.48231900	-3.75283000

H	6.20650100	1.07794400	-2.15900300
H	5.56251000	-0.56480800	-2.32998700
C	3.02596500	0.21443000	-3.29026400
H	3.14214800	-0.86871400	-3.19489900
H	2.00051400	0.49275000	-3.04196600
H	3.20528100	0.45871400	-4.34385700
C	4.40651200	-1.74420900	2.45081400
H	5.20844700	-1.14472800	2.89748300
H	4.20775400	-2.59550800	3.11162700
H	4.77137800	-2.13550700	1.49664300
C	2.61371500	-0.47238400	3.65438400
H	2.29470200	-1.35875900	4.21140500
H	3.39053000	0.02567900	4.24590000
H	1.75599600	0.20104000	3.56694700
C	5.79545300	4.41223700	1.31385000
H	5.99095700	5.38249700	1.78387300
H	6.51112300	3.68577100	1.71323900
H	5.98321000	4.51720200	0.23885400
C	3.34893100	5.00278500	1.04251600
H	3.48491500	5.15771400	-0.03416900
H	2.31726200	4.67462600	1.20456500
H	3.49067900	5.96879100	1.53982500
C	-2.26955400	3.09368500	-3.14765500
H	-1.68530900	3.13498500	-4.07254600
H	-3.14167600	3.74441300	-3.28217700
H	-1.65369800	3.49646300	-2.33907000
C	-3.66845500	1.17026700	-3.95247300
H	-3.91699200	0.11029600	-3.84536400
H	-4.60152900	1.74355400	-3.89702000
H	-3.23674500	1.31628200	-4.94910500
C	-6.72657400	3.14602500	1.39202100
H	-7.22680300	4.01892000	1.82590800
H	-7.26485800	2.85767900	0.48300200
H	-6.80981000	2.32272500	2.11105000
C	-4.50911500	3.89423900	2.35645100
H	-4.51652600	3.09094000	3.10255400
H	-3.46483600	4.13778500	2.13380200
H	-4.98085700	4.77513900	2.80609900
C	-4.88850800	-2.22832500	0.77239800
H	-5.82938700	-1.75011100	1.06934100
H	-4.93116300	-2.41393200	-0.30440700
H	-4.82279000	-3.19704200	1.28046000
C	-3.63246200	-1.21150700	2.68698300
H	-2.87121800	-0.48995200	2.99571700

H	-4.59614400	-0.89964700	3.10598300
H	-3.38049300	-2.18092500	3.12872300
O	0.04607500	3.11971200	-0.26089600
O	0.60066700	1.99354500	-2.17926900
H	-0.42814100	-5.35873000	4.28223000

<sup>s</sup>In2

ATOM	X	Y	Z
Fe	-0.24261600	0.59505900	-0.13089500
N	-1.63457100	2.00866200	-0.09362700
N	0.92474600	2.18723100	-0.07493700
C	-3.38301500	0.41946200	0.22132500
C	-3.95731600	-0.32545000	-0.82028100
C	-4.19978300	-1.68245700	-0.61128700
H	-4.62663900	-2.26925500	-1.42120300
C	-3.87759100	-2.31487900	0.58892700
C	-3.33288600	-1.54448300	1.61411900
H	-3.08138900	-2.02925200	2.55477700
C	-3.07608800	-0.18379800	1.45437100
C	-2.95402100	1.82954600	0.00848800
C	-3.84046200	2.92353600	-0.02716900
H	-4.90574800	2.73360500	0.04553700
C	-3.35721400	4.21145100	-0.13676200
H	-4.03735300	5.05742100	-0.16339600
C	-1.96373000	4.42093200	-0.18336600
C	-1.31561300	5.70372800	-0.24511900
H	-1.93246800	6.59658900	-0.28280800
C	0.04084900	5.80425000	-0.24730900
H	0.51838400	6.77848100	-0.28934600
C	0.87848000	4.63475100	-0.18577400
C	2.28582200	4.64981400	-0.14764100
H	2.82629100	5.59106400	-0.17190700
C	2.95789400	3.44919500	-0.06997100
H	4.04125800	3.42511800	-0.02680900
C	2.26196200	2.22330800	-0.03559600
C	0.26267300	3.37756500	-0.14358300
C	-1.15719100	3.27672300	-0.15076300
C	3.00697100	0.93205100	0.04886700
C	3.25048500	0.35147200	1.30373700
C	3.95880600	-0.85043300	1.35386500
H	4.14820200	-1.31990000	2.31533700
C	4.41806800	-1.48309300	0.20241400
C	4.15761300	-0.88383400	-1.02929800
H	4.49703100	-1.37573500	-1.93644700

C	3.44887700	0.31030600	-1.13206900
C	2.77040900	1.01688700	2.58691300
H	1.87785100	1.60521300	2.34418000
C	3.16341300	0.91604100	-2.49902400
H	2.25484300	1.52172400	-2.40691500
C	-4.27024500	0.29313600	-2.17418900
H	-3.87884800	1.31577000	-2.18078500
C	-2.44541900	0.60415900	2.59570200
H	-2.49956300	1.66964300	2.35181000
C	-4.06547400	-3.81097700	0.76344000
H	-3.84954900	-4.04563300	1.81372800
C	5.14931500	-2.81059300	0.28348100
H	5.26271900	-3.05654400	1.34717300
C	-0.07500100	-0.36651800	-1.67995100
C	0.14102200	-1.18689100	-0.66389100
H	-0.10708700	-0.41979000	-2.77059900
C	0.38221600	-2.61309000	-0.44878000
C	0.44688300	-3.52937200	-1.51191500
C	0.53817800	-3.11271100	0.85361500
C	0.64767000	-4.88657500	-1.28175000
H	0.32864900	-3.16032000	-2.52787600
C	0.73818700	-4.46977300	1.08977300
H	0.49624200	-2.41028900	1.68222100
C	0.79105900	-5.36425400	0.02125500
H	0.69001200	-5.57751700	-2.11960200
H	0.85349400	-4.83202900	2.10786900
C	4.31285300	1.83380500	-2.94265100
H	4.48041100	2.64686500	-2.22969300
H	5.24532800	1.26310300	-3.02827900
H	4.09565500	2.27909700	-3.92024300
C	2.88904700	-0.14151500	-3.57560400
H	2.48621400	0.33883500	-4.47393100
H	3.80444700	-0.66713600	-3.87111700
H	2.16450400	-0.88253500	-3.22521500
C	6.55458300	-2.72616300	-0.32666800
H	7.14575700	-1.93668300	0.14952000
H	7.08415000	-3.67703300	-0.19982700
H	6.50618700	-2.51226700	-1.40073100
C	4.32647700	-3.92950800	-0.37031600
H	4.19580100	-3.74466800	-1.44318600
H	4.83034500	-4.89611600	-0.25464700
H	3.33111300	-4.00218500	0.07950600
C	3.83498800	1.98261500	3.12939900
H	4.75476900	1.43819500	3.37406700

H	4.08477100	2.75639500	2.39666200
H	3.47783700	2.47726500	4.03970100
C	2.36133600	0.01383300	3.67099300
H	3.22902200	-0.50246500	4.09643500
H	1.86057500	0.53708800	4.49276200
H	1.67413400	-0.74183200	3.27691200
C	-5.78498300	0.37719600	-2.40477300
H	-6.23482900	-0.62255300	-2.42169900
H	-6.27503800	0.95256200	-1.61163200
H	-6.00097900	0.86091400	-3.36390700
C	-3.57379100	-0.45812600	-3.31651500
H	-3.97426500	-1.47158800	-3.43366000
H	-3.72549900	0.06946900	-4.26472200
H	-2.49816500	-0.53740800	-3.12989400
C	-3.06012200	-4.58344800	-0.10354100
H	-3.16253100	-5.66258800	0.05878600
H	-3.23244900	-4.38432600	-1.16813500
H	-2.03000500	-4.29498000	0.13001000
C	-5.50505300	-4.25428300	0.47469500
H	-5.76895500	-4.08914400	-0.57624300
H	-5.62384200	-5.32365000	0.68107300
H	-6.22032600	-3.70295200	1.09418500
C	-3.20523500	0.41710300	3.91653100
H	-4.26946400	0.64027000	3.78991500
H	-3.11563400	-0.60653000	4.29648400
H	-2.80182900	1.08988400	4.68107600
C	-0.96682100	0.24612800	2.78276800
H	-0.52512200	0.83568200	3.59309700
H	-0.84753900	-0.81541300	3.02312200
H	-0.34500400	0.43074200	1.88561200
H	0.94641600	-6.42406000	0.20136200

<sup>1</sup>In2

ATOM	X	Y	Z
Fe	-0.36327900	0.31799700	-0.06313600
N	0.78523600	2.08317400	0.03908100
N	-1.88389400	1.72734200	-0.04971400
C	2.99463500	1.04018500	0.17054400
C	3.16819700	0.34013100	1.37686800
C	4.10347100	-0.68834700	1.41250400
H	4.25312800	-1.23309400	2.34248200
C	4.87243900	-1.03794800	0.30156200
C	4.65690700	-0.34414400	-0.88452600
H	5.21751000	-0.61691300	-1.77276800

C	3.73155800	0.69816000	-0.97241800
C	2.10372600	2.23377700	0.14095900
C	2.69713300	3.51388400	0.24698300
H	3.77622200	3.57783300	0.33063800
C	1.91806500	4.64056300	0.23533700
H	2.36156600	5.62887000	0.31026900
C	0.51633300	4.50380900	0.13596200
C	-0.37603100	5.62689400	0.12979100
H	0.04918500	6.62395100	0.19076500
C	-1.71844700	5.44745800	0.05359200
H	-2.39402900	6.29734600	0.04963400
C	-2.27816800	4.12861900	-0.01252600
C	-3.66716500	3.88424500	-0.06992000
H	-4.36300400	4.71782100	-0.07661500
C	-4.11752100	2.58900900	-0.11234900
H	-5.17717300	2.36385100	-0.15531600
C	-3.19863500	1.51711100	-0.09810700
C	-1.42838600	3.01024200	-0.01052500
C	0.00151100	3.20062200	0.05139600
C	-3.71317200	0.11884500	-0.13935900
C	-3.91546500	-0.50361300	-1.37790200
C	-4.43931400	-1.79674400	-1.39397900
H	-4.60110700	-2.29268300	-2.34887400
C	-4.74997700	-2.48002000	-0.22124300
C	-4.52481100	-1.83709000	0.99623800
H	-4.74986400	-2.36047900	1.92301800
C	-4.00545400	-0.54599600	1.06113000
C	-3.56297300	0.18298600	-2.68874800
H	-3.08725500	1.14184600	-2.45782500
C	-3.75113200	0.09593100	2.41693700
H	-3.27573200	1.06877900	2.25343600
C	2.42608700	0.72769700	2.64861700
H	1.67968900	1.48711200	2.39627900
C	3.51196200	1.40569300	-2.30348100
H	2.95137100	2.32748600	-2.11446100
C	5.93526800	-2.11539500	0.45339600
H	5.45187000	-2.96661700	0.95003300
C	-5.28536200	-3.89958800	-0.27109700
H	-5.43342600	-4.15444900	-1.32826500
C	-0.94698300	-1.44650100	-0.03314000
C	0.37085100	-1.44147200	-0.16137600
H	-1.73567800	-2.19578600	0.01882500
C	1.42673300	-2.43993800	-0.29327800
C	1.83040400	-3.22638500	0.79817700

C	2.04671700	-2.67352200	-1.52985200
C	2.81213700	-4.20244100	0.65779800
H	1.36305400	-3.06502800	1.76528900
C	3.02022300	-3.65653400	-1.67355800
H	1.74860100	-2.07619900	-2.38612500
C	3.41243700	-4.42665900	-0.58006200
H	3.10699400	-4.79560100	1.52012600
H	3.47859700	-3.82035200	-2.64596600
C	-5.06675600	0.34931100	3.16475100
H	-4.87642900	0.84575600	4.12289400
H	-5.73683000	0.98493700	2.57538700
H	-5.58914500	-0.59219300	3.37094400
C	-2.77647400	-0.73948700	3.25789800
H	-2.54351200	-0.22199800	4.19553000
H	-3.20507600	-1.71556800	3.51324500
H	-1.84379500	-0.90923300	2.70952600
C	-4.26684900	-4.89070800	0.30975700
H	-3.30458900	-4.81335400	-0.20752700
H	-4.09392100	-4.69402500	1.37449500
H	-4.63025200	-5.91987600	0.21138700
C	-6.64244700	-4.02879300	0.43277200
H	-7.37075800	-3.32287300	0.01963300
H	-7.04106000	-5.04248000	0.31396700
H	-6.55132600	-3.83057200	1.50709400
C	-2.54341500	-0.63392400	-3.49382300
H	-1.65695000	-0.84775600	-2.88712500
H	-2.96802400	-1.58810600	-3.82671200
H	-2.23266200	-0.07882300	-4.38626600
C	-4.82182300	0.48452500	-3.51262100
H	-5.34405600	-0.44000200	-3.78529500
H	-5.51940100	1.11200900	-2.94690200
H	-4.56030300	1.00949800	-4.43823600
C	7.06675900	-1.61410900	1.36661500
H	6.68772600	-1.30547100	2.34642500
H	7.81507900	-2.39962000	1.52298700
H	7.56859800	-0.75092700	0.91254200
C	6.51439800	-2.61969400	-0.86864000
H	7.09126900	-1.83707700	-1.37681500
H	7.19361200	-3.45860200	-0.68196300
H	5.72647500	-2.96246300	-1.54565300
C	2.65150100	0.54283700	-3.23699700
H	2.47198500	1.06160100	-4.18582000
H	3.15162400	-0.40796900	-3.45526000
H	1.68359000	0.31762700	-2.77523800

C	4.82327200	1.81781400	-2.98308400
H	4.61107900	2.40826200	-3.88129800
H	5.44345500	2.42319500	-2.31323700
H	5.41118900	0.94740600	-3.29501600
C	3.39357000	1.35731900	3.66140500
H	4.16146600	0.63812400	3.96968800
H	3.90031100	2.22825800	3.23067900
H	2.85519500	1.68282900	4.55888300
C	1.66224000	-0.45137100	3.26157200
H	0.95285500	-0.85963100	2.53482700
H	2.33997000	-1.25483400	3.57218800
H	1.10687100	-0.12149700	4.14737100
H	4.18044200	-5.18724200	-0.68964600

<sup>99</sup>In2

ATOM	X	Y	Z
Fe	-0.32640800	0.36403600	-0.12731600
N	0.74388700	2.12364200	-0.01904800
N	-1.90885200	1.71978900	-0.29140000
C	2.89336100	1.08491900	0.41543700
C	2.77774000	0.33407400	1.60572300
C	3.57951600	-0.79096100	1.76163200
H	3.49977500	-1.37466300	2.67551700
C	4.50464200	-1.19075300	0.79362800
C	4.59372000	-0.43685400	-0.36940800
H	5.29932000	-0.72841400	-1.14097200
C	3.79562900	0.69141600	-0.58510100
C	2.06218700	2.31198800	0.23011700
C	2.61957600	3.57497900	0.32120000
H	3.67746500	3.67313300	0.53654600
C	1.81435300	4.71607000	0.12180000
H	2.24784600	5.71063800	0.17481900
C	0.45964800	4.55967100	-0.12302400
C	-0.45662900	5.66113900	-0.31199600
H	-0.05191500	6.66970000	-0.30044600
C	-1.78311800	5.45575500	-0.48910600
H	-2.45857200	6.29626000	-0.62476400
C	-2.34230100	4.12567200	-0.48826100
C	-3.69415100	3.85550400	-0.63122800
H	-4.39891400	4.67121800	-0.76792000
C	-4.14843200	2.52657400	-0.57816400
H	-5.20288900	2.29022200	-0.66352800
C	-3.23376900	1.49904600	-0.39243800
C	-1.44843500	3.02517900	-0.31960000

C	-0.07072500	3.23646900	-0.16276300
C	-3.67231200	0.07833700	-0.26079600
C	-3.67164900	-0.76403300	-1.38206800
C	-4.00725600	-2.10832200	-1.20853100
H	-4.00811500	-2.77267700	-2.07036200
C	-4.32523800	-2.63233400	0.04111700
C	-4.32857400	-1.76796100	1.13744600
H	-4.56358600	-2.16341800	2.12288900
C	-4.01004100	-0.41706500	1.01117700
C	-3.32818100	-0.24461000	-2.76993200
H	-2.99739900	0.79399300	-2.67044200
C	-3.97188300	0.46492600	2.25199600
H	-3.84073400	1.50168000	1.92765100
C	1.88719100	0.79764900	2.75319200
H	1.09584300	1.42885600	2.33830300
C	3.96640300	1.47682700	-1.87971900
H	3.16792700	2.22277800	-1.93511400
C	5.38783600	-2.39770900	1.07284400
H	4.71977500	-3.20811600	1.39541500
C	-4.60825500	-4.11355800	0.21332700
H	-4.65012400	-4.55852500	-0.78899700
C	-0.81948600	-1.40218600	0.47737800
C	0.23217400	-1.50742500	-0.24492900
H	-1.62894300	-1.89331300	0.99938200
C	1.26059400	-2.36908100	-0.80480300
C	1.83802100	-3.38291300	-0.02792800
C	1.65885300	-2.22492800	-2.13784100
C	2.78125700	-4.24058900	-0.58172800
H	1.54093900	-3.49002000	1.01097800
C	2.59805000	-3.08855300	-2.69288500
H	1.21129100	-1.43927900	-2.73971700
C	3.15993700	-4.10022100	-1.91714700
H	3.22280400	-5.02275500	0.02895700
H	2.89149000	-2.96860500	-3.73156400
C	-5.28390800	0.40517700	3.04431300
H	-5.25682800	1.12173500	3.87261700
H	-6.14004600	0.65132100	2.40700800
H	-5.45472800	-0.58890700	3.47300600
C	-2.76918800	0.10899100	3.13789100
H	-2.73487500	0.76127100	4.01821700
H	-2.83135600	-0.92887100	3.48746200
H	-1.83006800	0.22447300	2.58654900
C	-3.46166100	-4.79253700	0.97699500
H	-2.50456100	-4.63618500	0.46748300

H	-3.37403400	-4.38314400	1.99062200
H	-3.63556000	-5.87105500	1.06200500
C	-5.95754700	-4.37455200	0.89427300
H	-6.77665500	-3.90105500	0.34286400
H	-6.15585100	-5.45069200	0.94795700
H	-5.96971300	-3.98368900	1.91827100
C	-2.17422400	-1.02602000	-3.41055100
H	-1.29246400	-1.01796600	-2.76080900
H	-2.44625800	-2.07142600	-3.59622700
H	-1.90109200	-0.57656600	-4.37173600
C	-4.57101200	-0.24397200	-3.67065600
H	-4.95026200	-1.26174900	-3.82058300
H	-5.37438800	0.35405100	-3.22682400
H	-4.33370700	0.17691200	-4.65417200
C	6.35404600	-2.09661200	2.23061300
H	5.82019300	-1.78761600	3.13499800
H	6.95079900	-2.98293300	2.47462200
H	7.04151800	-1.28906800	1.95178700
C	6.16937800	-2.89662300	-0.14319500
H	6.92044300	-2.16368400	-0.46177400
H	6.69838000	-3.82232700	0.10763900
H	5.50711800	-3.10172300	-0.98971100
C	3.84502100	0.59443600	-3.12794700
H	3.92454300	1.20967800	-4.03125300
H	4.63444000	-0.16413800	-3.17216600
H	2.88258000	0.07621000	-3.14914700
C	5.30265600	2.23373900	-1.87930200
H	5.40991500	2.82582400	-2.79526400
H	5.37421500	2.91210300	-1.02270000
H	6.14592200	1.53473200	-1.82758900
C	2.70707100	1.66679700	3.71934200
H	3.52284800	1.08412300	4.16410600
H	3.14530700	2.52461700	3.19784000
H	2.07439800	2.04482600	4.53074500
C	1.19657600	-0.34934300	3.49860200
H	0.66297100	-1.00486400	2.80286200
H	1.90747700	-0.95641700	4.07087900
H	0.46930200	0.05634800	4.21096800
H	3.89339400	-4.77550700	-2.34781600

<sup>T</sup>In3

ATOM	X	Y	Z
N	-1.06560600	-1.26455000	-1.08566200
N	1.57466700	-1.27517100	-0.94062900

C	-3.07779900	0.04724100	-0.65490200
C	-3.79188700	0.07923900	0.55886000
C	-4.31221500	1.29654200	1.01041700
H	-4.85168900	1.32743300	1.95473200
C	-4.13782700	2.48146600	0.30596700
C	-3.45736600	2.42672400	-0.91128600
H	-3.32018900	3.34314400	-1.47805700
C	-2.92750100	1.23861700	-1.40582900
C	-2.44409200	-1.21084000	-1.15226600
C	-3.17098800	-2.24627500	-1.71559900
H	-4.25276900	-2.15182400	-1.76386300
C	-2.54533800	-3.37821000	-2.25016400
H	-3.12407700	-4.18225400	-2.69696100
C	-1.11445600	-3.44302400	-2.24422400
C	-0.35293700	-4.49393400	-2.78780600
H	-0.87268300	-5.33192500	-3.24930400
C	1.04358800	-4.47290400	-2.75738700
H	1.60864700	-5.29245300	-3.19801600
C	1.74511900	-3.40716000	-2.16443100
C	3.17236200	-3.29713600	-2.10786600
H	3.79499600	-4.06987700	-2.55069600
C	3.73965700	-2.16922400	-1.50189700
H	4.82037900	-2.05631500	-1.46213200
C	2.95227000	-1.18916700	-0.92864100
C	0.99187400	-2.34742500	-1.58015000
C	-0.42522600	-2.34651600	-1.64694700
C	3.46968400	0.01114500	-0.20750700
C	3.60515100	1.25227600	-0.87388700
C	3.87900300	2.39632200	-0.12304500
H	3.95722500	3.35039200	-0.64093300
C	4.01580700	2.36569000	1.26279800
C	3.95092400	1.12637200	1.88751100
H	4.09747100	1.07320800	2.96564700
C	3.69460000	-0.05646900	1.18466800
C	3.54623200	1.43966300	-2.39179700
H	3.65302800	2.52111700	-2.54671100
C	3.79113900	-1.34764700	2.00188500
H	3.71802100	-1.02783800	3.04968300
C	-4.03375700	-1.17819300	1.38190300
H	-3.27733100	-1.91136500	1.08667800
C	-2.27102000	1.21195600	-2.78149800
H	-1.47534000	0.46233400	-2.75032300
C	-4.66493300	3.79649700	0.85056600
H	-5.10024000	3.58944800	1.83740100

C	4.21808700	3.63773000	2.06473300
H	4.25763300	3.35075200	3.12413900
C	-3.90514200	-0.95735200	2.89526400
H	-3.86244300	-1.92478300	3.40873400
H	-2.99700900	-0.40090500	3.14057300
H	-4.76485200	-0.40918700	3.29959800
C	-5.41472300	-1.77685800	1.07155900
H	-6.20753700	-1.07185200	1.35176000
H	-5.52835300	-2.00363000	0.00761900
H	-5.57026300	-2.70405800	1.63650300
C	-3.29666300	0.75604800	-3.83270600
H	-4.11995400	1.47883100	-3.90161500
H	-2.82794400	0.68092100	-4.82161900
H	-3.71738100	-0.22200100	-3.57820200
C	-1.63223400	2.53971500	-3.19874400
H	-1.04048000	2.38692700	-4.10971500
H	-2.39131900	3.29725700	-3.43469800
H	-0.97585900	2.92730800	-2.41346700
C	-3.53650400	4.81978600	1.04174900
H	-3.90714700	5.70836500	1.56645400
H	-2.70131200	4.39164600	1.60532000
H	-3.13577700	5.14516100	0.07455900
C	-5.77884700	4.36717600	-0.03802700
H	-5.39688800	4.59520100	-1.04026400
H	-6.60206400	3.65219000	-0.14553800
H	-6.18082800	5.29409900	0.38798600
C	5.18577700	-1.97166500	1.83006800
H	5.31089000	-2.82112000	2.51260700
H	5.31856900	-2.33662700	0.80626600
H	5.97593000	-1.24231400	2.04058400
C	2.70250900	-2.40961000	1.80776000
H	1.71305700	-1.95479600	1.77423600
H	2.83915500	-2.97850700	0.88511500
H	2.73061800	-3.11244600	2.64989700
C	5.54808600	4.32140300	1.71982900
H	5.69315000	5.21760600	2.33419600
H	6.39496400	3.64704500	1.88866200
H	5.56715400	4.63032100	0.66784300
C	3.03741700	4.60289100	1.88540500
H	2.99844000	4.98733500	0.85965800
H	2.07935500	4.10851600	2.07842600
H	3.13999900	5.46070100	2.56110100
C	2.23198300	1.04792100	-3.08065100
H	2.09070100	-0.03551400	-3.10427700

H	1.37946300	1.49892000	-2.56377500
H	2.24797200	1.41208100	-4.11602600
C	4.74951300	0.78560200	-3.08831600
H	5.69208500	1.08981400	-2.61890200
H	4.67906100	-0.30478000	-3.04451700
H	4.78224800	1.08187200	-4.14398400
C	-0.35814800	0.38864900	2.12351600
O	0.26080000	1.99345100	-0.47999800
C	-0.51820500	-0.79525000	2.35479200
H	-0.27764600	1.49248700	1.92417700
C	0.03794300	3.15157100	0.16276100
C	-0.72370400	-2.17084300	2.70807800
O	-0.21231400	3.09567100	1.41943800
O	0.09334100	4.20838400	-0.50682600
C	-0.93816100	-3.14267200	1.72197200
C	-0.71363600	-2.54922900	4.05824000
C	-1.14197800	-4.46932200	2.08355800
H	-0.94408000	-2.84248700	0.68090700
C	-0.92178100	-3.87815100	4.41174000
H	-0.54666400	-1.79625600	4.82224100
C	-1.13598800	-4.84167900	3.42688100
H	-1.30529500	-5.21315200	1.30929600
H	-0.91520500	-4.16175300	5.46008700
Fe	0.26366400	0.13021500	-0.29549900
H	-1.29689300	-5.87890800	3.70557800

<sup>Q</sup>In3

ATOM	X	Y	Z
N	-1.21723700	-1.15701500	-1.01332600
N	1.43545400	-1.38191500	-0.78757200
C	-3.11004800	0.31424000	-0.73095600
C	-3.81980100	0.37912300	0.48276400
C	-4.27056200	1.62304800	0.93312800
H	-4.80398600	1.68912200	1.87848000
C	-4.02673400	2.79751000	0.22769000
C	-3.34078000	2.70576300	-0.98128700
H	-3.12629400	3.61366200	-1.53600200
C	-2.86741300	1.49057700	-1.47024300
C	-2.54735700	-0.98411300	-1.22532900
C	-3.34017800	-1.90466200	-1.87804100
H	-4.39193200	-1.69127400	-2.03440700
C	-2.76218100	-3.12403600	-2.35368700
H	-3.38293600	-3.87299200	-2.84181800
C	-1.41555800	-3.32956900	-2.20773400

C	-0.70583000	-4.50286700	-2.67462200
H	-1.28514100	-5.30464400	-3.13021700
C	0.64075300	-4.61134600	-2.57605500
H	1.14483300	-5.49885000	-2.95557100
C	1.45795200	-3.55749500	-2.00086000
C	2.82598700	-3.55868000	-1.97950100
H	3.38502700	-4.39484700	-2.39414400
C	3.51666500	-2.42209100	-1.42689600
H	4.59993600	-2.36817900	-1.45109500
C	2.80048600	-1.40276600	-0.85410100
C	0.74507600	-2.42169400	-1.45941800
C	-0.61456300	-2.30659300	-1.57123900
C	3.44851000	-0.21104500	-0.21841700
C	3.58880400	0.99468500	-0.94677800
C	4.03229200	2.13713200	-0.27818100
H	4.12381100	3.06417100	-0.84109200
C	4.33445200	2.14025300	1.08141700
C	4.24453300	0.93198600	1.75986200
H	4.50740000	0.90387700	2.81650200
C	3.82005700	-0.25053400	1.14254900
C	3.39250100	1.14383700	-2.45909600
H	3.51087300	2.21784500	-2.65173900
C	3.89857400	-1.51080300	2.00996800
H	4.01648500	-1.13889700	3.03634700
C	-4.11790200	-0.86994000	1.30392700
H	-3.35452900	-1.61671300	1.05928900
C	-2.13294000	1.44496600	-2.80380500
H	-1.41925000	0.61729500	-2.75189600
C	-4.40862600	4.14221800	0.82079300
H	-5.16777400	3.95719300	1.59303300
C	4.74128000	3.41401300	1.79910200
H	4.88635600	3.15861000	2.85724900
C	-4.05715000	-0.63041100	2.81738800
H	-4.11456200	-1.58870700	3.34459700
H	-3.12302700	-0.13805900	3.10367900
H	-4.89476900	-0.01483200	3.16644300
C	-5.48982500	-1.45250100	0.93162500
H	-6.28384200	-0.72717100	1.14980400
H	-5.54000900	-1.70482100	-0.13085000
H	-5.69303200	-2.36248900	1.50941600
C	-3.12203600	1.14347500	-3.94081900
H	-3.87408700	1.93943800	-4.01660700
H	-2.59810300	1.07986500	-4.90248200
H	-3.63955900	0.19414700	-3.76833200

C	-1.33156900	2.71657400	-3.10345600
H	-0.66319000	2.53555700	-3.95403600
H	-1.98758200	3.55183400	-3.38235400
H	-0.73126500	3.00907900	-2.23549300
C	-3.18326200	4.76805800	1.50739700
H	-3.43645400	5.73771500	1.95315600
H	-2.80596700	4.11211900	2.29922300
H	-2.36478500	4.91287900	0.79232500
C	-5.01609800	5.10928600	-0.20174700
H	-4.27929700	5.41254300	-0.95390400
H	-5.86606100	4.65519000	-0.72290100
H	-5.36644300	6.01921000	0.29851400
C	5.17300000	-2.30954400	1.69211500
H	5.31311000	-3.10898400	2.43015600
H	5.09966300	-2.76756200	0.70160900
H	6.05956400	-1.66554800	1.71220300
C	2.67279100	-2.42839100	2.03604100
H	1.76385800	-1.85686100	2.22822800
H	2.53851400	-2.96840000	1.09677100
H	2.79304100	-3.16594500	2.83987400
C	6.07224700	3.96201200	1.26634900
H	6.37084200	4.85936600	1.82091100
H	6.87164100	3.21823500	1.35714000
H	5.98444700	4.23576200	0.20819100
C	3.63410200	4.47445700	1.72062400
H	3.50688800	4.82888300	0.69085400
H	2.66992700	4.06845000	2.04459700
H	3.89002300	5.34117600	2.34242100
C	2.01943800	0.77050000	-3.03343000
H	1.84822000	-0.30812000	-3.02710900
H	1.21592500	1.25217500	-2.46749100
H	1.96270300	1.11951000	-4.07267600
C	4.51987200	0.43993000	-3.23132900
H	5.50392900	0.75751400	-2.86769000
H	4.44300500	-0.64518400	-3.11720300
H	4.45510900	0.67994300	-4.29968200
C	-0.23200500	0.28450300	2.40587700
O	0.21121600	1.97601500	-0.20610600
C	-0.55493400	-0.88162000	2.52816300
H	0.04497500	1.35931200	2.26797500
C	0.29233600	3.09572800	0.53104600
C	-0.93351900	-2.25400200	2.70690700
O	0.40765200	2.96703800	1.79998700
O	0.25006000	4.19415600	-0.07469100

C	-0.71185600	-3.18841900	1.68585100
C	-1.52432100	-2.67338900	3.90745900
C	-1.09217000	-4.51406300	1.86156100
H	-0.24510800	-2.87105000	0.76064200
C	-1.89818000	-4.00234000	4.07629900
H	-1.69486800	-1.94996400	4.69865600
C	-1.68702800	-4.92592600	3.05320200
H	-0.92092600	-5.22586500	1.05899900
H	-2.35790700	-4.31683700	5.00860800
Fe	0.19468300	0.10147800	-0.17098700
H	-1.98185100	-5.96268000	3.18688600

<sup>T</sup>In4

ATOM	X	Y	Z
Fe	0.42829300	-0.47346100	0.07364000
N	-0.26877100	-2.45603600	-0.14026800
N	2.22041300	-1.53944300	-0.02595700
C	-2.61337200	-1.87003500	-0.04065600
C	-3.21721000	-1.63342700	1.21066600
C	-4.19576200	-0.63960600	1.29637800
H	-4.65424700	-0.45084300	2.26543000
C	-4.60137000	0.11238100	0.19505000
C	-4.00171800	-0.15773900	-1.03017200
H	-4.30986800	0.41847300	-1.89950800
C	-3.00043600	-1.11992400	-1.16592000
C	-1.53727800	-2.89774500	-0.20131100
C	-1.86089500	-4.23429300	-0.42144300
H	-2.90403300	-4.52219000	-0.49351400
C	-0.83729400	-5.18792400	-0.53816900
H	-1.07265200	-6.23697300	-0.69857000
C	0.48479600	-4.77716400	-0.44726900
C	1.61746200	-5.66582000	-0.54536700
H	1.42856400	-6.72748100	-0.68546000
C	2.88824200	-5.20033500	-0.47011200
H	3.72827500	-5.88676600	-0.54655500
C	3.17084200	-3.79390000	-0.29285100
C	4.45034300	-3.26176700	-0.22408000
H	5.31781200	-3.91257700	-0.29577400
C	4.60587600	-1.86716900	-0.06884400
H	5.59084800	-1.41471400	-0.02192500
C	3.48402500	-1.05946900	0.01846000
C	2.06109900	-2.90464700	-0.18984000
C	0.74486900	-3.38686800	-0.25902200
C	3.58890500	0.42425300	0.15250800

C	3.56263300	1.22479700	-1.00346100
C	3.55040800	2.61064000	-0.85981500
H	3.51521300	3.23268700	-1.75172700
C	3.54394800	3.22074500	0.39481300
C	3.59204600	2.40595900	1.52263600
H	3.59248600	2.87225200	2.50601100
C	3.60850800	1.01284500	1.42577800
C	3.52597800	0.61163400	-2.39591100
H	3.38960400	-0.46788100	-2.28346300
C	3.63114100	0.16895000	2.69171200
H	3.51782200	-0.87903700	2.39836900
C	-2.92298500	-2.40298700	2.49962100
C	-2.36558100	-1.35266400	-2.53015900
H	-1.42358000	-1.88591100	-2.37402600
C	-5.66777700	1.18645800	0.31591800
H	-5.69583300	1.72200900	-0.64196500
C	3.42174500	4.72762000	0.53053700
H	3.49623700	4.96655400	1.59938700
C	-3.72329200	-3.71366600	2.55782400
H	-3.61142200	-4.18428600	3.54196200
H	-4.78954300	-3.53298400	2.38299700
H	-3.36585000	-4.42096000	1.80279300
C	-3.26785600	-2.24211500	-3.39698400
H	-4.23894000	-1.76114500	-3.56756300
H	-2.80481100	-2.42961000	-4.37290000
H	-3.44652900	-3.20746500	-2.91060100
C	-2.01624100	-0.04452800	-3.25106300
H	-1.42760900	-0.25838800	-4.15070400
H	-2.91309100	0.49971600	-3.57083100
H	-1.42966800	0.60999100	-2.59730900
C	-7.05113300	0.56199100	0.54753000
H	-7.82677000	1.33601600	0.57517300
H	-7.30226900	-0.14848900	-0.24744000
H	-7.07835700	0.02314800	1.50243600
C	-5.34105500	2.21617000	1.40468600
H	-5.34128900	1.75586300	2.39980600
H	-4.36003500	2.67047800	1.23538800
H	-6.09165200	3.01478200	1.40782500
C	2.46336500	0.50346900	3.62819400
H	2.45987600	-0.17743400	4.48729100
H	2.53352500	1.52680200	4.01513300
H	1.50663000	0.40104400	3.10372700
C	4.98087400	0.30256200	3.40941500
H	5.80341900	0.00530100	2.74948900

H	5.15777200	1.33764000	3.72569800
H	5.00930700	-0.33318900	4.30208400
C	4.55086400	5.47280100	-0.19241400
H	4.46326700	6.55293400	-0.02924400
H	5.53227200	5.14843600	0.16991900
H	4.51373700	5.29569300	-1.27361600
C	2.04419500	5.19997800	0.04106200
H	1.92892700	5.01702200	-1.03393600
H	1.23919800	4.66419000	0.55575200
H	1.91573400	6.27426400	0.21668900
C	4.85905200	0.83471200	-3.12237200
H	5.05392000	1.90441400	-3.26616500
H	5.69162600	0.41257200	-2.54876400
H	4.84594800	0.35785700	-4.10928600
C	2.34360700	1.13025100	-3.22466600
H	1.39877200	0.97038400	-2.69333400
H	2.43728000	2.20162800	-3.43772700
H	2.29419500	0.60397400	-4.18492900
C	-0.38438800	1.32748000	0.14111700
C	-1.07931200	2.33976600	0.04806500
C	-2.00773800	3.41942300	-0.10110300
C	-2.92642200	3.40821800	-1.16658300
C	-2.06275900	4.48162400	0.81702100
C	-3.87343600	4.41660500	-1.29883200
H	-2.89431300	2.58747500	-1.87614200
C	-3.01396000	5.48849500	0.68019300
H	-1.35877100	4.50179500	1.64383700
C	-3.92458800	5.46017300	-0.37474900
H	-4.58017300	4.38542000	-2.12350000
H	-3.04537900	6.29755200	1.40456100
C	-1.44627300	-2.65243300	2.83650100
H	-1.01985700	-3.46921800	2.24800600
H	-0.83832700	-1.75949400	2.65780000
H	-1.36127300	-2.92514000	3.89502300
H	-3.31236100	-1.76502000	3.30328100
H	-4.66903700	6.24449400	-0.47554700

<sup>99</sup>In4

ATOM	X	Y	Z
Fe	-0.08639200	-0.60869100	-0.03313300
N	1.15667800	-2.32422900	0.12486900
N	-1.51080900	-2.17261000	0.02544600
C	3.20930100	-1.06877800	0.05477500
C	3.66427300	-0.57397900	-1.18377500

C	4.26996500	0.68474800	-1.21138200
H	4.60266300	1.07541600	-2.17112200
C	4.45637100	1.45404600	-0.06375100
C	4.01199300	0.93226700	1.14631400
H	4.14907600	1.52019100	2.05122900
C	3.37371800	-0.30602400	1.22526500
C	2.49728400	-2.38053400	0.16061900
C	3.19963000	-3.57121200	0.32605800
H	4.28250400	-3.54941600	0.37920100
C	2.49095800	-4.78287900	0.42357100
H	3.02036700	-5.72431400	0.54732800
C	1.10654500	-4.76957600	0.36174900
C	0.28061200	-5.95196400	0.44398300
H	0.77227900	-6.91555400	0.55508900
C	-1.07087400	-5.87570700	0.38782400
H	-1.67407700	-6.77842000	0.45150600
C	-1.75204800	-4.60887000	0.24401600
C	-3.12963600	-4.47159400	0.18494200
H	-3.76702900	-5.35028400	0.24422100
C	-3.69239000	-3.18521400	0.04980400
H	-4.76657000	-3.04266600	0.00272400
C	-2.85240700	-2.08130400	-0.02249400
C	-0.94921000	-3.42989300	0.15993900
C	0.45030500	-3.50848200	0.21509900
C	-3.39491400	-0.69484600	-0.15135100
C	-3.62391400	0.06979200	1.00615200
C	-4.04996600	1.38908000	0.86599900
H	-4.21517000	1.98676000	1.75966800
C	-4.23894400	1.97307500	-0.38679100
C	-4.01979000	1.18927200	-1.51628600
H	-4.16528400	1.63471400	-2.49866800
C	-3.59311300	-0.13740800	-1.42314600
C	-3.40873900	-0.51024300	2.39655400
H	-2.91718000	-1.48099900	2.28312100
C	-3.33682000	-0.93711600	-2.69193000
H	-2.89957700	-1.89719600	-2.40175800
C	3.58695400	-1.31938800	-2.51676900
C	2.88496600	-0.80922300	2.57699800
H	2.18362100	-1.62843000	2.39690600
C	5.07004600	2.84181600	-0.12680000
H	5.29322000	3.14260000	0.90529600
C	-4.60477300	3.44067300	-0.51999100
H	-4.80077800	3.63340300	-1.58282900
C	4.72087300	-2.34842000	-2.64603500

H	4.72758800	-2.78338800	-3.65251200
H	5.69665100	-1.88368600	-2.46673000
H	4.58977000	-3.16219700	-1.92603100
C	4.05385100	-1.36999800	3.39851600
H	4.79953700	-0.59109000	3.59982700
H	3.69945200	-1.75822300	4.36070600
H	4.55079400	-2.18620600	2.86239300
C	2.11767400	0.26478200	3.35923500
H	1.65614800	-0.17777200	4.24935600
H	2.77567100	1.07338100	3.69850900
H	1.32760100	0.70276000	2.73949300
C	6.38520800	2.87521000	-0.91434100
H	6.84319300	3.86845300	-0.84757900
H	7.09974500	2.14111800	-0.52667900
H	6.22074400	2.65941800	-1.97627800
C	4.06133000	3.85073500	-0.69606600
H	3.79212400	3.58890700	-1.72662600
H	3.14049300	3.86676900	-0.10465800
H	4.48562700	4.86169600	-0.70303800
C	-2.32556600	-0.24323000	-3.61332800
H	-2.09401700	-0.88310300	-4.47269400
H	-2.71433700	0.70598700	-4.00043500
H	-1.39282300	-0.03611100	-3.07669200
C	-4.65109400	-1.23377300	-3.42613700
H	-5.34021600	-1.79069800	-2.78169800
H	-5.14858600	-0.30601200	-3.73322300
H	-4.46458200	-1.83060500	-4.32649100
C	-5.87337800	3.80531500	0.26087700
H	-6.13664700	4.85557300	0.09208200
H	-6.72078200	3.18400600	-0.04837900
H	-5.72966200	3.66878400	1.33890000
C	-3.42128300	4.32401100	-0.09641700
H	-3.18805600	4.17683300	0.96500600
H	-2.52071900	4.07900000	-0.66874300
H	-3.65116200	5.38488600	-0.24964500
C	-4.75405900	-0.75185500	3.09450100
H	-5.29354000	0.19183200	3.24078800
H	-5.38858100	-1.41609100	2.49735800
H	-4.60372800	-1.21226500	4.07793000
C	-2.48439800	0.36447000	3.25321400
H	-1.53227600	0.53947800	2.74013900
H	-2.93647700	1.33848600	3.47377200
H	-2.27721200	-0.12867200	4.20990200
C	0.07379100	1.35656500	-0.09461200

C	0.19963400	2.57961800	-0.02860900
C	0.36722400	3.99796400	0.05529300
C	0.55216100	4.62593000	1.29959000
C	0.36620800	4.79630100	-1.10238500
C	0.73264800	6.00266700	1.38022000
H	0.55610100	4.01831500	2.19981200
C	0.54698800	6.17240200	-1.01579700
H	0.22548500	4.32143600	-2.06872800
C	0.73210700	6.78248000	0.22430700
H	0.87571000	6.46949500	2.35070700
H	0.54477100	6.77161500	-1.92211000
C	2.23503900	-1.95258500	-2.87501000
H	2.05562900	-2.88198100	-2.32815700
H	1.40450000	-1.27215100	-2.65899700
H	2.22290600	-2.18792600	-3.94590300
H	3.77311200	-0.55374200	-3.28075600
H	0.87504400	7.85699500	0.29016300

<sup>T</sup>In5

ATOM	X	Y	Z
Fe	-0.12080600	0.60343300	0.24438100
N	1.19973800	2.21514200	-0.26521700
N	-1.44090700	2.18667100	0.04241800
C	3.10402000	0.79705000	-0.52114400
C	3.88230700	0.38125100	0.57042700
C	4.24010900	-0.96679300	0.66004000
H	4.81758000	-1.29763800	1.51756800
C	3.83077400	-1.89995000	-0.28454500
C	3.12515300	-1.44437900	-1.39910700
H	2.82654900	-2.17035700	-2.15024500
C	2.75677800	-0.11162300	-1.54516200
C	2.51241200	2.16916300	-0.53963200
C	3.25126200	3.32081500	-0.81415700
H	4.31031200	3.23293700	-1.02915300
C	2.62140800	4.56968900	-0.79159200
H	3.18965200	5.47563600	-0.98567500
C	1.25703300	4.64865200	-0.53783200
C	0.49756100	5.87229700	-0.52330800
H	1.02327600	6.81009300	-0.68362400
C	-0.84483100	5.86411200	-0.32481600
H	-1.40250800	6.79728400	-0.32232500
C	-1.57838300	4.63327100	-0.13159200
C	-2.95824100	4.56175800	0.02162300
H	-3.55663800	5.46832600	0.02004800

C	-3.57125900	3.29225300	0.14706200
H	-4.64902300	3.19959500	0.22968900
C	-2.79598000	2.15135200	0.14012500
C	-0.83607400	3.42077900	-0.11964600
C	0.55626200	3.43102900	-0.30163500
C	-3.35845800	0.77025200	0.19062700
C	-3.55495400	0.07405900	-1.01301500
C	-3.93543900	-1.26988800	-0.96143800
H	-4.06283500	-1.80849300	-1.89590700
C	-4.13992400	-1.92923700	0.24808700
C	-3.98837900	-1.19462200	1.42663100
H	-4.17955000	-1.68883900	2.37668900
C	-3.58504800	0.13843500	1.42662500
C	-3.37949900	0.75743400	-2.36375700
C	-3.44653600	0.89615500	2.73923900
H	-2.91957100	1.83301100	2.53095800
C	4.38363600	1.35814100	1.62706600
C	2.04665000	0.36883100	-2.80710400
H	1.28474700	1.09680400	-2.50821400
C	4.13347600	-3.38247700	-0.15084100
H	3.29452100	-3.91301400	-0.62076000
C	-4.50021600	-3.40630000	0.34451700
H	-5.38907500	-3.47548300	0.98795500
C	5.85467300	1.70477000	1.34706500
H	6.22108100	2.44392800	2.06892000
H	6.48300400	0.80944100	1.42913300
H	5.98601100	2.11499400	0.33967700
C	3.04570800	1.09006600	-3.72776000
H	3.83657200	0.39913400	-4.04420800
H	2.54036200	1.46409600	-4.62578000
H	3.51627500	1.93966300	-3.22341500
C	1.33341700	-0.73987400	-3.58401000
H	0.71746000	-0.29919800	-4.37559300
H	2.04647600	-1.42068400	-4.06429300
H	0.68389000	-1.33342400	-2.93479200
C	5.41077300	-3.74810700	-0.92137100
H	5.60387100	-4.82573200	-0.86427700
H	5.32983000	-3.46953700	-1.97779500
H	6.27629200	-3.22435300	-0.49746900
C	4.21453100	-3.85400600	1.30448900
H	5.13121400	-3.49744100	1.79006700
H	3.36029900	-3.49162100	1.88607000
H	4.23100000	-4.94902700	1.34434000
C	-2.62772300	0.14128400	3.79221000

H	-2.56226800	0.74014400	4.70818600
H	-3.09087000	-0.81509800	4.06107800
H	-1.60701800	-0.04946200	3.44694400
C	-4.83756000	1.26322700	3.27764500
H	-5.39951800	1.85413100	2.54590500
H	-5.41795700	0.35979200	3.50148600
H	-4.75269900	1.84854500	4.20040300
C	-4.84558900	-4.05516700	-0.99659800
H	-5.16478800	-5.09065800	-0.83776500
H	-5.65558600	-3.52662300	-1.51130700
H	-3.97169600	-4.07688300	-1.65890500
C	-3.37022300	-4.19153000	1.03198600
H	-2.46022900	-4.16182600	0.42426300
H	-3.13181500	-3.77592900	2.01616400
H	-3.66021000	-5.23994700	1.16744800
C	-2.21328100	0.17318500	-3.16851000
H	-1.27677100	0.22982000	-2.60302200
H	-2.39313900	-0.87692700	-3.42883900
H	-2.07639500	0.72716500	-4.10430000
C	0.47189700	-0.80051300	1.46762400
C	0.05098200	-1.36097900	0.39322200
C	-0.10466800	-2.66560800	-0.23337900
C	0.47858500	-3.78396600	0.38344500
C	-0.81154300	-2.84285300	-1.42622500
C	0.36682100	-5.04298900	-0.19719800
H	1.00181000	-3.63388500	1.32483600
C	-0.92283100	-4.10335000	-2.00622700
H	-1.28373000	-1.98350400	-1.88650000
C	-0.32976400	-5.20726100	-1.39580700
H	0.82386100	-5.90175300	0.28703900
H	-1.47301800	-4.22296000	-2.93556800
C	1.02231600	-0.95063000	2.87038700
O	1.48261900	-2.08442400	3.13953000
O	0.94809600	0.05551100	3.61529500
H	3.80655500	2.28384600	1.53895200
C	4.21041300	0.85820500	3.06584600
H	4.80982900	-0.03840600	3.26236500
H	4.54967900	1.63250500	3.76444800
H	3.16305900	0.62985700	3.28554200
C	-4.68084100	0.71898800	-3.17692900
H	-4.96836700	-0.30986800	-3.42328600
H	-5.50553800	1.17587500	-2.61943200
H	-4.55844500	1.26564900	-4.11887800
H	-3.14797200	1.81037900	-2.17945200

H	-0.41466900	-6.19112600	-1.84820400
<sup>Q</sup> In5			
ATOM	X	Y	Z
Fe	-0.07543200	0.58850400	0.22767200
N	1.21209100	2.21544000	-0.28842500
N	-1.44252700	2.17783500	0.03435100
C	3.13520400	0.81798500	-0.47960000
C	3.82880000	0.39013100	0.66567600
C	4.18546900	-0.95533400	0.76222000
H	4.68724600	-1.29974300	1.66002400
C	3.87606800	-1.87372600	-0.23800800
C	3.25521900	-1.40446700	-1.39377800
H	3.03833700	-2.11234600	-2.19135000
C	2.87508600	-0.07273100	-1.53678300
C	2.53275900	2.18365400	-0.53476500
C	3.25785700	3.33069000	-0.84600200
H	4.31683000	3.24992700	-1.06134000
C	2.60613800	4.57212000	-0.87947900
H	3.16126300	5.47851400	-1.10698300
C	1.24115600	4.63997300	-0.63812500
C	0.46852700	5.85677600	-0.67343000
H	0.98732800	6.79254200	-0.86546400
C	-0.87331100	5.84396600	-0.48138400
H	-1.44050700	6.77073400	-0.51647800
C	-1.59451100	4.61379200	-0.24124300
C	-2.97052700	4.53918600	-0.08106100
H	-3.57384300	5.44203500	-0.11641600
C	-3.57692400	3.27579200	0.10346300
H	-4.65348200	3.18151700	0.19600900
C	-2.79305300	2.13784900	0.14171200
C	-0.84143800	3.40589200	-0.18152200
C	0.55039300	3.42229600	-0.36266300
C	-3.35707000	0.76060800	0.27234000
C	-3.73116600	0.05464400	-0.88410000
C	-4.08854500	-1.29103400	-0.75987100
H	-4.34745900	-1.84622600	-1.65526600
C	-4.11148700	-1.93607900	0.47443500
C	-3.80770400	-1.18590400	1.61284000
H	-3.86681300	-1.67020500	2.58443000
C	-3.41886500	0.14897900	1.53860900
C	-3.74370300	0.73810200	-2.24886000
C	-3.15135000	0.95725400	2.80128500
H	-2.48603300	1.78444500	2.53083600
C	4.24068600	1.37254200	1.75538000

C	2.25555900	0.40593100	-2.84336800
H	1.83294600	1.40116600	-2.67740000
C	4.20423600	-3.35269000	-0.11860700
H	3.38926200	-3.89141600	-0.62099000
C	-4.44008200	-3.41452500	0.63602600
H	-5.20110100	-3.48657800	1.42599400
C	5.66326500	1.88411300	1.47448300
H	5.96004100	2.62918700	2.22171600
H	6.38075700	1.05547300	1.51741200
H	5.74145300	2.34338900	0.48394200
C	3.34655500	0.54555100	-3.91508500
H	3.81511100	-0.42424400	-4.12153100
H	2.92275400	0.92641100	-4.85168300
H	4.12995600	1.23729300	-3.58609400
C	1.10996100	-0.48546300	-3.32825100
H	0.63618300	-0.04612200	-4.21376300
H	1.45342500	-1.49051600	-3.59845800
H	0.35205900	-0.59131500	-2.54796300
C	5.50772300	-3.67943000	-0.86275300
H	5.71926100	-4.75435100	-0.82131800
H	5.44979900	-3.38171800	-1.91552400
H	6.35207400	-3.14852100	-0.40621700
C	4.25920400	-3.84983700	1.32910600
H	5.15604300	-3.48127600	1.84254600
H	3.38246200	-3.51759900	1.89574300
H	4.30258900	-4.94479200	1.34752400
C	-2.45912300	0.17191900	3.91853300
H	-2.26211200	0.84151000	4.76372500
H	-3.08611200	-0.64509900	4.29431800
H	-1.49844800	-0.23602700	3.59193700
C	-4.46876100	1.56814200	3.30550200
H	-4.93653300	2.19099800	2.53575500
H	-5.17758900	0.77805800	3.58206200
H	-4.29121100	2.19097100	4.18983700
C	-5.01299300	-4.06771500	-0.62291300
H	-5.30115900	-5.10228700	-0.40841500
H	-5.89745400	-3.53818700	-0.99350200
H	-4.26572300	-4.09386500	-1.42519000
C	-3.20270900	-4.19378500	1.11332800
H	-2.42060300	-4.17421200	0.34771100
H	-2.78538900	-3.76579200	2.03049500
H	-3.46301800	-5.23978100	1.31324100
C	-2.41244700	0.56854900	-2.99355800
H	-1.57003100	0.89022100	-2.37356600

H	-2.25202100	-0.47783700	-3.27757200
H	-2.40803200	1.16534000	-3.91325700
C	0.47812600	-0.89508600	1.35564600
C	0.03867700	-1.38201500	0.25412000
C	-0.15226200	-2.63990700	-0.45215600
C	0.51164100	-3.78561400	0.01432100
C	-0.98704800	-2.74840600	-1.56799500
C	0.35019400	-5.00424100	-0.63661600
H	1.13133200	-3.69452200	0.90293400
C	-1.15271500	-3.96934100	-2.21501100
H	-1.52121900	-1.86933800	-1.90767300
C	-0.48056300	-5.10031900	-1.75444400
H	0.86789500	-5.88508700	-0.26667800
H	-1.81039400	-4.03768100	-3.07729700
C	1.03461300	-1.12727700	2.74282700
O	1.48263100	-2.27775900	2.95080200
O	0.97707700	-0.15945500	3.53957900
H	3.56292000	2.23218200	1.70593800
C	4.15626900	0.81126200	3.17897000
H	4.88936200	0.01249000	3.34385600
H	4.38660400	1.60816600	3.89626500
H	3.15681000	0.42503600	3.39997500
C	-4.91376000	0.29067800	-3.13286500
H	-4.79826500	-0.74544500	-3.47103000
H	-5.86905700	0.37126200	-2.60350500
H	-4.96389000	0.92012500	-4.02832800
H	-3.87374700	1.81003600	-2.06830200
H	-0.60787300	-6.05393500	-2.25881300

<sup>1</sup>Ts1

ATOM	X	Y	Z
N	-1.08947100	-1.27598600	-1.07225800
N	1.55613700	-1.24710900	-0.95772100
C	-3.12930200	-0.00415000	-0.62563400
C	-3.82664600	0.00578300	0.59733500
C	-4.40559700	1.19886900	1.04326900
H	-4.93975200	1.21019100	1.99131100
C	-4.29485100	2.38403700	0.32678200
C	-3.60801400	2.35470800	-0.88848300
H	-3.50727300	3.27480200	-1.45697100
C	-3.02868600	1.18944700	-1.38079100
C	-2.46901200	-1.24637500	-1.12679300
C	-3.18704800	-2.29415700	-1.67865900
H	-4.27165300	-2.21963500	-1.70374500

C	-2.54896600	-3.41118800	-2.22865300
H	-3.11827500	-4.22543800	-2.66901900
C	-1.11707900	-3.44348900	-2.25217300
C	-0.34681200	-4.47117000	-2.82648900
H	-0.85990800	-5.31272700	-3.28905000
C	1.04861900	-4.42201900	-2.82567700
H	1.62112700	-5.22180700	-3.29232800
C	1.74065000	-3.35208000	-2.22894900
C	3.16600400	-3.21506400	-2.20701000
H	3.79186400	-3.96709200	-2.67997200
C	3.72385000	-2.08203100	-1.60367400
H	4.80231100	-1.94245400	-1.59434600
C	2.93102100	-1.12959500	-0.99244900
C	0.98002600	-2.31835700	-1.60787500
C	-0.43792400	-2.34106100	-1.65286300
C	3.45645400	0.07399600	-0.28433700
C	3.53199600	1.32326700	-0.94675900
C	3.83543700	2.46444200	-0.20344600
H	3.87066300	3.42394000	-0.71622100
C	4.05961000	2.42231300	1.17140300
C	4.04763700	1.17768100	1.78738400
H	4.25595000	1.11729800	2.85498900
C	3.76267100	-0.00271700	1.09042000
C	3.38913100	1.52066300	-2.45823900
H	3.44528500	2.60679900	-2.60752800
C	3.91822500	-1.29734600	1.89398000
H	3.83406700	-0.99146100	2.94506000
C	-3.96883800	-1.24886900	1.44732700
H	-3.21150900	-1.96077600	1.10695300
C	-2.36329400	1.18781000	-2.75208600
H	-1.53031700	0.48030000	-2.70916800
C	-4.86933600	3.68064000	0.86875700
H	-5.41114900	3.43786500	1.79278100
C	4.29349300	3.69024200	1.97114900
H	4.41605500	3.39391200	3.02140800
C	-3.72440800	-0.99719100	2.94092200
H	-3.63033200	-1.95375800	3.46804400
H	-2.80222100	-0.43109200	3.09812400
H	-4.55256900	-0.44530800	3.40213300
C	-5.34552300	-1.89817100	1.24257000
H	-6.14362400	-1.21674200	1.56326700
H	-5.51770300	-2.14686800	0.19074700
H	-5.43018700	-2.82031800	1.83032800
C	-3.35712200	0.67922300	-3.80967800

H	-4.21423100	1.36073800	-3.88678000
H	-2.87770400	0.62523900	-4.79481600
H	-3.73154800	-0.31767300	-3.55645100
C	-1.78629300	2.54276100	-3.17137600
H	-1.18399900	2.41516500	-4.07921800
H	-2.57747300	3.26531500	-3.41149400
H	-1.15048400	2.95691700	-2.38353100
C	-3.74806900	4.66512700	1.23065000
H	-4.16175700	5.58206400	1.66713700
H	-3.05179100	4.21997800	1.94869300
H	-3.16541500	4.93987100	0.34400500
C	-5.87141700	4.31858100	-0.10227700
H	-5.38048500	4.61935300	-1.03504800
H	-6.67541200	3.61880100	-0.35506100
H	-6.32117200	5.21475800	0.34079800
C	5.34097900	-1.85008200	1.70687400
H	5.50566800	-2.71517400	2.36071900
H	5.48935500	-2.17427500	0.67106600
H	6.09763700	-1.09292200	1.94081600
C	2.88705700	-2.41549900	1.69351700
H	1.87719900	-2.01521300	1.61343500
H	3.08528600	-3.00088600	0.79229000
H	2.92325200	-3.09435100	2.55485100
C	5.57771700	4.41049800	1.53906800
H	5.74841800	5.30017300	2.15632700
H	6.45014100	3.75430000	1.63191400
H	5.51007200	4.73674100	0.49441800
C	3.07984800	4.62722200	1.88795500
H	2.96543300	5.02834700	0.87379400
H	2.15100600	4.10204700	2.13363000
H	3.20282000	5.47586400	2.57152700
C	2.06332500	1.08126100	-3.09458400
H	1.96557200	-0.00639300	-3.12974700
H	1.21364000	1.48868800	-2.53837000
H	2.02046200	1.46009200	-4.12404300
C	4.58661800	0.92062600	-3.21185400
H	5.53512800	1.27605800	-2.79297600
H	4.57293200	-0.17165000	-3.15629300
H	4.55039100	1.20808700	-4.26983400
C	-0.04704800	0.39793700	2.10268200
O	0.09484400	1.98111700	-0.49824000
C	-0.25060700	-0.78117300	2.36824000
H	-0.03768900	1.62804300	1.86343000
C	-0.06056600	3.07613500	0.23345000

C	-0.49691300	-2.14256900	2.74989900
O	-0.10609800	2.93284200	1.52766100
O	-0.15418600	4.18539500	-0.32521500
C	-0.84340900	-3.10466900	1.79070200
C	-0.40073200	-2.52082500	4.09715900
C	-1.09602900	-4.41629600	2.17610000
H	-0.91433500	-2.80736900	0.75038100
C	-0.65609600	-3.83495800	4.47476600
H	-0.12875400	-1.77839400	4.84101600
C	-1.00585300	-4.78630600	3.51718500
H	-1.36475800	-5.15048200	1.42232900
H	-0.58019700	-4.11655200	5.52103400
Fe	0.23190100	0.09840800	-0.21144800
H	-1.20387700	-5.81186900	3.81470400

<sup>Q</sup>Ts1

ATOM	X	Y	Z
N	-1.17830300	-1.21982400	-1.04927500
N	1.48105200	-1.32624500	-0.88604400
C	-3.14141400	0.16059100	-0.69860000
C	-3.84634200	0.18605800	0.51882100
C	-4.35276100	1.40332500	0.98510900
H	-4.88999300	1.43037200	1.93116200
C	-4.16025200	2.59428800	0.29354500
C	-3.46869900	2.54586500	-0.91701800
H	-3.29562200	3.46903800	-1.46098300
C	-2.95359100	1.35707700	-1.42620700
C	-2.53686500	-1.11046700	-1.20524500
C	-3.29768600	-2.08482000	-1.81199300
H	-4.36814600	-1.92893200	-1.91156800
C	-2.69043700	-3.26133300	-2.32905700
H	-3.28286500	-4.03440800	-2.81158200
C	-1.28862700	-3.37821900	-2.25992800
C	-0.54711400	-4.46904500	-2.79888600
H	-1.09349700	-5.28102000	-3.27614000
C	0.82745700	-4.50444200	-2.74650200
H	1.36713800	-5.34060800	-3.18803300
C	1.57335500	-3.45767000	-2.14027200
C	2.98509000	-3.39993000	-2.11975000
H	3.57196000	-4.19259300	-2.57647200
C	3.60508000	-2.26995400	-1.54423600
H	4.68683500	-2.16950600	-1.55285400
C	2.85023000	-1.27999400	-0.94750800
C	0.84089500	-2.38495900	-1.55173500

C	-0.55141000	-2.32942700	-1.63119000
C	3.43549600	-0.07873600	-0.27984200
C	3.51917100	1.15317800	-0.97339700
C	3.89124000	2.29837900	-0.26861700
H	3.94097400	3.24430700	-0.80474900
C	4.17737400	2.27784300	1.09525600
C	4.14135000	1.04911700	1.74089700
H	4.39122400	1.00500400	2.80028600
C	3.78604100	-0.13590800	1.08494300
C	3.33109600	1.32577900	-2.48379400
H	3.40988800	2.40721100	-2.65457300
C	3.91785700	-1.41402600	1.91933100
H	3.90335600	-1.07257500	2.96281400
C	-4.07126500	-1.07841400	1.33660100
H	-3.34082100	-1.81964100	0.99947000
C	-2.24453700	1.34592800	-2.77491900
H	-1.46100800	0.58447200	-2.71861500
C	-4.61337300	3.91452100	0.89162100
H	-5.34463400	3.68393000	1.67820400
C	4.51943200	3.54959600	1.84972500
H	4.65823000	3.27517600	2.90386900
C	-3.85423900	-0.87074400	2.84099100
H	-3.82623800	-1.84115200	3.34993500
H	-2.90770400	-0.35853600	3.03535900
H	-4.66392800	-0.28451800	3.29248800
C	-5.47092200	-1.65596600	1.08118800
H	-6.24449300	-0.94275500	1.39273100
H	-5.62124800	-1.87691300	0.01998500
H	-5.61640300	-2.58372900	1.64782500
C	-3.22775300	0.93209700	-3.88197800
H	-4.03585500	1.66996500	-3.97033600
H	-2.71607500	0.87400700	-4.85060000
H	-3.67351300	-0.04488600	-3.67036200
C	-1.56484500	2.67100000	-3.13210700
H	-0.92739400	2.52654400	-4.01299800
H	-2.29833800	3.44613300	-3.39087000
H	-0.94507000	3.02595600	-2.30349300
C	-3.42028500	4.62261300	1.55374200
H	-3.73001700	5.57380500	2.00347200
H	-2.98366200	3.99518100	2.33797500
H	-2.62937300	4.82257000	0.82143800
C	-5.30183300	4.83514500	-0.12277600
H	-4.60176700	5.17606900	-0.89385300
H	-6.13396000	4.32629300	-0.62175500

H	-5.69591900	5.72634700	0.37881700
C	5.29905300	-2.04818000	1.68545900
H	5.45925000	-2.88221200	2.37957600
H	5.37322600	-2.43672100	0.66431100
H	6.10203100	-1.31760900	1.83466000
C	2.81743600	-2.47578400	1.80843700
H	1.82751500	-2.02095000	1.83383300
H	2.89755000	-3.05723900	0.88728200
H	2.90260100	-3.16738500	2.65616300
C	5.83610500	4.16057500	1.35083200
H	6.09346600	5.05469800	1.93082200
H	6.66094500	3.44456100	1.43628300
H	5.75337200	4.45614700	0.29815400
C	3.37376100	4.56850300	1.77851500
H	3.24363200	4.93974900	0.75510200
H	2.42312100	4.11954100	2.08395400
H	3.58742100	5.43062800	2.42180700
C	1.97858900	0.90969300	-3.07908300
H	1.85239100	-0.17522700	-3.09673400
H	1.15041200	1.34618500	-2.51239200
H	1.92018600	1.27552800	-4.11255000
C	4.49197100	0.68124700	-3.25844300
H	5.45998400	1.02720100	-2.87792600
H	4.45673000	-0.40862200	-3.17139400
H	4.42866900	0.94178000	-4.32204000
C	-0.02919300	0.35343800	2.19125400
O	0.13502600	1.95306300	-0.38546700
C	-0.33107200	-0.81278500	2.41913600
H	0.10978100	1.58890400	1.97167700
C	0.11076800	3.04285500	0.36584500
C	-0.67483100	-2.16370300	2.76187500
O	0.17539700	2.88365800	1.65846700
O	0.03221200	4.16550300	-0.16981600
C	-1.02094500	-3.09087000	1.76876900
C	-0.67249000	-2.56765000	4.10538600
C	-1.36368500	-4.39257900	2.11709300
H	-1.02517600	-2.77201400	0.73226900
C	-1.01741000	-3.87144800	4.44560100
H	-0.40230200	-1.85199200	4.87580100
C	-1.36523600	-4.78806000	3.45397800
H	-1.63137500	-5.09957600	1.33715300
H	-1.01432000	-4.17234300	5.48933000
Fe	0.23703500	0.05675200	-0.14409400
H	-1.63280900	-5.80607000	3.72187000

<sup>T</sup>Ts2

ATOM	X	Y	Z
Fe	-0.13776400	0.57242200	0.50932500
N	1.10797300	1.98000500	-0.46515300
N	-1.57118100	1.91744700	-0.26099500
C	3.17701800	0.69013700	-0.42537800
C	3.82801900	0.49493700	0.80542800
C	4.62332600	-0.63835600	0.97386800
H	5.14099900	-0.78290500	1.91918200
C	4.77687200	-1.58656200	-0.03790000
C	4.08260100	-1.39323600	-1.22874000
H	4.17033200	-2.14292600	-2.01160600
C	3.27013400	-0.27779600	-1.43908400
C	2.43698800	1.96549700	-0.68428100
C	3.13371100	3.07093400	-1.15506400
H	4.20231800	2.99192900	-1.32281300
C	2.44623800	4.27452900	-1.40555800
H	2.97895200	5.15354200	-1.75863600
C	1.07404800	4.32156500	-1.21816800
C	0.26760000	5.49191900	-1.47882500
H	0.77194100	6.40066700	-1.79825600
C	-1.08011900	5.46685900	-1.34715300
H	-1.67012800	6.35514600	-1.55966400
C	-1.77346400	4.26511900	-0.94856900
C	-3.15357700	4.15705100	-0.87444500
H	-3.77866900	5.01708700	-1.10064700
C	-3.73401300	2.91695200	-0.55199700
H	-4.81026600	2.78386000	-0.55728900
C	-2.91245400	1.83129000	-0.27011600
C	-0.98780000	3.11173100	-0.64340400
C	0.41157700	3.14007400	-0.76672100
C	-3.48568100	0.46432100	-0.07008900
C	-3.58383600	-0.38302800	-1.19021000
C	-4.10817700	-1.66305300	-1.01945600
H	-4.17609800	-2.32399200	-1.88082000
C	-4.53056000	-2.12550000	0.22718300
C	-4.41396100	-1.26977000	1.31945600
H	-4.73388000	-1.62666000	2.29533000
C	-3.88900400	0.01923000	1.19792800
C	-3.08519600	0.04847500	-2.56317200
C	-3.77190400	0.92143800	2.41764900
H	-2.99087200	1.66008600	2.20557400
C	3.68338400	1.50181300	1.93755900

C	2.53158800	-0.11512500	-2.75981800
H	1.77723500	0.66668200	-2.62563300
C	5.68104300	-2.79370800	0.14395200
H	5.56391500	-3.42471500	-0.74675900
C	-5.10983200	-3.51993700	0.38988700
H	-5.30296100	-3.67099900	1.45969300
C	4.90625000	2.42663400	2.00842200
H	4.78584700	3.16809600	2.80696800
H	5.81581900	1.84928300	2.21508900
H	5.04921100	2.96090400	1.06352200
C	3.49345700	0.34954800	-3.86173900
H	4.27899500	-0.39720100	-4.03113700
H	2.95875500	0.49955000	-4.80691700
H	3.97473900	1.29417700	-3.58583400
C	1.78367900	-1.38920200	-3.17364600
H	1.16738900	-1.18846700	-4.05754500
H	2.47349700	-2.20142500	-3.43074200
H	1.13002500	-1.74399900	-2.37038600
C	7.15365200	-2.36567300	0.22122200
H	7.80954100	-3.24104800	0.29153500
H	7.44228400	-1.78978900	-0.66461300
H	7.33062300	-1.73938300	1.10373300
C	5.29557100	-3.63936500	1.36465600
H	5.40568500	-3.07067600	2.29509700
H	4.25779800	-3.98272000	1.30171200
H	5.94157700	-4.52182200	1.43563500
C	-3.34344300	0.16492800	3.68001500
H	-3.08324800	0.87831600	4.46965600
H	-4.14739500	-0.47229300	4.06686700
H	-2.46987700	-0.46325900	3.48021800
C	-5.08604900	1.67819000	2.65932600
H	-5.35947400	2.28544200	1.79032100
H	-5.90314200	0.97286200	2.85456100
H	-4.99529900	2.34275100	3.52640800
C	-6.44885700	-3.65065600	-0.34945900
H	-6.88659800	-4.64225200	-0.18719900
H	-7.16492900	-2.89781000	-0.00306100
H	-6.31250800	-3.51482000	-1.42894400
C	-4.12647300	-4.60794300	-0.06180800
H	-3.91243700	-4.52586700	-1.13416800
H	-3.17546000	-4.53188300	0.47482900
H	-4.54803000	-5.60334600	0.11821400
C	-1.75392700	-0.64106700	-2.89053200
H	-1.01495400	-0.45076000	-2.10420300

H	-1.88013000	-1.72735400	-2.97189400
H	-1.35064200	-0.27180800	-3.84100700
C	-0.01217600	-0.65017500	1.98240300
C	0.07581400	-1.42061000	0.96912500
C	0.29844400	-2.62976300	0.20811200
C	1.57110700	-3.22134600	0.17690900
C	-0.72668200	-3.21209900	-0.55411500
C	1.81236100	-4.35229500	-0.59483800
H	2.37426000	-2.75992700	0.74248600
C	-0.48472900	-4.35033900	-1.31657500
H	-1.71096800	-2.75303800	-0.55084200
C	0.78583800	-4.92558000	-1.34532100
H	2.80967300	-4.78502800	-0.61612700
H	-1.29457400	-4.78699700	-1.89560700
C	0.00672100	0.56389500	3.95508600
O	0.18474800	-0.28938800	4.75139700
O	-0.16106600	1.66556900	3.55818000
H	2.80717200	2.12110300	1.71751300
C	3.42895400	0.82455400	3.28983000
H	4.32378700	0.31283700	3.66329900
H	3.14381200	1.57332000	4.03712900
H	2.62228800	0.08866800	3.21357200
C	-4.12255100	-0.18855800	-3.66757100
H	-4.31874700	-1.25575300	-3.82184000
H	-5.07327400	0.29984100	-3.42784200
H	-3.75854300	0.21902100	-4.61753000
H	-2.89446200	1.12491300	-2.53175600
H	0.97475400	-5.80902100	-1.94841300

<sup>9</sup>Ts2

ATOM	X	Y	Z
Fe	-0.15080400	0.53564500	0.44893000
N	1.10416200	1.99016800	-0.46465500
N	-1.57862500	1.91805300	-0.26070000
C	3.17083400	0.70146700	-0.42600000
C	3.82962400	0.51282700	0.80159000
C	4.62238500	-0.62190000	0.97289700
H	5.14556700	-0.76130700	1.91593000
C	4.76505000	-1.57823700	-0.03253600
C	4.06328400	-1.39093500	-1.22001400
H	4.14285400	-2.14692400	-1.99754200
C	3.25393000	-0.27398100	-1.43356000
C	2.42960200	1.97631000	-0.68573600
C	3.12659600	3.08497500	-1.15532200

H	4.19533400	3.00866300	-1.32266800
C	2.43565300	4.28633200	-1.40064500
H	2.96652400	5.16781000	-1.75086800
C	1.06414300	4.33208300	-1.21232000
C	0.25561000	5.50161300	-1.46816700
H	0.75744600	6.41249100	-1.78564800
C	-1.09163900	5.47351000	-1.33322600
H	-1.68324200	6.36190400	-1.54108300
C	-1.78433700	4.26917900	-0.93726300
C	-3.16322200	4.16072700	-0.85866200
H	-3.78932600	5.02148300	-1.07928000
C	-3.74363500	2.91704100	-0.53862900
H	-4.81990500	2.78392800	-0.54066600
C	-2.92072800	1.83172600	-0.26551300
C	-0.99543400	3.11479200	-0.63989900
C	0.40204900	3.14717000	-0.76451900
C	-3.48818500	0.46211400	-0.06654600
C	-3.57745800	-0.38833100	-1.18507100
C	-4.09216800	-1.67219000	-1.01330400
H	-4.15393800	-2.33484600	-1.87388900
C	-4.51385800	-2.13565200	0.23322700
C	-4.40600800	-1.27705900	1.32410400
H	-4.72533600	-1.63465400	2.29994800
C	-3.89013400	0.01550000	1.20148900
C	-3.08190600	0.04546800	-2.55837100
C	-3.78032600	0.91923200	2.42071300
H	-3.00836400	1.66656700	2.20639900
C	3.69390600	1.52588600	1.92928500
C	2.50793500	-0.11754100	-2.75094300
H	1.74607200	0.65632700	-2.61248400
C	5.66757200	-2.78656600	0.14988900
H	5.52849900	-3.43141500	-0.72766100
C	-5.08455200	-3.53347500	0.39740700
H	-5.27660500	-3.68447600	1.46742600
C	4.92414000	2.44113200	1.99585000
H	4.81033200	3.18614400	2.79203300
H	5.82940700	1.85744900	2.20357800
H	5.07035400	2.97121200	1.04907300
C	3.46107600	0.35898700	-3.85553600
H	4.25304200	-0.38005500	-4.02867700
H	2.92157500	0.50539000	-4.79854600
H	3.93406100	1.30776000	-3.57957200
C	1.77199700	-1.39841500	-3.16506300
H	1.14553000	-1.20050100	-4.04232500

H	2.46919900	-2.20070200	-3.43315600
H	1.12958200	-1.76551000	-2.35822000
C	7.14295700	-2.36257600	0.18765000
H	7.79751200	-3.23862700	0.26181500
H	7.41445700	-1.80574100	-0.71559500
H	7.34010000	-1.71884900	1.05323500
C	5.30679700	-3.61176600	1.39181500
H	5.44284700	-3.03095400	2.31121300
H	4.26595200	-3.94996200	1.35937700
H	5.94934500	-4.49695000	1.45986500
C	-3.33932200	0.16754500	3.68166100
H	-3.08758500	0.88365100	4.47165100
H	-4.13339000	-0.48131900	4.06957000
H	-2.45747100	-0.44832400	3.47956400
C	-5.10227900	1.66101100	2.66557100
H	-5.38446400	2.26450500	1.79674400
H	-5.91095600	0.94674900	2.86342700
H	-5.01681100	2.32723100	3.53194300
C	-6.42310600	-3.67256300	-0.34129100
H	-6.85543200	-4.66629400	-0.17756500
H	-7.14305600	-2.92311900	0.00443200
H	-6.28783700	-3.53732000	-1.42099100
C	-4.09517200	-4.61641000	-0.05312900
H	-3.88111500	-4.53426500	-1.12548300
H	-3.14475900	-4.53470800	0.48370900
H	-4.51139300	-5.61391000	0.12771800
C	-1.75080800	-0.64159100	-2.89093100
H	-1.00816600	-0.45073800	-2.10804300
H	-1.87439600	-1.72823000	-2.97162200
H	-1.35141300	-0.27146600	-3.84264100
C	-0.00538400	-0.64003900	1.96358300
C	0.07900300	-1.42839900	0.96348300
C	0.30992900	-2.64660800	0.21866200
C	1.58024000	-3.24377500	0.21875400
C	-0.70192300	-3.23079200	-0.55936500
C	1.83227700	-4.38267600	-0.53766300
H	2.37339700	-2.78032700	0.79671900
C	-0.44949300	-4.37678000	-1.30705700
H	-1.68424300	-2.76779800	-0.57967700
C	0.81868800	-4.95764800	-1.30433800
H	2.82748500	-4.82067700	-0.53351800
H	-1.24896900	-4.81481400	-1.89925700
C	0.00787300	0.60489200	3.93233500
O	0.18962800	-0.24082100	4.73535900

O	-0.16519500	1.69844300	3.51800500
H	2.82263300	2.15137400	1.70771500
C	3.43475300	0.85505300	3.28392400
H	4.32582300	0.33768300	3.65860100
H	3.15551400	1.60814600	4.02910500
H	2.62276900	0.12478900	3.21000700
C	-4.12187400	-0.19210300	-3.66026400
H	-4.31825500	-1.25942500	-3.81349600
H	-5.07198200	0.29608100	-3.41776700
H	-3.76078200	0.21548800	-4.61133300
H	-2.89289600	1.12214400	-2.52582600
H	1.01584200	-5.84744000	-1.89534700

MECP

ATOM	X	Y	Z
Fe	0.18398461	-0.31302809	0.03230475
N	1.26848574	-1.48934164	-1.34405861
N	-1.45153955	-1.44005611	-1.17234819
C	3.34157620	-0.41722832	-0.55210344
C	3.72262788	0.53758558	-1.51962363
C	4.46155108	1.65085256	-1.12457146
H	4.76337355	2.37428831	-1.87594739
C	4.83207755	1.85549449	0.20520248
C	4.44050228	0.90734765	1.14486050
H	4.72482513	1.05835333	2.18368270
C	3.69699165	-0.22507382	0.79862621
C	2.60257540	-1.64833809	-0.97948769
C	3.25941027	-2.84822723	-1.11079050
H	4.32031966	-2.89334201	-0.88456142
C	2.58248821	-3.99456966	-1.58382878
H	3.10383138	-4.93506450	-1.73197722
C	1.19150333	-3.91053551	-1.79087923
C	0.39110333	-5.03303493	-2.19104970
H	0.89807508	-5.97501616	-2.38489483
C	-0.96245125	-4.94068526	-2.33329734
H	-1.54833344	-5.79871530	-2.65203534
C	-1.63194309	-3.72189575	-2.02874589
C	-3.02488110	-3.56030806	-2.09095182
H	-3.64510080	-4.38209308	-2.43953866
C	-3.59440766	-2.36822155	-1.70051387
H	-4.66564935	-2.21213902	-1.75587100
C	-2.77072238	-1.33530699	-1.19294129
C	-0.86092808	-2.59754684	-1.61356555
C	0.55611987	-2.66217538	-1.58170250

C	-3.41016653	-0.08471713	-0.66952838
C	-3.96241877	-0.07192184	0.62352378
C	-4.59299686	1.09240012	1.06846885
H	-5.02700528	1.11470279	2.06457055
C	-4.68052636	2.23496780	0.27994962
C	-4.12068979	2.19716373	-0.99729295
H	-4.18793727	3.07922401	-1.62832792
C	-3.49465890	1.05473176	-1.49408888
C	-3.90873332	-1.29102004	1.53744178
H	-3.04656605	-1.89712383	1.23554007
C	-3.00531915	1.02017650	-2.93596681
H	-2.17719757	0.30669222	-2.98976787
C	3.42095127	0.31571604	-2.99557526
H	2.54427425	-0.33550286	-3.05850971
C	3.32311040	-1.22182697	1.88872719
H	2.52559303	-1.86351296	1.50027036
C	5.66988970	3.04790039	0.63360478
H	5.52284800	3.17173214	1.71457476
C	-5.36811142	3.48405572	0.80158655
H	-5.76906526	3.24361907	1.79457602
C	-0.87038186	0.53398359	1.43304273
H	-1.44299419	1.43131803	1.60683610
C	-0.46350275	-0.60733501	1.82102938
C	0.27418411	1.96741713	-0.88397716
C	0.23044795	1.12992964	-1.76641389
H	0.24315211	0.51149777	-2.63705362
C	0.33638938	3.07843948	0.02266451
C	-0.76139719	3.93704650	0.15758124
C	1.50295116	3.30953418	0.76240608
C	-0.67836741	5.03225141	1.01189373
H	-1.67136251	3.73688804	-0.40059659
C	1.57321129	4.40303904	1.61728051
H	2.34240738	2.62883851	0.65959348
C	0.48655053	5.26918123	1.73897743
H	-1.52697389	5.70253001	1.10853048
H	2.47916624	4.57916031	2.18941884
C	-0.31665603	-1.72600563	2.73547949
C	-0.49544264	-1.55622098	4.11523469
C	0.01606857	-2.99429389	2.24208652
C	-0.34683143	-2.63481860	4.97996697
H	-0.74408824	-0.57261852	4.50157890
C	0.16000216	-4.07266612	3.10877095
H	0.15849085	-3.12869176	1.17258993
C	-0.02028557	-3.89545624	4.47905144

H	-0.48553195	-2.49304638	6.04776347
H	0.41431961	-5.05105146	2.71242060
C	-5.17565491	-2.14912993	1.39116586
H	-6.06370563	-1.56400107	1.65917850
H	-5.30635741	-2.51657669	0.37043518
H	-5.12654804	-3.01604215	2.06013862
C	-3.71704589	-0.92686409	3.01561072
H	-2.91308685	-0.19855527	3.14916809
H	-4.63341022	-0.51099244	3.45032622
H	-3.46111685	-1.82434044	3.58800545
C	-2.48653210	2.36741573	-3.44969548
H	-1.99987857	2.22902031	-4.42123432
H	-3.29935422	3.08821767	-3.59489516
H	-1.75591561	2.80513906	-2.76324321
C	-4.12537586	0.50437414	-3.85461855
H	-4.45832195	-0.49500825	-3.55795105
H	-4.99010909	1.17765748	-3.81524221
H	-3.77887012	0.45385045	-4.89311040
C	-6.54771759	3.90267689	-0.08593461
H	-6.20850746	4.18751644	-1.08861643
H	-7.27018071	3.08679234	-0.19288398
H	-7.06529046	4.76544469	0.34821226
C	-4.37156483	4.63791906	0.97248821
H	-4.86423950	5.51349763	1.40989514
H	-3.54409030	4.34469192	1.62711852
H	-3.94998783	4.93864578	0.00530723
C	4.51201432	-2.12927447	2.23591286
H	5.35216328	-1.53719089	2.61899063
H	4.22562527	-2.85192200	3.00898769
H	4.85985710	-2.68599870	1.36055359
C	2.79174531	-0.54565779	3.15851618
H	2.39188413	-1.30375523	3.84013088
H	3.58100930	-0.00418518	3.69249345
H	1.98604145	0.15926550	2.92835296
C	4.59593297	-0.41586612	-3.66285945
H	4.37624548	-0.61715927	-4.71794949
H	5.50568156	0.19536585	-3.61557552
H	4.79763956	-1.37026162	-3.16552507
C	3.09173077	1.60597186	-3.75562901
H	2.71557058	1.36162339	-4.75531001
H	2.32790090	2.19244361	-3.23491228
H	3.97611509	2.23982264	-3.88927363
C	7.16144113	2.76443186	0.39921155
H	7.77542337	3.60061401	0.75219932

H	7.47761269	1.85858463	0.92753485
H	7.36230636	2.62108689	-0.66936017
C	5.25050343	4.35751358	-0.04293816
H	5.46685900	4.34283421	-1.11702339
H	4.17938893	4.54791761	0.08349047
H	5.80237399	5.19891623	0.39030871
H	0.54582002	6.12598414	2.40279672
H	0.09388474	-4.73677416	5.15596228

<sup>Q</sup>In7

ATOM	X	Y	Z
Fe	-0.46001000	-0.57359800	-0.54875000
N	0.26990000	-2.44173500	0.12650400
N	-2.16968200	-1.35789500	0.39824400
C	2.62845200	-1.93268700	-0.04507600
C	3.31093900	-1.74584100	-1.26504000
C	4.27753100	-0.73827500	-1.33468400
H	4.79144800	-0.58341000	-2.28162600
C	4.60877800	0.06447400	-0.24444700
C	3.95153000	-0.17289900	0.95670300
H	4.21526600	0.42885300	1.82259700
C	2.95724900	-1.14251000	1.07531600
C	1.53104900	-2.93444600	0.14465700
C	1.80253600	-4.25354200	0.46299500
H	2.83299800	-4.58795200	0.50438100
C	0.74441500	-5.13660800	0.77645500
H	0.94560700	-6.17817200	1.01132900
C	-0.55001000	-4.64640200	0.83406700
C	-1.69797800	-5.43518200	1.22523700
H	-1.54487300	-6.49200200	1.42921200
C	-2.92853600	-4.88372300	1.35868700
H	-3.77378400	-5.49274100	1.66957100
C	-3.15035100	-3.48069800	1.11018900
C	-4.36585700	-2.83799500	1.29011100
H	-5.23061800	-3.40034500	1.63276300
C	-4.47033000	-1.46045600	1.04123000
H	-5.40445000	-0.93342800	1.19771900
C	-3.35498800	-0.76259700	0.58340500
C	-2.03636700	-2.70027900	0.67667400
C	-0.76259800	-3.26930100	0.53067100
C	-3.38896600	0.69838200	0.26605300
C	-2.85804300	1.61961400	1.19166500
C	-2.82262100	2.96627100	0.84293600
H	-2.39551700	3.68098700	1.53975700

C	-3.27077800	3.41921600	-0.39800900
C	-3.80092200	2.49116900	-1.28853600
H	-4.15042500	2.83883400	-2.25761200
C	-3.86579900	1.12885100	-0.98366000
C	-2.34680400	1.15950700	2.55147700
H	-1.91601100	0.16123900	2.41855300
C	-4.45622200	0.14704100	-1.98776800
H	-4.06349300	-0.84780600	-1.75379100
C	3.12378700	-2.59385800	-2.52253100
C	2.29886000	-1.36700400	2.43168400
H	1.36237000	-1.90576500	2.27013000
C	5.66036000	1.15418800	-0.35115200
H	5.68524500	1.67448900	0.61508800
C	-3.09921400	4.87233500	-0.80198500
H	-3.62179000	5.01237300	-1.75710400
C	3.78245100	-3.97597300	-2.38850800
H	3.82790000	-4.46670700	-3.36777300
H	4.80343200	-3.89146000	-2.00016800
H	3.20962300	-4.62049100	-1.71619700
C	3.19616900	-2.25016400	3.31093600
H	4.16193000	-1.76239000	3.49209000
H	2.72214100	-2.43783000	4.28158400
H	3.38620900	-3.21546100	2.82917800
C	7.05309200	0.55972500	-0.60214900
H	7.81405300	1.34844500	-0.61514800
H	7.32040000	-0.16296800	0.17630100
H	7.08896800	0.04288200	-1.56867200
C	5.30379100	2.19471700	-1.42023000
H	5.27929300	1.74306800	-2.41911100
H	4.32506200	2.64197800	-1.22142600
H	6.05047700	2.99706300	-1.43436200
C	-4.06299400	0.44772000	-3.43910600
H	-4.38780100	-0.37565800	-4.08481000
H	-4.54120100	1.36121800	-3.81163900
H	-2.97934800	0.55452700	-3.54046400
C	-5.98552900	0.09747800	-1.85054800
H	-6.28758100	-0.18632700	-0.83771600
H	-6.42253700	1.07894300	-2.07183100
H	-6.41068900	-0.63029500	-2.55147600
C	-3.70874900	5.84890700	0.21073700
H	-3.61157900	6.87958300	-0.14846700
H	-4.77168300	5.64012100	0.37217900
H	-3.20097800	5.78714200	1.18004100
C	-1.61089000	5.17673100	-1.03637400

H	-1.03732200	5.05527200	-0.10978400
H	-1.18770900	4.49323200	-1.78041000
H	-1.47258600	6.20477300	-1.39061000
C	-3.50862800	1.04231700	3.55054900
H	-3.98054500	2.02055500	3.70426100
H	-4.27343000	0.34577800	3.19241700
H	-3.14588700	0.68234600	4.52050600
C	-1.23791100	2.05094500	3.11990000
H	-0.45225600	2.21417700	2.37546200
H	-1.62408300	3.02484400	3.44448500
H	-0.79075500	1.57009800	3.99699200
C	0.48765800	1.17773700	-0.13548600
C	1.17904400	2.17879000	0.03666300
C	2.05691500	3.28935100	0.25073200
C	2.93563000	3.29942900	1.34784900
C	2.09675600	4.36976000	-0.64724400
C	3.83606700	4.34328200	1.52703700
H	2.90879600	2.47098600	2.04772800
C	2.99868600	5.41313600	-0.46235500
H	1.42045400	4.37431300	-1.49687700
C	3.87567600	5.40293900	0.62119000
H	4.51391500	4.32829300	2.37609200
H	3.01931000	6.23542900	-1.17203600
C	1.68283400	-2.71642500	-3.02402500
H	1.05027400	-3.28268400	-2.33606900
H	1.23308700	-1.72982200	-3.16350900
H	1.67321400	-3.23442400	-3.99045900
H	3.67701900	-2.06560500	-3.30967800
H	4.58435200	6.21430000	0.75915700
C	-1.18837600	-1.25394200	-2.31203200
O	-1.77902300	-2.22370600	-2.74005100
O	-0.74533200	-0.16056200	-2.72051100
C	1.93482300	-0.06186000	3.14815200
H	1.36509000	0.59471100	2.48356900
H	1.32637300	-0.27966000	4.03374900
H	2.82448500	0.47959800	3.49260900

<sup>Q</sup>In8

ATOM	X	Y	Z
Fe	1.06187400	-0.33941700	0.04707600
N	3.07221300	-0.07479600	-0.21871000
N	1.57430900	-2.23982400	-0.08661500
C	2.99497100	2.29648600	-0.03755400
C	2.31917200	2.87376800	-1.13275500

C	1.41399000	3.90667800	-0.89923500
H	0.88089000	4.34388200	-1.73929300
C	1.14516100	4.37249900	0.38964700
C	1.83420800	3.79927000	1.45293100
H	1.62802400	4.15230100	2.46204300
C	2.74831000	2.75807300	1.26558000
C	3.82404700	1.07118900	-0.24415000
C	5.18476500	1.06246400	-0.42403700
H	5.72386800	2.00561800	-0.43258800
C	5.88014200	-0.17540300	-0.57986200
H	6.95736400	-0.19451300	-0.72146300
C	5.15019200	-1.37426400	-0.52661700
C	5.71148300	-2.68551100	-0.63437500
H	6.78591200	-2.77849900	-0.78107700
C	4.93456100	-3.81597100	-0.54908500
H	5.39775500	-4.79773100	-0.62767800
C	3.52312800	-3.74330300	-0.35376200
C	2.66808800	-4.85555600	-0.22891400
H	3.06964700	-5.86389500	-0.28190400
C	1.28537900	-4.63314700	-0.02636200
H	0.60032800	-5.47039500	0.07502900
C	0.77767400	-3.35116100	0.03314500
C	2.95452600	-2.44134700	-0.26724300
C	3.73920600	-1.29805500	-0.34191800
C	-0.67377000	-3.03897300	0.20099400
C	-1.16681500	-2.63121900	1.45788300
C	-2.50496300	-2.26306500	1.56981700
H	-2.88833000	-1.93135700	2.53244400
C	-3.37473400	-2.28082600	0.47697000
C	-2.86771700	-2.69017200	-0.75193800
H	-3.51919700	-2.70298700	-1.62006200
C	-1.52581500	-3.04503100	-0.91591400
C	-0.26332500	-2.63541000	2.68350500
H	0.76876700	-2.55525300	2.32907200
C	-1.01179300	-3.42216900	-2.29769800
H	0.08048500	-3.36117300	-2.26672700
C	2.58828400	2.38313600	-2.54846000
H	2.92632200	1.34488800	-2.47086100
C	3.41968400	2.12667800	2.47611500
H	4.07748100	1.33162900	2.11369400
C	0.07231800	5.41783900	0.63525300
H	0.10695800	5.67545100	1.70193600
C	-4.81997100	-1.84522500	0.67322800
H	-4.78828400	-0.89859000	1.23061900

O	-0.58290600	0.71210900	0.79914200
C	-1.18473300	0.71153500	-0.32134900
O	-0.63387100	0.30652900	-1.37252300
C	-2.56232200	1.17298300	-0.34811800
C	-3.72646200	1.50289900	-0.33760100
C	-5.11540100	1.84515300	-0.31022800
C	-5.81507400	2.07031700	-1.50429200
C	-5.79482100	1.91237900	0.91483600
C	-7.17532300	2.35441900	-1.46968400
H	-5.28791300	2.01129500	-2.45102800
C	-7.15624700	2.19232000	0.94059400
H	-5.25050900	1.73680500	1.83730000
C	-7.84779700	2.41309900	-0.24974100
H	-7.71222500	2.52544600	-2.39744800
H	-7.67803200	2.23859400	1.89127900
C	-0.39429200	-3.97162700	3.42841700
H	-1.41939600	-4.11364300	3.79268500
H	-0.14588600	-4.80852100	2.76681200
H	0.28178100	-4.00341800	4.29120400
C	-0.50958400	-1.45039800	3.62385400
H	-1.47110900	-1.53395000	4.14451000
H	0.27276200	-1.41334000	4.39048400
H	-0.50111300	-0.50589600	3.07030200
C	-5.58480200	-2.86456800	1.53183500
H	-5.09534200	-3.02381100	2.49824400
H	-6.60840500	-2.52059900	1.72038700
H	-5.63956200	-3.83182000	1.01778700
C	-5.57563800	-1.57889300	-0.62979900
H	-5.75958100	-2.50942400	-1.18075200
H	-6.54680000	-1.12095100	-0.41272400
H	-5.02144100	-0.89748800	-1.28241900
C	-1.49136200	-2.45598000	-3.38866900
H	-0.97170100	-2.66697300	-4.33052800
H	-2.56605000	-2.55972200	-3.58068700
H	-1.29272800	-1.41885700	-3.10163900
C	-1.38402200	-4.87072400	-2.64156000
H	-0.97930500	-5.56632200	-1.89867700
H	-2.47374000	-4.99622000	-2.66724200
H	-0.98724000	-5.15005900	-3.62479200
C	4.29764000	3.14242800	3.21898300
H	5.05337000	3.56652000	2.54872800
H	3.70091200	3.96934700	3.62204600
H	4.81421800	2.66265600	4.05836200
C	2.39362500	1.48288600	3.41876900

H	2.89882900	1.00014300	4.26348300
H	1.69682100	2.22604700	3.82451500
H	1.80514700	0.72172600	2.89484200
C	0.30691100	6.70646300	-0.16203500
H	0.23909000	6.52478000	-1.24091000
H	-0.44810400	7.45798000	0.09492900
H	1.29575900	7.12770200	0.04802300
C	-1.31741100	4.83105200	0.34298000
H	-2.10528000	5.54822200	0.60082200
H	-1.41933200	4.58472900	-0.72074900
H	-1.48410400	3.91102900	0.91314700
C	3.72684100	3.19430100	-3.18373700
H	4.63813000	3.12237300	-2.58072400
H	3.95096600	2.82283100	-4.19067900
H	3.45023600	4.25289900	-3.26496300
C	1.34473400	2.38813600	-3.44447800
H	1.01602100	3.40681100	-3.68326800
H	1.57137200	1.89131000	-4.39471000
H	0.51374700	1.85828600	-2.96736400
H	-8.91150500	2.62947700	-0.22639500

<sup>9</sup>In9

ATOM	X	Y	Z
Fe	0.63628700	-0.75083500	0.38076600
N	2.42296000	-1.17969300	-0.66226800
N	0.17340000	-2.60184300	-0.52110300
C	3.42023000	0.91519400	-0.10097200
C	2.85200700	1.97991900	-0.82260500
C	2.62276500	3.18906900	-0.16991200
H	2.16741700	4.00813900	-0.72260800
C	2.93732000	3.36973000	1.17728500
C	3.52512900	2.30926100	1.86160400
H	3.77782200	2.44093800	2.91197100
C	3.76417900	1.07627000	1.24982500
C	3.53368200	-0.42912800	-0.74495800
C	4.69185200	-0.86151700	-1.38125200
H	5.55856800	-0.21032500	-1.41520600
C	4.71627400	-2.14335700	-1.96828100
H	5.61329800	-2.50448800	-2.46504100
C	3.58509000	-2.94328900	-1.91370500
C	3.48899800	-4.26713700	-2.48687700
H	4.36338200	-4.67395100	-2.98949100
C	2.34719400	-4.99375100	-2.40931800
H	2.29899000	-5.98617800	-2.85136300

C	1.16559500	-4.48296500	-1.75036500
C	-0.03303200	-5.17099400	-1.64539000
H	-0.12896100	-6.16546200	-2.07396800
C	-1.12624000	-4.56685300	-0.98940200
H	-2.08102200	-5.07418000	-0.90400900
C	-0.97745900	-3.29297200	-0.45424000
C	1.24698700	-3.17878600	-1.17416700
C	2.42848700	-2.42907800	-1.25195300
C	-2.10164900	-2.57701000	0.22316500
C	-2.24615100	-2.64992600	1.61736300
C	-3.24307300	-1.88675300	2.22945300
H	-3.36136800	-1.93319700	3.31004600
C	-4.07825800	-1.04377000	1.50054900
C	-3.92324500	-1.00221600	0.11514300
H	-4.56462500	-0.34759700	-0.47151500
C	-2.94673100	-1.75142900	-0.53873200
C	-1.34452300	-3.53608800	2.46346700
H	-0.52767100	-3.88766200	1.82547400
C	-2.80023700	-1.63641500	-2.04891400
H	-1.95050600	-2.25363600	-2.35527500
C	2.47842500	1.83820700	-2.29040100
H	2.65525400	0.80022500	-2.58655600
C	4.36803000	-0.06162000	2.05904100
H	4.37566700	-0.95519000	1.42714600
C	2.61462500	4.67299000	1.88599100
H	2.99534500	4.58951400	2.91217500
C	-5.10563600	-0.17056900	2.19899000
H	-5.05050700	-0.39725300	3.27169200
O	-1.08504800	1.97998600	2.98218700
C	-0.79926200	1.49763900	1.88338200
O	-0.01633600	0.50715600	1.68640300
C	-1.41379800	2.11159300	0.69308200
C	-2.00926300	2.66439100	-0.20598800
C	-2.77254900	3.33376200	-1.21632800
C	-2.45737300	3.20456000	-2.57679500
C	-3.86928500	4.12490000	-0.83901400
C	-3.22486200	3.85383400	-3.53717500
H	-1.61741300	2.58571100	-2.87212300
C	-4.63424300	4.76909300	-1.80486500
H	-4.11166100	4.22586300	0.21432300
C	-4.31399200	4.63573500	-3.15515400
H	-2.97501100	3.74424500	-4.58804400
H	-5.48181000	5.37677400	-1.50278100
C	-2.11107700	-4.77181000	2.95435900

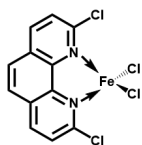
H	-2.95396600	-4.48064800	3.59290500
H	-2.50807700	-5.34540800	2.10953600
H	-1.45540600	-5.42809600	3.53836800
C	-0.70569900	-2.77250900	3.63063400
H	-1.45256500	-2.46274300	4.37086500
H	0.02312900	-3.40987600	4.14426900
H	-0.19194500	-1.87495100	3.26991300
C	-6.53346800	-0.48187600	1.73135100
H	-6.77506500	-1.53958500	1.88175200
H	-7.25982400	0.11991100	2.28933000
H	-6.65948400	-0.25505100	0.66616400
C	-4.77741000	1.31964100	2.02352600
H	-4.82096200	1.60940100	0.96657500
H	-5.49778200	1.93745300	2.57268900
H	-3.77174000	1.54964700	2.39030500
C	-2.49259400	-0.19504500	-2.46833300
H	-2.30279500	-0.13716100	-3.54664900
H	-3.32676400	0.47774700	-2.23997400
H	-1.61030500	0.18092600	-1.93837700
C	-4.04099000	-2.17724800	-2.77090500
H	-4.22156000	-3.22527500	-2.50756000
H	-4.93665300	-1.60246600	-2.50638400
H	-3.91019100	-2.11443500	-3.85739500
C	5.82382900	0.24665800	2.43377800
H	6.42542600	0.43473300	1.53761300
H	5.88649200	1.13349900	3.07590300
H	6.26942000	-0.59517400	2.97614700
C	3.52785100	-0.39240700	3.29932500
H	3.93422500	-1.27455400	3.80724300
H	3.52614900	0.43494400	4.01862600
H	2.48943300	-0.60026200	3.01905900
C	3.30941700	5.87185800	1.22706900
H	2.94261500	6.02845900	0.20588000
H	3.11407900	6.78910400	1.79411000
H	4.39328200	5.72231300	1.17685400
C	1.09633300	4.89132300	1.96641000
H	0.86911600	5.81000600	2.51995400
H	0.66182300	4.98780700	0.96400300
H	0.59738100	4.05405200	2.46531300
C	3.36933600	2.72486000	-3.17045900
H	4.42837400	2.49122300	-3.01520700
H	3.13649300	2.57393800	-4.23085600
H	3.21994100	3.78656400	-2.94018000
C	0.99261300	2.13033500	-2.52754700

H	0.74749800	3.17697500	-2.31056400
H	0.72720600	1.93394900	-3.57339800
H	0.36841600	1.50056900	-1.88324500
H	-4.91239400	5.13967900	-3.90817700
CO <sub>2</sub>			
ATOM	X	Y	Z
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16509200
O	0.00000000	0.00000000	-1.16509200
CO <sub>3</sub> <sup>2-</sup>			
ATOM	X	Y	Z
C	0.00000000	0.00000000	-0.00055500
O	0.00000000	0.00000000	1.29821500
O	0.00000000	1.12525000	-0.64889900
O	0.00000000	-1.12525000	-0.64889900
HCO <sub>3</sub> <sup>-</sup>			
ATOM	X	Y	Z
C	0.00000000	0.15355800	0.00000000
O	1.21678700	0.44146500	0.00000000
O	-1.00900600	0.87799200	0.00000000
O	-0.28176000	-1.22929900	0.00000000
H	0.59182700	-1.64261200	0.00000000
Phenylacetylene			
ATOM	X	Y	Z
C	3.23061400	-0.00000100	-0.00000800
H	4.29873700	-0.00001600	-0.00011300
C	2.02295100	0.00000400	0.00001100
C	0.58762900	-0.00000800	0.00008300
C	-0.11960000	-1.21100400	-0.00000800
C	-0.11958700	1.21099600	-0.00000800
C	-1.51024300	-1.20671000	-0.00002500
H	0.42653600	-2.14897200	-0.00004500
C	-1.51023100	1.20671600	-0.00002500
H	0.42656200	2.14895800	-0.00004500
C	-2.20791600	0.00000700	0.00003300
H	-2.04993900	-2.14865000	-0.00006800
H	-2.04991600	2.14866300	-0.00006800
H	-3.29367700	0.00001300	0.00001700

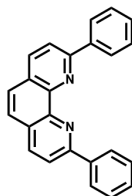
DMF

ATOM	X	Y	Z
O	1.95118600	-0.09296300	0.00004400
C	0.85905200	-0.64551000	-0.00001700
H	0.75858400	-1.74515000	-0.00006900
N	-0.34033500	-0.02204900	-0.00014800
C	-1.58719500	-0.75885700	0.00004700
H	-2.17840500	-0.51336400	-0.88973500
H	-1.38588600	-1.83282200	0.00021700
H	-2.17830700	-0.51309600	0.88983200
C	-0.42404800	1.42452600	0.00000200
H	-0.95930500	1.77527100	0.88975400
H	0.58729600	1.83069800	0.00090100
H	-0.95797700	1.77556000	-0.89040600

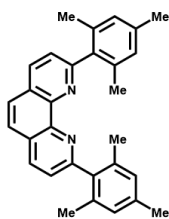
### <sup>1</sup>H NMR and <sup>13</sup>C NMR data for the various targeted products



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 2.19 (s, 2H), 1.6-0.89 (s, 4H).

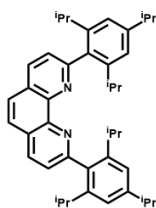


<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 8.50 (d, *J* = 7.1 Hz, 4H), 8.31 (d, *J* = 8.4 Hz, 2H), 8.16 (d, *J* = 8.4 Hz, 2H), 7.79 (s, 2H), 7.70 – 7.58 (m, 4H), 7.57 – 7.49 (m, 2H). <sup>13</sup>C NMR (76 MHz, CDCl<sub>3</sub>) δ 156.82, 146.15, 139.50, 136.91, 129.44, 128.85, 127.82 (d, *J* = 16.8 Hz), 126.03, 120.02.

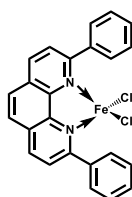


<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 8.31 (d, *J* = 8.2 Hz, 2H), 7.88 (s, 2H), 7.60 (d, *J* = 8.2 Hz, 2H), 6.95 (s, 4H), 2.34 (s, 6H), 2.17 (s, 12H). <sup>13</sup>C NMR (76 MHz, CDCl<sub>3</sub>) δ 160.10, 146.22, 138.12, 137.40, 136.26, 135.67, 128.49, 127.09, 126.16, 125.02, 20.87 (d, *J* =

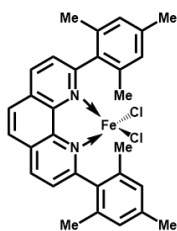
37.7 Hz).



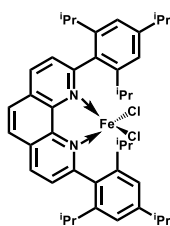
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.29 (d,  $J = 8.1$  Hz, 2H), 7.90 (s, 2H), 7.62 (d,  $J = 8.1$  Hz, 2H), 7.08 (s, 4H), 2.95 (p,  $J = 6.9$  Hz, 2H), 2.53 (p,  $J = 6.8$  Hz, 4H), 1.31 (d,  $J = 6.9$  Hz, 12H), 1.10 (dd,  $J = 6.8, 1.7$  Hz, 24H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CDCl}_3$ )  $\delta$  160.59, 148.63, 146.14 (d,  $J = 21.0$  Hz), 136.91, 135.28, 127.24, 126.21, 124.97, 120.60, 34.41, 30.53, 24.00.



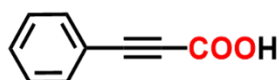
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  57.35 (s, 2H), 26.71 (s, 2H), 2.53 (s, 2H), 1.29 (s, 4H), 0.87 (s, 4H) -14.76 (s, 2H).



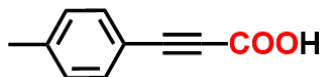
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  52.16 (s, 2H), 27.29 (s, 2H), 1.68 (s, 4H), 0.74 (s, 6H), -10.67 (s, 12H), -16.53 (s, 2H).



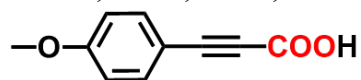
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  53.90 (s, 2H), 29.10 (s, 2H), 2.43 (s, 4H), 2.04 (s, 2H), 1.26 (s, 12H), -6.0 – -4.0 (m, 24H), -7.77 (s, 2H), -20.01 (s, 2H).



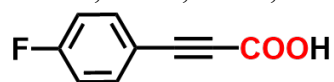
$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  10.51 (s, 1H), 7.83 – 7.08 (m, 5H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  155.38, 132.48, 130.47, 128.51, 119.52, 85.40, 80.65.



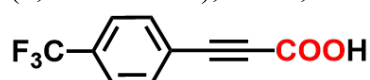
$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  10.08 (s, 1H), 7.54 (d,  $J = 8.1$  Hz, 2H), 7.37 – 7.11 (m, 2H), 2.37 (s, 3H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  155.43, 141.35, 132.47, 129.18, 116.44, 85.82, 80.18, 20.32.



$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  10.10 (s, 1H), 7.51 (d,  $J = 9.0$  Hz, 2H), 6.94 (d,  $J = 9.0$  Hz, 2H), 3.82 (s, 3H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  161.77, 155.65, 134.47, 114.16, 111.11, 86.39, 79.89, 54.60.



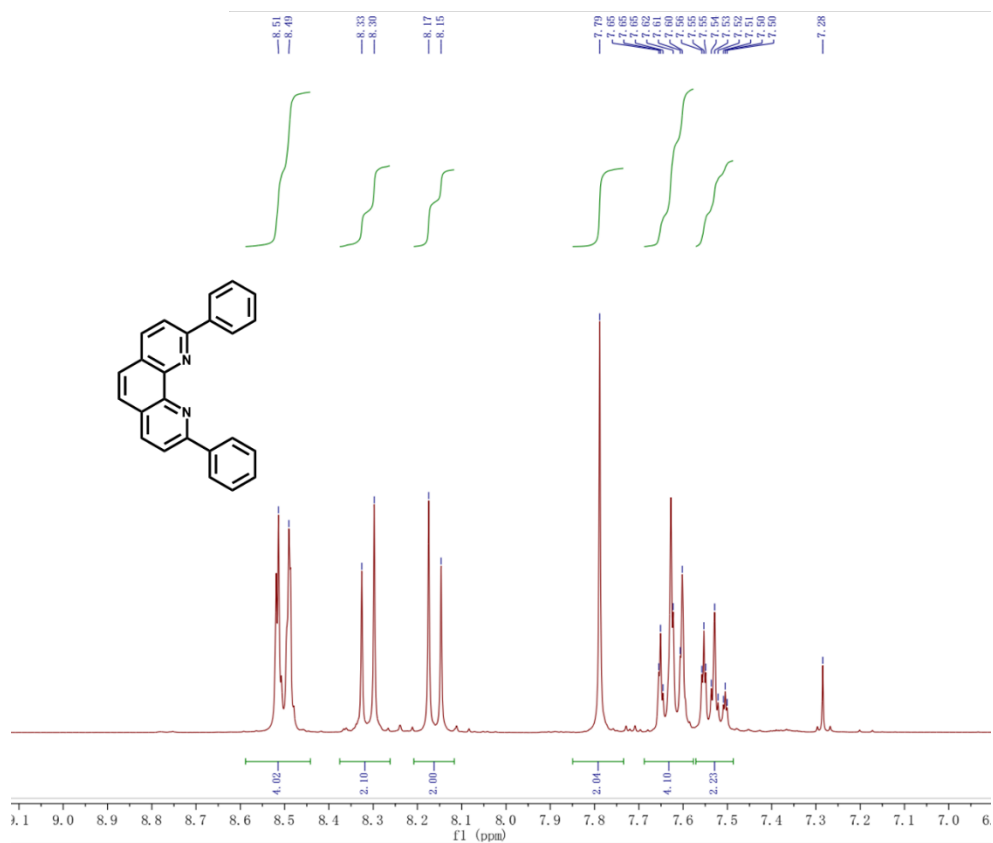
$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  10.38 (s, 1H), 7.72–7.49 (m, 2H), 7.30–6.99 (m, 2H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  165.58, 162.24, 155.15, 134.98 (d,  $J = 9.0$  Hz), 115.79 (d,  $J = 22.7$  Hz), 84.19, 80.53.



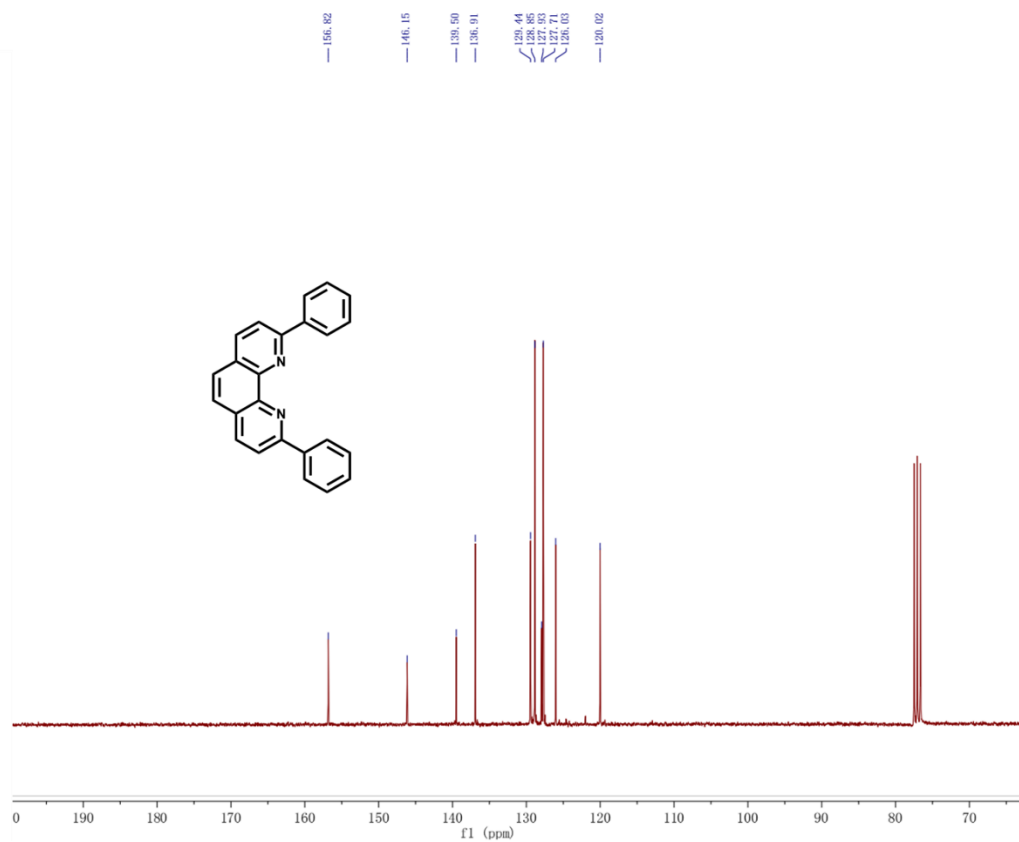
$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  10.38 (s, 1H), 8.00 – 7.62 (m, 4H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  156.09, 134.49, 133.42, 132.98, 132.55, 130.68, 126.90 (q,  $J = 3.9$  Hz), 125.95 – 124.43 (m), 123.49, 84.25.



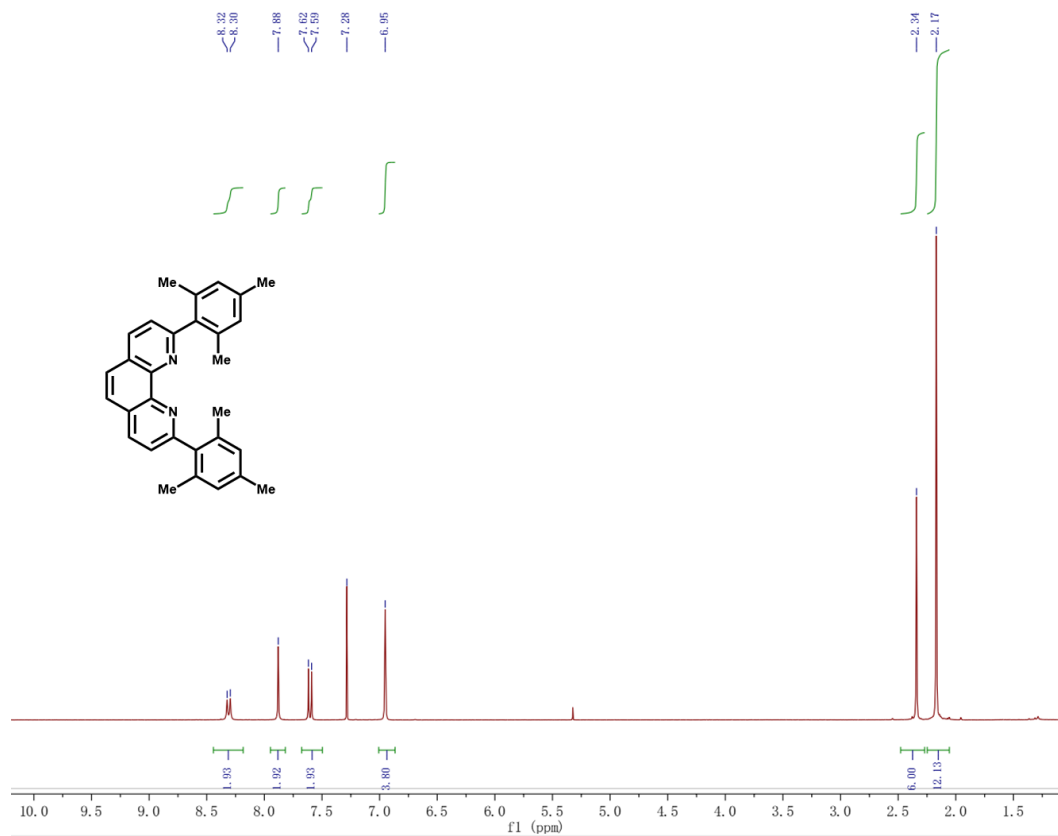
$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  10.08 (s, 1H), 2.35 (t,  $J = 7.0$  Hz, 2H), 1.62 (h,  $J = 7.2$  Hz, 2H), 1.04 (t,  $J = 7.4$  Hz, 3H).  $^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  153.50 (d,  $J = 8.8$  Hz), 91.06 – 83.09 (m), 75.31 – 66.68 (m), 18.47 (dd,  $J = 92.8, 9.0$  Hz), 10.49 (d,  $J = 8.1$  Hz).



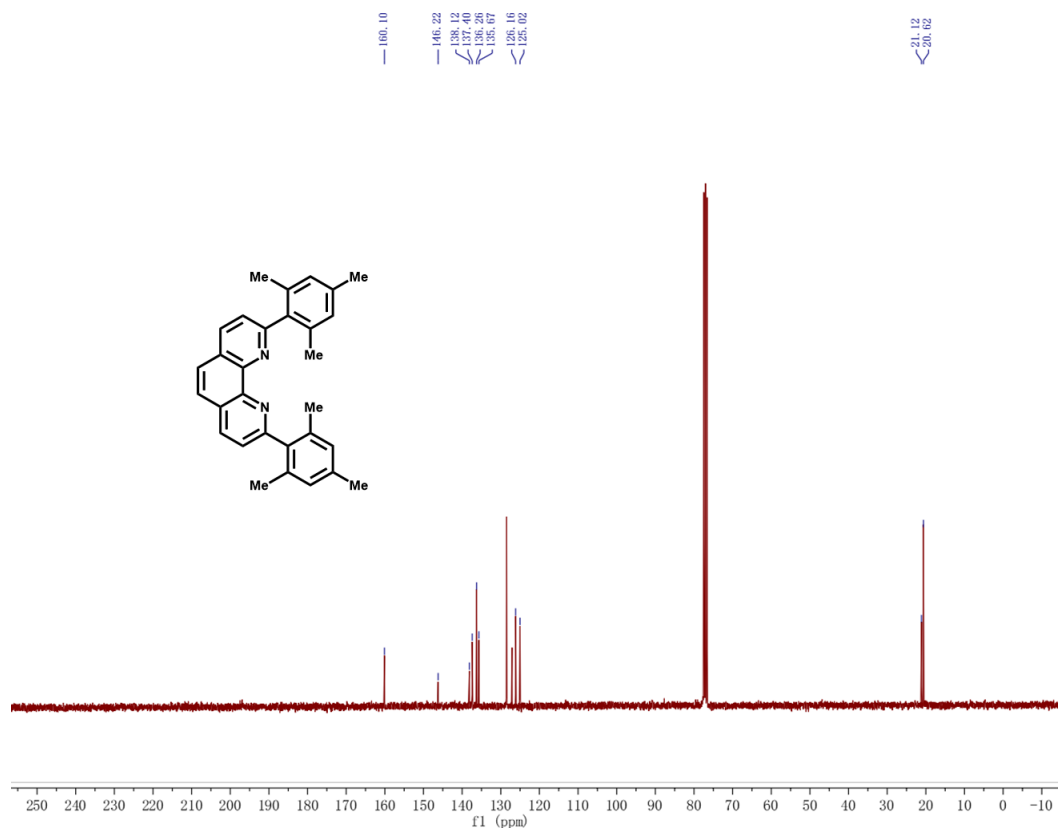
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



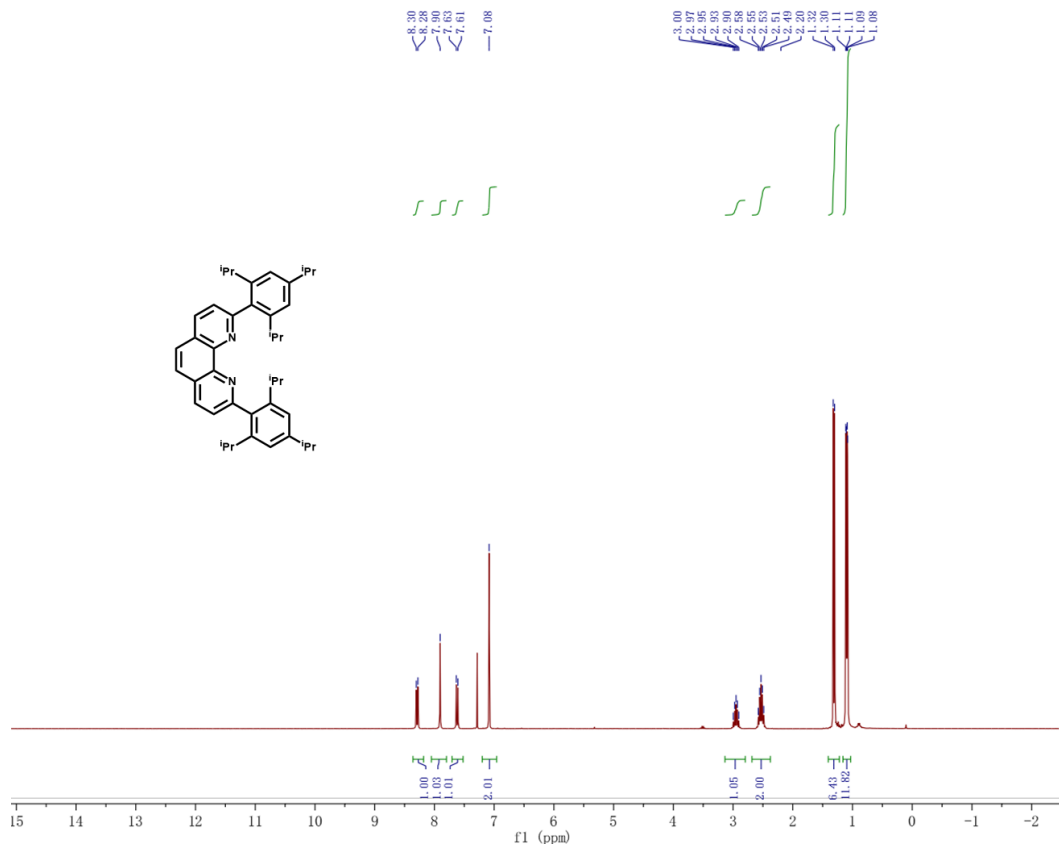
<sup>13</sup>C NMR (76 MHz, CDCl<sub>3</sub>)



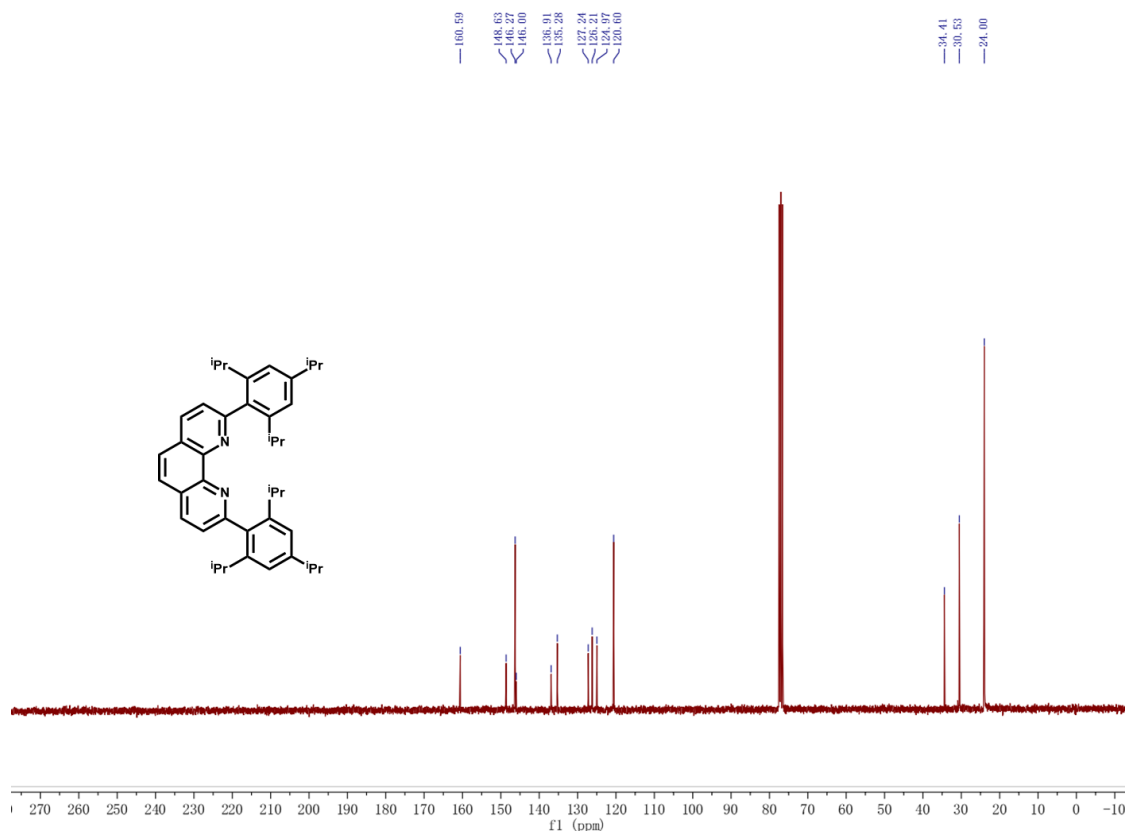
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



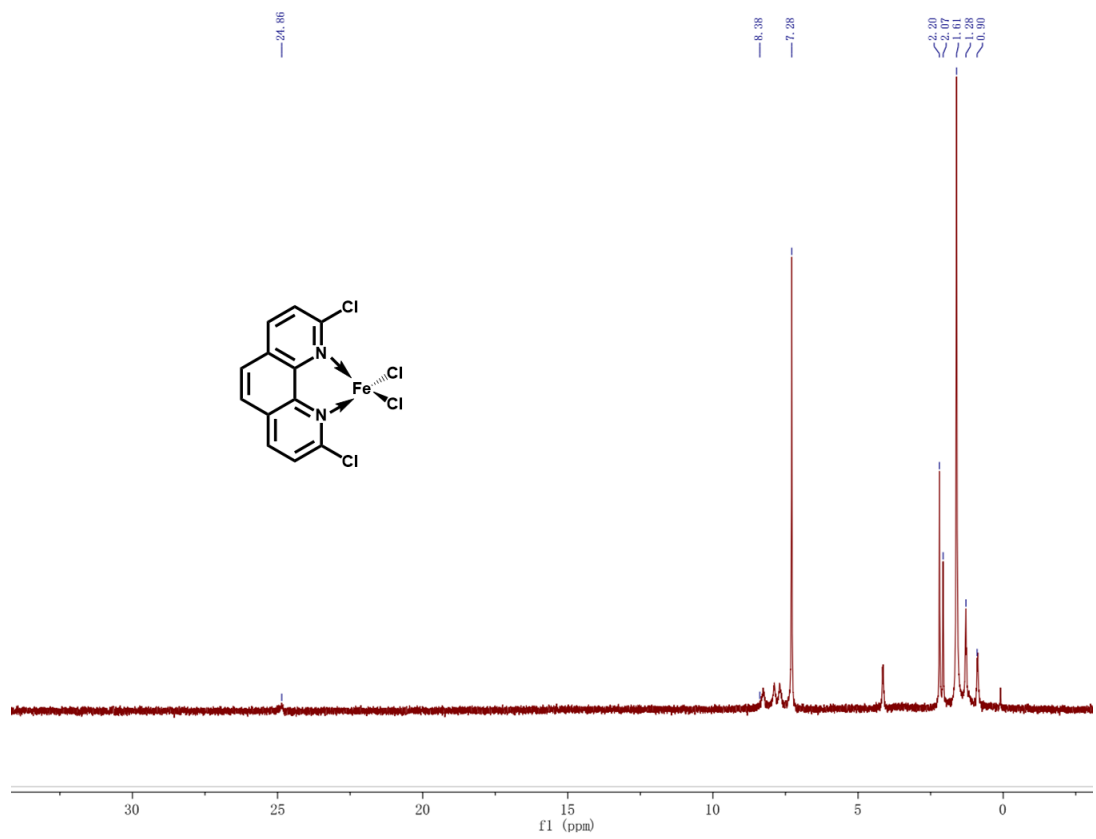
<sup>13</sup>C NMR (76 MHz, CDCl<sub>3</sub>)



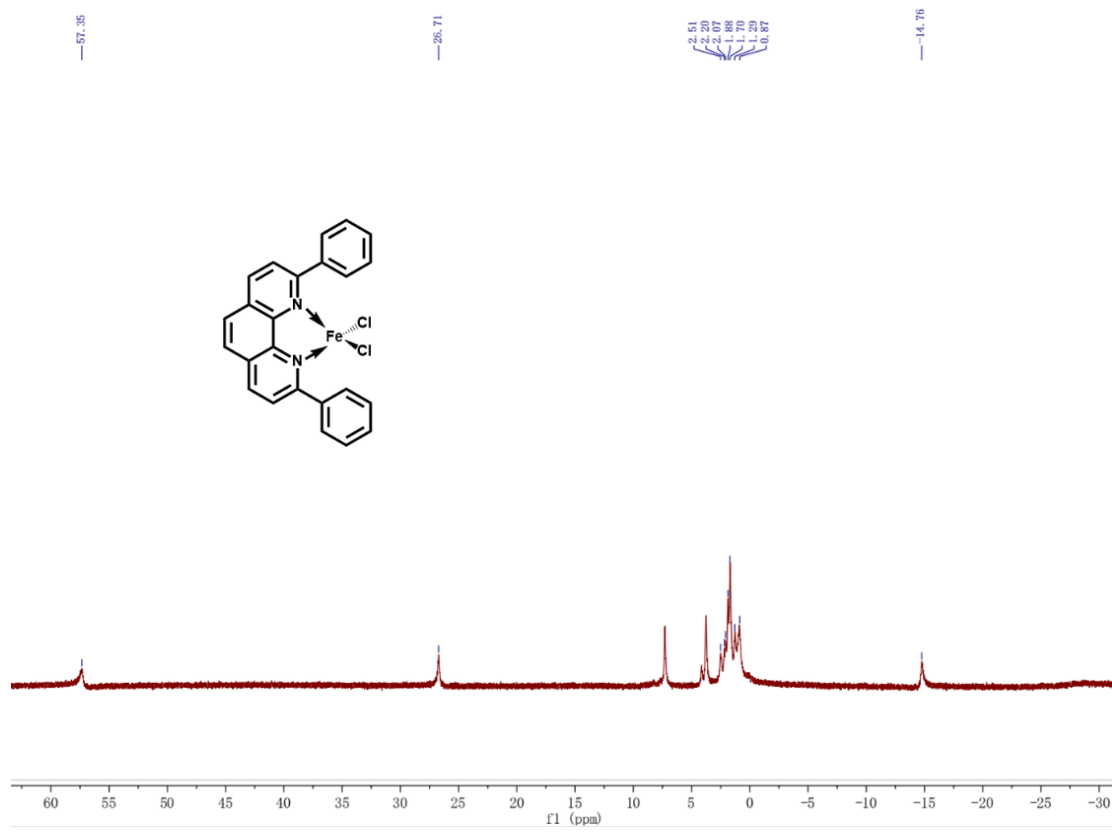
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)**



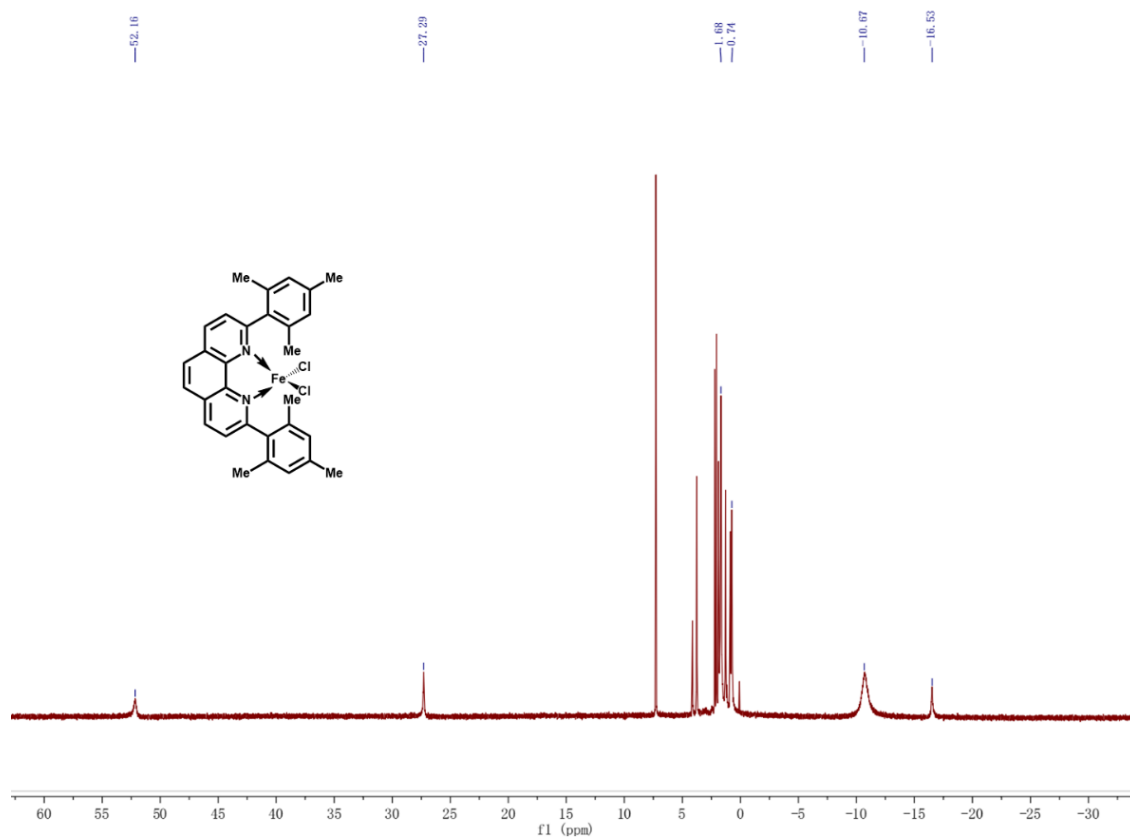
**<sup>13</sup>C NMR (76 MHz, CDCl<sub>3</sub>)**



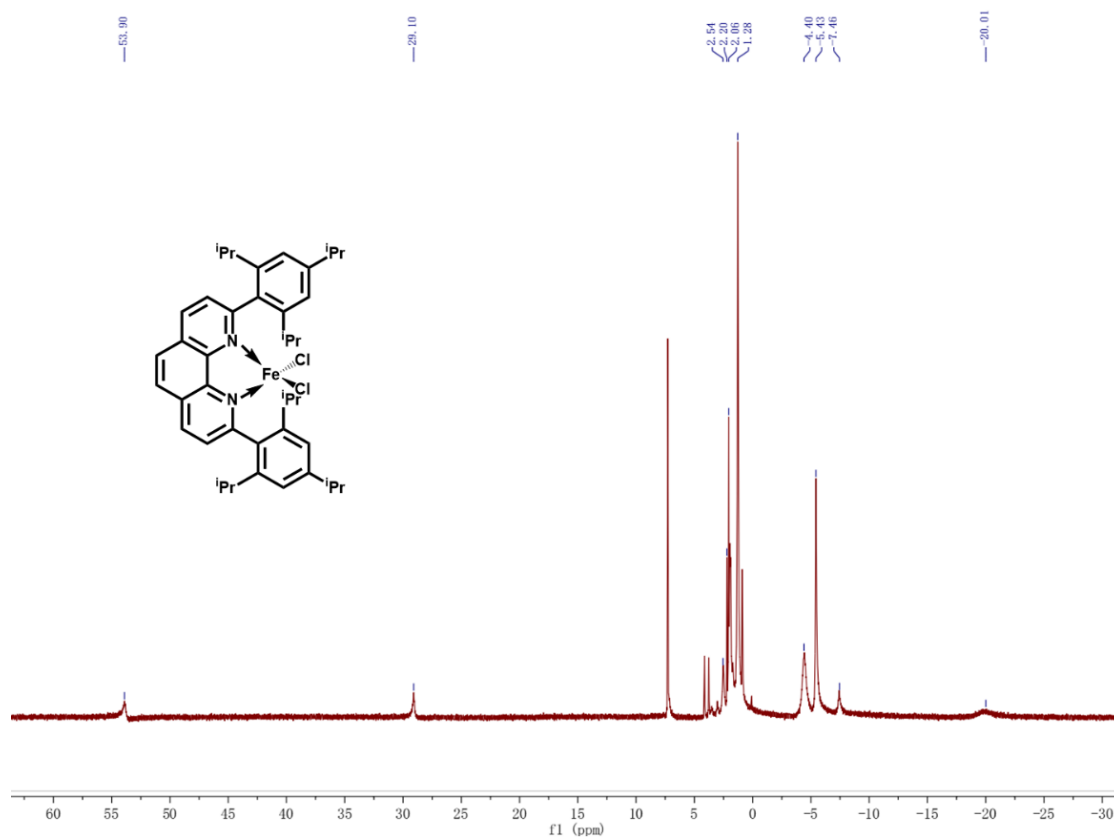
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



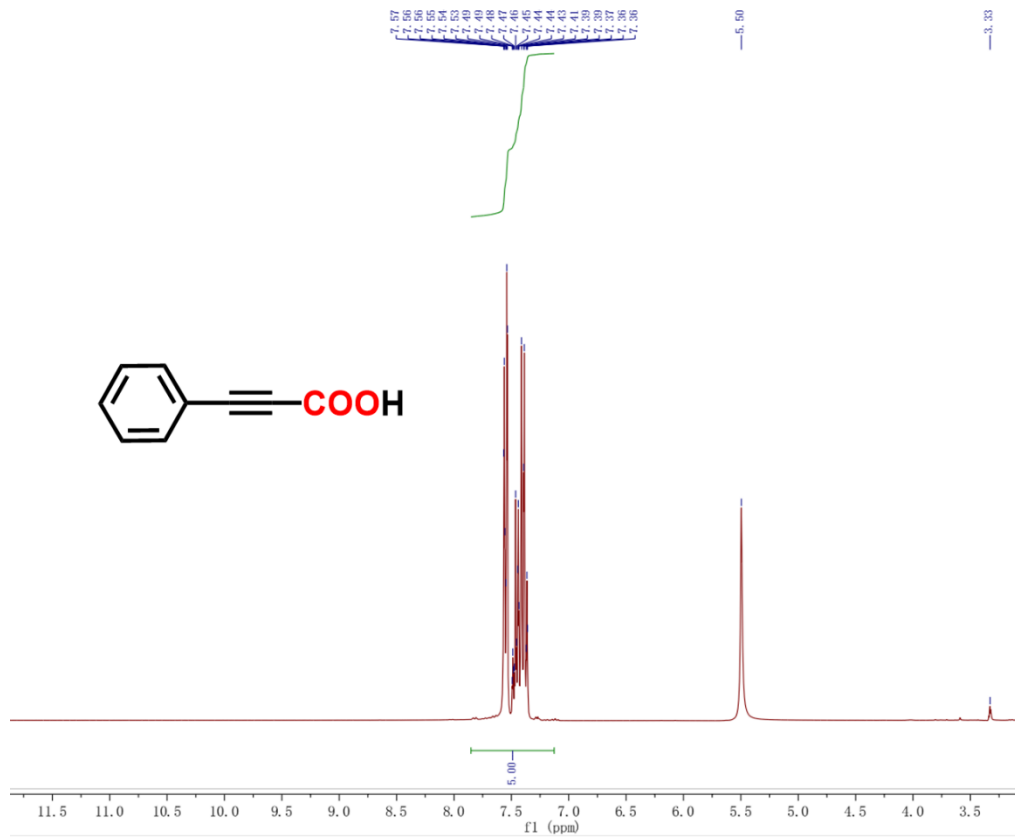
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



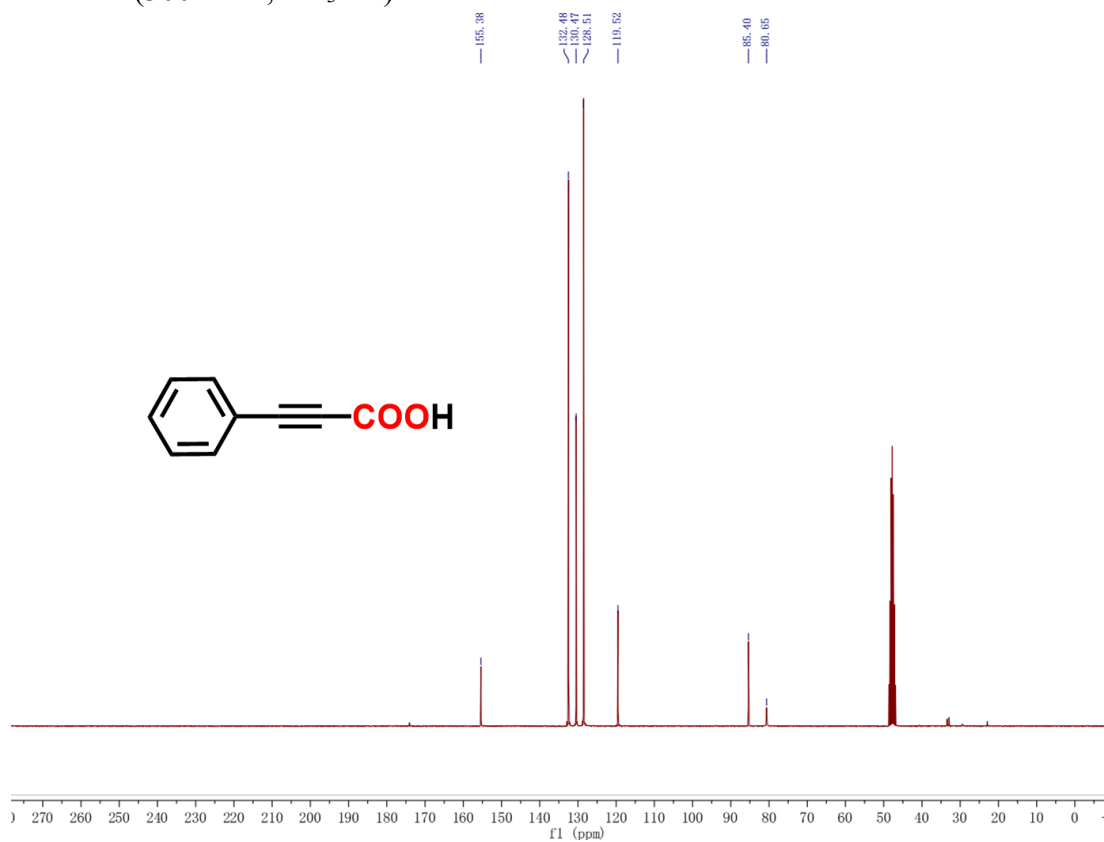
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



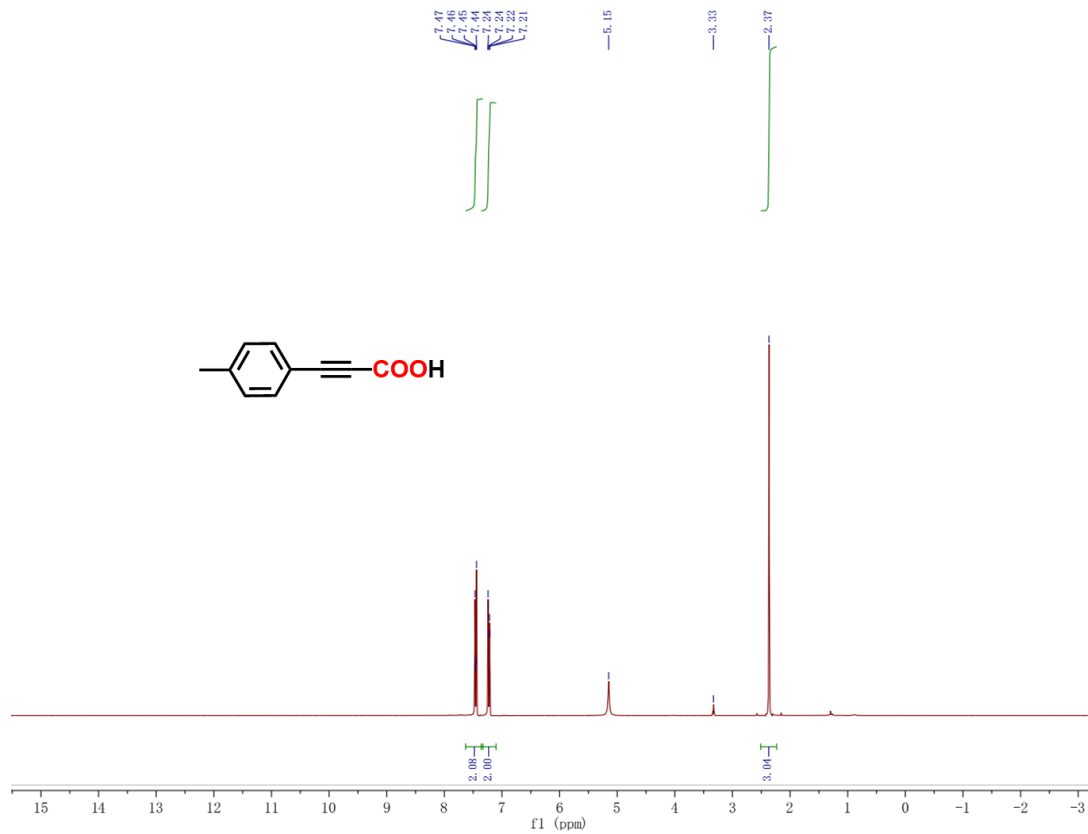
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



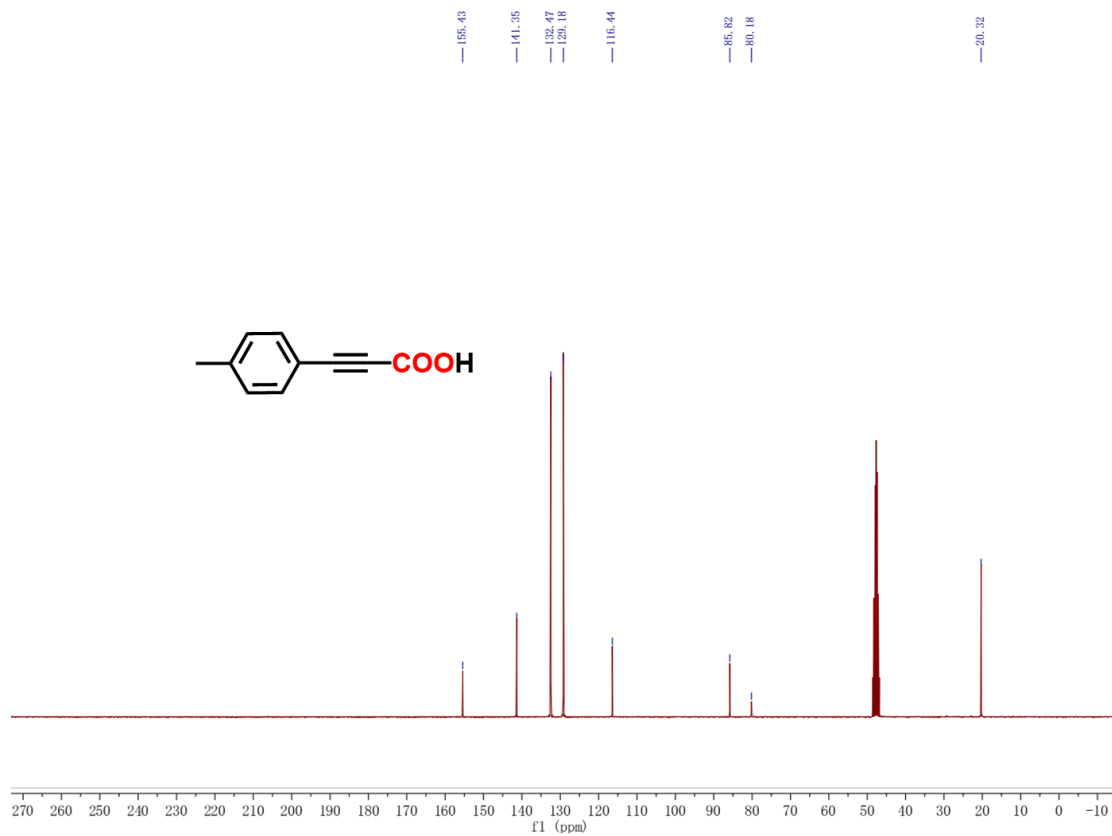
$^1\text{H}$  NMR (300 MHz,  $\text{CD}_3\text{OD}$ )



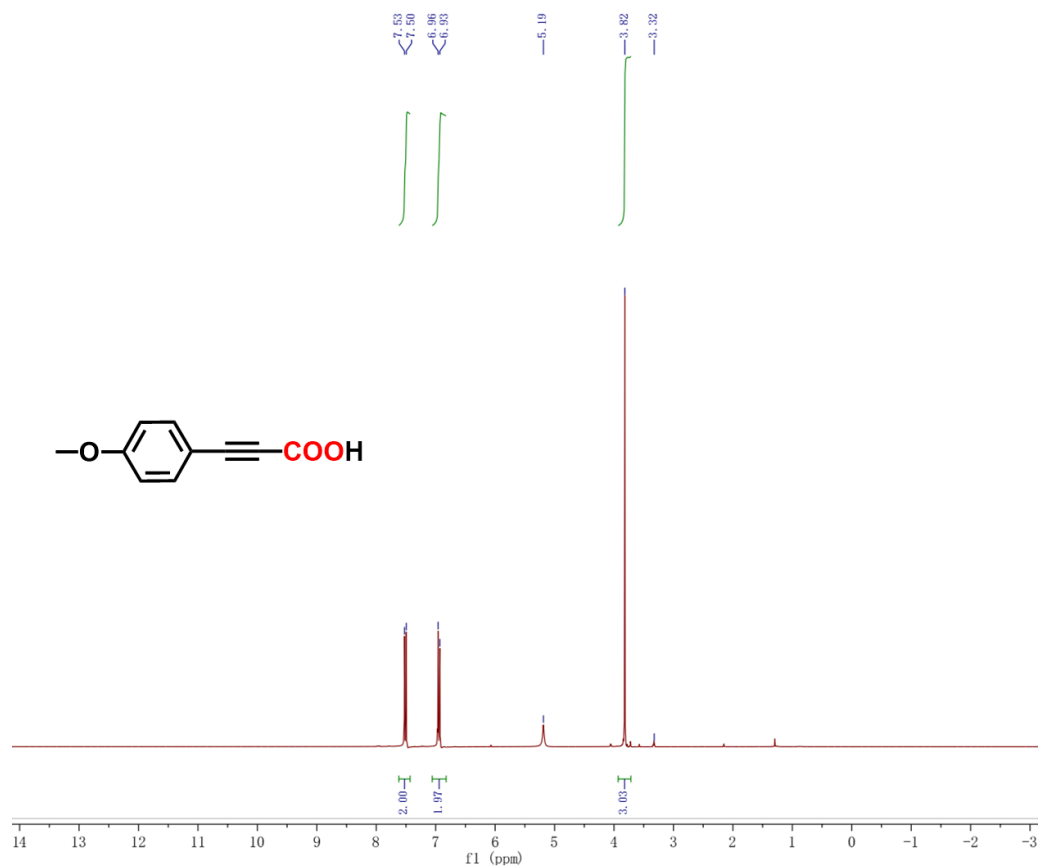
$^{13}\text{C}$  NMR (76 MHz,  $\text{CD}_3\text{OD}$ )



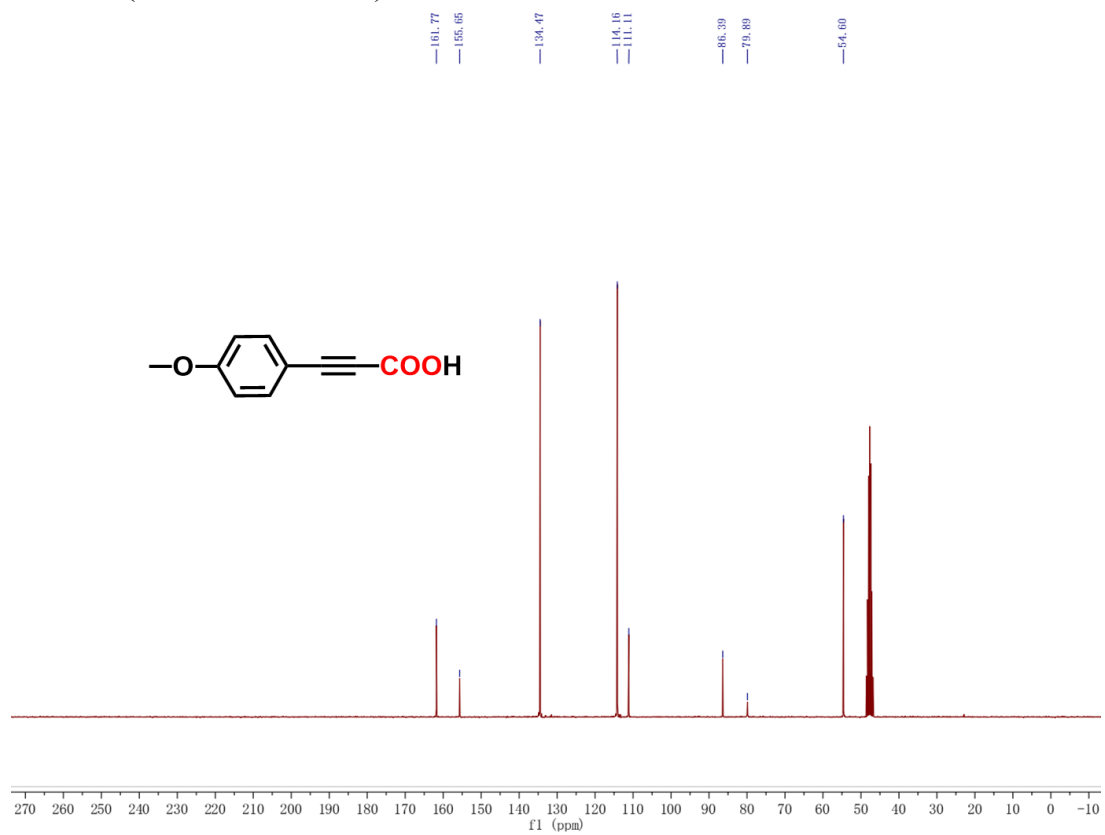
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD)



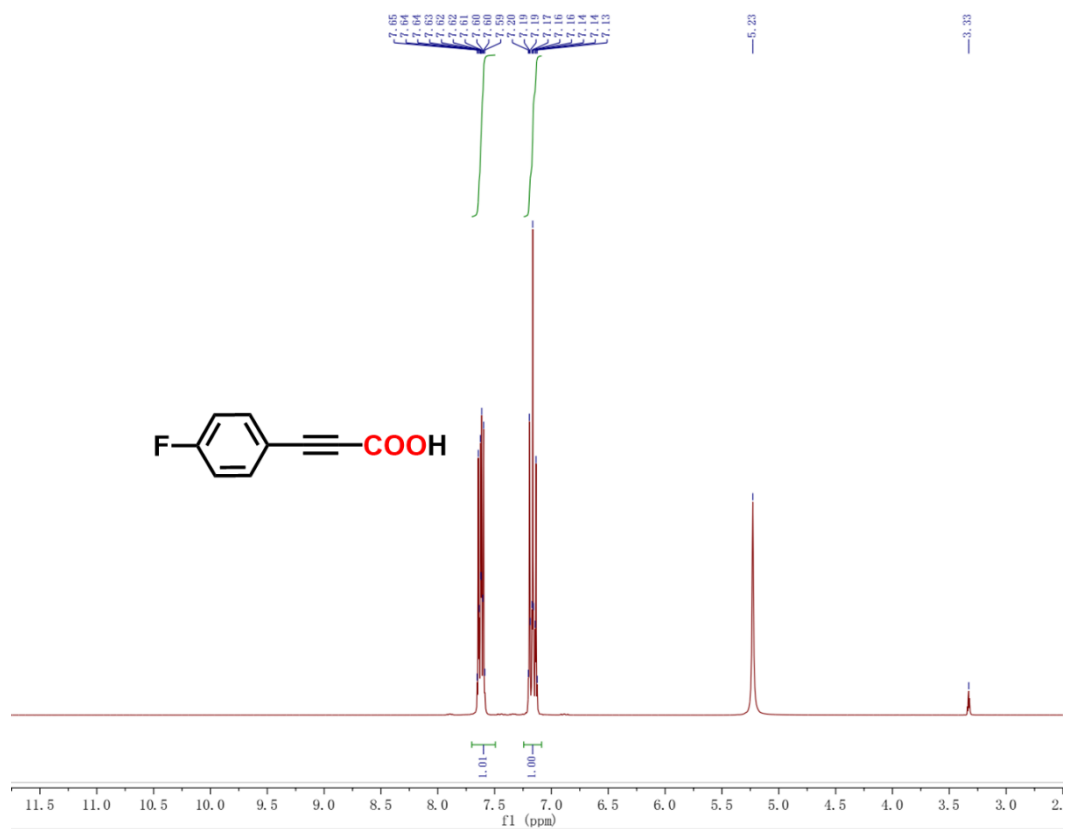
<sup>13</sup>C NMR (76 MHz, CD<sub>3</sub>OD)



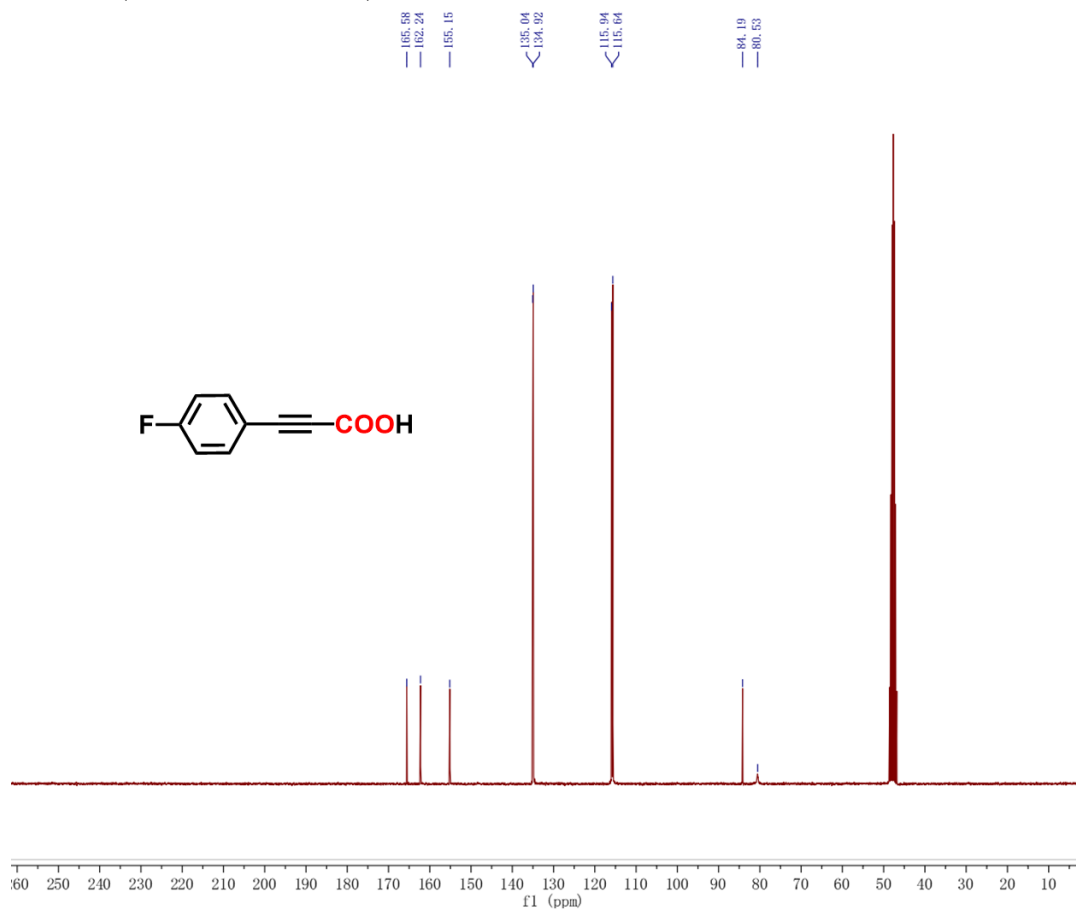
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD)



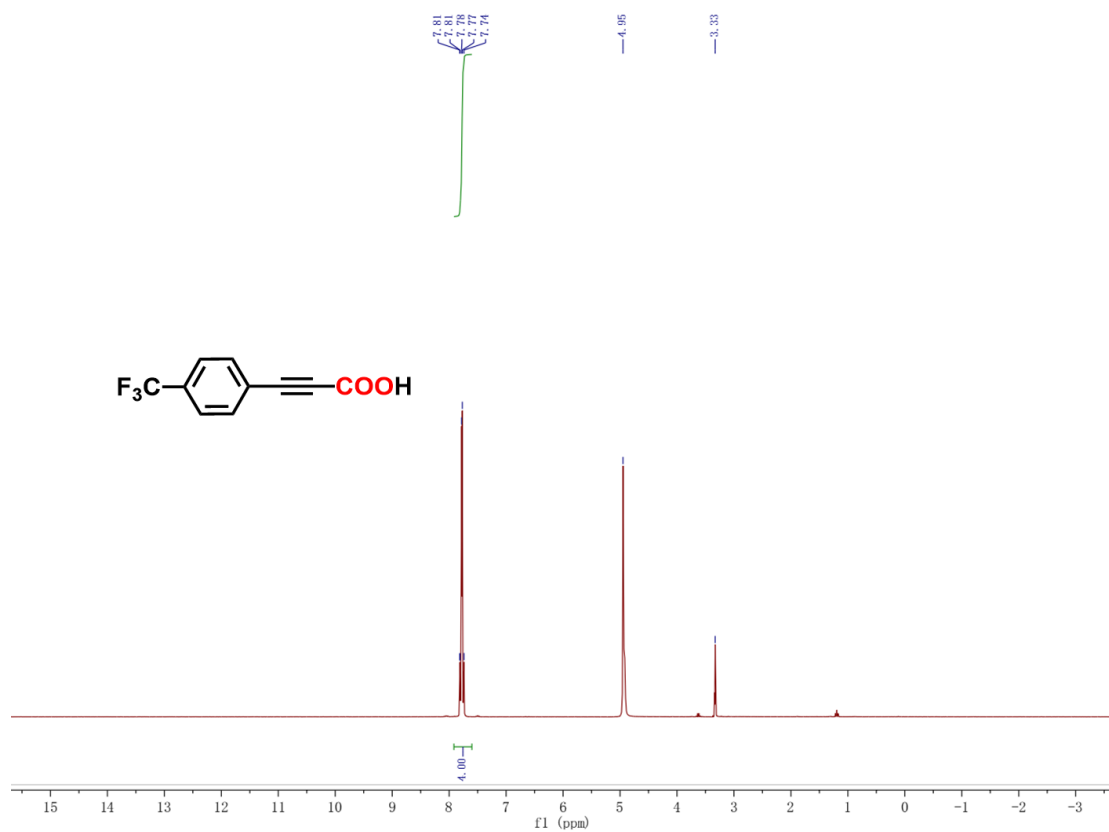
<sup>13</sup>C NMR (76 MHz, CD<sub>3</sub>OD)



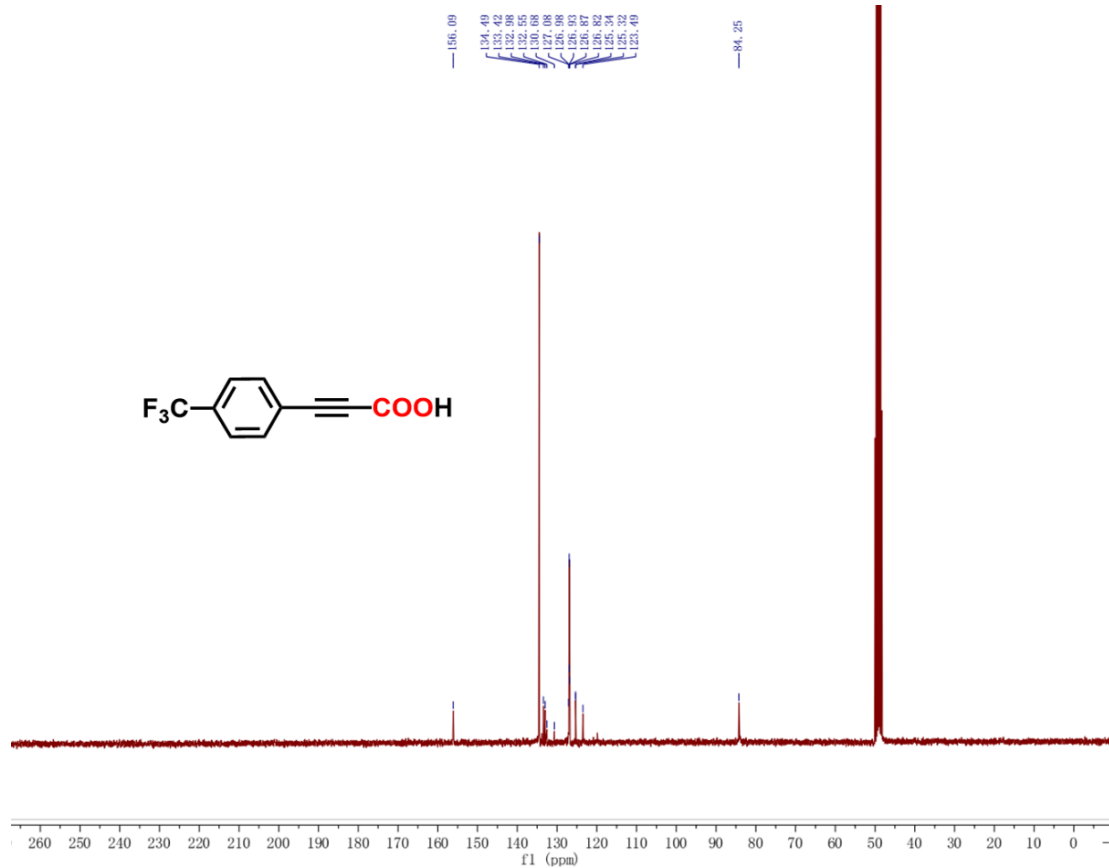
<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD)



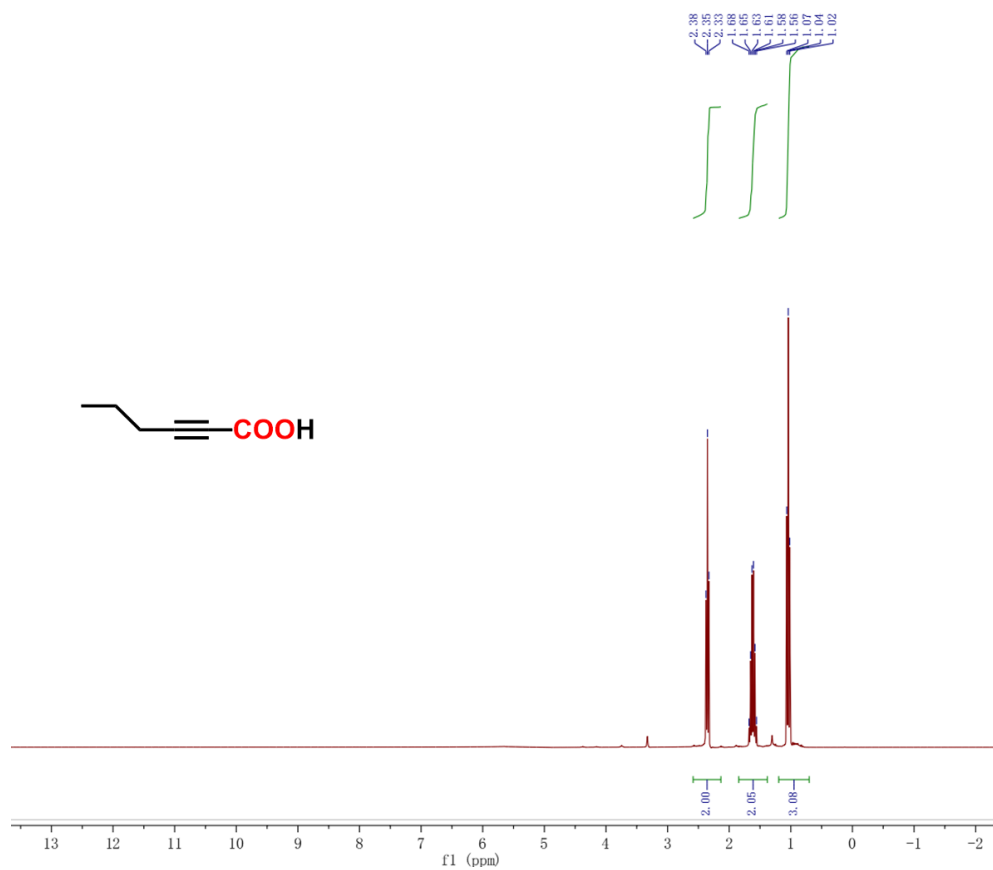
<sup>13</sup>C NMR (76 MHz, CD<sub>3</sub>OD)



$^1\text{H NMR}$  (300 MHz,  $\text{CD}_3\text{OD}$ )



$^{13}\text{C NMR}$  (76 MHz,  $\text{CD}_3\text{OD}$ )



<sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD)



<sup>13</sup>C NMR (76 MHz, CD<sub>3</sub>OD)

## Reference:

- 1 M. Hu, Q. He, S. Fan, Z. Wang, L. Liu, Y. Mu, Q. Peng and S. Zhu, Ligands with 1, 10-phenanthroline scaffold for highly regioselective iron-catalyzed alkene hydrosilylation. *Nat. Commun.*, 2018, **9**, 221.
- 2 P. He, M.-Y. Hu, J.-H. Li, T.-Z. Qiao, Y.-L. Lu and S.-F. Zhu, Spin effect on redox acceleration and regioselectivity in Fe-catalyzed alkyne hydrosilylation. *Natl. Sci. Rev.*, 2024, **11**, nwad324.
- 3 M.-Y. Hu, P. He, T.-Z. Qiao, W. Sun, W.-T. Li, J. Lian, J.-H. Li and S.-F. Zhu, Iron-catalyzed regiodivergent alkyne hydrosilylation. *J. Am. Chem. Soc.*, 2020, **142**, 16894-16902.
- 4 M.-Y. Hu, J. Lian, W. Sun, T.-Z. Qiao and S.-F. Zhu, Iron-catalyzed dihydrosilylation of alkynes: efficient access to geminal bis (silanes). *J. Am. Chem. Soc.*, 2019, **141**, 4579-4583.
- 5 Q. Huang, Y.-X. Su, W. Sun, M.-Y. Hu, W.-N. Wang and S.-F. Zhu, Iron-catalyzed vinylzincation of terminal alkynes. *J. Am. Chem. Soc.*, 2021, **144**, 515-526.
- 6 Q. Huang, W.-N. Wang and S.-F. Zhu, Iron-catalyzed alkylzincation of terminal alkynes. *ACS Catal.*, 2022, **12**, 2581-2588.
- 7 W.-T. Li, M.-Y. Hu, J.-W. Xiong, X.-Y. Zhang and S.-F. Zhu, Iron-catalysed hydroalumination of internal alkynes. *Chem. Sci.*, 2022, **13**, 7873-7879.
- 8 W. Sun, M.-P. Li, L.-J. Li, Q. Huang, M.-Y. Hu and S.-F. Zhu, Phenanthroline-imine ligands for iron-catalyzed alkene hydrosilylation. *Chem. Sci.*, 2022, **13**, 2721-2728.
- 9 Y. A. Mikheev and Y. A. Ershov, Assignment of the  $\pi \rightarrow \pi^*$  and  $n \rightarrow \pi^*$  transitions to the spectral bands of azobenzene and dimethylaminoazobenzene. *Russ. J. Phys. Chem. A*, 2018, **92**, 1499-1507.
- 10 Y. Hirose, H. Yui and T. Sawada, Effect of Potential Energy Gap between the  $n-\pi^*$  and the  $\pi-\pi^*$  State on Ultrafast Photoisomerization Dynamics of an Azobenzene Derivative. *J. Phys. Chem. A*, 2002, **106**, 3067-3071.
- 11 A. Vogler and H. Kunkely, Photoreactivity of metal-to-ligand charge transfer excited states. *Coord. Chem. Rev.*, 1998, **177**, 81-96.
- 12 A. M. May and J. L. Dempsey, A new era of LMCT: leveraging ligand-to-metal charge transfer excited states for photochemical reactions. *Chem. Sci.*, 2024, **15**, 6661-6678.