Supporting information for

Fluorinated 2,6-Bis(imino)pyridyl Iron Complexes Targeting Bimodal Dispersive Polyethylene; probing chain termination pathway via a combined experimental and DFT study

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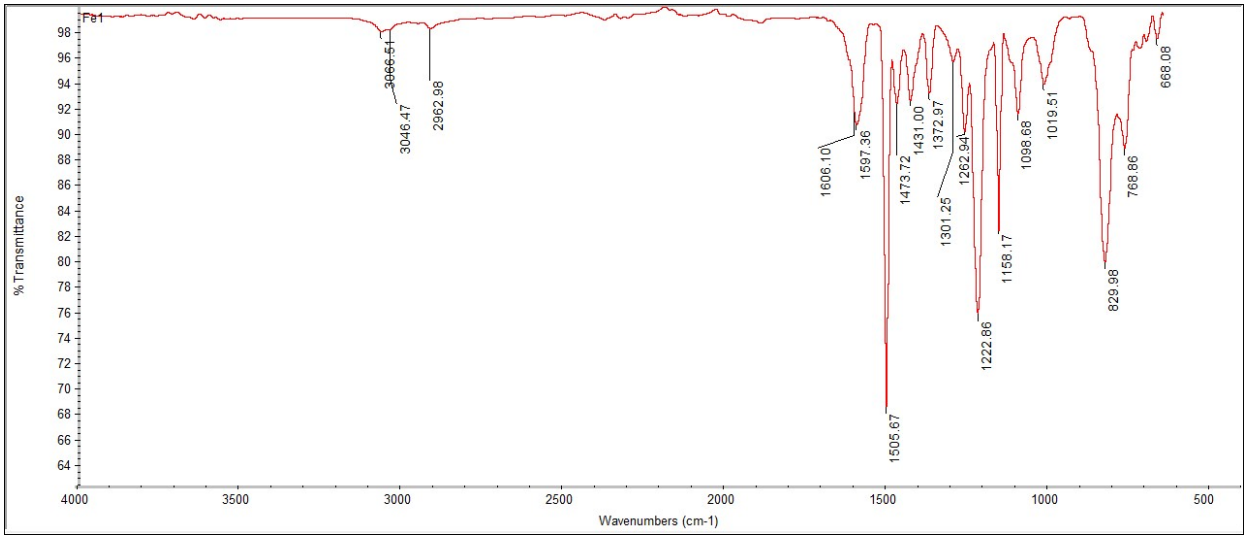


Figure S1. FT-IR spectrum of **Fe1**.

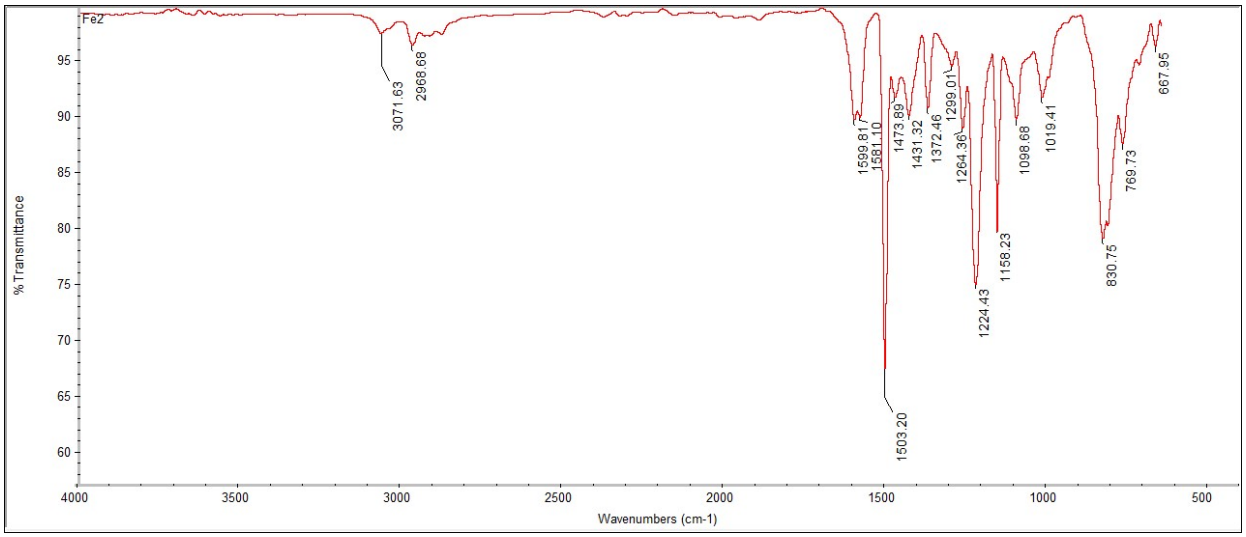


Figure S2. FT-IR spectrum of **Fe2**.

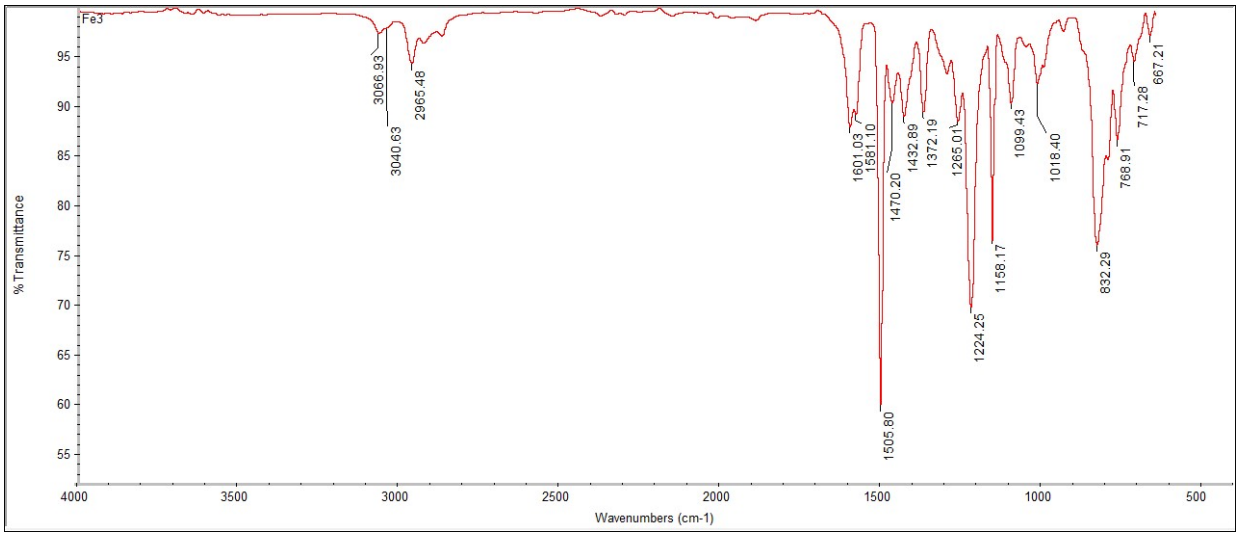


Figure S3. FT-IR spectrum of **Fe3**.

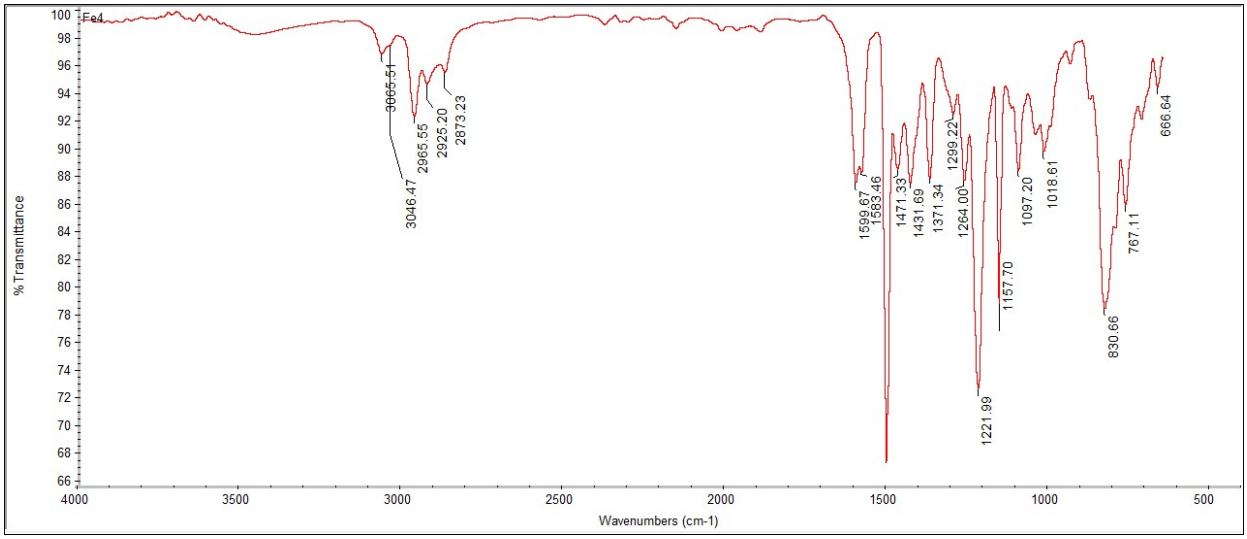


Figure S4. FT-IR spectrum of **Fe4**.

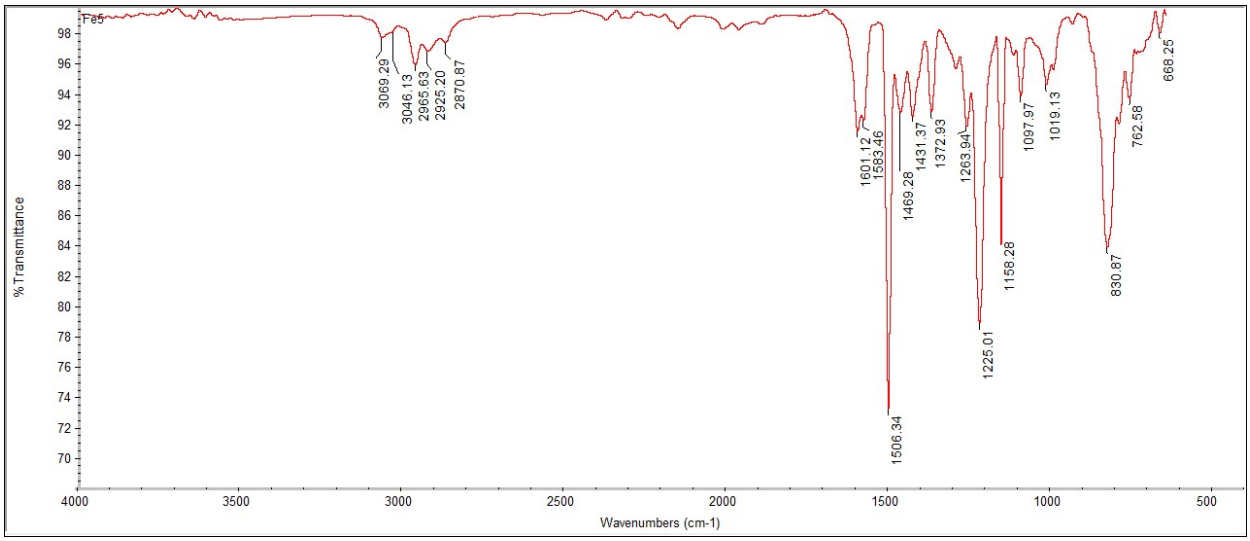


Figure S5. FT-IR spectrum of **Fe5**.

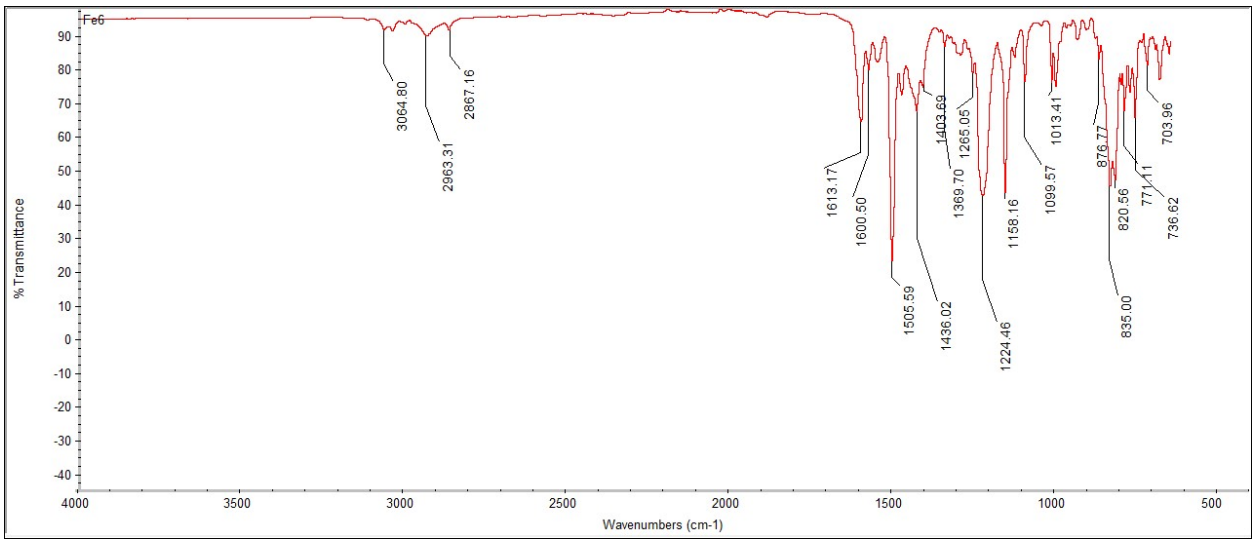


Figure S6. FT-IR spectrum of **Fe6**.

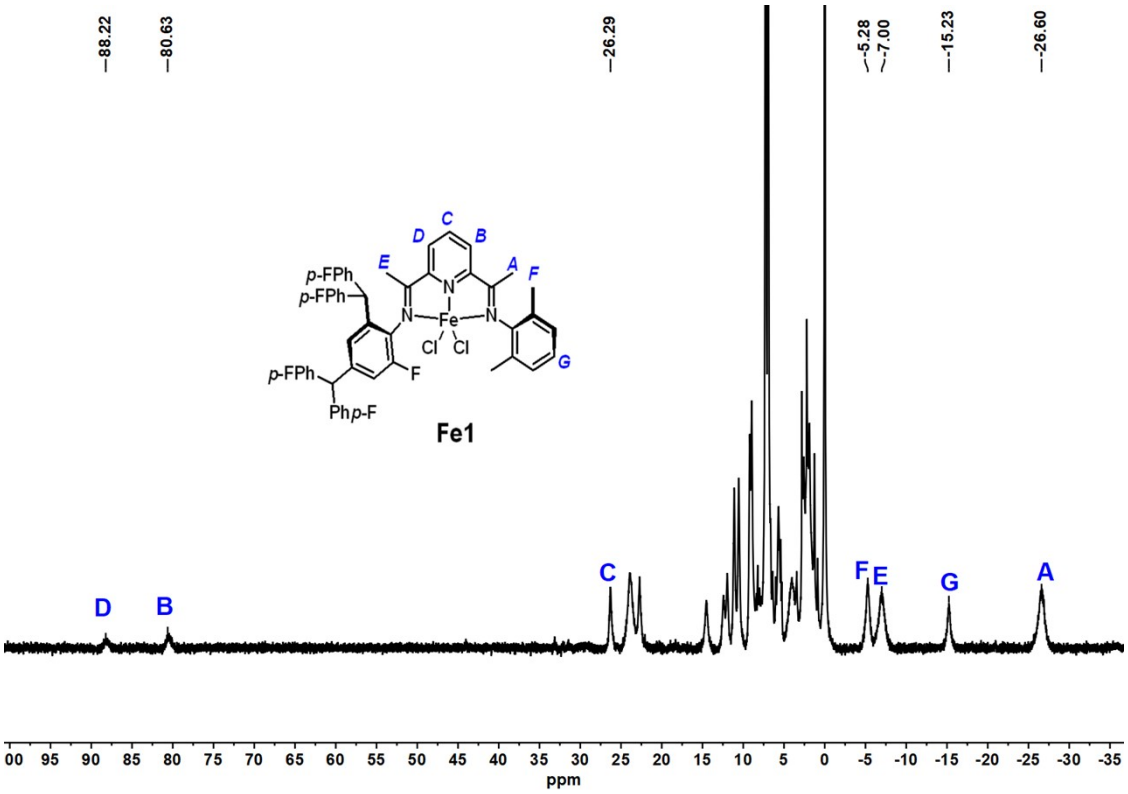


Figure S7. ^{1}H NMR spectrum of **Fe1** (recorded in $CDCl_3$ at ambient temperature).

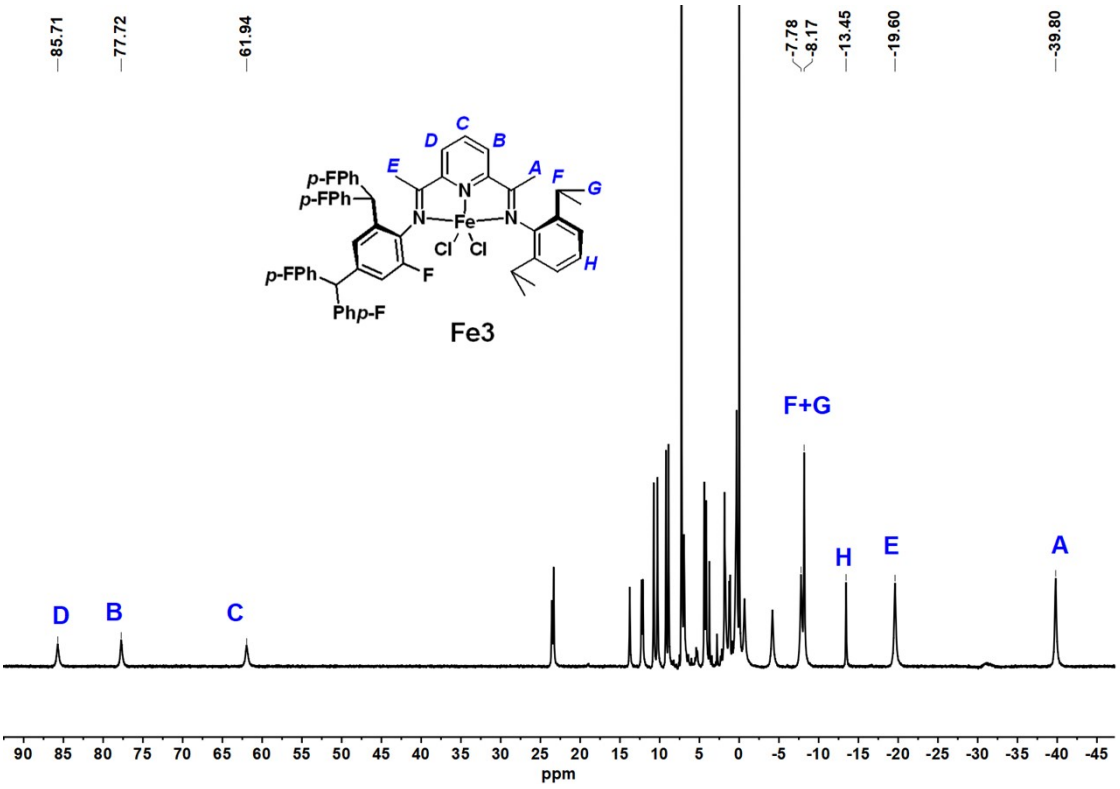


Figure S8. ^{1}H NMR spectrum of **Fe3** (recorded in $CDCl_3$ at ambient temperature).

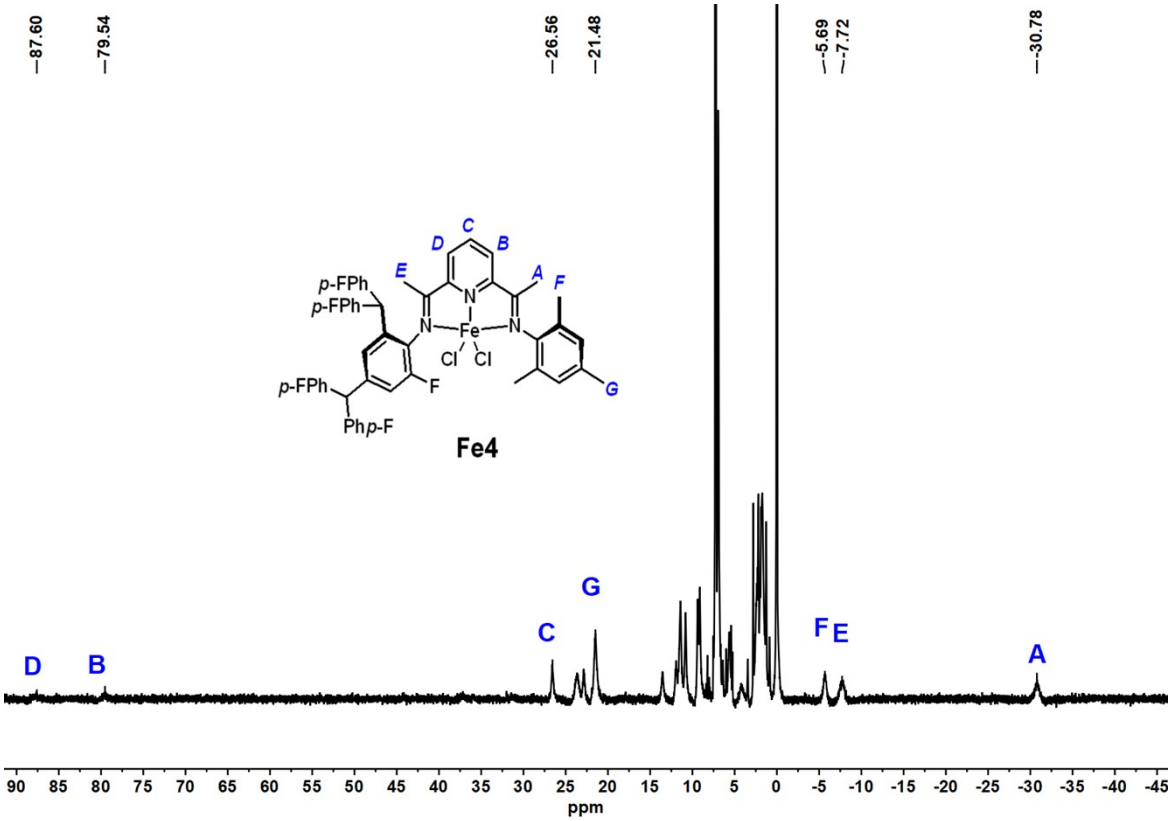


Figure S9. ^{1}H NMR spectrum of **Fe4** (recorded in $CDCl_3$ at ambient temperature).

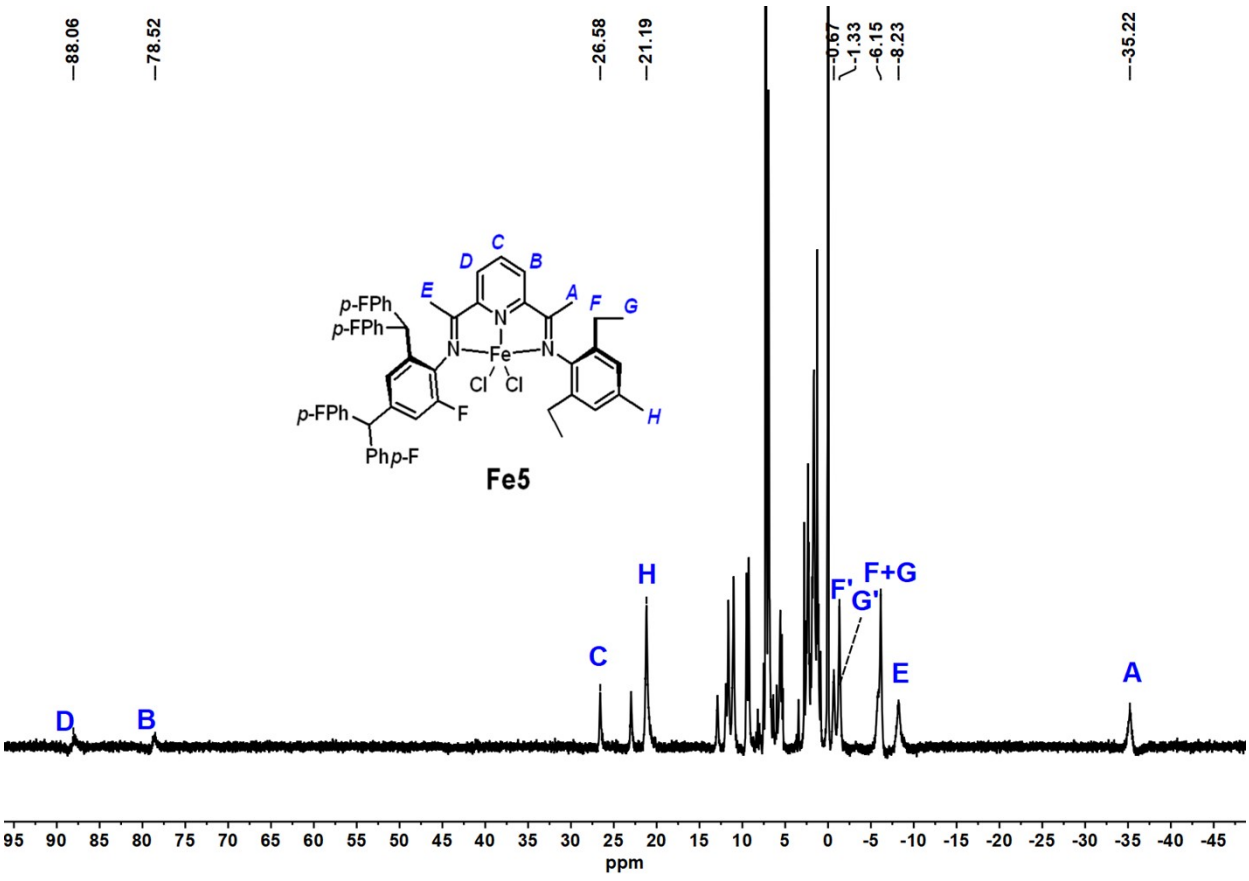


Figure S10. ^{1}H NMR spectrum of **Fe5** (recorded in $CDCl_3$ at ambient temperature).

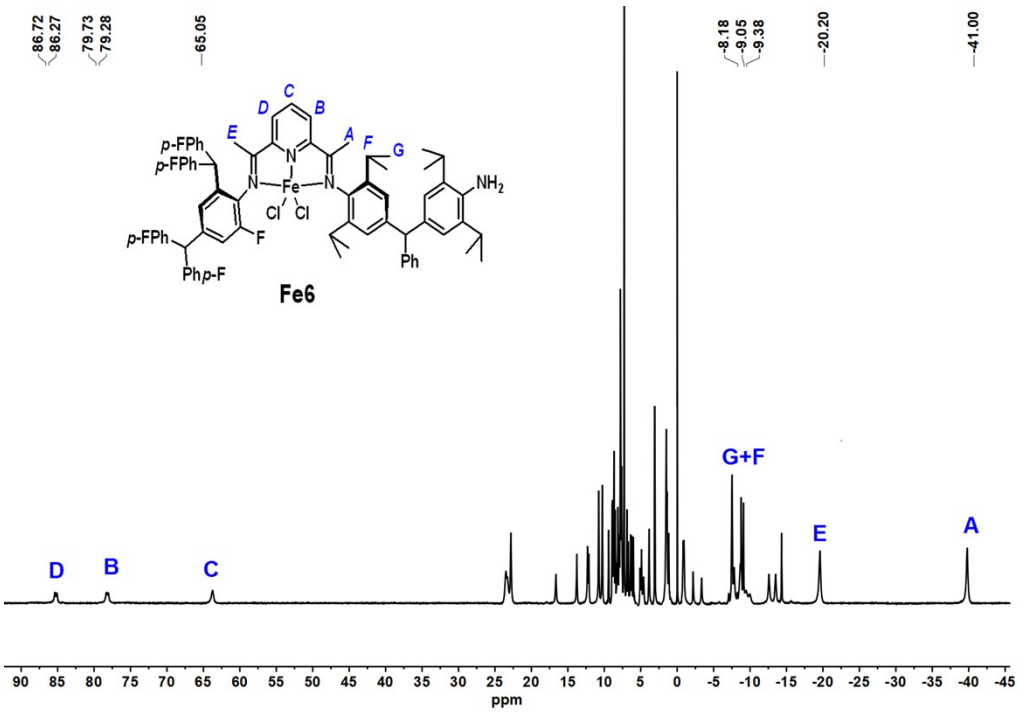


Figure S11. ^{1}H NMR spectrum of **Fe6** (recorded in $CDCl_3$ at ambient temperature).

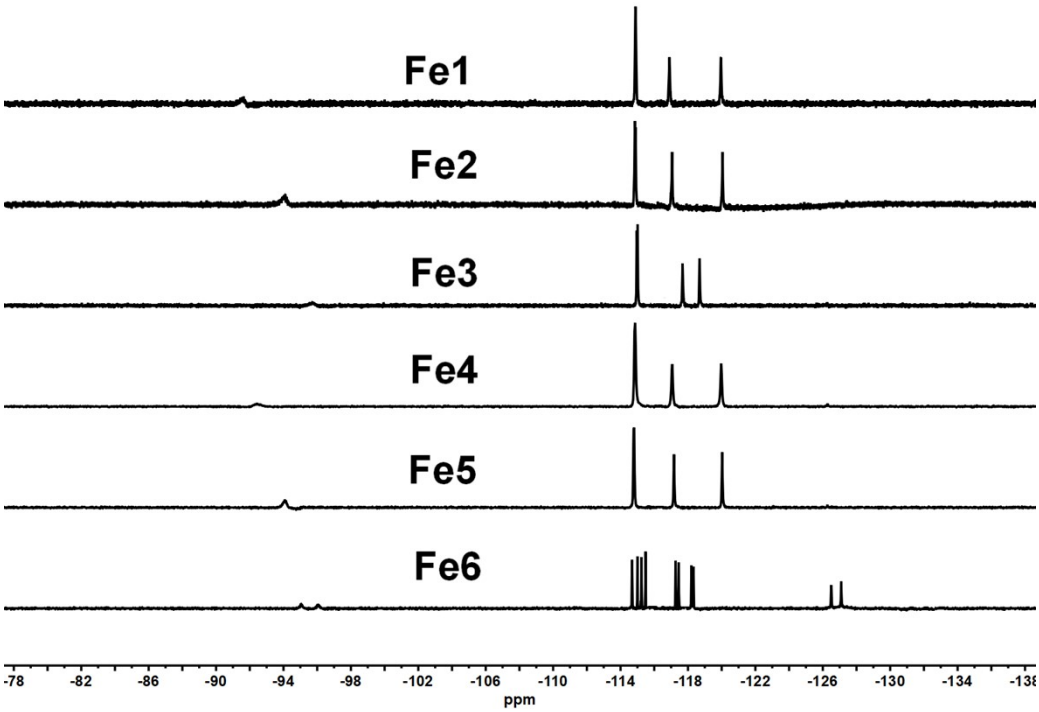


Figure S12. ^{19}F NMR spectra of **Fe1**–**Fe6**; recorded in $CDCl_3$ at ambient temperature.

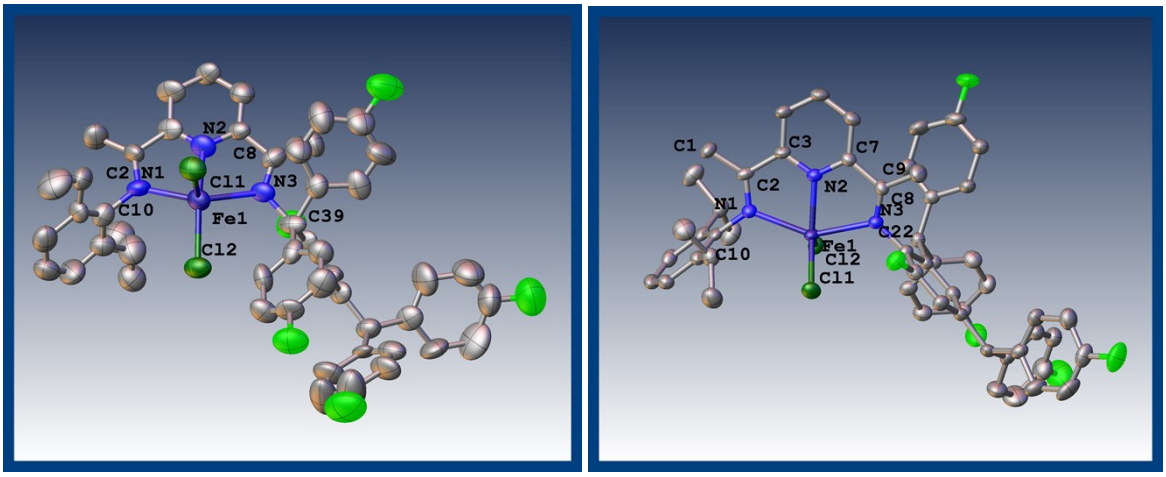


Figure S13. X-ray crystal structural drawing showing ADPs of **Fe2** (left) and **Fe3** (right) made by Olex2.

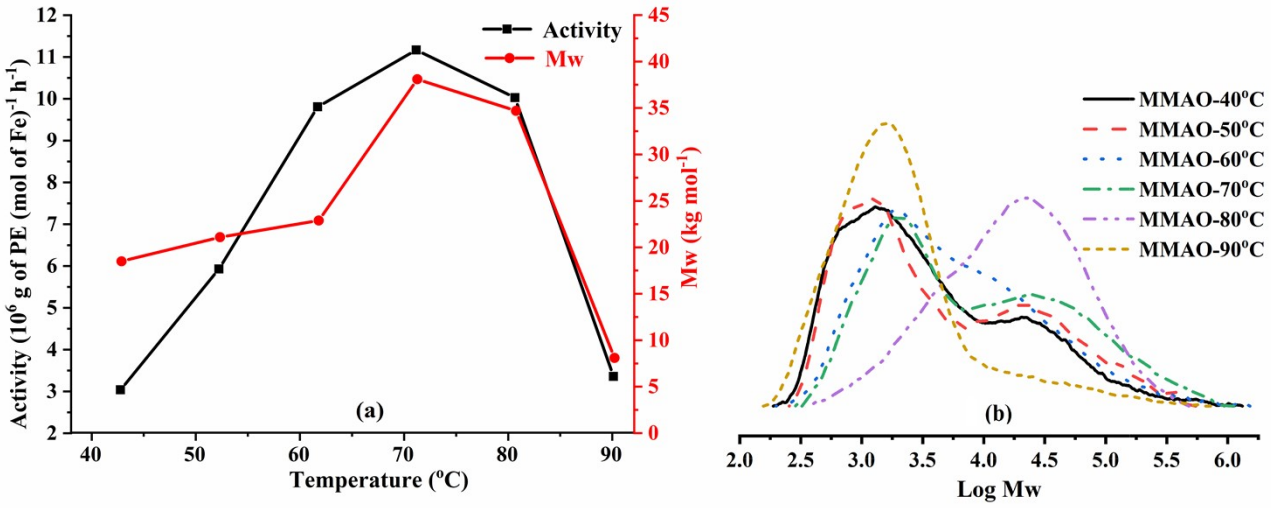


Figure S14. Activity and M_w as a function of reaction temperature (a); GPC curves of the obtained polyethylene at different run temperatures (b) for the **Fe2**/MMAO system (entries 1–6, Table 2).

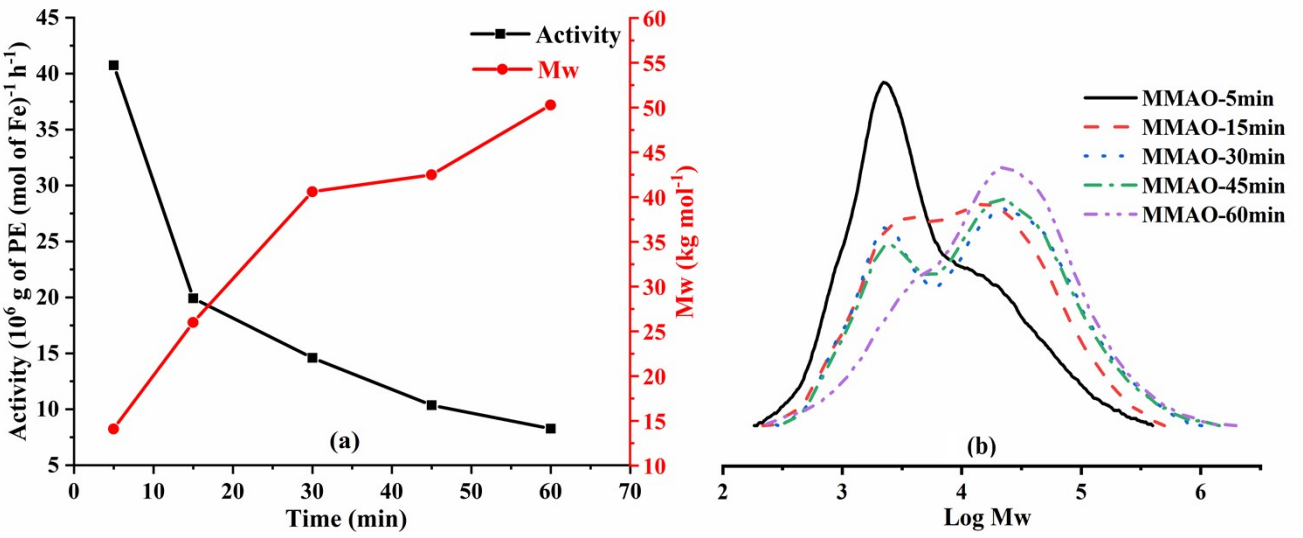


Figure S15. Activity and M_w as a function of reaction time (a); GPC curves of the obtained polyethylene at different run time (b) for the **Fe2**/MMAO system (entries 8, 11–14, Table 2).

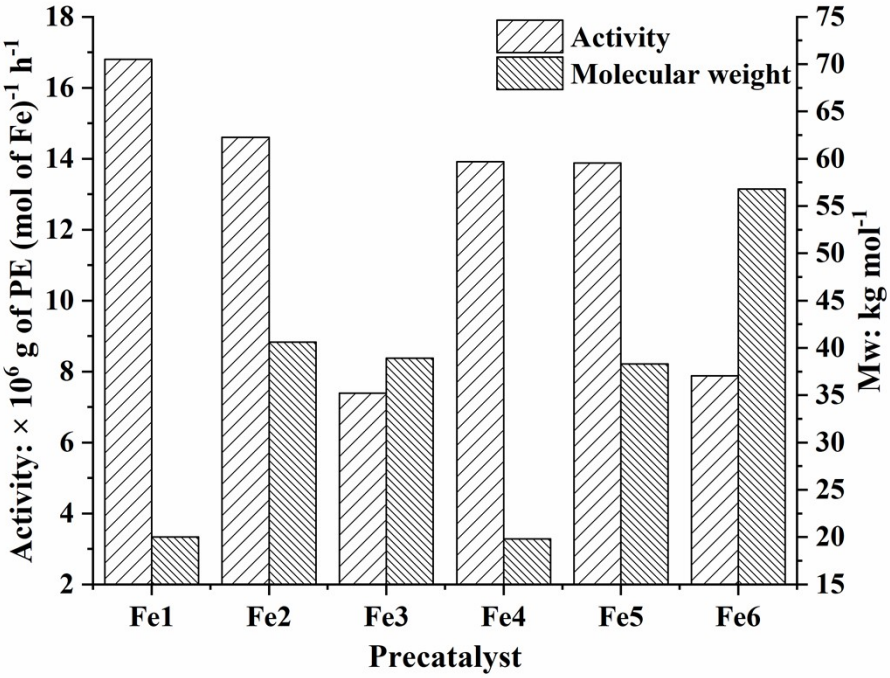


Figure S16. Catalytic activities and molecular weight of resultant polyethylenes by **Fe1–Fe6**/MMAO (entries 8, 17–21, Table 2).

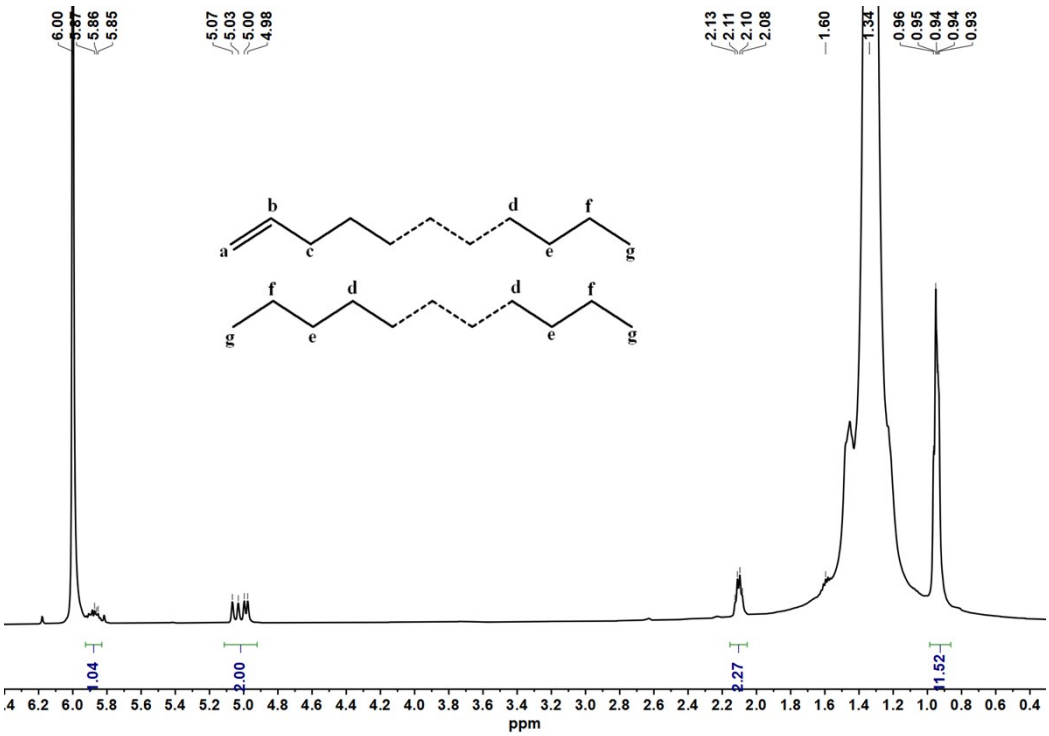


Figure S17. [1]H NMR spectrum of the polyethylene prepared with catalyst **Fe1**/MMAO at 70 °C (entry 17, Table 2).

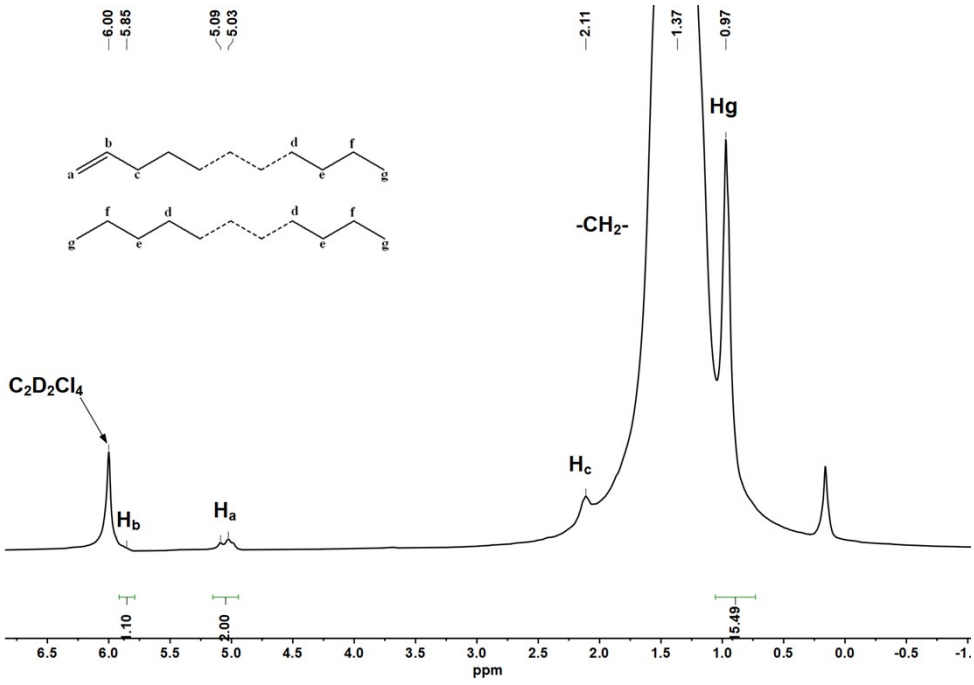


Figure S18. [1]H NMR spectrum of the polyethylene prepared with catalyst **Fe6**/MMAO at 70 °C (entry 21, Table 2).

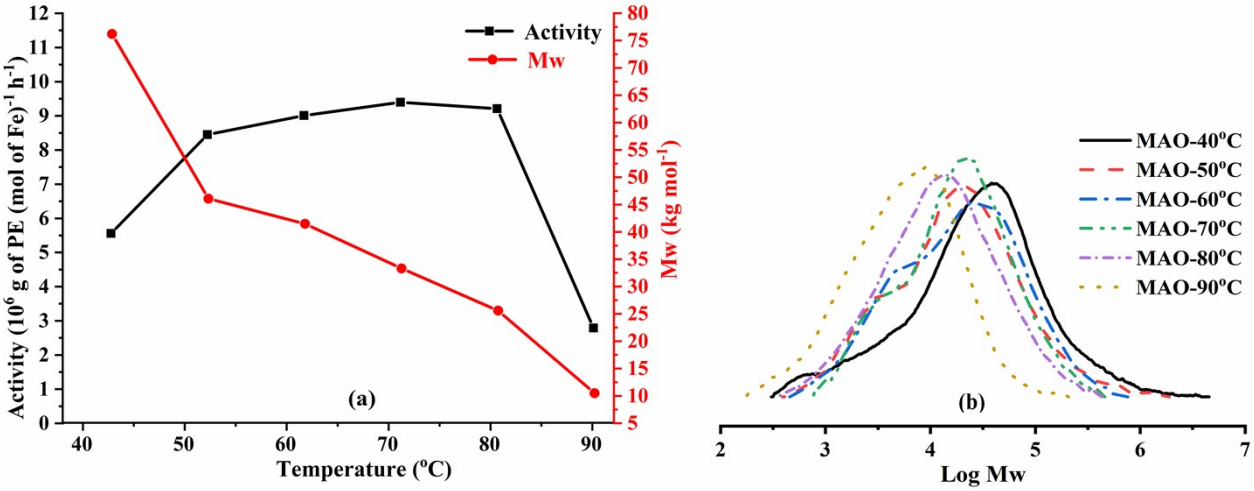


Figure S19. Activity and M_w as a function of reaction temperature (a); GPC curves of the obtained polyethylene at different run temperatures (b) for the **Fe2**/MAO system (entries 1–6, Table 3).

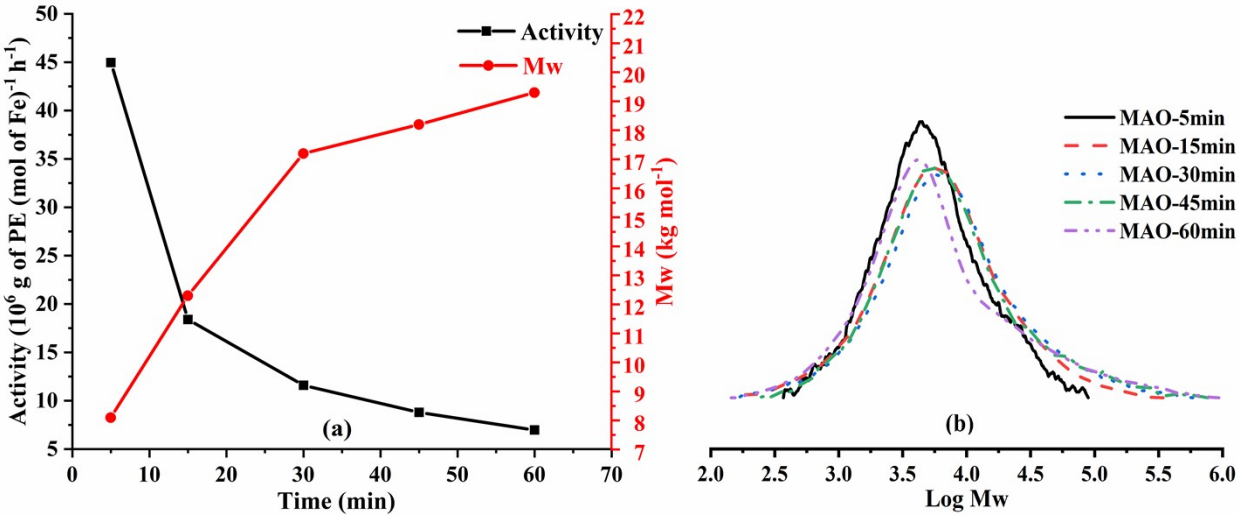


Figure S20. Activity and M_w as a function of reaction time (a); GPC curves of the obtained polyethylene at different run time (b) for the **Fe2**/MAO system (entries 10, 12–15, Table 3).

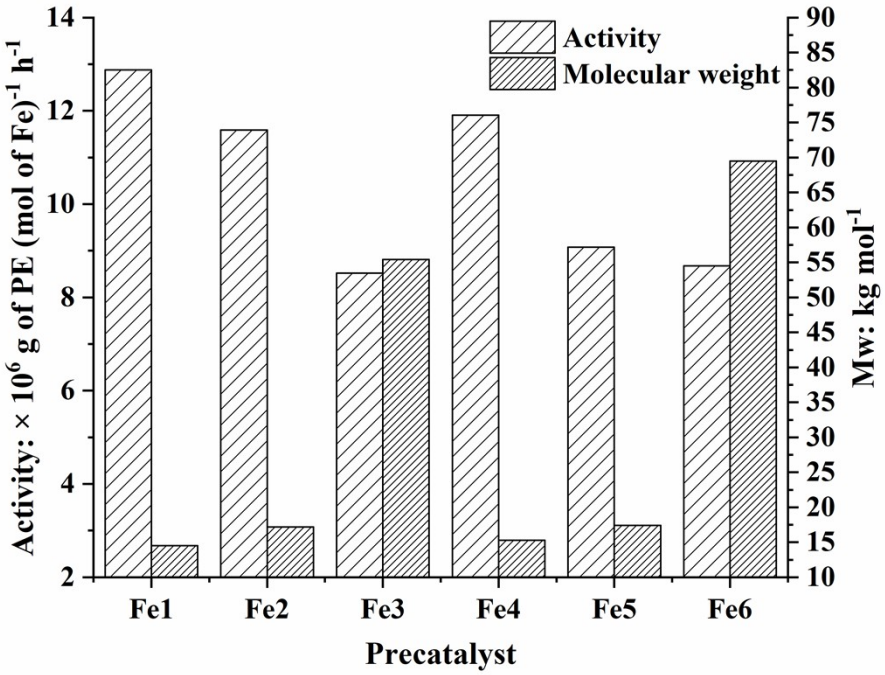


Figure S21. Catalytic activities and molecular weight of resultant polyethylenes by **Fe1**–**Fe6**/MAO (entries 10, 17–21, Table 3).

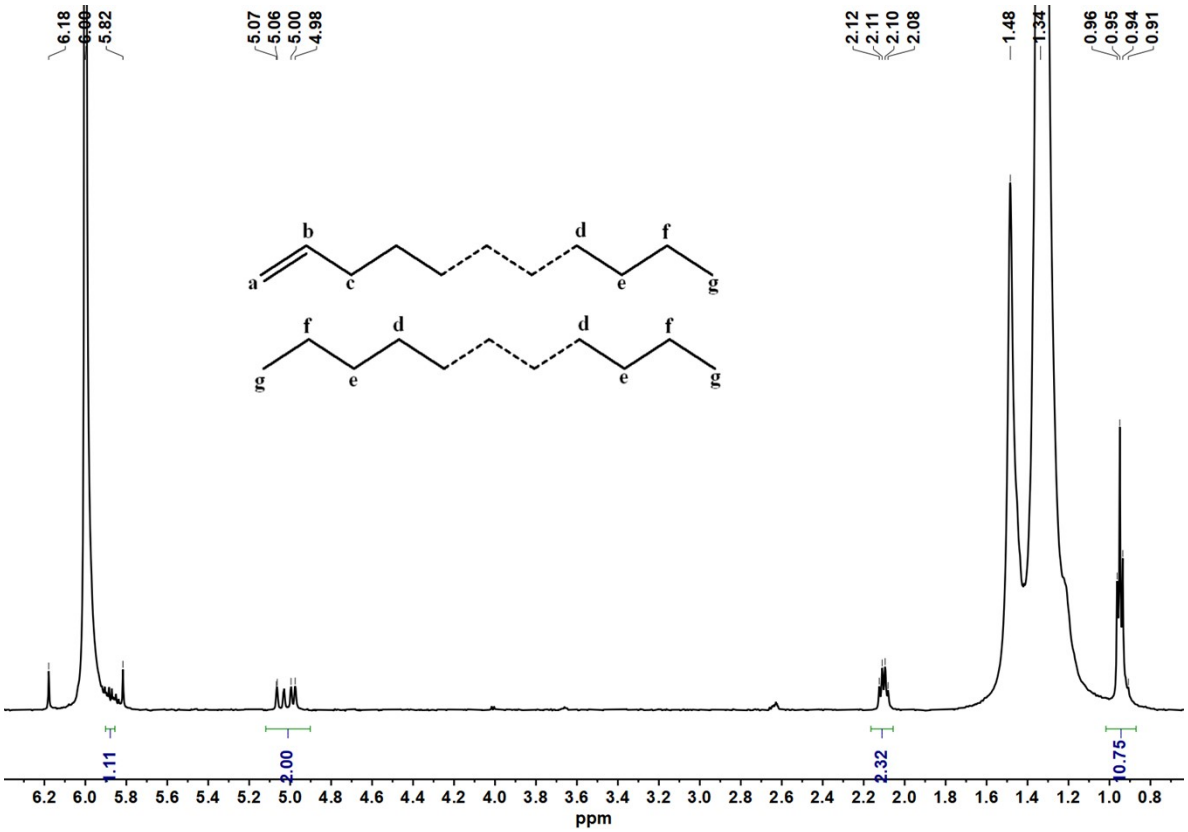


Figure S22. ^{1}H NMR spectrum of the polyethylene prepared with catalyst **Fe1**/MAO at 70 °C (entry 17, Table 3).

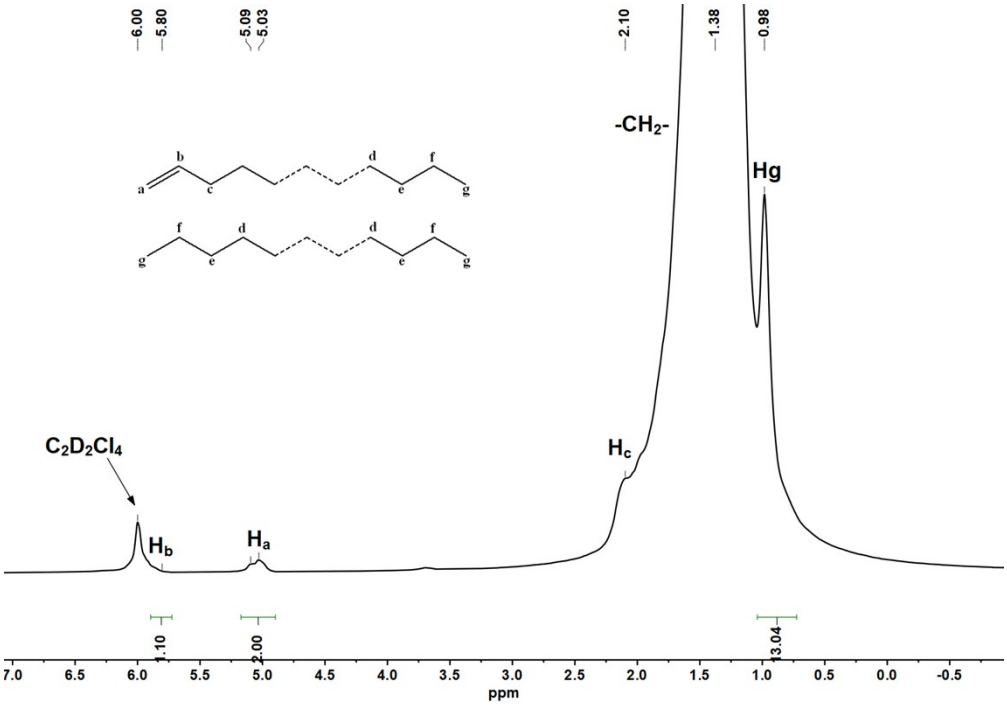


Figure S23. ^{1}H NMR spectrum of the polyethylene prepared with catalyst **Fe6**/MAO at 70 °C (entry 21, Table 3).

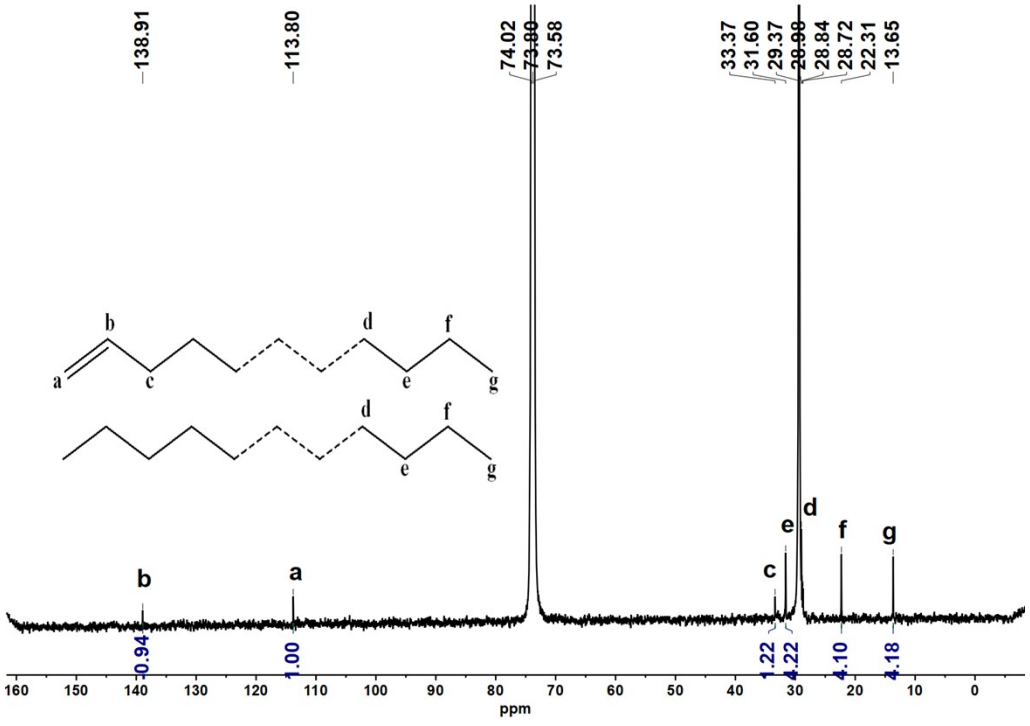
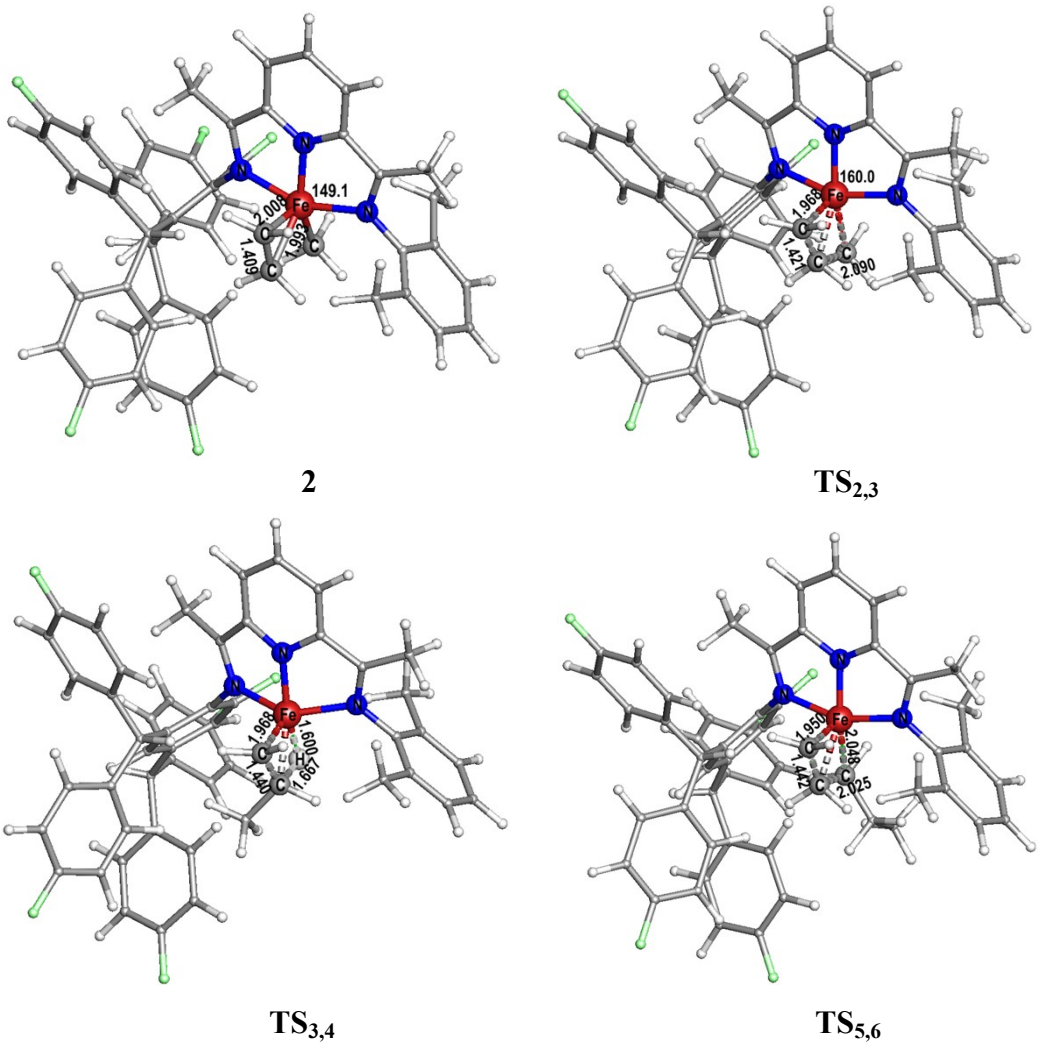


Figure S24. 1D sequence inverse-gated decoupled ^{13}C NMR spectrum of the polyethylene obtained using **Fe2**/MAO (δ C 73.8, tetrachloroethane-d_2) (entry 10, Table 3).

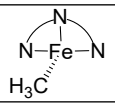
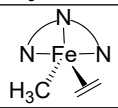
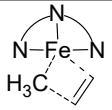
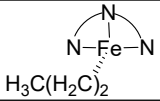


2 **$TS_{2,3}$**

$TS_{3,4}$ **$TS_{5,6}$**

Figure S25. Optimized structures of **2**, **$TS_{2,3}$** (287*i* cm^{-1}), **$TS_{3,4}$** (313*i* cm^{-1}), and **$TS_{5,6}$** (442*i* cm^{-1}). Mesitylene groups are omitted for clarity. Bond lengths are in Å.

Table S1 Calculation data of the optimized structures as well as their total electronic energy (E), total free energy (G), and total enthalpy (H).

Complexes	Structure	Electronic energy (Hartree)	Free energy (Hartree)	Enthalpy (Hartree)
1		-3855.353607	-3854.666068	-3854.521542
2		-3933.867877	-3933.124743	-3932.977638
$TS_{2,3}$		-3933.843842	-3933.103653	-3932.955144
3		-3933.916439	-3933.174389	-3933.024148

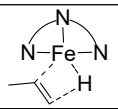
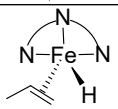
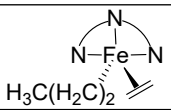
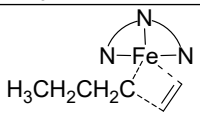
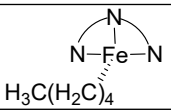
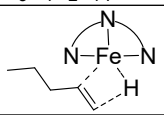
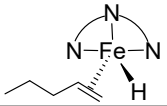
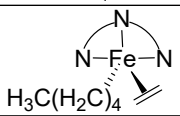
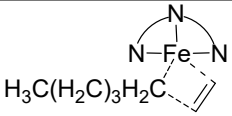
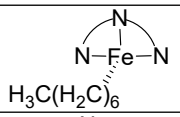
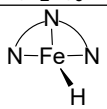
$TS_{3,4}$		-3933.869566	-3933.129786	-3932.983415
4		-3933.876521	-3933.137829	-3932.988136
5		-4012.446943	-4011.653591	-4011.497991
$TS_{5,6}$		-4012.418101	-4011.620463	-4011.468928
6		-4012.485495	-4011.688819	-4011.534009
$TS_{6,7}$		-4012.427279	-4011.631314	-4011.481755
7		-4012.432784	-4011.639443	-4011.484927
8		-4091.000237	-4090.148986	-4089.991351
$TS_{8,9}$		-4090.986592	-4090.136838	-4089.978347
9		-4091.052728	-4090.203188	-4090.043022
10		-3816.058251	-3815.400408	-3815.257244

Table S2 Crystal data and structure refinement for **Fe2** and **Fe3**.

Identification Code	**Fe2**	**Fe3**
CCDC number	2160181	2160182
Empirical formula	C51H42Cl2F5FeN3	$C_{53}H_{46}Cl_2F_5FeN_3 \cdot CH_2Cl_2$
Formula weight	918.62	1031.60
Temperature/K	169.98(14)	170.00(10)
Crystal system	orthorhombic	orthorhombic
Space group	Pna21	$P2_12_12_1$
a/Å	16.1979(8)	12.8077(5)
b/Å	42.047(3)	15.7660(6)
c/Å	15.3322(9)	24.8093(10)
α/°	90	90
β/°	90	90
γ/°	90	90

Volume/Å^3	10442.3(12)	5009.6(3)
Z	8	4
ρ_{calc}g/cm^3	1.169	1.368
μ/mm^{-1}	3.685	0.572
F(000)	3792.0	2128.0
Crystal size/mm^3	0.15 × 0.12 × 0.1	0.22 × 0.182 × 0.135
Radiation	Cu Kα (λ = 1.54184)	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.848 to 131.968	6.902 to 61.44
Index ranges	-19 ≤ h ≤ 18, -48 ≤ k ≤ 49, -18 ≤ l ≤ 7	-15 ≤ h ≤ 18, -16 ≤ k ≤ 22, -34 ≤ l ≤ 35
Reflections collected	37481	33959
Independent reflections	12010 [R_{int} = 0.1700, R_{sigma} = 0.1565]	13013 [R_{int} = 0.0558, R_{sigma} = 0.0984]
Data/restraints/parameters	12010/59/1137	13013/0/610
Goodness-of-fit on F^2	1.092	0.985
Final R indexes [I>=2σ (I)]	R_1 = 0.1198, wR_2 = 0.3120	R_1 = 0.0530, wR_2 = 0.1053
Final R indexes [all data]	R_1 = 0.1842, wR_2 = 0.3516	R_1 = 0.1051, wR_2 = 0.1201
Largest diff. peak/hole / e Å^{-3}	0.60/-0.73	0.43/-0.51
Flack parameter	0.43(2)	-0.006(11)

General Considerations

All manipulations of air- and/ or moisture-sensitive compounds were performed under an atmosphere of nitrogen using standard Schlenk techniques or using high-purity nitrogen-protected glove box. The ligand synthesis was performed using a high throughput (HT) automated workstation-FLEX MULTIPLANT (Chemspeed technologies, Füllinsdorf, Basel, Switzerland). The FLEX MULTIPLANT contains a reactor module consisting of six 100 mL process developing reactors (PD-reactors) equipped with a condenser which can be operated in parallel. The steps involved in the synthesis including the solvent feeding (via peristaltic pumps), gradient heating, stirring of the reactant mixture, were completely automated and executed using Chemspeed AutoSuite software. FT-IR spectra were recorded using a PerkinElmer System 2000 FT-IR spectrometer. Elemental analyses were performed by a Flash EA 1112 microanalyzer. High temperature ^{1}H NMR and ^{13}C NMR spectra of polyethylene were taken in 1,1,2,2-tetrachloroethane-d_2 (2 mL) at 100 °C with TMS as an internal standard. ^{13}C spectra of polymers obtained by **Fe2**/MMAO and **Fe2**/MAO were recorded on a Bruker DMX 300 spectrometer at 75.47 MHz in 5 mm standard glass tubes at 100 °C with the number of scans between 3000 and 5000. Operating conditions used for ^{13}C spectra: spectral width 18.8324 kHz; acquisition time 0.87 s; relaxation delay 2.0 s. While ^{1}H spectra of these samples as well as polymers obtained by

Fe1 were measured using a Bruker AVANCE III 500WB spectrometer at 499.92 MHz with 32 scans. Operating conditions used for ^{1}H spectra: spectral width 15.0 kHz; acquisition time 2.1845 s; relaxation delay 2.0 s. ^{1}H spectra of polymers obtained by **Fe6**/MMAO and **Fe6**/MAO were recorded on a Bruker DMX 300 spectrometer at 300 MHz. Operating conditions used for ^{1}H spectra: spectral width 14.9701 kHz; acquisition time 2.1889 s; relaxation delay 1.0 s. Moreover, 1D sequence inverse-gated decoupled ^{13}C NMR spectra of the polymers were measured by a Bruker AVANCE III 500WB spectrometer maintained at 100 °C and its operating conditions were set as follows: spectral frequency 125.70 MHz; pulse width 10.0 Ms; spectral width 21.3675 kHz; acquisition time 0.7668 s; relaxation delay 5.0 s; number of scans 2500. High-temperature gel permeation chromatography (GPC) was performed on PL-GPC 220 instrument in 1,2,4-trichlorobenzene at 150 °C. Melting temperatures of preheated samples were determined by differential scanning calorimetry (DSC) with a PerkinElmer TA-Q2000 DSC analyzer. The program was set as follows: a sample (4.0 – 6.0 mg) was heated to 150 °C at a rate of 20 °C min^{-1} and kept for 5 min at 150 °C to remove the thermal history and cooled to −20 °C at a rate of 20 °C min^{-1}. Other reagents were purchased from Aldrich, Acros or local suppliers and used as received. Cocatalysts MAO (1.46 M in toluene) and MMAO (1.93 M in heptane) were purchased from Akzo Nobel corporation. Toluene used as solvent in polymerization was distilled over sodium for 8 hours and distilled under nitrogen atmosphere prior to use.

Typical procedures for ethylene polymerization.

Ethylene polymerization at 1 atm C_2H_4. A 100 mL oven-dried Schlenk flask containing pre-catalyst (1.5 μmol) equipped with a stirrer was placed in a water bath and purged with ethylene (1atm), followed by charging with 30 mL of freshly distilled toluene and the required amount of cocatalyst via syringe. The optimum experimental temperature has already been set based on the results of 10 atm polymerization. After the reaction mixture was stirred under 1 atm of ethylene pressure for 30 min, the pressure was vented and the solution was quenched with 10% hydrochloric acid in ethanol. The polymer was further precipitated by pouring the reaction mixture into large volume of acidified ethanol (10% HCl), filtered, washed with ethanol, and then dried under vacuum at 80 °C to a constant weight.

Ethylene polymerization at 5 or 10 atm C_2H_4. The 5 or 10 atm ethylene polymerization was carried out in a stainless-steel autoclave (250 mL) which was equipped with an ethylene pressure control system, a temperature controller and a mechanical stirrer. The oven-dried stainless-steel autoclave was placed under vacuum and backfilled with nitrogen two times and ethylene one time. After that, the autoclave allowed to cool to the required reaction temperature under ethylene atmosphere, then the toluene solution (25 mL) with dissolved precatalyst (1.5 μmol) was injected into the autoclave. More toluene (25 mL) was then added to completely wash the residual precatalyst into the autoclave. Then the required amount of cocatalyst was introduced by syringe followed by more toluene (50 mL) to complete the addition. Afterwards, the reactor was sealed and pressurized to 5 or 10 atm of ethylene pressure. After the reaction was carried out for 30 min, the pressure was released and 10 mL of methanol was immediately injected to stop the reaction. The reaction mixture was poured into a large amount of acidified ethanol (10% HCl) to precipitate the resulting polymer, filtered, washed with ethanol, and then dried under vacuum at 100 °C to a constant weight.

Computational Part

1. Computational Details

All DFT calculations in this study were performed using the Gaussian 09[1] suite of ab initio programs for the M06 functional[2] with the all-electron 6-31G(d,p) basis set[3,4]. All structures were optimized with solvent effect corrections using the integral equation formalism polarizable continuum model (IEFPCM)[5] with the SMD[6] (Solvation Model Based on Density) atomic radii for isopropanol. Thermal corrections were obtained by frequency calculations using the same method on optimized structures within the harmonic potential approximation under 298.15 K and 1 atm pressure. The energies reported in the text are Gibbs free energies with solvent effect corrections. The spin multiplicities of ground states were verified as doublet by comparing the relative energies of optimized structures at different spin states. The optimized structures were confirmed to have no imaginary vibrational mode for all intermediates and only one imaginary vibrational mode for each transition state (TS). All TSs were also confirmed to connect correct intermediates by intrinsic reaction coordinate (IRC) calculations. The 3D molecular structures shown in this paper were drawn by using the JIMP2 molecular visualizing and manipulating

program.[7]

2. Evaluation of density functionals

In order to evaluate the dependence of density functionals of this catalytic system, we calculated the relative electronic energies between key intermediates and transition states using other widely-used and/or recently developed density functionals, including B3LYP[8,9], B3LYP-D3[10], B3PW91[11,12], B3PW91-D3[11-13], HSE06[14,15], HSE06-D3[13-15], M06-L[16], PBEh1PBE[17], PBEh1PBE-D3[13,17], TPSSh[18,19], TPSSh-D3[13,18,19], ωB97X[20] and ωB97X-D[20] with the same basis sets introduced above. The calculation results are listed in Table S3. We can see that the largest difference of relative electronic energies obtained by different functionals is near 25 kcal/mol, which indicates a strong functional dependency of this iron catalytic system. Some functionals without dispersion corrections, such as B3LYP, B3PW91, HSE06, PBEh1PBE, TPSS and ωB97X, lead to obviously smaller relative electronic energies. The results of M06 are in the middle of those functionals and very close to the results of B3LYP-D3, M06-L, PBEh1PBE-D3 functionals. More importantly, the free energy barrier obtained by the M06 functional matches well with the experimental conditions. Therefore, we believe M06 is a suitable functional for computational study of this system.

Table S3. Absolute and relative electronic energies of ^{D}**3** and ^{D}**TS$_{3,4}$** with different functionals of polymerization.

Functionals	Absolute electronic energies (Hartree)		Relative electronic energies (kcal/mol)
	^{D}**3**	^{D}**TS$_{3,4}$**	^{D}**3** → ^{D}**TS$_{3,4}$**
B3LYP	-3935.73562078	-3935.70234929	20.9
B3LYP-D3	-3935.90310857	-3935.86236798	25.6
B3PW91	-3934.73051519	-3934.67053164	37.6
B3PW91-D3	-3934.91894657	-3934.85063380	42.9
HSE06	-3932.77093386	-3932.70606175	40.7
HSE06-D3	-3932.76937852	-3932.70050967	43.2
M06	-3933.91638258	-3933.86956648	29.4
M06-L	-3935.47764847	-3935.42573318	32.6
PBEh1PBE	-3932.78785343	-3932.75885601	18.2
PBEh1PBE-D3	-3932.80072862	-3932.75329159	29.8
TPSSh	-3935.94609773	-3935.91628147	18.7
TPSSh-D3	-3935.94155728	-3935.91093876	19.3
ωB97X	-3935.08908036	-3935.05277633	22.8
ωB97X-D	-3934.94653646	-3934.90739931	24.6

3. Evaluation of spin states

In order to find out correct spin-states in those reactions, we optimized the structures of quartet states of key intermediates and transition states using the same methods described above. As shown in Table S4, the quartet states are less stable than the corresponding doublet states. Therefore, we believe those polymerization reactions go through low-spin pathways without spin crossover.

Table S4. Absolute and relative free energies of doublet and quartet states of key intermediates and transition states of polymerization catalyzed by iron complex.

Complexes	Absolute free energies (Hartree)		Relative energies (kcal/mol)
	Doublet	**Quartet**	**Doublet → Quartet**
1	-3855.353606	-3855.341654	7.5
$TS_{2,3}$	-3933.843842	-3933.828724	9.5

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5. Atomic coordinates and solvent corrected absolute free energies of all optimized structures

1 Gsolv= -3854.666068

C	-3.14212300	-2.74845000	-0.83172700
C	-4.07741500	-3.79270700	-0.77759000
C	-5.42826400	-3.48691200	-0.94110100
C	-5.86649500	-2.17810100	-1.15369200
C	-4.90808700	-1.15732800	-1.20039000
N	-3.59157500	-1.47615000	-1.04328500
H	-6.16002800	-4.29096800	-0.90297000
H	-3.75754900	-4.81838400	-0.61484700
H	-6.92251800	-1.95437800	-1.28147300
C	-5.07587600	0.25245200	-1.37256900
C	-1.72499000	-2.76302900	-0.65289800
C	-6.42782000	0.87180600	-1.46654100
H	-6.92897100	0.60971400	-2.40971100
H	-7.07677600	0.51548700	-0.65594800
H	-6.37754600	1.96274100	-1.40574600
C	-0.95022600	-3.98800900	-0.32204200
H	-0.32115900	-3.82393000	0.56408000
H	-1.61325000	-4.83154600	-0.10903200
H	-0.28360100	-4.27910800	-1.14508800
N	-3.91029300	0.94240200	-1.40831200
N	-1.15078600	-1.53755800	-0.75908200
C	-3.91063700	2.36036600	-1.47644200
C	-3.65741400	3.07761600	-0.29633500
C	-4.04846500	3.01565300	-2.70888900

C	-3.56889700	4.46728100	-0.36075700
C	-3.95699000	4.40815900	-2.73340300
C	-3.72341400	5.13348700	-1.57120100
H	-3.37176700	5.02693400	0.55297400
H	-4.06035600	4.92411600	-3.68742100
H	-3.65062200	6.21811500	-1.61057100
C	0.22612400	-1.37609000	-0.50472300
C	1.18519200	-1.74534800	-1.43932300
C	0.66563900	-0.70309600	0.65187900
C	2.53788200	-1.48441100	-1.28172200
C	2.02158100	-0.45948800	0.82605200
C	2.97005500	-0.83044300	-0.13270700
H	3.22564700	-1.78908100	-2.06698800
H	2.35466500	0.07908000	1.71394700
C	-3.46158700	2.34027200	0.99180800
H	-4.36370100	1.78896600	1.29269100
C	-4.24470800	2.23057600	-3.96835000
H	-5.20404200	1.69676900	-3.98305400
C	-0.38182200	-0.26021000	1.65820800
H	-1.22325600	0.11006600	1.04719400
C	4.41713800	-0.43112000	0.09888000
H	4.66982600	-0.76779900	1.11795600
C	-0.92369700	-1.44793900	2.42742500
C	-0.06574100	-2.36888300	3.03594300
C	-2.29984500	-1.66787500	2.50308800
C	-0.56368600	-3.48133500	3.70540000
H	1.01190300	-2.21922700	2.97262500
C	-2.81842400	-2.78253600	3.15311900
H	-2.98358900	-0.96353700	2.02686900
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H	0.09158400	-4.20524600	4.18217100
H	-3.88724000	-2.97332300	3.19738900
C	0.06608300	0.91640600	2.50322600
C	0.29326200	0.83644400	3.87561700
C	0.26974100	2.14572000	1.86176900
C	0.71726100	1.94956300	4.59890100
H	0.13087500	-0.10343300	4.39893100
C	0.69333600	3.26401200	2.56409400
H	0.09215400	2.22324700	0.78747500
C	0.91169100	3.14317800	3.92904800
H	0.89507800	1.90021200	5.66974700
H	0.85688200	4.22022200	2.07452400
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C	5.74937000	-0.58056800	-2.06655100

C	5.89462900	-2.38273300	-0.48605800
C	6.60067600	-1.25998700	-2.93111500
H	5.36288800	0.39593200	-2.35453800
C	6.74997300	-3.07638200	-1.33377200
H	5.61257100	-2.82510600	0.46901400
C	7.08818400	-2.49797400	-2.54610700
H	6.89309100	-0.84361800	-3.89120100
H	7.15724400	-4.04869300	-1.07042700
C	4.60044100	1.07973000	0.09785700
C	3.72966200	1.94562300	-0.56584300
C	5.70470000	1.62268400	0.76113400
C	3.94715300	3.32056600	-0.56569600
H	2.86223200	1.54617000	-1.08951900
C	5.93738900	2.99132000	0.77587100
H	6.39619000	0.95578600	1.27594600
C	5.04759700	3.81910500	0.10891000
H	3.27472800	4.00432500	-1.07673600
H	6.78790000	3.42446600	1.29517600
F	0.77505200	-2.35939400	-2.55995800
F	-2.42303800	-4.75117700	4.37010800
F	1.31853600	4.21833800	4.61767000
F	7.91534900	-3.15524700	-3.37031900
F	5.25993400	5.14236100	0.12058400
C	-0.97949500	1.11684900	-1.99069600
H	-1.27984000	2.15938800	-2.16904500
H	-0.78810400	0.66310900	-2.98139100
H	-3.18532700	3.01602500	1.80772300
H	-2.65967300	1.59026300	0.89119400
H	-4.21689600	2.88375800	-4.84670700
H	-3.46060400	1.47001700	-4.08344300
H	-0.00110700	1.11901500	-1.48416700
Fe	-2.32920200	-0.09489700	-1.18096100

2 Gsolv= -3933.124743

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C	3.96890500	2.49875500	-2.78929800
C	5.32316000	2.19285700	-2.89630200
C	5.84693300	1.07827200	-2.23216600
C	4.99751300	0.30175800	-1.45649600
N	3.68018700	0.62213600	-1.34080600
H	5.97192400	2.81366200	-3.50814500
H	3.55522200	3.35133500	-3.32200600
H	6.89856100	0.81920800	-2.32923000
C	5.30183200	-0.92758000	-0.75431300

C	1.72394100	1.76053400	-1.81563700
C	6.66201600	-1.53342400	-0.85391600
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H	7.42449600	-0.83816700	-0.47971200
H	6.73803600	-2.46394300	-0.28640200
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H	1.42470900	3.61201400	-2.85948400
H	0.55780100	2.23102600	-3.54731800
N	4.27347000	-1.44889300	-0.11537700
N	1.24871100	0.84198600	-0.97993700
C	4.41752000	-2.73858100	0.48073300
C	4.87497200	-2.87721300	1.80097700
C	4.05433800	-3.85820700	-0.28547700
C	4.90360700	-4.15719600	2.35839200
C	4.09171500	-5.11716800	0.31338600
C	4.50150400	-5.27028100	1.63149600
H	5.25654600	-4.27240600	3.38258400
H	3.79695600	-5.98617100	-0.27387900
H	4.52187200	-6.25751000	2.08769700
C	-0.15881800	0.66974400	-0.92295500
C	-0.75743900	-0.12515500	-1.89841500
C	-0.97665100	1.17447300	0.10182600
C	-2.09268000	-0.48471000	-1.87760700
C	-2.32891500	0.83644300	0.10698500
C	-2.89791200	-0.00500700	-0.84941600
H	-2.47439500	-1.13837600	-2.65833800
H	-2.96043600	1.20318800	0.91681800
C	5.37653300	-1.70443700	2.59082200
H	6.13436500	-1.13361000	2.03805500
C	3.67869600	-3.71018300	-1.72849800
H	4.57239700	-3.64538100	-2.36620800
C	-0.39667000	2.12129800	1.13877900
H	0.65356000	1.82699700	1.27567000
C	-4.34257700	-0.43329300	-0.66457700
H	-4.91059700	0.48092300	-0.42638100
C	-0.35978800	3.53957500	0.59727200
C	-1.49788200	4.14065000	0.05076400
C	0.82724200	4.27268200	0.63472400
C	-1.45397100	5.43247900	-0.45872400
H	-2.43331200	3.58388400	0.01384300
C	0.89396700	5.56699600	0.12747600
H	1.72069700	3.81928800	1.06364600
C	-0.25193300	6.12236200	-0.41503200

H	-2.33010600	5.90967800	-0.88935300
H	1.81462100	6.14379400	0.14632300
C	-1.05966800	2.00053800	2.50481000
C	-1.41551900	3.11609000	3.26319100
C	-1.27336300	0.73056000	3.05880300
C	-1.97079600	2.98010300	4.53342000
H	-1.25652800	4.11558000	2.86439400
C	-1.82900500	0.57411700	4.32042000
H	-1.01639300	-0.15864100	2.48365400
C	-2.16918500	1.70932400	5.04000600
H	-2.25053000	3.84534400	5.12836700
H	-2.00450400	-0.40925600	4.74823000
C	-4.95940300	-1.00703000	-1.92600000
C	-4.96243400	-2.37743900	-2.19256600
C	-5.49125800	-0.13917600	-2.88309600
C	-5.48588500	-2.87556300	-3.38119500
H	-4.55256500	-3.06955400	-1.45875900
C	-6.02242500	-0.61657700	-4.07478500
H	-5.48707800	0.93334000	-2.69004700
C	-6.00921100	-1.98347800	-4.30170200
H	-5.49679000	-3.93986900	-3.59981100
H	-6.44520900	0.04819100	-4.82317000
C	-4.49932900	-1.35469900	0.53620300
C	-3.45700000	-2.15491300	1.00866500
C	-5.74095000	-1.43057700	1.17336500
C	-3.64163000	-3.00521300	2.09513700
H	-2.48006700	-2.11524400	0.52784600
C	-5.94457800	-2.27074100	2.26010200
H	-6.56467900	-0.81706100	0.80877700
C	-4.88403500	-3.04534100	2.70358600
H	-2.83709200	-3.63076600	2.47235800
H	-6.90314800	-2.33117600	2.76818700
F	0.01104800	-0.58479300	-2.89815800
F	-0.19989900	7.36495900	-0.91365500
F	-2.70843900	1.56892900	6.25908700
F	-6.52183200	-2.45577700	-5.44621600
F	-5.06858200	-3.85571600	3.75494600
C	1.29560400	-1.90568000	0.00545000
H	1.65046400	-2.76685800	0.59042000
H	1.13283200	-2.26749400	-1.02971000
H	5.83535600	-2.04072200	3.52649800
H	4.57891200	-0.99853800	2.85067900
H	3.09404400	-4.56892200	-2.07498800
H	3.09499900	-2.79971200	-1.90477700

H	0.29857000	-1.63692900	0.39005900
Fe	2.58144500	-0.39950400	-0.21887100
C	3.12285300	0.77858700	1.31417100
C	2.24945800	-0.24149500	1.73957600
H	1.21705300	-0.00269100	1.99873700
H	2.62723300	-1.10393200	2.29103900
H	4.19580300	0.72252700	1.50887100
H	2.75956700	1.80163300	1.18402600

3 Gsolv= -3933.174389

C	-2.87309000	-3.04582100	-1.03703300
C	-3.68858100	-4.18431600	-1.14498400
C	-5.05177400	-4.00921200	-1.37564000
C	-5.62045100	-2.73911400	-1.48598200
C	-4.77938800	-1.62352400	-1.36871400
N	-3.44333100	-1.81322000	-1.17726000
H	-5.68959200	-4.88580200	-1.46655200
H	-3.26562800	-5.18096200	-1.05511400
H	-6.68667900	-2.61497600	-1.65584300
C	-5.10586100	-0.23246500	-1.37023200
C	-1.48072600	-2.93693000	-0.75306100
C	-6.51872600	0.23418700	-1.44798200
H	-6.92893400	0.12590700	-2.46271100
H	-7.15862500	-0.36082300	-0.78420200
H	-6.61408900	1.28500800	-1.15907100
C	-0.63449900	-4.10952600	-0.40029700
H	-0.03020600	-3.89717600	0.49228900
H	-1.25126400	-4.98604500	-0.18083700
H	0.06007000	-4.37792300	-1.20731200
N	-4.03066400	0.58270100	-1.24578100
N	-1.01289000	-1.65766200	-0.75170100
C	-4.19144600	1.99038600	-1.16385500
C	-3.94102400	2.60721500	0.07490800
C	-4.47027200	2.75487300	-2.30801400
C	-3.97841800	3.99719800	0.15617100
C	-4.50325200	4.14567000	-2.18451600
C	-4.26055000	4.76730800	-0.96703700
H	-3.77646000	4.47569700	1.11382100
H	-4.71133800	4.74455000	-3.07069200
H	-4.28135000	5.85242600	-0.89447000
C	0.34353800	-1.43103600	-0.43709600
C	1.36027800	-1.80858500	-1.30952900
C	0.71774400	-0.71082100	0.71468900
C	2.69536600	-1.50283400	-1.10405500

C	2.05737000	-0.41139800	0.93275100
C	3.05780900	-0.78488100	0.03145700
H	3.42454300	-1.81374400	-1.84862100
H	2.33199300	0.17568700	1.81029500
C	-3.62315200	1.77076200	1.27567500
H	-4.46969500	1.13192600	1.56453500
C	-4.71420600	2.10870700	-3.63800400
H	-5.74523100	1.74045500	-3.73173800
C	-0.36879400	-0.29312300	1.68374600
H	-1.25303500	-0.10655400	1.05528100
C	4.47763500	-0.31159200	0.29265600
H	4.70001700	-0.56305700	1.34265200
C	-0.75323100	-1.45315300	2.57838100
C	0.20300400	-2.12279700	3.34738300
C	-2.07624200	-1.89508500	2.62381400
C	-0.14764000	-3.20688400	4.14244800
H	1.24097200	-1.79319400	3.31756900
C	-2.44666400	-2.98513200	3.40484300
H	-2.83353700	-1.38600000	2.02598100
C	-1.47072300	-3.62153000	4.15228600
H	0.58437800	-3.73666600	4.74595400
H	-3.47144100	-3.34423200	3.43915100
C	-0.10732700	1.02345400	2.39028800
C	-0.26242000	1.18833900	3.76544600
C	0.19675900	2.15110700	1.61349100
C	-0.11590200	2.43994900	4.36089500
H	-0.51201700	0.33254600	4.38896100
C	0.34610800	3.40436800	2.18795000
H	0.31588600	2.04358900	0.53423400
C	0.18519400	3.52625500	3.56070700
H	-0.23477500	2.57946500	5.43198000
H	0.58465100	4.28119100	1.59189200
C	5.51234200	-1.03235300	-0.55044800
C	5.93295000	-0.53769900	-1.78648100
C	6.02302400	-2.25675100	-0.11276800
C	6.84290500	-1.24059900	-2.56891300
H	5.54742900	0.41557900	-2.14431800
C	6.93628000	-2.97272600	-0.87713400
H	5.69649100	-2.65808700	0.84632900
C	7.33050000	-2.44753200	-2.09731300
H	7.18001900	-0.86512600	-3.53121800
H	7.34552800	-3.92241600	-0.54354100
C	4.59200500	1.20193500	0.18684600
C	3.76339500	1.95895800	-0.64415500

C	5.58359100	1.86077900	0.91806200
C	3.90885500	3.33945700	-0.73962900
H	2.98458400	1.46623600	-1.22612900
C	5.74476400	3.23817900	0.83811500
H	6.24281200	1.28084800	1.56372300
C	4.89823800	3.95538000	0.00764200
H	3.26656900	3.93696000	-1.38196000
H	6.50751700	3.76141700	1.40832400
F	1.02322700	-2.46057800	-2.43375100
F	-1.81327400	-4.67327500	4.90820200
F	0.32545400	4.73359800	4.12524600
F	8.21334200	-3.12766600	-2.84128000
F	5.04180500	5.28526300	-0.07254600
C	-1.29624700	1.24028200	-1.87779900
H	-1.46449600	2.11860700	-1.22536300
H	-1.89002100	1.46811500	-2.78378100
C	0.16953600	1.17737800	-2.27239300
H	0.79423600	0.93952000	-1.39756100
H	0.33700600	0.35144900	-2.98264100
C	0.67015400	2.47977300	-2.88448000
H	1.72063400	2.41767300	-3.20317500
H	0.07532000	2.75995200	-3.76429100
H	0.58402900	3.30599100	-2.16310300
H	-3.35040500	2.38958900	2.13742000
H	-2.78030100	1.09229600	1.07116500
H	-4.55278200	2.82241000	-4.45288900
H	-4.05422700	1.24845200	-3.80172300
Fe	-2.33222200	-0.29140100	-1.10426800

4 Gsolv= -3933.137829

C	3.18708500	1.42544100	-1.93008400
C	3.99593800	2.11956000	-2.84241200
C	5.36003900	1.88676000	-2.86371400
C	5.90683000	0.88520700	-2.03747600
C	5.07778600	0.23366800	-1.14611600
N	3.77081000	0.59264400	-1.00898400
H	5.99551200	2.42026900	-3.56489600
H	3.54703200	2.81435200	-3.54898900
H	6.95247000	0.60278900	-2.12994000
C	5.40014600	-0.96818700	-0.39276200
C	1.76894400	1.34746800	-1.89583700
C	6.77389100	-1.54808500	-0.45595100
H	7.03646900	-1.77918300	-1.49578600
H	7.51907400	-0.83209000	-0.08793600

H	6.85494900	-2.46847100	0.12622500
C	0.92610500	1.96345300	-2.96081600
H	-0.05761600	2.26987300	-2.59573800
H	1.40923100	2.84199200	-3.39900300
H	0.76092900	1.23521400	-3.76896000
N	4.37777700	-1.50975200	0.22192700
N	1.29381500	0.52038100	-0.94862800
C	4.51051900	-2.75874400	0.89400400
C	5.10719700	-2.85187500	2.16298300
C	3.97699400	-3.88921500	0.25129700
C	5.14378300	-4.10357800	2.78195600
C	4.03848500	-5.11781700	0.90620800
C	4.61235800	-5.22898400	2.16684000
H	5.60282100	-4.18531500	3.76645500
H	3.62716400	-5.99683500	0.41163700
H	4.65049500	-6.19380800	2.66761100
C	-0.10283100	0.29182200	-0.92265800
C	-0.60600700	-0.79156500	-1.64048900
C	-1.01980300	1.09740600	-0.21681300
C	-1.94725500	-1.13042400	-1.67188900
C	-2.37541900	0.78376600	-0.29350700
C	-2.85384600	-0.33003700	-0.98465600
H	-2.25716900	-2.00903500	-2.23302900
H	-3.09160900	1.39287100	0.25791900
C	5.69438000	-1.65824800	2.85728000
H	6.39265800	-1.10005700	2.22138200
C	3.36654500	-3.76692000	-1.10914000
H	4.08437500	-3.37796200	-1.84436300
C	-0.52228300	2.28949400	0.59113700
H	0.47419900	1.99637700	0.96119800
C	-4.32571800	-0.67724300	-0.85177600
H	-4.88412300	0.25923000	-1.01423200
C	-0.28521800	3.50014800	-0.29387000
C	-1.32034000	4.05634300	-1.05112600
C	0.97941100	4.08549900	-0.35914800
C	-1.10073800	5.16077600	-1.86489400
H	-2.31481900	3.61349300	-1.00609400
C	1.22271800	5.18981000	-1.17139300
H	1.79528300	3.66147400	0.22630500
C	0.17367500	5.70643800	-1.91233700
H	-1.89493300	5.60285200	-2.46035100
H	2.20548100	5.64940600	-1.23470000
C	-1.37251500	2.62012800	1.81721400
C	-1.54568900	3.94026200	2.24214000

C	-1.93531900	1.60534600	2.60434000
C	-2.26045000	4.24714600	3.39615900
H	-1.11448100	4.75541100	1.66572200
C	-2.65806100	1.89019900	3.75516200
H	-1.82198000	0.56459700	2.30893000
C	-2.80969900	3.21420700	4.13324200
H	-2.39663400	5.27395300	3.72466200
H	-3.10476100	1.10099300	4.35415500
C	-4.80487900	-1.65402100	-1.90856100
C	-4.86160200	-3.02975000	-1.67966400
C	-5.14460500	-1.17341200	-3.17602300
C	-5.25279900	-3.90862900	-2.68486100
H	-4.59981700	-3.42408300	-0.69919900
C	-5.54055700	-2.03359800	-4.19227700
H	-5.09437500	-0.10228900	-3.37054500
C	-5.58760800	-3.39263400	-3.92497400
H	-5.30369400	-4.98121200	-2.51861100
H	-5.81310400	-1.67052800	-5.17950600
C	-4.65735800	-1.12724700	0.56338600
C	-3.71212400	-1.72764300	1.39845200
C	-5.95971900	-0.96110400	1.04166000
C	-4.05013100	-2.14299600	2.68334100
H	-2.68938000	-1.86673100	1.04841600
C	-6.31677200	-1.36705000	2.32105100
H	-6.70870900	-0.50209900	0.39665300
C	-5.34894400	-1.95164300	3.12266200
H	-3.32195700	-2.60828700	3.34248500
H	-7.32422100	-1.23442600	2.70596100
F	0.25707900	-1.54167300	-2.33916900
F	0.39412700	6.76787300	-2.70029300
F	-3.50854600	3.50056600	5.24029400
F	-5.97204100	-4.23167400	-4.89656900
F	-5.68129100	-2.34097600	4.36104500
H	6.24316700	-1.96780200	3.75271000
H	4.92088900	-0.94786100	3.17689600
H	3.00803300	-4.73681900	-1.46893400
H	2.52068300	-3.06486700	-1.09604600
Fe	2.66253100	-0.35059700	0.20498300
C	3.09752500	0.76270000	1.88405600
C	2.35554200	-0.36713100	2.26487200
H	2.90419500	-1.24355300	2.61870000
H	4.18390300	0.80250500	1.97702600
H	2.60849000	1.74093300	1.88331200
H	1.71664000	-1.52706600	0.53421300

C	0.97350300	-0.25153600	2.83405200
H	0.49000000	0.67673600	2.51389300
H	0.32705900	-1.09008600	2.54403000
H	1.00893300	-0.22166200	3.93320600

5 Gsolv= -4011.653591

C	-3.09270500	-1.98393200	-1.94558800
C	-3.92298000	-2.77673300	-2.76468400
C	-5.24650600	-2.43355300	-2.93632400
C	-5.75574400	-1.26666100	-2.32710800
C	-4.91218400	-0.53210600	-1.51727200
N	-3.63977900	-0.91797800	-1.27695700
H	-5.88820800	-3.03725800	-3.57240200
H	-3.51158800	-3.64258600	-3.27811000
H	-6.77590000	-0.94265600	-2.51262100
C	-5.22619000	0.76780600	-0.92005300
C	-1.68722100	-2.05975200	-1.78760900
C	-6.57864800	1.36499800	-1.12369700
H	-6.76460500	1.51831600	-2.19401900
H	-7.35823300	0.68658000	-0.75684000
H	-6.68089000	2.32674800	-0.61649600
C	-0.84880100	-3.04651100	-2.52892500
H	0.01720300	-3.36532300	-1.93792100
H	-1.41773600	-3.94384900	-2.79231800
H	-0.46268200	-2.60812300	-3.46102700
N	-4.23841200	1.34317300	-0.29791100
N	-1.16573900	-1.08018900	-1.01857200
C	-4.38976300	2.66792500	0.20333300
C	-4.92240000	2.89725000	1.48204900
C	-3.93012600	3.72313200	-0.60037300
C	-4.93583000	4.20743700	1.96308300
C	-3.95656900	5.01553700	-0.07617100
C	-4.44328100	5.26008800	1.20162700
H	-5.34147700	4.39464900	2.95650000
H	-3.58730400	5.83713200	-0.68913400
H	-4.45120900	6.27226300	1.59940400
C	0.23484600	-0.91352600	-1.01080700
C	0.81352100	-0.12840400	-2.00707800
C	1.07385000	-1.37710600	0.01806800
C	2.13622200	0.27744300	-1.99081400
C	2.41458600	-0.99990200	0.01813400
C	2.95210200	-0.14760800	-0.94672500
H	2.49562100	0.93993000	-2.77499200
H	3.05231700	-1.31738300	0.84410200

C	-5.47734800	1.78006900	2.31339600
H	-6.25039000	1.21131100	1.77964500
C	-3.45878600	3.47103100	-2.00031900
H	-4.30613700	3.31506300	-2.68391700
C	0.50389800	-2.27165400	1.10386800
H	-0.55675700	-1.99418000	1.19474100
C	4.35107200	0.39497300	-0.72138300
H	4.98288800	-0.46346900	-0.43992900
C	0.51047400	-3.72479200	0.66652400
C	1.66217100	-4.32669300	0.15089800
C	-0.65259600	-4.48984700	0.76696300
C	1.65369900	-5.65076000	-0.27033700
H	2.57862900	-3.74457900	0.06412900
C	-0.68424300	-5.81610700	0.34732300
H	-1.55552000	-4.03510000	1.17412100
C	0.47379000	-6.37163400	-0.16895900
H	2.54015900	-6.12884600	-0.67823800
H	-1.58681400	-6.41754200	0.41281600
C	1.13741600	-2.03147200	2.46686100
C	1.54330000	-3.07307200	3.30072600
C	1.27988400	-0.71672700	2.93353700
C	2.07893300	-2.82176700	4.56200800
H	1.44076900	-4.10392200	2.96866900
C	1.81431600	-0.44578500	4.18487100
H	0.98328700	0.11477800	2.29295400
C	2.20623600	-1.51082100	4.98180000
H	2.39835000	-3.62841000	5.21635800
H	1.93652200	0.57252900	4.54456400
C	4.96757800	0.99506100	-1.96995200
C	4.89069100	2.35971100	-2.25363300
C	5.58191100	0.15292100	-2.90035700
C	5.41749900	2.87792000	-3.43240100
H	4.41414400	3.03121400	-1.54124200
C	6.11709000	0.65065500	-4.08173500
H	5.63917200	-0.91568600	-2.69442100
C	6.02409800	2.01161200	-4.32574100
H	5.36690100	3.93836300	-3.66393500
H	6.60303100	0.00647800	-4.80950200
C	4.37636700	1.34711800	0.46757600
C	3.24044800	2.02943000	0.91035500
C	5.58498900	1.56418400	1.13467500
C	3.30052500	2.89546600	1.99853900
H	2.28385600	1.88076000	0.40812200
C	5.66625400	2.42449200	2.22202600

H	6.48069300	1.04487400	0.79410500
C	4.51492700	3.07497000	2.63792100
H	2.41820400	3.42416800	2.35328500
H	6.59929100	2.59303500	2.75286200
F	0.02528000	0.30292700	-3.00446600
F	0.45531600	-7.64567800	-0.58428300
F	2.72626600	-1.26024800	6.19171600
F	6.54031400	2.50369800	-5.46052500
F	4.58157100	3.90060800	3.69155600
C	-1.15269400	1.56581000	0.20171900
H	-1.23966000	2.08395200	-0.77664000
H	-5.93162200	2.17110100	3.22947000
H	-4.70608100	1.05912600	2.61182700
H	-2.88466500	4.32217900	-2.38178800
H	-2.83193700	2.57375200	-2.07081000
H	-0.13835500	1.13442400	0.20471600
Fe	-2.50656500	0.08773700	-0.08282900
C	-3.24673700	-1.07048800	1.47971500
C	-2.33633600	-0.13983800	1.97772400
H	-1.33356700	-0.43582500	2.28580000
H	-2.68676100	0.76929500	2.46648800
H	-4.32363700	-0.91747600	1.56519200
H	-2.95298400	-2.10955000	1.31628400
C	-1.18974800	2.62207400	1.29747200
H	-2.22051400	2.92151900	1.54038900
H	-0.77597900	2.20241700	2.23023800
C	-0.40629700	3.87546100	0.92700700
H	0.63059900	3.63319300	0.64969200
H	-0.85927100	4.37165600	0.05656200
H	-0.37545700	4.60902800	1.74438100

6 Gsolv= -4011.688819

C	3.23613000	2.62662300	-1.33722700
C	4.16704000	3.66805200	-1.48797300
C	5.51924500	3.34628100	-1.58421800
C	5.96437000	2.02434200	-1.52558800
C	5.00803900	1.01009700	-1.37615800
N	3.68765500	1.33871500	-1.30844900
H	6.24650400	4.14675200	-1.70216100
H	3.84010000	4.70338900	-1.52744000
H	7.02242400	1.78450700	-1.59029400
C	5.19373400	-0.39772100	-1.22465500
C	1.82805700	2.67704000	-1.13300600
C	6.55785700	-0.99308500	-1.14201800

H	7.09957500	-0.89022900	-2.09313300
H	7.16028100	-0.48013700	-0.38032200
H	6.52504900	-2.05565300	-0.88635600
C	1.07478100	3.95266100	-0.99835700
H	0.44904800	3.94589200	-0.09543800
H	1.75625900	4.80508400	-0.92302900
H	0.40824400	4.12610300	-1.85411200
N	4.03825300	-1.09632800	-1.10882500
N	1.24128100	1.45428900	-0.99780600
C	4.08428100	-2.49071500	-0.83836700
C	3.85840500	-2.91900000	0.47991100
C	4.26592500	-3.41328100	-1.87981000
C	3.82046100	-4.28713000	0.74443100
C	4.22369500	-4.77501600	-1.57518000
C	4.00297300	-5.21386400	-0.27572400
H	3.64281100	-4.62302800	1.76544400
H	4.35988200	-5.49713800	-2.37952300
H	3.96759300	-6.27910100	-0.05829600
C	-0.12270800	1.40610000	-0.63930300
C	-1.12304000	1.66292000	-1.56899100
C	-0.52158600	0.99928800	0.64927800
C	-2.47283700	1.51132400	-1.29640500
C	-1.87548700	0.87045700	0.93648200
C	-2.86506700	1.10285200	-0.02509900
H	-3.19027800	1.70545300	-2.08983800
H	-2.17647800	0.53846600	1.93091600
C	3.65634400	-1.91078400	1.56862900
H	4.56165700	-1.31197800	1.74364500
C	4.49799500	-2.94824600	-3.28465700
H	5.48652900	-2.48486000	-3.40637300
C	0.55919900	0.72268400	1.67990000
H	1.36614700	0.22212100	1.11953300
C	-4.31838700	0.87218300	0.35552600
H	-4.50134300	1.48375400	1.25502000
C	1.14978000	2.02318200	2.18699900
C	0.33104500	3.04755400	2.67235500
C	2.52729500	2.23997200	2.13398900
C	0.86860800	4.25678800	3.09839100
H	-0.74811000	2.89943700	2.70524900
C	3.08476500	3.44766000	2.54085100
H	3.18046300	1.45565700	1.74849000
C	2.24074200	4.43623100	3.01790600
H	0.24386600	5.06089100	3.47767900
H	4.15419900	3.63205100	2.48466200

C	0.12945700	-0.26099600	2.75142600
C	0.01884800	0.06811900	4.10090300
C	-0.16265800	-1.57453200	2.35899100
C	-0.37755300	-0.88033400	5.04191300
H	0.25262600	1.07685800	4.43433600
C	-0.55923100	-2.53233300	3.28020000
H	-0.07855000	-1.84738900	1.30516800
C	-0.66126900	-2.16376100	4.61393800
H	-0.46531300	-0.63486200	6.09682100
H	-0.78712200	-3.55292500	2.98507700
C	-5.28917500	1.36354400	-0.70064100
C	-5.68639900	0.54765300	-1.76280100
C	-5.75618200	2.67824800	-0.65643000
C	-6.52976100	1.02722300	-2.75812100
H	-5.33234200	-0.48156800	-1.81050400
C	-6.60422200	3.17611400	-1.63943500
H	-5.44692000	3.32674100	0.16283500
C	-6.97556200	2.33658100	-2.67631500
H	-6.84746200	0.40374100	-3.58939000
H	-6.97934000	4.19552000	-1.61297700
C	-4.61081600	-0.56734400	0.75901600
C	-3.78350200	-1.64045400	0.42616100
C	-5.79008800	-0.83121600	1.46326700
C	-4.11786000	-2.94456800	0.78317500
H	-2.85287200	-1.46321300	-0.11146700
C	-6.13988200	-2.12267900	1.83171400
H	-6.44972900	-0.00330000	1.72302800
C	-5.29196700	-3.16244400	1.48105800
H	-3.47754800	-3.78676800	0.53275000
H	-7.05130400	-2.33588400	2.38360200
F	-0.75922100	2.03398000	-2.80656100
F	2.76492600	5.60534200	3.41004400
F	-1.04159700	-3.08217000	5.51252700
F	-7.79450600	2.80386400	-3.62838100
F	-5.61929100	-4.41309500	1.83343500
C	1.21002200	-1.62126300	-1.48024900
H	1.24569800	-2.25259700	-0.57087700
H	1.76908600	-2.21374000	-2.22862800
C	-0.22506000	-1.49049400	-1.95988900
H	-0.84177100	-0.97135800	-1.21039600
H	-0.26661300	-0.85278600	-2.86074000
C	-0.90234300	-2.81924800	-2.27942800
H	-0.25403700	-3.42014800	-2.93901900
H	-1.00272000	-3.40748900	-1.34900900

H	3.37588100	-2.38745800	2.51359100
H	2.86104300	-1.19753000	1.30387400
H	4.44041500	-3.78495300	-3.98858000
H	3.76038500	-2.19486300	-3.58926300
Fe	2.42113400	-0.05952900	-1.16627900
C	-2.26701500	-2.65158800	-2.93362000
H	-2.89516900	-1.99708900	-2.30632300
H	-2.14041100	-2.11246600	-3.88516300
C	-2.97881200	-3.97027600	-3.17856200
H	-3.16105700	-4.50597100	-2.23732400
H	-3.94884000	-3.83090300	-3.66993400
H	-2.37677100	-4.63166400	-3.81566900

7 Gsolv= -4011.639443

C	3.18528600	1.70891200	-1.84286800
C	3.98188000	2.57898700	-2.58646700
C	5.36750700	2.44591700	-2.52721200
C	5.94602000	1.41614400	-1.77583200
C	5.11617400	0.57094100	-1.05237100
N	3.76814900	0.76370800	-1.05230400
H	6.00059600	3.12291100	-3.09446200
H	3.52893700	3.34701700	-3.20895400
H	7.02335000	1.26890400	-1.77462700
C	5.46529500	-0.64871300	-0.35515800
C	1.75229800	1.58139400	-1.82631400
C	6.86503200	-1.16371900	-0.39068000
H	7.17876900	-1.35144400	-1.42638600
H	7.56365700	-0.42699500	0.02599700
H	6.97377000	-2.09558400	0.16898400
C	0.91477600	2.23698900	-2.87070800
H	-0.08537600	2.49437400	-2.51219100
H	1.38540400	3.15038000	-3.24623000
H	0.79232000	1.55505300	-3.72549500
N	4.42719900	-1.27507400	0.16741800
N	1.29889300	0.69606800	-0.93553600
C	4.60216300	-2.58755200	0.70243400
C	5.06590900	-2.78936000	2.01213400
C	4.25469800	-3.66926000	-0.12465900
C	5.14997200	-4.10117700	2.48586700
C	4.35242600	-4.96100300	0.38999600
C	4.79132900	-5.18080200	1.69022000
H	5.50804700	-4.26653400	3.50135800
H	4.08007900	-5.80188900	-0.24666400
H	4.86089000	-6.19374300	2.08044800

C	-0.09891700	0.44129500	-0.95521300
C	-0.56409900	-0.60092000	-1.75403300
C	-1.04576500	1.17905800	-0.21569700
C	-1.89675900	-0.96920000	-1.83094900
C	-2.39137700	0.84070400	-0.34020900
C	-2.83344600	-0.23462200	-1.11212900
H	-2.17569000	-1.81292900	-2.45798300
H	-3.13191400	1.40090000	0.23028800
C	5.47619100	-1.64761800	2.89479600
H	6.17038400	-0.95982000	2.39587000
C	3.80218100	-3.42762000	-1.53096400
H	4.59828900	-2.98077900	-2.14320700
C	-0.59739200	2.33051000	0.67582400
H	0.39669500	2.04341200	1.05238900
C	-4.30902000	-0.59530900	-1.05277600
H	-4.86350700	0.34070000	-1.22960800
C	-0.37037600	3.59733000	-0.12980000
C	-1.40179000	4.18079700	-0.87121300
C	0.88629500	4.20362700	-0.14025700
C	-1.18610600	5.33320700	-1.61687200
H	-2.39008400	3.72212000	-0.86772100
C	1.12533800	5.35614300	-0.88396300
H	1.69859300	3.75987900	0.43566900
C	0.08036600	5.89897800	-1.61195100
H	-1.97751000	5.79740100	-2.19904300
H	2.10186000	5.83275200	-0.90401400
C	-1.47875200	2.56037400	1.90338700
C	-1.67283800	3.84544400	2.41714800
C	-2.04597700	1.48746300	2.60613100
C	-2.40955500	4.06406800	3.57740700
H	-1.23960500	4.70287300	1.90728100
C	-2.79017900	1.68454400	3.76174400
H	-1.92480700	0.46989600	2.23956500
C	-2.96034800	2.97683300	4.23047000
H	-2.56075400	5.06398900	3.97503500
H	-3.23794300	0.85124200	4.29693600
C	-4.73195100	-1.55729400	-2.14723200
C	-4.82885600	-2.93402200	-1.94138000
C	-4.97907800	-1.05568600	-3.42850000
C	-5.16806300	-3.79339700	-2.98209900
H	-4.64436300	-3.34725800	-0.95160400
C	-5.32082800	-1.89580800	-4.48018400
H	-4.89715800	0.01671400	-3.60478300
C	-5.40940900	-3.25717900	-4.23474000

H	-5.25023800	-4.86656400	-2.83300900
H	-5.52026500	-1.51587700	-5.47847000
C	-4.69635600	-1.05936100	0.34155700
C	-3.83390300	-1.82788200	1.12854100
C	-5.95286700	-0.73222900	0.85479100
C	-4.21153400	-2.26157300	2.39491900
H	-2.84393600	-2.08660000	0.75210700
C	-6.34736900	-1.15057300	2.12048400
H	-6.63598000	-0.13493000	0.25165900
C	-5.46521500	-1.91146000	2.86970500
H	-3.54963800	-2.86217200	3.01411500
H	-7.31923300	-0.89389400	2.53305200
F	0.32618700	-1.27911500	-2.49222700
F	0.29698400	7.00653200	-2.33457700
F	-3.67966100	3.17812000	5.34309800
F	-5.74209100	-4.07692100	-5.24106900
F	-5.83359700	-2.31769100	4.09205800
H	5.97103800	-2.01935500	3.79815000
H	4.61463600	-1.04739600	3.21378100
H	3.49052800	-4.35941500	-2.01363100
H	2.95666600	-2.72465100	-1.54951100
Fe	2.69545500	-0.37258400	-0.03644600
C	2.86609600	0.55949100	1.69872500
C	2.17083500	-0.66555000	1.88629800
H	2.74283500	-1.50665900	2.28920100
H	3.91377800	0.66780300	1.99009600
H	2.30198700	1.49516800	1.77069900
H	1.81701000	-1.60193400	0.21687600
C	0.74356800	-0.65627300	2.36436900
H	0.24417100	0.24106500	1.98169300
H	0.76386300	-0.53363800	3.46277200
C	-0.10192800	-1.87895900	2.03553700
H	-1.10160800	-1.73510100	2.47765900
H	-0.24776600	-1.93504400	0.94456600
C	0.49163000	-3.18326400	2.54053800
H	-0.19359900	-4.02574200	2.38705000
H	1.42724800	-3.42540800	2.02043900
H	0.71441500	-3.12780500	3.61530000

8 Gsolv= -4090.148986

C	3.10681700	2.25856400	-1.84749700
C	3.94067900	3.15143100	-2.52003700
C	5.29419900	2.85444900	-2.64961100
C	5.80133800	1.66389200	-2.11781500

C	4.93671500	0.80202200	-1.45893700
N	3.61599700	1.10431500	-1.32609600
H	5.95456100	3.54238400	-3.17029600
H	3.53695900	4.06769800	-2.94337800
H	6.85421900	1.41383800	-2.22429800
C	5.23722800	-0.50109200	-0.90891200
C	1.68506500	2.33694800	-1.65816000
C	6.59934900	-1.08881200	-1.07626000
H	6.85368200	-1.18045300	-2.14023300
H	7.35846500	-0.43908100	-0.62224600
H	6.67847300	-2.07844800	-0.62050700
C	0.86517600	3.38786900	-2.32640400
H	-0.04285000	3.61528200	-1.75859800
H	1.42944600	4.31834900	-2.44491800
H	0.55641100	3.05704100	-3.32829400
N	4.20769400	-1.09933100	-0.34277800
N	1.18272500	1.33621100	-0.94282200
C	4.36135300	-2.45896500	0.06415400
C	4.79938300	-2.77549500	1.36030900
C	4.02523600	-3.46354700	-0.85775400
C	4.81973800	-4.11824400	1.74067400
C	4.05005500	-4.79227000	-0.43257700
C	4.43013500	-5.12244500	0.86222900
H	5.15261100	-4.37157100	2.74652900
H	3.76796700	-5.57408900	-1.13739400
H	4.43967200	-6.16216900	1.18182400
C	-0.22907600	1.19896200	-0.91789200
C	-0.83157700	0.52935000	-1.98133500
C	-1.04222300	1.57153000	0.16510400
C	-2.15773000	0.13753800	-1.98465100
C	-2.38794000	1.20995300	0.14625400
C	-2.94948000	0.46000600	-0.88720800
H	-2.53557100	-0.44189200	-2.82383800
H	-3.01165100	1.45828900	1.00533500
C	5.28027200	-1.71533800	2.30564000
H	6.07170200	-1.09984700	1.85730500
C	3.68936200	-3.12833000	-2.28019400
H	4.60062200	-3.03371300	-2.88864600
C	-0.45753800	2.38087100	1.30999700
H	0.58878100	2.05978200	1.41327200
C	-4.34043600	-0.11046500	-0.68521500
H	-4.95833300	0.69791500	-0.26137500
C	-0.40100600	3.85399700	0.94802700
C	-1.51400200	4.52309200	0.43000100

C	0.78194700	4.57157400	1.13129600
C	-1.44805900	5.86848800	0.08763500
H	-2.44544200	3.97837900	0.28059600
C	0.87045800	5.91830600	0.79253400
H	1.65386300	4.06481500	1.54442900
C	-0.25019200	6.54191000	0.27139300
H	-2.30398100	6.39945100	-0.32016100
H	1.78848000	6.48423600	0.92536500
C	-1.13170700	2.09968900	2.64625600
C	-1.54656200	3.11592600	3.50659100
C	-1.31114200	0.77144400	3.05812900
C	-2.12653800	2.82695300	4.73999600
H	-1.41594300	4.15679400	3.21878500
C	-1.89099500	0.46284600	4.27971400
H	-1.00872100	-0.04180000	2.39790000
C	-2.29038000	1.50377100	5.10450000
H	-2.45244800	3.61415500	5.41445800
H	-2.04113000	-0.56597700	4.59583900
C	-5.00732400	-0.53473100	-1.97953900
C	-4.95572100	-1.84911500	-2.44694900
C	-5.64815200	0.42828800	-2.76346400
C	-5.53165900	-2.20064000	-3.66370800
H	-4.46086000	-2.61408500	-1.85084900
C	-6.23270500	0.09727800	-3.97935800
H	-5.68806800	1.45930500	-2.41273600
C	-6.16265500	-1.21873100	-4.40804900
H	-5.50067400	-3.22041600	-4.03750400
H	-6.73963900	0.83622800	-4.59393200
C	-4.31355000	-1.21926800	0.35963500
C	-3.16115300	-1.95732800	0.64096500
C	-5.48747000	-1.52962100	1.05133200
C	-3.17035500	-2.97090000	1.59475300
H	-2.22981900	-1.73783500	0.11807600
C	-5.51772200	-2.53704100	2.00716700
H	-6.39635100	-0.96802100	0.83591900
C	-4.35142900	-3.24104400	2.26433800
H	-2.27296800	-3.54437800	1.82204300
H	-6.42299700	-2.78004700	2.55688600
F	-0.06165900	0.18994500	-3.02713900
F	-0.17632500	7.83651200	-0.06628200
F	-2.85416900	1.21681600	6.28622500
F	-6.72625400	-1.55040900	-5.57774600
F	-4.36977500	-4.20897000	3.19069200
C	1.16286900	-1.51744900	-0.24427700

H	1.37348100	-1.90142700	-1.26873900
H	5.68909700	-2.16749600	3.21519000
H	4.48271300	-1.02690100	2.60855900
H	3.07641900	-3.91266900	-2.73787600
H	3.15202500	-2.17712900	-2.36497900
H	0.14510900	-1.09827800	-0.29505300
Fe	2.50395300	-0.02887000	-0.31199700
C	3.05084100	0.99882000	1.31454800
C	2.16544700	-0.04565400	1.64848400
H	1.13422200	0.17443600	1.92933500
H	2.53996500	-0.94886900	2.13151300
H	4.12168300	0.90773400	1.51023800
H	2.70442100	2.03501400	1.27466200
C	1.08908100	-2.69653900	0.71297200
H	2.08778600	-3.05905900	0.99993300
H	0.61225600	-2.36936200	1.65567100
C	0.29937400	-3.88125500	0.16800300
H	-0.71478500	-3.55241900	-0.12397000
H	0.77263600	-4.23271200	-0.76560100
C	0.19678800	-5.04504100	1.14256000
H	-0.25242700	-4.69266500	2.08615000
H	1.21338500	-5.37754900	1.40663400
C	-0.60712200	-6.20989100	0.59177900
H	-1.63425700	-5.90402000	0.34975200
H	-0.15830100	-6.59557300	-0.33330900
H	-0.66979500	-7.04306400	1.30161500

9 Gsolv= -4090.203188

C	-3.66299800	-1.96775500	-1.94270000
C	-4.71714500	-2.79459100	-2.36492600
C	-5.99735000	-2.25222200	-2.45305700
C	-6.25230500	-0.91910500	-2.12580300
C	-5.17712300	-0.12244800	-1.70924100
N	-3.92695000	-0.66099900	-1.64862500
H	-6.81914400	-2.88526400	-2.78075800
H	-4.53818500	-3.83574800	-2.61874500
H	-7.25623900	-0.50778100	-2.18945600
C	-5.17264400	1.23542000	-1.26642900
C	-2.29514100	-2.27813300	-1.69696800
C	-6.43999700	2.00825900	-1.13062700
H	-6.90648500	2.19075100	-2.10927200
H	-7.17301700	1.45032100	-0.53267300
H	-6.27858600	2.97619800	-0.64850600
C	-1.74264400	-3.65460500	-1.81068500

H	-1.18428400	-3.92870500	-0.90515900
H	-2.54177700	-4.39016300	-1.94166800
H	-1.05200500	-3.74863300	-2.65938800
N	-3.94345500	1.70492500	-0.94253100
N	-1.55198700	-1.21681900	-1.27784400
C	-3.81326800	3.00798600	-0.38988100
C	-3.63481400	3.12285600	0.99816500
C	-3.77868800	4.13785700	-1.22114700
C	-3.42322500	4.38622300	1.54736700
C	-3.56743500	5.38689700	-0.63395700
C	-3.39051200	5.51597900	0.73782500
H	-3.28129700	4.47754400	2.62362400
H	-3.53516400	6.26838900	-1.27342200
H	-3.22131600	6.49706700	1.17611300
C	-0.22193100	-1.45097300	-0.86892000
C	0.79732800	-1.64356200	-1.79275000
C	0.13886400	-1.38361800	0.49109500
C	2.13511900	-1.72340400	-1.44209300
C	1.47662700	-1.49209700	0.85208500
C	2.49362700	-1.63178000	-0.09996200
H	2.87308500	-1.83317200	-2.23273600
H	1.74679500	-1.41566400	1.90576800
C	-3.66301400	1.89596200	1.85550600
H	-4.65405900	1.42006700	1.85607800
C	-3.96299700	4.00810800	-2.70208600
H	-5.00043000	3.76237100	-2.96705800
C	-0.96889900	-1.17599300	1.50759800
H	-1.65697400	-0.46125300	1.02511000
C	3.94110200	-1.65785200	0.36615600
H	4.03750300	-2.52632200	1.03939900
C	-1.76636100	-2.45051400	1.69931400
C	-1.13297300	-3.67120500	1.95114800
C	-3.15717800	-2.43320400	1.58381600
C	-1.86421800	-4.84619100	2.08605900
H	-0.04643200	-3.70440300	2.02906000
C	-3.90654600	-3.59909400	1.69896900
H	-3.66812200	-1.49095600	1.38046800
C	-3.24222800	-4.78801700	1.94945700
H	-1.38437000	-5.80147000	2.28097200
H	-4.98752100	-3.59766600	1.58853400
C	-0.49871000	-0.50362400	2.78249100
C	-0.48679100	-1.13268000	4.02586900
C	-0.05863600	0.82459100	2.70166500
C	-0.04738400	-0.46257000	5.16586800

H	-0.83479600	-2.15936700	4.11739200
C	0.37962200	1.50919400	3.82553100
H	-0.06397200	1.33051200	1.73367300
C	0.37853700	0.84711700	5.04473400
H	-0.03599300	-0.94225400	6.14080800
H	0.71740400	2.54073100	3.77422100
C	4.92265500	-1.88051500	-0.76838100
C	5.34119700	-0.81955300	-1.57651500
C	5.38704800	-3.16361000	-1.05720400
C	6.20112700	-1.02779500	-2.64687400
H	4.98604600	0.18869700	-1.36283100
C	6.25333100	-3.39369900	-2.12162700
H	5.06378500	-4.00088700	-0.43944700
C	6.64438100	-2.31703600	-2.89904100
H	6.53329700	-0.21023900	-3.28144200
H	6.62712600	-4.38718600	-2.35378500
C	4.33848100	-0.43620700	1.18763700
C	3.63380700	0.76790200	1.16712400
C	5.50527600	-0.50773700	1.95570600
C	4.07761000	1.87625600	1.88438300
H	2.71277200	0.84899600	0.59251600
C	5.96207000	0.58278100	2.68267200
H	6.07177000	-1.43880100	1.97571300
C	5.23676900	1.76374100	2.63034600
H	3.52944100	2.81538800	1.87583600
H	6.86519500	0.53396400	3.28487300
F	0.47383200	-1.69761400	-3.09439600
F	-3.95227100	-5.91898300	2.05861800
F	0.79786800	1.50034300	6.13687000
F	7.47981300	-2.52657100	-3.92542100
F	5.67012700	2.82224800	3.32820400
C	-1.05679900	1.85575200	-1.08815700
H	-1.09861000	2.32124700	-0.08364500
H	-1.45938200	2.64251900	-1.75390400
C	0.38972400	1.60162300	-1.47244300
H	0.84099000	0.84909400	-0.80882500
H	0.44248200	1.16319200	-2.48465700
C	1.28280400	2.83750300	-1.43142200
H	0.83114000	3.65123400	-2.02282400
H	1.32562000	3.21365300	-0.39276000
H	-3.39156500	2.12012400	2.89219200
H	-2.95776400	1.14104300	1.47684200
H	-3.70912600	4.94345400	-3.21173000
H	-3.33609100	3.21052000	-3.12040600

Fe	-2.49329700	0.46274900	-1.14147800
C	2.69389500	2.56087500	-1.93052700
H	3.10581600	1.69360200	-1.38632300
H	2.65330300	2.24940900	-2.98748800
C	3.64747800	3.73492400	-1.78234900
H	3.63828500	4.08643100	-0.73653400
H	3.28555500	4.58487900	-2.38456900
C	5.07785000	3.40113600	-2.17920600
H	5.45134900	2.59657600	-1.52455300
H	5.08509500	2.98865700	-3.20068700
C	6.00750800	4.59881000	-2.09585500
H	7.03668900	4.34191600	-2.37177600
H	5.67614900	5.40417600	-2.76444200
H	6.03085200	5.00896100	-1.07770600

10 Gsolv= -3815.398739

C	-2.95502600	-2.80213900	-1.09736400
C	-3.79470500	-3.91976000	-1.18446700
C	-5.15464100	-3.71741200	-1.41745500
C	-5.69234400	-2.43488400	-1.55668700
C	-4.82852200	-1.34013800	-1.46280500
N	-3.49879700	-1.55851000	-1.25250800
H	-5.81370600	-4.57960700	-1.48915500
H	-3.39299100	-4.92376400	-1.07724500
H	-6.75535900	-2.28944600	-1.73102000
C	-5.11099000	0.06322300	-1.52550400
C	-1.55300100	-2.71639000	-0.83365700
C	-6.50297100	0.57373700	-1.67029500
H	-6.93646600	0.28650300	-2.63865800
H	-7.15577500	0.15126000	-0.89483100
H	-6.54549300	1.66346200	-1.59132200
C	-0.70926600	-3.90940200	-0.55747200
H	0.04782200	-3.68624700	0.20408600
H	-1.31807800	-4.74144500	-0.18883400
H	-0.17688800	-4.25033100	-1.45597100
N	-4.01391200	0.84141400	-1.40280800
N	-1.08290600	-1.44471300	-0.81383700
C	-4.13677400	2.25726900	-1.34900300
C	-4.09371200	2.87546500	-0.09035700
C	-4.21544400	3.00885600	-2.52933100
C	-4.15912000	4.26612800	-0.02575700
C	-4.28423400	4.39866800	-2.42471600
C	-4.26174400	5.02682500	-1.18507400
H	-4.12347500	4.75227000	0.94848200

H	-4.34563700	4.99168600	-3.33662400
H	-4.31210600	6.11166300	-1.12301000
C	0.28051200	-1.19960300	-0.54836200
C	1.26740000	-1.53804400	-1.46776000
C	0.68009200	-0.53113900	0.62501400
C	2.60665100	-1.23706800	-1.28545300
C	2.02384400	-0.22969700	0.81432700
C	2.99783700	-0.56687100	-0.13039600
H	3.31874800	-1.52255100	-2.05642200
H	2.32536400	0.31038200	1.71281400
C	-3.94965100	2.03659100	1.14058600
H	-4.83491600	1.40992300	1.32056600
C	-4.19132800	2.32835400	-3.86236000
H	-5.06436700	1.68039200	-4.01569800
C	-0.39069200	-0.19139400	1.64475400
H	-1.24512300	0.16149100	1.04515900
C	4.42586800	-0.10580500	0.09506500
H	4.62913500	-0.24082400	1.17010300
C	-0.87047000	-1.43843600	2.35992900
C	0.02749600	-2.38049700	2.86917400
C	-2.23855200	-1.68500700	2.48948000
C	-0.42258000	-3.54063200	3.49059500
H	1.09868200	-2.21090800	2.76217900
C	-2.71028200	-2.84454100	3.09388300
H	-2.95312400	-0.96132700	2.09423100
C	-1.78814300	-3.75385500	3.58566400
H	0.26514500	-4.28148400	3.88933000
H	-3.77280900	-3.05289000	3.18446600
C	-0.01866200	0.96862500	2.54577700
C	0.33423700	0.81996600	3.88583000
C	-0.01520700	2.25346500	1.98811200
C	0.68656300	1.92346000	4.66001400
H	0.32628500	-0.16755000	4.34315000
C	0.33210900	3.36387300	2.74376900
H	-0.29093500	2.37732200	0.93946100
C	0.67987900	3.17592700	4.07329500
H	0.96022400	1.82319100	5.70686700
H	0.33625300	4.36554800	2.32273900
C	5.44155800	-0.95793700	-0.64351300
C	5.92620000	-0.60869500	-1.90551500
C	5.86892500	-2.15958800	-0.07328000
C	6.81757700	-1.43284500	-2.58494100
H	5.60530000	0.32470700	-2.36543600
C	6.76238400	-2.99432400	-0.73284900

H	5.49214100	-2.44669900	0.90815600
C	7.22173600	-2.61233700	-1.98317000
H	7.20380400	-1.17187300	-3.56646600
H	7.10781100	-3.92726400	-0.29583800
C	4.59863700	1.38014900	-0.18609500
C	3.70307300	2.11266300	-0.96600300
C	5.72106100	2.03338300	0.33330700
C	3.91584800	3.46470300	-1.22281600
H	2.81762100	1.63037300	-1.37630600
C	5.94938900	3.38056200	0.09057900
H	6.43156400	1.46979600	0.93789300
C	5.03606200	4.07481100	-0.68854300
H	3.22292100	4.04560000	-1.82535100
H	6.81504300	3.89892800	0.49389400
F	0.89822300	-2.17039100	-2.59256900
F	-2.23042400	-4.87703600	4.16744300
F	1.01452500	4.24270800	4.81308000
F	8.08651800	-3.40814400	-2.62724900
F	5.24633900	5.37696600	-0.92722100
H	-3.77768100	2.64970900	2.03107400
H	-3.09678200	1.34739300	1.03114000
H	-4.17226700	3.05894600	-4.67760100
H	-3.30421300	1.68738200	-3.95887700
Fe	-2.37459000	-0.07336000	-1.13095500
H	-1.38493400	1.18980500	-1.22249500

C2H4 Gsolv= -78.487958

C	0.00000000	0.66346200	0.00001200
C	0.00000000	-0.66346200	0.00001200
H	0.00000000	1.23772300	0.92485100
H	0.00000000	-1.23772300	0.92485100
H	0.00000000	1.23804700	-0.92492100
H	0.00000000	-1.23804700	-0.92492100

CH2=CHCH2CH3 Gsolv= -157.008870

C	-1.84951400	0.01578000	-0.27374800
C	-0.71085600	-0.29571700	0.33913100
H	-2.72655100	-0.62592500	-0.22290400
H	-0.64848200	-1.22993000	0.90514600
H	-1.94903700	0.93460700	-0.85239200
C	0.53795000	0.52539000	0.30179300
H	0.35604700	1.44373800	-0.27370000
H	0.79793200	0.84344000	1.32299600
C	1.71071600	-0.24707200	-0.29111700

H	2.62860700	0.35137400	-0.29085300
H	1.91064400	-1.16224400	0.28058400
H	1.50106600	-0.54534800	-1.32523000

CH2=CHCH3 Gsolv= -117.752485

C	1.27535500	-0.22019000	0.00000100
C	0.13045600	0.45728500	-0.00000200
H	2.24077500	0.28105500	0.00000300
H	0.16296400	1.54918700	-0.00000300
H	1.28968900	-1.31044700	-0.00000400
C	-1.22504000	-0.16289100	-0.00000000
H	-1.80625300	0.14618000	-0.87885400
H	-1.16557600	-1.25733800	-0.00002600
H	-1.80622400	0.14614000	0.87889100

CH3CH2CH2CH2CH2CH2CH3 Gsolv= -275.994044

C	-2.54282500	0.49467400	0.00007400
H	-2.53945400	1.15894100	-0.87789600
H	-2.53943700	1.15873700	0.87819800
C	-1.27081400	-0.33968900	-0.00003400
H	-1.27177400	-1.00610600	0.87859800
H	-1.27184600	-1.00598500	-0.87875800
C	-3.80166600	-0.35472100	-0.00001300
H	-4.71112500	0.25690800	0.00009500
H	-3.84004900	-1.00473900	-0.88398700
H	-3.84000600	-1.00498700	0.88378100
C	-0.00003800	0.49491900	-0.00003200
H	-0.00003800	1.16096100	0.87878300
H	-0.00001400	1.16092500	-0.87887500
C	1.27080300	-0.33970000	0.00000200
H	1.27175800	-1.00615400	-0.87863900
H	1.27176300	-1.00606300	0.87871000
C	2.54279300	0.49461200	-0.00004400
H	2.53938400	1.15890000	0.87794500
H	2.53941000	1.15876300	-0.87813600
C	3.80173500	-0.35467500	0.00004400
H	3.84018100	-1.00489600	-0.88379700
H	4.71115700	0.25703100	0.00000900
H	3.84015400	-1.00475700	0.88398700

CH3CH2CH2CH2CH3 Gsolv= -197.479521

C	-1.27213700	0.52416900	0.00003500
H	-1.26882800	1.18839500	-0.87798700
H	-1.26883200	1.18830300	0.87812600

C	0.00004900	-0.30991100	-0.00000100
H	0.00002300	-0.97667700	0.87856700
H	-0.00003300	-0.97667300	-0.87857400
C	-2.53102100	-0.32518100	-0.00001400
H	-3.44061300	0.28629000	0.00004900
H	-2.56934700	-0.97527300	-0.88392200
H	-2.56932100	-0.97541300	0.88379300
C	1.27196200	0.52406200	-0.00003500
H	1.26849600	1.18839600	0.87793900
H	1.26850900	1.18826400	-0.87810500
C	2.53114200	-0.32507500	0.00001700
H	2.56962800	-0.97547000	-0.88393900
H	3.44070600	0.28678400	-0.00004800
H	2.56964400	-0.97531100	0.88408900

CH3CH2CH2CH3 Gsolv= -158.222358

C	-0.56009900	-0.51488800	-0.00001400
H	-0.44793600	-1.16977600	0.87795100
H	-0.44799400	-1.16971600	-0.87802800
C	0.56017400	0.51487000	-0.00002400
H	0.44773800	1.16984700	-0.87792300
H	0.44769500	1.16992400	0.87781400
C	-1.94066200	0.11789700	0.00002500
H	-2.73858900	-0.63372200	-0.00015000
H	-2.08478600	0.75313500	0.88413700
H	-2.08471000	0.75346200	-0.88386600
C	1.94073000	-0.11793200	0.00001100
H	2.08450800	-0.75343200	-0.88393200
H	2.73862800	0.63369700	-0.00017100
H	2.08459200	-0.75310000	0.88417600

CH3CH2CH3 Gsolv= -118.965062

C	-0.00012200	0.58965100	0.00000100
H	0.00018700	1.25184300	0.87735600
H	0.00018900	1.25174800	-0.87742300
C	-1.26019800	-0.258981	0.00000200
H	-2.17000000	0.35239800	-0.00004500
H	-1.29775600	-0.90962600	-0.88370500
H	-1.29778600	-0.90954300	0.88376700
C	1.26027000	-0.25904900	0.00000100
H	2.16987600	0.35282100	-0.00016700
H	1.29786500	-0.90954700	0.88397900
H	1.29772000	-0.90981200	-0.88378600

HCl Gsolv= -460.776010

Cl	0.00000000	0.00000000	0.07148600
H	0.00000000	0.00000000	-1.21526600

TS2,3 Gsolv= -3933.103653

C	3.28212100	1.50839600	-2.02877000
C	4.14968000	2.22696900	-2.84868800
C	5.49536300	1.86801600	-2.89642300
C	5.96293500	0.78544500	-2.14576800
C	5.07237700	0.08764500	-1.33907500
N	3.75942800	0.46443200	-1.28153400
H	6.18146000	2.42289700	-3.53059800
H	3.78078900	3.05471000	-3.44934200
H	7.00915800	0.49364600	-2.19494300
C	5.29409600	-1.10188500	-0.55622400
C	1.85975800	1.63310400	-1.89143600
C	6.59292600	-1.83575800	-0.55666100
H	7.26292500	-1.46429900	-1.33653800
H	7.11507100	-1.74059200	0.40478000
H	6.43941500	-2.90846800	-0.72474300
C	1.05458200	2.52146800	-2.77612500
H	0.15421900	2.88790000	-2.27123200
H	1.63455000	3.39132000	-3.10042800
H	0.73220400	1.98189700	-3.67848100
N	4.21157500	-1.51206300	0.08919000
N	1.33538800	0.79036700	-0.99802600
C	4.23927200	-2.77968100	0.74051900
C	4.67488800	-2.91028100	2.06881900
C	3.75384600	-3.88645400	0.02141000
C	4.57814300	-4.16533700	2.67456300
C	3.67033200	-5.11948800	0.66639400
C	4.07114500	-5.26149400	1.98932100
H	4.91268600	-4.27405600	3.70576700
H	3.28540300	-5.97668000	0.11499800
H	3.99729100	-6.22798200	2.48294200
C	-0.07337300	0.62944800	-0.98584300
C	-0.63945600	-0.24552200	-1.91100300
C	-0.92941100	1.21644600	-0.03708100
C	-1.97954100	-0.59149200	-1.91998600
C	-2.28496300	0.89856700	-0.06872600
C	-2.82386000	-0.01339300	-0.97762400
H	-2.33421800	-1.30944500	-2.65581300
H	-2.94610600	1.33551900	0.68003300
C	5.23702400	-1.75245600	2.84100000

H	5.92108800	-1.14021300	2.24158100
C	3.36114500	-3.74748600	-1.41856500
H	4.24095500	-3.74743300	-2.07786000
C	-0.37020900	2.20124000	0.97559600
H	0.65069400	1.86039400	1.19878700
C	-4.28596600	-0.39735200	-0.82511600
H	-4.85045100	0.54726200	-0.76110200
C	-0.22419300	3.57750400	0.35221900
C	-1.29856700	4.20195200	-0.28925300
C	1.00014600	4.24490500	0.40362300
C	-1.15682700	5.45467800	-0.87381900
H	-2.26124800	3.69442400	-0.33935600
C	1.16506200	5.49774600	-0.17943400
H	1.84609300	3.77099500	0.90049100
C	0.07949600	6.07928700	-0.81122800
H	-1.98246600	5.95011700	-1.37744100
H	2.11604500	6.02255200	-0.15124700
C	-1.12800300	2.19648900	2.29677800
C	-1.53064400	3.36799600	2.93737400
C	-1.40106800	0.97420800	2.92673100
C	-2.19178200	3.33142800	4.16330600
H	-1.32613500	4.33355500	2.48031600
C	-2.06588500	0.91519600	4.14264700
H	-1.10243300	0.04340700	2.44448700
C	-2.45168500	2.10403500	4.74343200
H	-2.50769700	4.24097000	4.66704100
H	-2.29325800	-0.03324100	4.62239500
C	-4.83484300	-1.14489200	-2.02536500
C	-4.87361500	-2.53894500	-2.08145800
C	-5.26236300	-0.41979400	-3.14092200
C	-5.33107300	-3.19874900	-3.21773000
H	-4.54689400	-3.12255400	-1.22249700
C	-5.72509100	-1.05900700	-4.28403300
H	-5.22823400	0.66915200	-3.11308200
C	-5.75061700	-2.44450400	-4.30004000
H	-5.36986000	-4.28325700	-3.27268400
H	-6.06576400	-0.50546200	-5.15479700
C	-4.52799500	-1.12446500	0.48823700
C	-3.55792400	-1.93949600	1.07689000
C	-5.76746400	-0.99987600	1.11995000
C	-3.81075700	-2.60873100	2.27007600
H	-2.58414900	-2.05164000	0.60073900
C	-6.03884100	-1.65719600	2.31352900
H	-6.53467700	-0.37180400	0.66784800

C	-5.04911800	-2.45162500	2.86952700
H	-3.06344100	-3.24383000	2.73832200
H	-6.99574000	-1.55922100	2.81885400
F	0.17033200	-0.81199200	-2.82113300
F	0.22611100	7.28312600	-1.38142800
F	-3.09642600	2.05964900	5.91768700
F	-6.19844400	-3.07205400	-5.39595800
F	-5.29766200	-3.08534600	4.02374200
C	1.09690300	-1.79160700	0.62836600
H	1.34514900	-2.58120300	1.34242200
H	1.04430100	-2.25805500	-0.37607000
H	5.78795000	-2.10759100	3.71844900
H	4.45108400	-1.07612300	3.20078600
H	2.71490300	-4.57285500	-1.73515500
H	2.83659200	-2.80154600	-1.60547200
H	0.10412900	-1.38300100	0.84107200
Fe	2.62278600	-0.39334300	-0.11764900
C	2.98673400	0.67817300	1.49216900
C	2.11488500	-0.39839000	1.80709700
H	1.12366500	-0.11823400	2.17168800
H	2.52598000	-1.20248200	2.42010400
H	4.04014000	0.63799400	1.78118200
H	2.60007300	1.69996100	1.44999600

TS3,4 Gsolv= -3933.129786

C	3.20817500	1.44948100	-1.84374200
C	4.01951600	2.17442800	-2.71841200
C	5.39571600	1.97975800	-2.69801700
C	5.93661600	0.97472200	-1.88328100
C	5.10303800	0.27606300	-1.02406700
N	3.78520300	0.63590100	-0.89662400
H	6.03838700	2.54079000	-3.37032700
H	3.57367500	2.86162400	-3.43438100
H	6.99013300	0.71915200	-1.96279500
C	5.40376900	-0.94261600	-0.31527900
C	1.78890200	1.33243700	-1.86506300
C	6.76179800	-1.56238000	-0.33782600
H	6.75408000	-2.46798100	-0.95990900
H	7.51598700	-0.88308400	-0.74164000
H	7.08841400	-1.87505900	0.65918500
C	0.97005400	1.93261100	-2.95736000
H	0.82678800	1.18663100	-3.75339700
H	-0.02348000	2.24033700	-2.62201600
H	1.46013300	2.80331100	-3.40193600

N	4.34946100	-1.51341500	0.24302900
N	1.29963400	0.48833600	-0.94678700
C	4.49115900	-2.77906600	0.88002900
C	5.01079800	-2.89791700	2.18130900
C	4.04026300	-3.90710900	0.17151000
C	5.07120000	-4.17118500	2.75312800
C	4.12091200	-5.15771000	0.78128700
C	4.63158000	-5.29459700	2.06628700
H	5.47434300	-4.27146100	3.76031700
H	3.77365400	-6.03279600	0.23324600
H	4.68830500	-6.27620100	2.53151700
C	-0.10039200	0.27441300	-0.93422700
C	-0.60367600	-0.82461500	-1.62727700
C	-1.01950900	1.10436200	-0.25643500
C	-1.94658100	-1.15733900	-1.66155800
C	-2.37566400	0.79703700	-0.34121400
C	-2.85417100	-0.33413000	-1.00419300
H	-2.25608000	-2.05043700	-2.19961800
H	-3.09365700	1.42363900	0.18762800
C	5.48145400	-1.71167200	2.97259700
H	6.09061600	-1.01563100	2.38452200
C	3.47746600	-3.75825900	-1.20763100
H	4.19039300	-3.28831800	-1.89799500
C	-0.52374500	2.30507500	0.54165400
H	0.46236600	2.00627100	0.93372500
C	-4.32488800	-0.67902500	-0.85849300
H	-4.88559000	0.25342500	-1.03540900
C	-0.25511900	3.50181600	-0.35306700
C	-1.26981200	4.06536700	-1.13187100
C	1.01903200	4.06778100	-0.40222000
C	-1.02046900	5.15840400	-1.95247500
H	-2.27139200	3.63763100	-1.09805700
C	1.29190000	5.16012600	-1.22132600
H	1.81839600	3.63787700	0.20169200
C	0.26265800	5.68467100	-1.98427900
H	-1.79811400	5.60641500	-2.56509400
H	2.28286800	5.60333800	-1.27360000
C	-1.38682400	2.66847200	1.75104400
C	-1.52141800	3.99785500	2.16244100
C	-1.99507700	1.68163400	2.54002900
C	-2.24021900	4.34032900	3.30359400
H	-1.05508900	4.79292300	1.58544300
C	-2.72189100	2.00245600	3.67898400
H	-1.91668200	0.63392300	2.25847000

C	-2.83342000	3.33392500	4.04333700
H	-2.34520600	5.37444600	3.62035600
H	-3.20142000	1.23509800	4.28094200
C	-4.80926600	-1.67831600	-1.89138900
C	-4.84589600	-3.05046400	-1.63732000
C	-5.17633500	-1.22411800	-3.16082800
C	-5.24316000	-3.95150500	-2.62003200
H	-4.56333600	-3.42397900	-0.65440900
C	-5.57930100	-2.10684200	-4.15486800
H	-5.14338000	-0.15605200	-3.37453900
C	-5.60522500	-3.46130800	-3.86313600
H	-5.27864900	-5.02149200	-2.43419200
H	-5.87345400	-1.76454500	-5.14332200
C	-4.64613300	-1.10299000	0.56771800
C	-3.68940100	-1.66634900	1.41552300
C	-5.95112500	-0.95049600	1.04357600
C	-4.01886600	-2.05936600	2.70971300
H	-2.66385200	-1.79310500	1.06881300
C	-6.29964300	-1.33396200	2.33213100
H	-6.70891500	-0.52042200	0.38896900
C	-5.32075500	-1.88251400	3.14588300
H	-3.28134400	-2.49523600	3.37865200
H	-7.30913500	-1.21136500	2.71499900
F	0.26166800	-1.59887100	-2.29651500
F	0.51150600	6.73459800	-2.77901100
F	-3.53571000	3.65415000	5.13870700
F	-5.99606200	-4.32186600	-4.81291000
F	-5.64522700	-2.24991400	4.39285800
H	6.08303100	-2.03627600	3.82821300
H	4.64132400	-1.12669000	3.36953600
H	3.19503300	-4.73073600	-1.62419500
H	2.58734300	-3.11403400	-1.20058700
Fe	2.68441900	-0.35606200	0.23162000
C	2.97286800	0.66006400	1.89186100
C	2.19001200	-0.51843300	2.16064100
H	2.72606000	-1.35433500	2.62215300
H	4.03511500	0.69911600	2.13787300
H	2.47239500	1.63189300	1.93223400
H	1.71709200	-1.46007700	0.86835200
C	0.80519900	-0.35754700	2.73294000
H	0.31749800	0.53117600	2.32323900
H	0.15619800	-1.22070100	2.52617700
H	0.85195800	-0.21875900	3.82157100

TS5,6 Gsolv= -4011.620463

C	3.15632000	1.87659600	-1.96316900
C	4.02445000	2.70037900	-2.67991000
C	5.37777400	2.38662700	-2.75341800
C	5.86104800	1.23953600	-2.11159900
C	4.98179700	0.43419600	-1.40556800
N	3.64339600	0.74683200	-1.33512300
H	6.05632900	3.02643700	-3.31081500
H	3.64117200	3.58607500	-3.18173300
H	6.91529300	0.97672900	-2.16842900
C	5.25429800	-0.80935200	-0.75301600
C	1.74939800	1.97951300	-1.81177500
C	6.60028800	-1.45155800	-0.83886300
H	6.86079600	-1.68000100	-1.88090500
H	7.37947200	-0.78022100	-0.45590200
H	6.64688500	-2.38341000	-0.26960200
C	0.92338000	2.95612100	-2.57801200
H	0.06793200	3.31335500	-1.99340100
H	1.51108600	3.83020900	-2.87534900
H	0.52469300	2.49750600	-3.49483400
N	4.18697800	-1.34022700	-0.16386200
N	1.23137500	1.03221200	-1.01235100
C	4.27498100	-2.67205200	0.33702300
C	4.70496200	-2.93007700	1.65028800
C	3.87642300	-3.71985600	-0.51192600
C	4.66752100	-4.24643000	2.11465000
C	3.84368700	-5.01914200	-0.00409200
C	4.22388100	-5.28513600	1.30520700
H	4.99841100	-4.45099500	3.13227600
H	3.51900300	-5.82967800	-0.65607500
H	4.19127100	-6.30223100	1.68933500
C	-0.17786900	0.89145100	-1.00039500
C	-0.76578400	0.10265600	-1.98933400
C	-1.01590900	1.38026100	0.01965900
C	-2.09726900	-0.27523200	-1.98104000
C	-2.36616400	1.03809600	0.00454000
C	-2.91482900	0.18701700	-0.95492100
H	-2.46304700	-0.93968500	-2.76062200
H	-3.00798300	1.38502900	0.81485800
C	5.22717600	-1.83790200	2.53594500
H	5.98441700	-1.22553800	2.03023400
C	3.53159000	-3.45788700	-1.94744000
H	4.43868100	-3.34218300	-2.55787700
C	-0.44081500	2.27491400	1.10437900

H	0.59827100	1.94608900	1.24756200
C	-4.33234900	-0.31051500	-0.74038800
H	-4.94198200	0.57125700	-0.48393500
C	-0.35542100	3.71110900	0.62034900
C	-1.47070800	4.36685400	0.09007700
C	0.85378200	4.40367900	0.69166000
C	-1.38290500	5.67497100	-0.37035800
H	-2.42250000	3.84079200	0.02666300
C	0.96472100	5.71243900	0.23193400
H	1.73117300	3.90606200	1.10348100
C	-0.15975800	6.32372000	-0.29496300
H	-2.24037700	6.19517500	-0.78855100
H	1.90369400	6.25747800	0.27450500
C	-1.13351900	2.11970200	2.45263200
C	-1.46664100	3.21542100	3.24962400
C	-1.39962100	0.83790400	2.95498100
C	-2.04980000	3.04919400	4.50364600
H	-1.26713900	4.22370100	2.89381000
C	-1.98519400	0.65044400	4.19882000
H	-1.16454400	-0.03843700	2.35038900
C	-2.30122900	1.76760200	4.95659100
H	-2.31120500	3.90009900	5.12690700
H	-2.20356200	-0.34270900	4.58220900
C	-4.94867000	-0.91615800	-1.98661900
C	-4.92580100	-2.28911700	-2.23689400
C	-5.50758300	-0.07075400	-2.94882200
C	-5.45176400	-2.81224400	-3.41403200
H	-4.49453200	-2.96441900	-1.49975700
C	-6.04046500	-0.57307600	-4.12899700
H	-5.52231000	1.00388700	-2.76856300
C	-6.00220100	-1.94239900	-4.33956600
H	-5.44347600	-3.87913600	-3.61978300
H	-6.48352900	0.07389300	-4.88119900
C	-4.39865600	-1.23786700	0.46569900
C	-3.29685300	-1.97698600	0.90307700
C	-5.60748400	-1.37867700	1.15194900
C	-3.38843100	-2.82798200	2.00048200
H	-2.34222300	-1.88394300	0.38446800
C	-5.72006300	-2.21992500	2.25167800
H	-6.47820100	-0.81515500	0.81738900
C	-4.60203200	-2.93091400	2.65894000
H	-2.53452100	-3.40682100	2.34588800
H	-6.65311100	-2.32918200	2.79768900
F	0.01995100	-0.36516400	-2.97246800

F	-0.06559300	7.58179700	-0.74661800
F	-2.86887800	1.59838000	6.15874300
F	-6.51684200	-2.43869900	-5.47274800
F	-4.69982900	-3.74033300	3.72203600
C	1.12336700	-1.54607500	0.39751400
H	1.43476100	-1.85545300	-0.63375200
H	5.68663200	-2.25982400	3.43602000
H	4.43879800	-1.14872300	2.86291300
H	2.95649000	-4.28618200	-2.37543800
H	2.95908100	-2.53066000	-2.07441400
H	0.13095400	-1.08679700	0.30969600
Fe	2.55434800	-0.23224100	-0.25082100
C	2.93608600	0.73007700	1.40165200
C	2.03039900	-0.33806400	1.74671000
H	1.04545500	-0.05214400	2.12619600
H	2.44690300	-1.16164200	2.32870600
H	3.98150700	0.64766000	1.70937600
H	2.56885100	1.75982900	1.41980500
C	1.00101600	-2.79804200	1.24305700
H	1.99076800	-3.19043700	1.51238900
H	0.49805100	-2.54605400	2.19130000
C	0.21324800	-3.88388700	0.52412500
H	-0.77811200	-3.52661500	0.20918600
H	0.73929300	-4.21319000	-0.38219700
H	0.06681400	-4.76610800	1.15947300

TS6,7 Gsolv= -4011.631314

C	3.18015300	1.70297700	-1.85931100
C	3.96377200	2.56293200	-2.62448500
C	5.35191900	2.42728200	-2.57964500
C	5.93879800	1.40628200	-1.82750400
C	5.11972100	0.56634000	-1.07989500
N	3.77264500	0.77236400	-1.06113000
H	5.97902700	3.09614900	-3.16308300
H	3.50440500	3.32129100	-3.25388900
H	7.01623800	1.26249300	-1.84367200
C	5.46396000	-0.64376500	-0.36969300
C	1.74528900	1.56746300	-1.83454800
C	6.84005700	-1.21920300	-0.41244200
H	6.88152000	-2.07122500	-1.10580900
H	7.57205000	-0.48114700	-0.75110700
H	7.16316600	-1.59474200	0.56390200
C	0.90357800	2.21045300	-2.88337800
H	-0.10205500	2.45273000	-2.52994800

H	1.36271600	3.13041200	-3.25693100
H	0.79579300	1.52616200	-3.73829300
N	4.42098400	-1.25244000	0.17613600
N	1.29614800	0.68827500	-0.93642000
C	4.61173400	-2.55205700	0.73624000
C	5.08686800	-2.72345600	2.04667600
C	4.25740700	-3.65449600	-0.06080900
C	5.19176900	-4.02477300	2.54455200
C	4.37582700	-4.93499900	0.47752400
C	4.83751500	-5.12427200	1.77461500
H	5.55983300	-4.16590900	3.56021300
H	4.09913500	-5.79111400	-0.13665400
H	4.92394300	-6.12840900	2.18379300
C	-0.10148400	0.43044100	-0.95332300
C	-0.56702900	-0.61608400	-1.74577600
C	-1.04797500	1.16961700	-0.21460400
C	-1.90003300	-0.98393900	-1.82196800
C	-2.39344800	0.83106900	-0.33715700
C	-2.83665400	-0.24543200	-1.10721800
H	-2.17909900	-1.82987100	-2.44595300
H	-3.13327200	1.39387000	0.23168200
C	5.46748000	-1.56209500	2.91812400
H	6.06972800	-0.81304600	2.39032200
C	3.75976400	-3.44612900	-1.45757500
H	4.51948900	-2.98014300	-2.10029300
C	-0.59784400	2.32394900	0.67198800
H	0.39433200	2.03533200	1.05202700
C	-4.31436900	-0.59914000	-1.05392900
H	-4.86298300	0.33667000	-1.24916600
C	-0.36599900	3.58497800	-0.14149800
C	-1.39607600	4.16810100	-0.88512900
C	0.89327100	4.18569900	-0.15783900
C	-1.17694200	5.31535900	-1.63764000
H	-2.38632400	3.71363300	-0.87719300
C	1.13581300	5.33291200	-0.90868100
H	1.70479300	3.74200900	0.41918900
C	0.09185000	5.87603700	-1.63786500
H	-1.96738000	5.77945000	-2.22121100
H	2.11452200	5.80479400	-0.93344500
C	-1.48001600	2.56354400	1.89695400
C	-1.67503300	3.85297800	2.39938500
C	-2.04643900	1.49639400	2.60911500
C	-2.41227600	4.08162200	3.55730200
H	-1.24184700	4.70601700	1.88225300

C	-2.79123200	1.70358100	3.76263500
H	-1.92381700	0.47555300	2.25185300
C	-2.96258300	2.99988100	4.21968800
H	-2.56400700	5.08495600	3.94601200
H	-3.23848300	0.87550100	4.30614500
C	-4.73299200	-1.57498400	-2.13769500
C	-4.83746900	-2.94816200	-1.91284000
C	-4.96775300	-1.09079200	-3.42799000
C	-5.17193200	-3.82099500	-2.94384000
H	-4.66298100	-3.34780000	-0.91569300
C	-5.30423100	-1.94454800	-4.47031100
H	-4.87994100	-0.02136200	-3.61884600
C	-5.40055900	-3.30189500	-4.20605600
H	-5.26011000	-4.89152500	-2.77994100
H	-5.49376200	-1.57826600	-5.47560600
C	-4.71527600	-1.04094400	0.34352600
C	-3.86204600	-1.80179100	1.14762800
C	-5.97403000	-0.70078600	0.84251400
C	-4.25034300	-2.21472300	2.41758700
H	-2.87091200	-2.06991400	0.78090600
C	-6.37937100	-1.09869100	2.11136200
H	-6.65001600	-0.10941800	0.22568000
C	-5.50580500	-1.85194100	2.87809500
H	-3.59624400	-2.80850200	3.05123500
H	-7.35297000	-0.83171500	2.51313800
F	0.32415200	-1.30077900	-2.47785200
F	0.31168600	6.97860900	-2.36706800
F	-3.68240400	3.21033500	5.33025900
F	-5.72828400	-4.13466700	-5.20320700
F	-5.88433100	-2.23806800	4.10382400
H	6.04385400	-1.90399900	3.78431500
H	4.58263500	-1.03597500	3.29938900
H	3.46374100	-4.39359400	-1.91926900
H	2.89240600	-2.77007100	-1.45994500
Fe	2.70135100	-0.36438900	-0.02745800
C	2.84763100	0.57822900	1.69364100
C	2.17103500	-0.66444500	1.86966400
H	2.75714600	-1.48853600	2.28857400
H	3.88813900	0.70119900	2.00399000
H	2.26698300	1.50360600	1.76550900
H	1.90785800	-1.48659700	0.23903800
C	0.73919000	-0.69892700	2.33423400
H	0.21553900	0.18732800	1.95772300
H	0.74140100	-0.59551200	3.43432900

C	-0.05503900	-1.94680100	1.96821100
H	-1.05743500	-1.86652400	2.41978800
H	-0.20737200	-1.97205400	0.87666900
C	0.60447100	-3.23922900	2.42146100
H	-0.04015600	-4.10766000	2.24125000
H	1.54780400	-3.41629800	1.88852900
H	0.83246900	-3.21214000	3.49625900

TS8,9 Gsolv= -4090.136838

C	3.15753500	2.16781400	-1.89242600
C	4.02576600	3.02521200	-2.56862800
C	5.37004100	2.69198400	-2.69887500
C	5.84416700	1.49193700	-2.15438600
C	4.96498800	0.65400100	-1.48752200
N	3.63534500	0.98529100	-1.36153000
H	6.04853400	3.35790100	-3.22487600
H	3.64922300	3.95242100	-2.99490600
H	6.89106600	1.21359400	-2.25568300
C	5.22894700	-0.63749900	-0.93177000
C	1.75726900	2.28670000	-1.69912100
C	6.56044400	-1.29440900	-1.09645900
H	6.78414400	-1.46862600	-2.15740600
H	7.36237800	-0.65707600	-0.70280500
H	6.60942200	-2.25715100	-0.58140000
C	0.93525900	3.33374200	-2.37117400
H	0.09832400	3.66109500	-1.74374300
H	1.53427300	4.21729600	-2.61293300
H	0.51039700	2.95438700	-3.31213800
N	4.16670100	-1.19030700	-0.35404200
N	1.23751600	1.29243100	-0.95974600
C	4.24684700	-2.55162800	0.06167500
C	4.70856900	-2.89460200	1.34445800
C	3.80695000	-3.54046700	-0.83628900
C	4.66247500	-4.23579600	1.73058900
C	3.76481200	-4.86703900	-0.40538700
C	4.17879900	-5.21730100	0.87395000
H	5.01800700	-4.50619800	2.72425400
H	3.40347200	-5.63167500	-1.09318900
H	4.13960000	-6.25513100	1.19767400
C	-0.17312600	1.17110600	-0.93241400
C	-0.79149900	0.47545900	-1.97184800
C	-0.98469700	1.58585700	0.14016100
C	-2.12837600	0.11850600	-1.96876000
C	-2.33988300	1.26177100	0.12622000

C	-2.91882300	0.50119200	-0.88960000
H	-2.51922500	-0.47337800	-2.79342100
H	-2.95931600	1.54777400	0.97677600
C	5.27042300	-1.86574600	2.28025400
H	6.01651800	-1.22738400	1.79056700
C	3.42629600	-3.18793200	-2.24289000
H	4.31771500	-3.04503800	-2.87034300
C	-0.37450800	2.38709300	1.27710300
H	0.66155700	2.03251500	1.37344200
C	-4.33018900	-0.01570300	-0.68394000
H	-4.92039800	0.82256300	-0.27911700
C	-0.27442200	3.85412700	0.89978600
C	-1.38744800	4.56230300	0.43651100
C	0.94531500	4.52364500	1.00575600
C	-1.28770500	5.90027200	0.07485700
H	-2.34697500	4.05439300	0.34674500
C	1.06808100	5.86184600	0.64447600
H	1.82110100	3.98475100	1.36620800
C	-0.05483800	6.52568300	0.18171100
H	-2.14341300	6.46158600	-0.29052700
H	2.01501100	6.39005400	0.71435100
C	-1.04353000	2.14385400	2.62434400
C	-1.34633700	3.18462300	3.50281400
C	-1.31629200	0.83278800	3.04074100
C	-1.90565600	2.93759800	4.75428900
H	-1.14101900	4.21294700	3.21409900
C	-1.87750500	0.56536500	4.28130300
H	-1.10570600	-0.00070800	2.37021100
C	-2.16330800	1.63022300	5.12193900
H	-2.14323400	3.74550000	5.44103500
H	-2.09922300	-0.44953600	4.60050200
C	-5.00476900	-0.43888700	-1.97486500
C	-5.02099500	-1.76568900	-2.40794200
C	-5.58162100	0.53755000	-2.79151400
C	-5.60213500	-2.11645200	-3.62266900
H	-4.57644000	-2.54123500	-1.78636500
C	-6.16966900	0.20789800	-4.00577200
H	-5.56692300	1.57809900	-2.46814800
C	-6.16872400	-1.12090800	-4.39977000
H	-5.62408200	-3.14571300	-3.97016900
H	-6.62692600	0.95763100	-4.64568800
C	-4.34983700	-1.10495100	0.38087600
C	-3.22221400	-1.86879200	0.68965100
C	-5.54044300	-1.37405400	1.06135800

C	-3.26973900	-2.86917000	1.65605600
H	-2.28113300	-1.67865500	0.17373100
C	-5.60950800	-2.36659100	2.03081600
H	-6.43143700	-0.79255600	0.82534400
C	-4.46641300	-3.09860000	2.31315700
H	-2.39218000	-3.46562700	1.90136900
H	-6.52816800	-2.57786900	2.57135000
F	-0.03165900	0.07937300	-3.00555100
F	0.05090300	7.81311600	-0.17463300
F	-2.70722300	1.38348300	6.32163400
F	-6.73669300	-1.45120900	-5.56753300
F	-4.52271300	-4.05355100	3.25094700
C	1.11277500	-1.37791200	0.27098900
H	1.38552200	-1.60541500	-0.79220100
H	5.75477100	-2.34855000	3.13553900
H	4.49941400	-1.19360100	2.67688300
H	2.82925200	-3.98242900	-2.70366100
H	2.86192300	-2.24882100	-2.29733000
H	0.12659300	-0.89818900	0.25232000
Fe	2.55121600	-0.04883200	-0.32337600
C	2.99150500	0.79376800	1.37931900
C	2.07771200	-0.28118000	1.67672400
H	1.10882400	-0.00761600	2.10402100
H	2.49571200	-1.14999400	2.18747700
H	4.04317800	0.67632900	1.65219700
H	2.64076300	1.82518300	1.47219500
C	1.00318600	-2.68913900	1.02106000
H	1.99646600	-3.10671900	1.24117900
H	0.51833100	-2.51130200	1.99737100
C	0.19940100	-3.73089800	0.25272400
H	-0.78613600	-3.31866500	-0.02697800
H	0.70984000	-3.94943300	-0.70075500
C	0.00763700	-5.02680000	1.02563900
H	-0.47806900	-4.80868000	1.99088300
H	0.99645300	-5.44090600	1.27763000
C	-0.80866800	-6.04938700	0.25573800
H	-0.93883300	-6.98125400	0.81767400
H	-1.80933200	-5.66103700	0.02158900
H	-0.32564900	-6.30134700	-0.69775600