Electronic Supplementary Material (ESI) for RSC Advances

Synthesis of both enantiomers of ferrocene[1,2-*c*]1H-quinolin-2-one by diastereoselective deproto-zincation of sugar-derived ferrocene esters

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General Procedures:

All reactions were performed in Schlenk tubes under argon atmosphere. THF was distilled over sodium/benzophenone. Liquid chromatography separations were achieved on silica gel Merck-Geduran Si 60 (63-200 μm). Nuclear magnetic resonance spectra were acquired using Bruker AC-300 (300 MHz and 75 MHz for ^{1}H and ^{13}C respectively) or Avance 500 spectrometer (500 MHz and 125 MHz for ^{1}H and ^{13}C respectively). ^{1}H chemical shifts (δ) are given in ppm relative to the solvent residual peak, and ^{13}C chemical shifts relative to the central peak of the solvent signal. High resolution mass spectra measurements were performed at the Centre Régional de Mesures Physiques de l'Ouest (CRMPO) in Rennes.

Experimental Procedures:

5-*O*-(*tert*-butyldiphenylsilyl)-1,2-*O*-isopropylidene-α-D-xylofuranose (**2a**) was prepared as previously described.[1]

2,3:5,6-di-*O*-cyclohexylidene-α-D-mannofuranose (**2b**), **1,2:5,6-di-*O*-isopropylidene-α-D-glucofuranose** (**2c**), **1,2:5,6-di-*O*-cyclohexylidene-α-D-glucofuranose** (**2d**) and **1,2:5,6-di-*O*-isopropylidene-α-D-allofuranose** (**2e**) are commercially available.

5-(*tert*-butoxycarbonylamino)-5-deoxy-1,2-*O*-isopropylidene-α-D-xylofuranose (**2f**) and **6-(*tert*-butoxycarbonylamino)-6-deoxy-3-*O*-methyl-1,2-*O*-isopropylidene-α-D-glucofuranose** (**2g**) were prepared as previously described.[2]

The starting ferrocene esters **3a-g** were prepared as previously described.[2]

General procedure for the deprotonation using the lithium-zinc base prepared from $ZnCl_2$·TMEDA (1 equiv) and TMPLi (3 equiv) before trapping with I_2. To a stirred cooled (0 °C) solution of 2,2,6,6-tetramethylpiperidine (1.1 mL, 6.0 mmol) in THF (5 mL) were successively added BuLi (1.6 M hexanes solution, 6.0 mmol) and, 5 min later, $ZnCl_2$·TMEDA[3] (0.60 g, 2.0 mmol). The mixture was stirred for 10 min at 0 °C before introduction of the required substrate 4 (2.0 mmol). After 2 h at rt, a solution of I_2 (1.5 g, 6.0 mmol) in THF (5 mL) was added. The mixture was stirred overnight before addition of an aq saturated solution of $Na_2S_2O_3$ (10 mL) and extraction with EtOAc (3 x 20 mL). After drying over anhydrous Na_2SO_4, the solvent was evaporated under reduced pressure, and the iodide was isolated by purification by flash chromatography on silica gel.

General procedure for the conversion of the 2-iodoferrocenecarboxylates 4 to 2-iodoferrocenemethanol (5).[4] The required diastereomeric mixture of the iodoferrocenecarboxylates **4** (0.30 mmol) was dissolved in THF (3 mL), and a 1.0 M DIBAL-H solution in heptane (1.2 mL, 1.2 mmol) was added dropwise at 0 °C. The mixture was stirred at this temperature for 1 h before quenching by addition of MeOH (0.5 mL), dilution with Et_2O (10 mL), and

addition of an aqueous saturated solution of sodium and potassium tartrate (10 mL) at 0 °C. After stirring for 30 min at rt, extraction with Et_2O and drying over anhydrous Na_2SO_4, the solvent was evaporated under reduced pressure, and 2-iodoferrocenemethanol (**5**) was isolated as orange crystals by purification by flash chromatography on silica gel (eluent: heptane/EtOAc 88/12). HPLC analysis on a chiral stationary phase (AS-H column, eluent: hexane/isopropanol 90/10, 1 mL/min, λ = 252 nm) gave two well separated peaks for the two enantiomers of 2-iodoferrocenemethanol (***R*-5**, 12.5 min, and ***S*-5**, 22.2 min).

3-*O*-(2-iodoferrocenecarbonyl)-5-*O*-(*tert*-butyldiphenylsilyl)-1,2-*O*-isopropylidene-α-D-xylofuranose (diastereomeric mixture) (**4a**)[2] was prepared from **3a** (1.3 g), and was isolated (eluent: heptane/EtOAc 93/7) as an orange solid (yield: 86%): mp 49-60 °C. ^{1}H NMR (300 MHz, $CDCl_3$): Common signals: δ 3.93-4.06 (m, 2H), 4.42-4.50 (m, 2H), 4.69-4.70 (m, 1H), 7.26-7.47 (m, 6H), 7.59-7.71 (m, 4H); major diastereomer signals: 1.03 (s, 9H), 1.34 (s, 3H), 1.54 (s, 3H), 4.15 (s, 5H), 4.60 (d, 1H, J = 3.7 Hz), 4.73 (dd, 1H, J = 1.5, 2.7 Hz), 5.48 (d, 1H, J = 3.0 Hz), 5.98 (d, J = 3.5 Hz, 1H); minor diastereomer signals: 1.04 (s, 9H), 1.33 (s, 3H), 1.53 (s, 3H), 4.13 (s, 5H), 4.57 (d, 1H, J = 3.7 Hz), 4.78 (dd, 1H, J = 1.5, 2.7 Hz), 5.50 (d, 1H, J = 3.0 Hz), 5.97 (d, 1H, J = 2.7 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 0.9, 19.0, 19.0, 26.3, 26.7, 26.8 (3C), 26.8, 38.9, 39.3, 61.0, 61.2, 69.6, 70.2, 70.4, 70.6, 72.5, 72.5, 72.6, 72.7 (5C), 75.7, 75.8, 79.3, 79.4, 80.0, 80.0, 83.3, 104.8, 104.9, 112.2, 112.3, 127.7 (4C), 129.6, 129.6, 129.7, 132.9, 132.9, 133.0, 133.0, 135.4, 135.6, 169.0, 169.2. HRMS: calcd for $C_{35}H_{39}{}^{56}FeINaO_6Si$ [$(M+Na)^{+\bullet}$] 789.0802, found 789.0804. A 20% de was estimated by NMR. Treatment with DIBAL-H (see above) afforded 2-iodoferrocenemethanol (**5**) in 61% yield, and 22% ee (*R*).[4]

1-*O*-(2-iodoferrocenecarbonyl)-2,3:5,6-di-*O*-cyclohexylidene-α-D-mannofuranose (diastereomeric mixture) (**4b**)[2] was prepared from **3b** (0.83 g), but could not be separated from the starting material (estimated yield: 50%). A 17% de was estimated by NMR. The treatment of one fraction containing only the main diastereomer with DIBAL-H (see above) afforded (*S*)-2-iodoferrocenemethanol (***S*-5**).[4]

3-*O*-(2-iodoferrocenecarbonyl)-1,2:5,6-di-*O*-isopropylidene-α-D-glucofuranose (diastereomeric mixture) (**4c**)[2] was prepared from **3c** (0.94 g), and was isolated (eluent: heptane/EtOAc 93/7) in 86% yield. A 54% de was determined by NMR. One fraction containing the major diastereomer ***S*$_P$-4c** was isolated as an orange solid: mp 61-66 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.30 (s, 3H), 1.34 (s, 3H), 1.45 (s, 3H), 1.54 (s, 3H), 4.11-4.28 (m, 3H), 4.28 (s, 5H), 4.38-4.45 (ddd, 1H, J = 9.9, 5.7, 4.2 Hz), 4.47 (t, 1H, J = 2.5 Hz), 4.57 (d, 1H, J = 3.6 Hz), 4.75 (br s, 1H), 4.84 (br s, 1H), 5.47 (d, 1H, J = 2.9 Hz), 5.89 (d, 1H, J = 3.6 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 25.3, 26.1, 26.7, 27.0, 39.5, 67.5, 69.1, 70.0, 72.4, 73.0, 73.1 (5C), 75.8, 80.1, 83.3, 105.1 (2 signals), 109.5, 112.3, 169.3; $[\alpha]_D$ = -63.4 ($CHCl_3$, c = 0.55, 20 °C); HRMS: calcd for $C_{23}H_{27}{}^{56}FeINaO_7$ [$(M+Na)^{+\bullet}$] 621.0049, found 621.0049.

Treatment with DIBAL-H (see above) afforded (*S*)-2-iodoferrocenemethanol (***S*-5**).[4]

3-*O*-(2-iodoferrocenecarbonyl)-1,2:5,6-di-*O*-cyclohexylidene-α-D-glucofuranose (diastereomeric mixture) (**4d**)[2] was prepared from **3d** (1.1 g), and was isolated (eluent: heptane/EtOAc 95/5) as an orange solid (87% yield): mp 68-80 °C. ^{1}H NMR (300 MHz, $CDCl_3$): Common signals: δ 1.34-1.73 (m, 20H), 4.07-4.26 (m, 3H), 4.26 (s, 5H), 4.37-4.47 (m, 2H), 4.51-6.63 (m, 1H); major diastereomer signals: 4.72 (dd, 1H, J = 1.4, 2.4 Hz), 4.83 (dd, 1H, J = 1.4, 2.7 Hz), 5.46 (d, 1H, J = 2.9 Hz), 5.87 (d, 1H, J = 3.6 Hz); minor diastereomer signals: 4.69 (dd, 1H, J = 1.5, 2.5 Hz), 4.88 (dd, 1H, J = 1.5, 2.7 Hz), 5.53 (d, 1H, J = 2.9 Hz), 5.95 (d, 1H, J = 3.5 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 23.4, 23.7, 23.8, 23.9, 24.8, 24.9, 25.0, 34.8, 34.9, 35.5, 35.6, 36.3, 36.4, 36.7, 39.4, 39.8, 67.2, 67.3, 69.2, 69.9, 70.1, 70.4, 70.8, 72.0, 72.1, 72.5, 72.6, 72.8, 73.0 (5C) 75.9, 76.0, 80.0, 80.1, 80.2, 82.8, 82.9, 104.7, 104.8, 110.1, 110.1, 112.9, 113.0, 169.0, 169.2. HRMS: calcd for $C_{29}H_{35}{}^{56}FeINaO_7$ $[(M+Na)^{+\bullet}]$ 701.0669, found 701.0669. A 56% de was determined by NMR. Treatment with DIBAL-H (see above) afforded 2-iodoferrocenemethanol (**5**) in 96% yield, and 57% ee (*S*).[4]

3-*O*-(2-iodoferrocenecarbonyl)-1,2:5,6-di-*O*-isopropylidene-α-D-allofuranose (diastereomeric mixture) (**4e**)[2] was prepared from **3e** (0.94 g), but could not be separated from the starting material (estimated yield: 64%). It was identified by HRMS: calcd for $C_{23}H_{27}{}^{56}FeINaO_7$ $[(M+Na)^{+\bullet}]$ 621.0043, found 621.0043. The mixture was treated with DIBAL-H (see above) to afford 2-iodoferrocenemethanol (**5**) in 86% yield, and 32% ee (*S*).[4]

5-(*tert*-butoxycarbonylamino)-5-deoxy-3-*O*-(2-iodoferrocenecarbonyl)-1,2-*O*-isopropylidene-α-D-xylofuranose (diastereomeric mixture) (**4f**)[2] was prepared from **3f** (2.0 g), but using 2,2,6,6-tetramethylpiperidine (1.7 mL, 9.0 mmol), BuLi (9.0 mmol) and $ZnCl_2$·TMEDA (0.90 g, 3.0 mmol), and was isolated (eluent: heptane/EtOAc 96/4 to 90/10) as an orange solid (yield: 70%): mp 72-77 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.33 and 1.34 (s, 3H), 1.43 (s, 9H), 1.55 (s, 3H), 3.47-3.53 (m, 2H), 4.24 (2s, 5H), 4.41-4.46 (m, 1H), 4.48-4.50 (m, 1H), 4.64-4.66 (m, 1H), 4.74-4.76 (m, 1H), 4.85-4.88 (m, 1H), 4.90-4.98 (m, 1H), 5.39-5.41 (m, 1H), 6.01 (2d, 1H, J = 3.7 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.4, 26.6, 26.9, 28.5 (3C), 39.4 (2 peaks), 39.7, 70.1, 70.6, 70.8, 72.9, 73.0, 73.1, 76.6, 78.4, 79.7, 80.4, 80.5, 83.7, 104.9, 112.5, 112.6, 155.9, 169.7, 169.9. Anal. Calcd for $C_{24}H_{30}FeINO_7$ (627.25): C, 45.96; H, 4.82; N, 2.23. Found: C, 46.14; H, 5.18; N, 2.13. Treatment with DIBAL-H (see above) afforded 2-iodoferrocenemethanol (**5**) in 91% yield, and 11% ee (*S*).[4]

6-(*tert*-butoxycarbonylamino)-6-deoxy-5-*O*-(2-iodoferrocenecarbonyl)-1,2-*O*-isopropylidene-3-*O*-methyl-α-D-glucofuranose (diastereomeric mixture) (**4g**)[2] was prepared similarly from **3g** (1.1 g): mp 72-77 °C. ^{1}H NMR (500 MHz, 340 K, C_6D_6): δ 1.18 (br s, 3H), 1.44 (br s, 9H), 3.02-3.21 (br m, 5H), 3.73 (br m, 2H), 4.09-4.27 (br m, 7H), 4.27 (br m, 1H), 4.34 (br m, 1H), 4.44 (br m, 1H), 4.60 (br m, 1H), 5.35 (br m, 1H), 5.80 (br m, 1H), 6.55 (br m, 1H). ^{13}C NMR (125 MHz, 340 K, C_6D_6): Common signals: δ 26.4, 27.4, 28.1 (3C), 40.9, 57.8, 70.3, 80.7, 81.9, 82.3, 84.7, 112.0, 153.4, 165.8;

major diastereomer signals: 39.0, 73.1, 76.0 (5C), 76.3, 78.1, 82.4, 105.9; minor diastereomer signals: 39.3, 73.3, 76.1, 76.2 (5C), 78.0, 81.9, 106.9. Anal. Calcd for $C_{26}H_{34}FeINO_8$ (671.30): C, 46.52; H, 5.11; N, 2.09. Found: C, 46.25; H, 4.88; N, 1.78. The main diastereomer ***R*$_P$-4g** was isolated (eluent: heptane/EtOAc 85/15 to 80/20) as an orange gum (35% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.32 (s, 3H), 1.41 (s, 9H), 1.49 (s, 3H), 3.37 (s, 3H), 3.46-3.55 (m, 1H), 3.73-3.81 (m, 2H), 4.25 (s, 5H), 4.32-4.41 (m, 1H), 4.44 (t, 1H, *J* = 2.6 Hz), 4.56 (d, 1H, *J* = 3.6 Hz), 4.70 (dd, 1H, J = 1.5, 2.5 Hz), 4.86 (br s, 1H), 5.01 (t, 1H, *J* = 5.1 Hz), 5.30-5.35 (m, 1H), 5.91 (d, 1H, *J* = 3.7 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.1, 26.7, 28.4 (3C), 39.7, 41.8, 57.9, 69.7, 70.1, 72.3, 72.8 (5C), 79.1, 79.8, 80.0, 81.0, 83.8, 105.0, 111.7, 155.7, 169.4. $[\alpha]_D$ = -2.0 ($CHCl_3$, *c* = 1.9, 20 °C). HRMS: calcd for $C_{26}H_{34}{}^{56}FeINNaO_8$ $[(M+Na)^{+\bullet}]$ 694.0571, found 694.0570. Treatment with DIBAL-H (see above) afforded (*R*)-2-iodoferrocenemethanol (***R*-5**) in 81% yield, and 96% ee (*R*).[4]

Reduction of another fraction (estimated yield for the minor diastereomer ***S*$_P$-4g**: 12%) allowed to obtain (*S*)-2-iodoferrocenemethanol (***S*-5**) in 88% yield, and 92% ee (*S*).[4]

Procedure for the deprotonation using the lithium-zinc base prepared from $ZnCl_2$·TMEDA (1 equiv) and LiTMP (2+2 equiv) in THF (sequential addition) before trapping with I_2. To a stirred cooled (0 °C) solution of 2,2,6,6-tetramethylpiperidine (1.1 mL, 4.0 mmol) in THF (5 mL) were successively added BuLi (1.6 M hexanes solution, 4.0 mmol) and, 5 min later, $ZnCl_2$·TMEDA[3] (0.60 g, 2.0 mmol). The mixture was stirred for 10 min at 0 °C before introduction of the required **3** (2.0 mmol). After 10 min at rt, a cooled (0 °C) solution prepared in THF (5 mL) from 2,2,6,6-tetramethylpiperidine (1.1 mL, 4.0 mmol) and BuLi (1.6 M hexanes solution, 4.0 mmol) was added, and the resulting mixture was stirred for 2 h at rt before a solution of I_2 (2.0 g, 6.0 mmol) in THF (5 mL) was added. The mixture was stirred overnight before addition of an aq saturated solution of $Na_2S_2O_3$ (10 mL) and extraction with EtOAc (3 x 20 mL). After drying over anhydrous Na_2SO_4, the solvent was evaporated under reduced pressure, and the iodide was isolated by purification by flash chromatography on silica gel. Under these conditions, **4c** was isolated in 87% yield and 72% de (S_P) using **3c** as substrate, and ***R*$_P$-4g** was isolated in 51% yield (57% if $ZnCl_2$ is used instead of $ZnCl_2$·TMEDA) using **3g** as substrate.

Procedure for the deprotonation using the mixed lithium-zinc base prepared from the Simpkins' amine (sequential addition) followed by trapping using I_2. To a stirred cooled (0 °C) solution of bis[(*R*)-1-phenylethyl]amine (0.90 g, 4.0 mmol) in THF (5 mL) were successively added BuLi (1.6 M hexanes solution, 4.0 mmol) and, 5 min later, $ZnCl_2$·TMEDA[3] (0.60 g, 2.0 mmol). The mixture was stirred for 10 min at 0 °C before introduction of **3c** (2.0 mmol). After 10 min at rt, a cooled (0 °C) solution prepared in THF (5 mL) from bis[(*R*)-1-phenylethyl]amine (0.90 g, 4.0 mmol) and BuLi (1.6 M hexanes solution, 4.0 mmol) was added, and the resulting mixture was stirred for 2 h at rt before a solution of I_2 (2.0 g, 6.0 mmol) in THF (5 mL) was added. The mixture was stirred overnight before

addition of an aq saturated solution of $Na_2S_2O_3$ (10 mL) and extraction with EtOAc (3 x 20 mL). After drying over anhydrous Na_2SO_4, the solvent was evaporated under reduced pressure, and the iodide was isolated by purification by flash chromatography on silica gel. Under these conditions, **4c** was isolated in 85% yield and 91% de (S_P).

Procedure for the Suzuki coupling. A solution of the required iodoferrocene **4** (0.5 mmol), 2-aminophenylboronic acid (0.27 g, 2.0 mmol), and CsF (0.15 g, 1.0 mmol) in dioxane (5 mL) was degassed with Ar for 30 min before addition of $Pd(dba)_2$ (14 mg, 25 μmol), and PPh_3 (26 mg, 0.10 mmol). The resulting mixture was heated for 12 h at 105 °C before cooling and dilution with Et_2O (30 mL), washing with H_2O, and extraction with CH_2Cl_2 (3 x 20 mL). After drying over anhydrous Na_2SO_4, the solvent was evaporated under reduced pressure, and the iodide was isolated by purification by flash chromatography on silica gel.

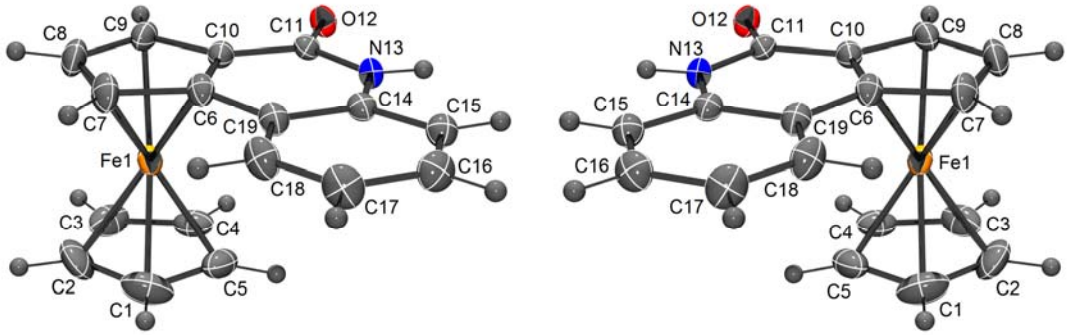
(R_P)-Ferrocene[1,2-*c*]1H-quinolin-2-one (***R*P-1**) was prepared from ***S*P-4c** (0.30 g). It was isolated (eluent: heptane/EtOAc/Et_3N 70/28/2) as an orange solid (yield: 92%): mp 218 °C (dec.); ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.98 (s, 5H), 4.53 (t, 1H, J = 2.5 Hz), 5.17 (dd, 1H, J = 1.1, 2.5 Hz), 5.24 (dd, 1H, J = 1.1, 2.5 Hz), 7.14 (ddd, 1H, J = 1.1, 7.6, 8.4 Hz), 7.24 (dd, 1H, J = 0.8, 8.0 Hz), 7.32 (ddd, 1H, J = 1.4, 7.2, 8.5 Hz), 7.68 (dd, 1H, J = 1.3, 7.5 Hz), 10.05 (br s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 64.1, 66.5, 70.5 (5C), 71.1, 71.7, 84.7, 116.1, 121.9, 122.6, 123.1, 127.1, 136.0, 169.7; $[\alpha]_D$ = +19 ($CHCl_3$, c = 0.21, 20 °C); HRMS: calcd for $C_{17}H_{13}{}^{56}FeNNaO$ $[(M+Na)^{+\bullet}]$ 326.0239 and $C_{17}H_{13}{}^{56}FeNO$ ($M^{+\bullet}$) 303.0341, found 326.0239 and 303.0338.

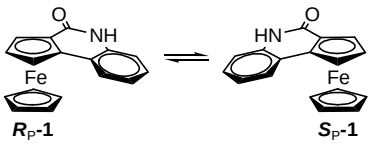
(S_P)- Ferrocene[1,2-*c*]1H-quinolin-2-one (***S*P-1**) was prepared from ***R*P-4g** (0.34 g). It was isolated (crystallization from $CHCl_3$) as an orange solid (yield: 84%): mp 218 °C (dec.); ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.98 (s, 5H), 4.53 (t, 1H, J = 2.5 Hz), 5.17 (dd, 1H, J = 1.1, 2.5 Hz), 5.22 (dd, 1H, J = 1.1, 2.5 Hz), 7.11-7.20 (m, 2H), 7.31 (ddd, 1H, J = 1.4, 7.2, 8.5 Hz), 7.68 (dd, 1H, J = 1.1, 7.7 Hz), 9.46 (br s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 64.1, 66.5, 70.5 (5C), 71.0, 71.7, 84.7, 115.9, 121.9, 122.6, 123.1, 127.1, 135.9, 169.4; $[\alpha]_D$ = -21 ($CHCl_3$, c = 0.30, 20 °C); HRMS: calcd for $C_{17}H_{13}{}^{56}FeNNaO$ $[(M+Na)^{+\bullet}]$ 326.0239 and $C_{17}H_{13}{}^{56}FeNO$ ($M^{+\bullet}$) 303.0341, found 326.0239 and 303.0340.

X-ray diffraction analysis of compounds R_P-1 and S_P-1

The sample was studied with graphite monochromatized $Mo_{K\alpha}$ radiation (λ = 0.71073 Å). X-ray diffraction data were collected at T = 150(2) K using APEXII Bruker-AXS diffractometer. The structure was solved by direct methods using the SIR97 program,[5] and then refined with full-matrix least-square methods based on F^2 (SHELX-97)[6] with the aid of the WINGX program.[7] The contribution of the disordered solvents to the calculated structure factors was estimated following the BYPASS algorithm,[8] implemented as the SQUEEZE option in PLATON.[9] A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 3349 unique intensities and 172 parameters converged at $\omega R(F^2)$ = 0.0856 ($R(F)$ = 0.0288) for 3068 observed reflections with $I > 2\sigma(I)$.

ORTEP figure





R_P-1 S_P-1

Crystal data

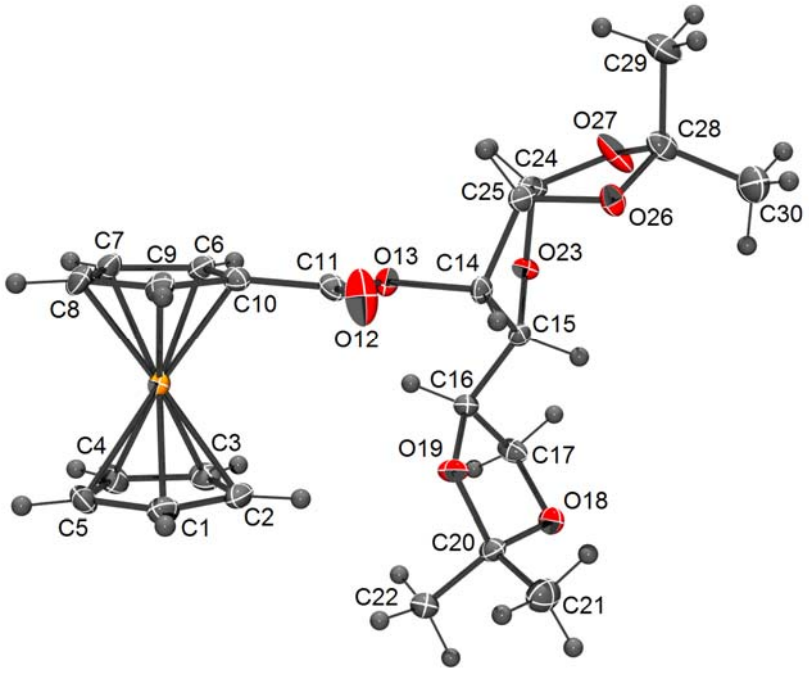
1: $C_{17}H_{13}FeNO$; M = 303.13; trigonal; space group R -3, $a = b$ = 27.0951(7) Å, c = 10.3490(3) Å, $\alpha = \beta$ = 90 °; γ = 120 °; V = 6579.8(3) Å^3, Z = 18; d = 1.38 g.cm^{-3}; μ = 1.025 mm^{-1}.

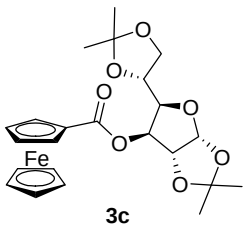
CCDC 872139 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray diffraction analysis of compound 3c

The sample was studied with graphite monochromatized $Mo_{K\alpha}$ radiation (λ = 0.71073 Å). X-ray diffraction data were collected at T = 100(2) K using APEXII Bruker-AXS diffractometer. The structure was solved by direct methods using the SIR97 program,[5] and then refined with full-matrix least-square methods based on F^2 (SHELX-97)[6] with the aid of the WINGX program.[7] All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 9694 unique intensities and 567 parameters converged at $\omega R(F^2)$ = 0.055 (R(F) = 0.0249) for 9093 observed reflections with $I > 2\sigma(I)$.

ORTEP figure





3c

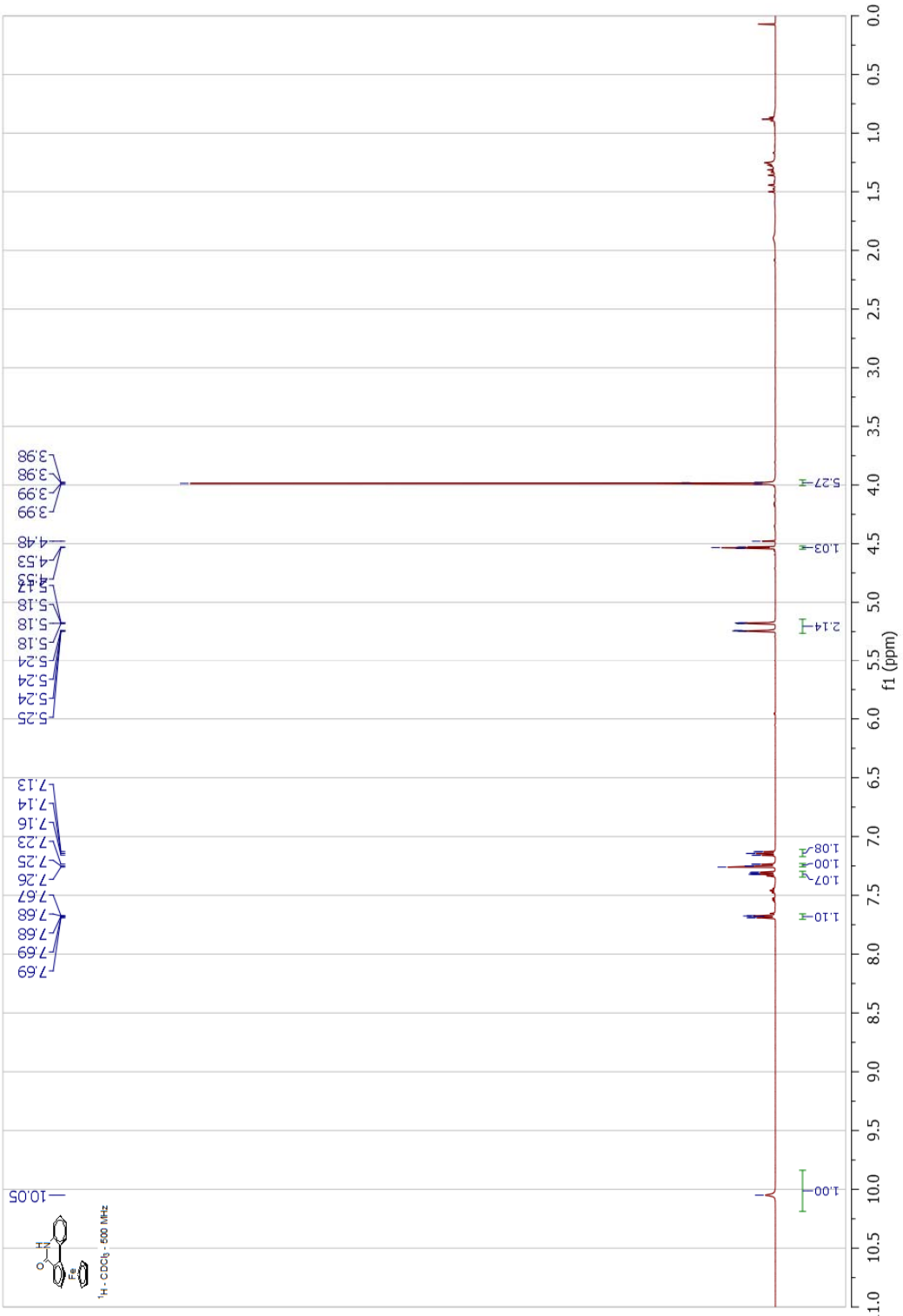
Crystal data

3c: $2(C_{23}H_{28}FeO_7)$; M = 944.61; monoclinic; space group $P2_1$, a = 11.1999(4) Å, b = 12.2306(4) Å, c = 16.1208(6) Å, β = 97.150(2) °, V = 2191.1(1) Å^3, Z = 2; d = 1.43 g.cm^{-3}; μ = 0.730 mm^{-1}.

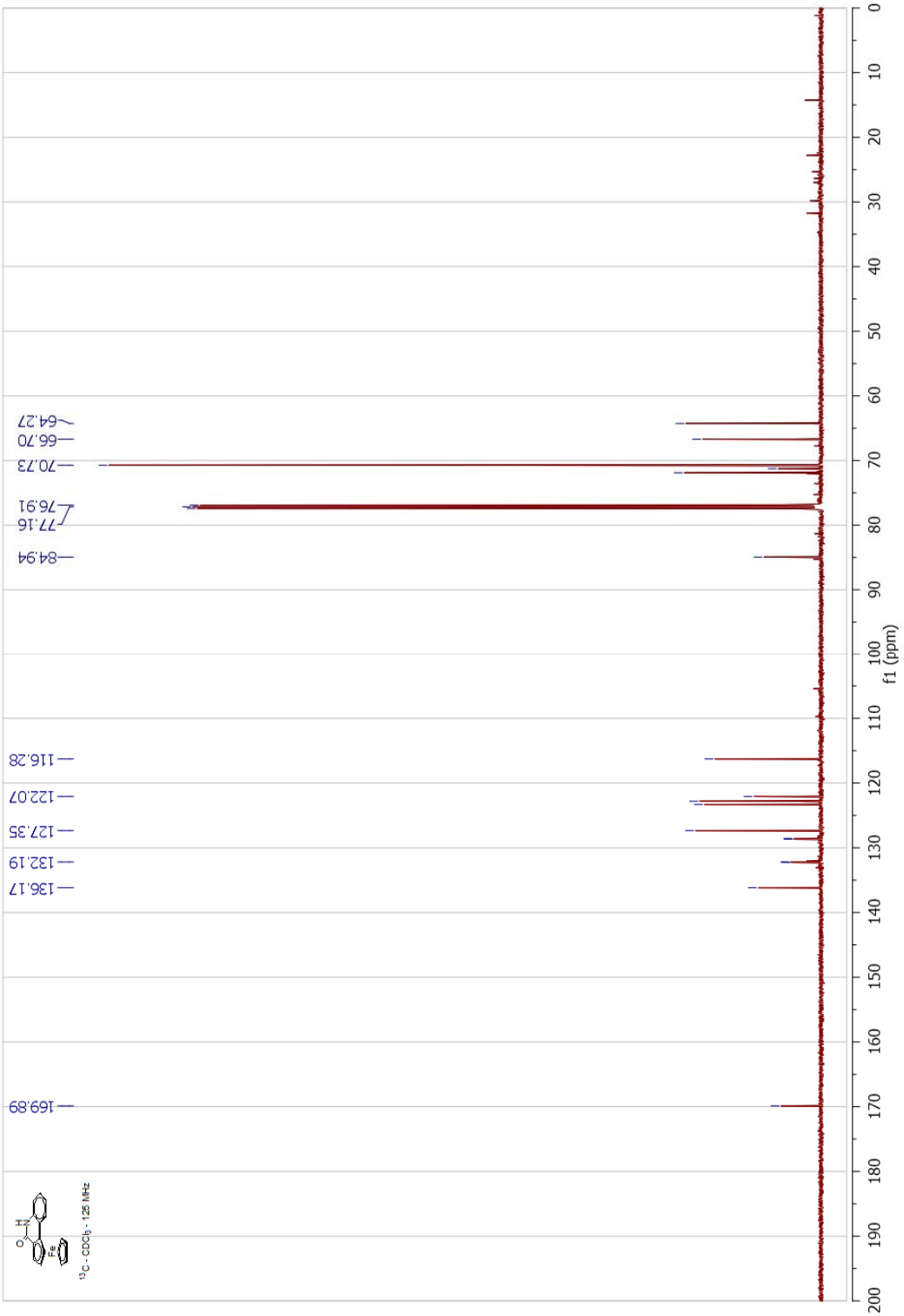
CCDC 798963 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

NMR spectra:

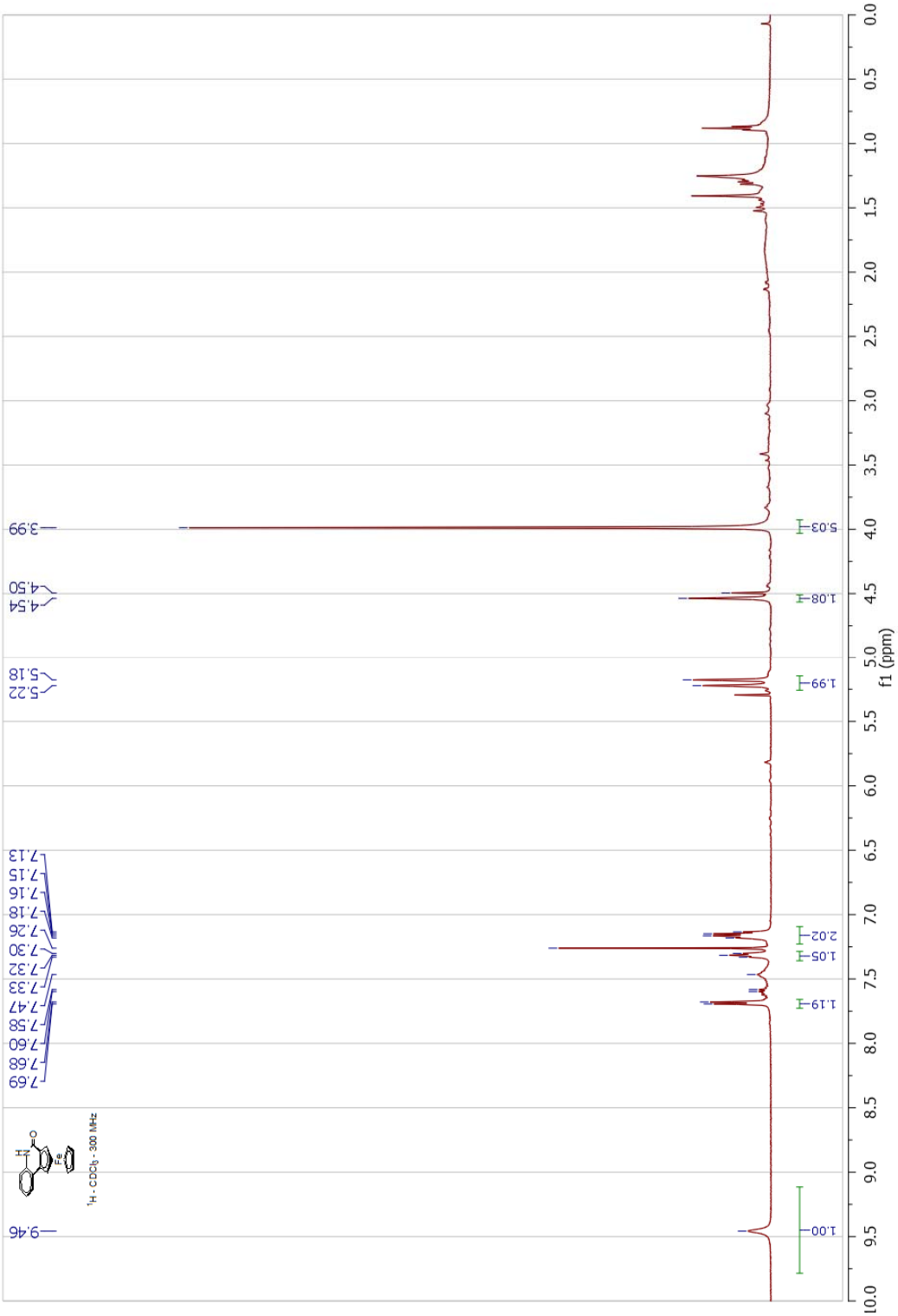
Compound R_P-1, ^{1}H-NMR



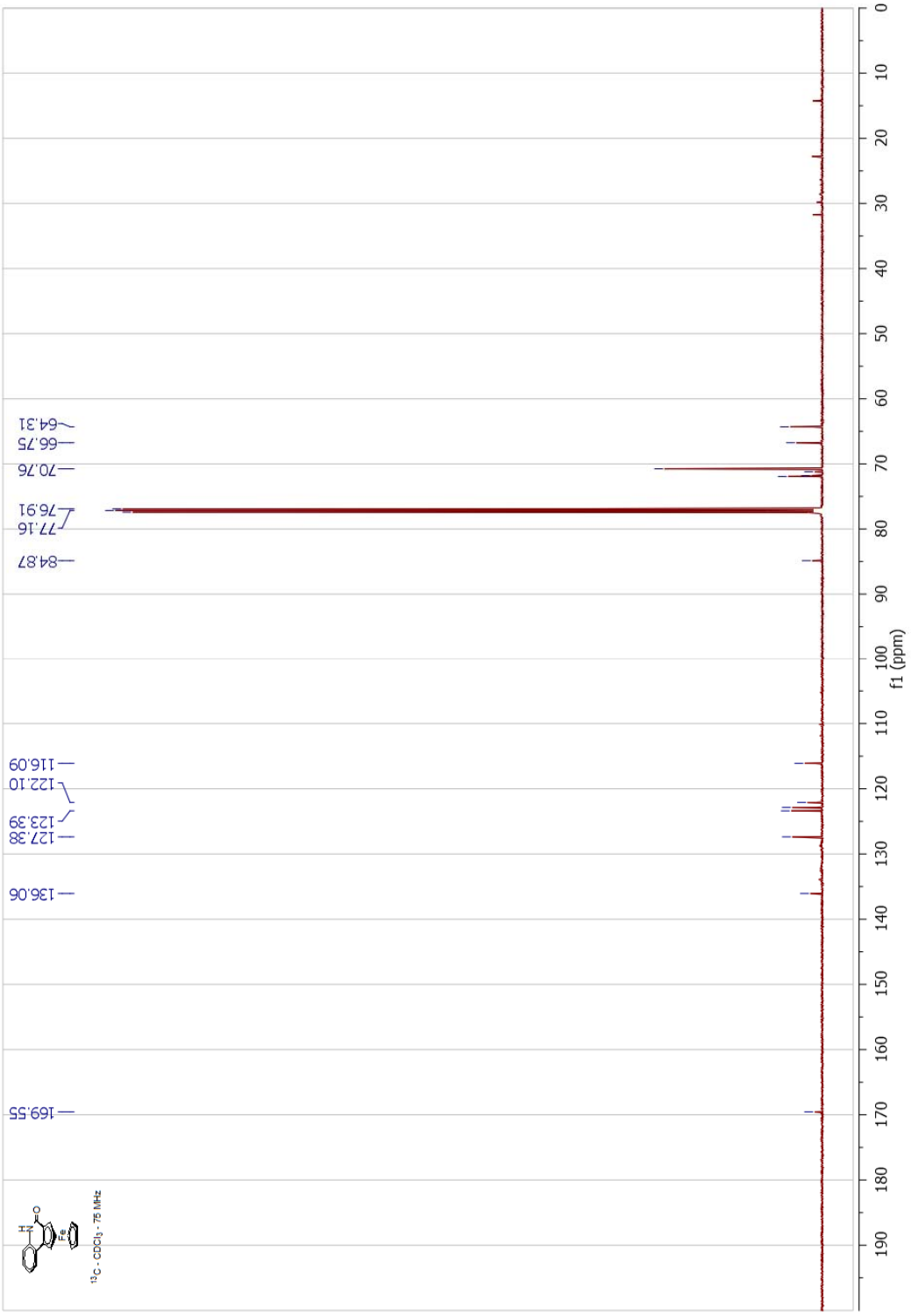
Compound R_P-1, ^{13}C-NMR



Compound S_P-1, ^{1}H-NMR

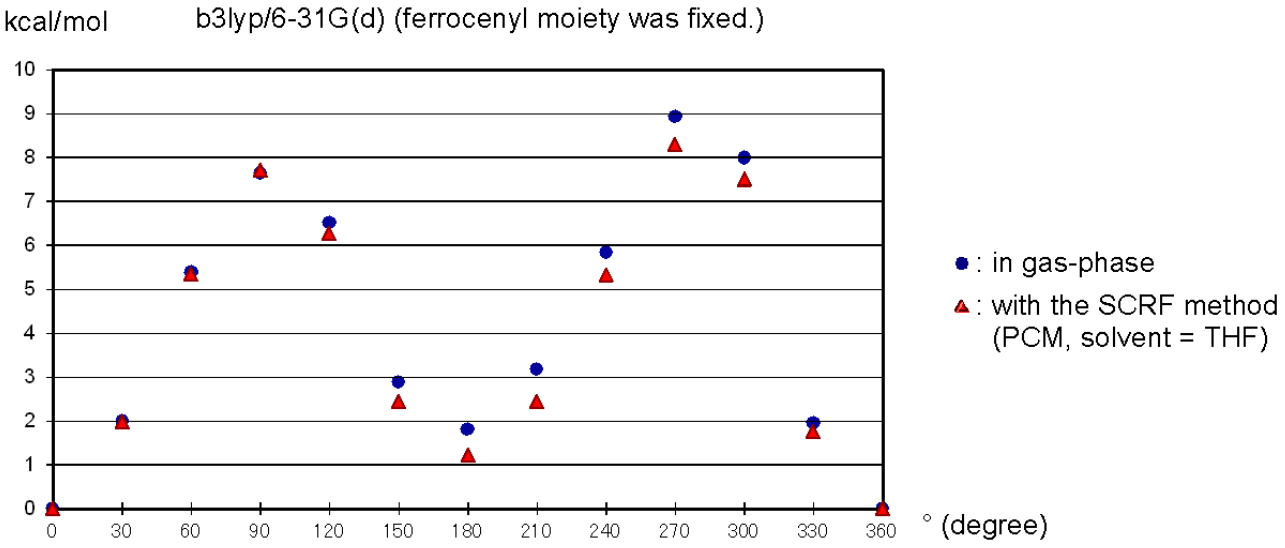


Compound S_P-1, ^{13}C-NMR

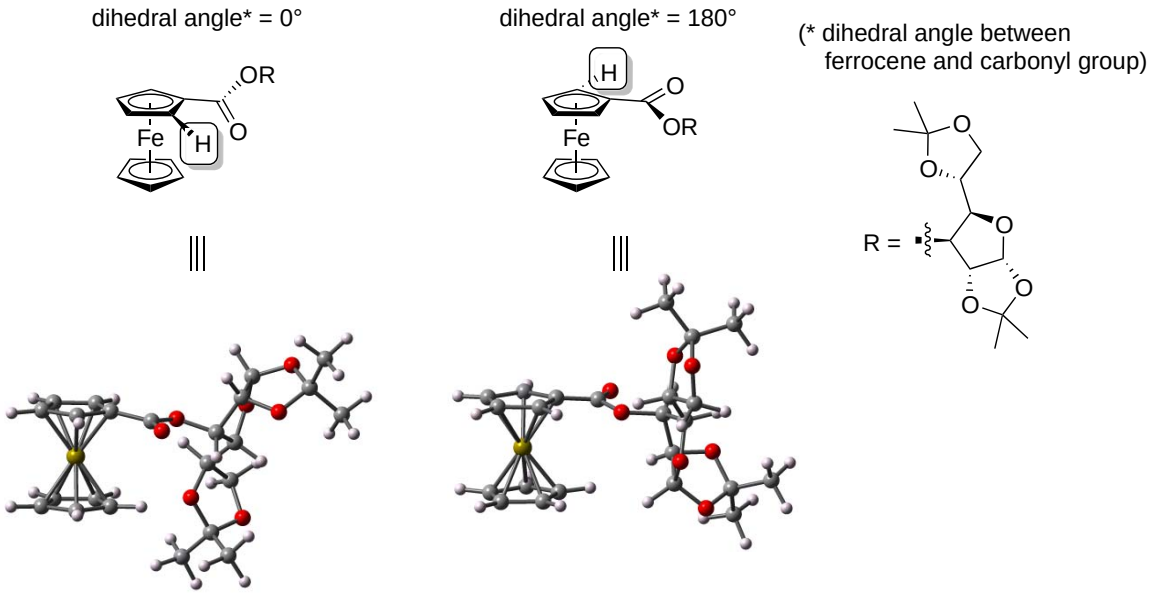


Geometrical Optimization of 3c:

The geometrical (local stabilization) optimization on **3c** was performed by changing the dihedral angle between the upper plane of ferrocenyl moiety and the ester carbonyl group (B3LYP/6-31G(d), the structure of ferrocenyl group was fixed). The dihedral angle was fixed with 30° intervals from 0°, which was defined as the conformation to give the major diastereomer of **4c**. The calculations were done both in gas-phase and with the SCRF method (PCM, solvent = THF), and both gave the similar results as shown in the following graph.



Two conformations were obtained as similarly most stable structures, which had the dihedral angles of 0° and 180° (to give the minor diastereomer).



More detailed calculation was performed starting from these structures (B3LYP or M06/LanL2DZ(Fe)&6-31G(d)). The conformation with the dihedral angle of approx. 0° possessed 2.2 (with B3LYP) or 4.6 (with M06) kcal/mol lower energy than those of approx. 180°, respectively. In THF (with the SCRF method, PCM), the similar differences (1.6 kcal/mol with B3LYP, and 4.0 kcal/mol with M06) were observed. These calculated results were in accordance with the observed diastereoselectivity in deprotonative metalation of **3c** using the lithium-zinc combination.

Computational Details

All calculations were carried with the Gaussian 09 program package.[10] The molecular structures and harmonic vibrational frequencies were obtained using the hybrid density functional method based on Becke's three–parameter exchange function and the Lee–Yang–Parr nonlocal correlation functional (B3LYP)[11] or M06.[12] We used LanL2DZ for Fe and 6–31G(d) for the other atoms. Geometry optimization and vibrational analysis were performed at the same level. All stationary points were optimized without any symmetry assumptions, and characterized by normal coordinate analysis at the same level of theory (number of imaginary frequencies, NIMAG, 0 for minima). The self-consistent reaction field (SCRF) method based on the Polarizable Continuum Model (PCM)[13] was employed to evaluate the solvent reaction field (THF; ε = 7.58).

Cartesian Coordinates and Total Electron Energies

<in gas-phase>

3c (dihedral angle = 0°)
Energy (RB+HF-LYP) = –2683.50292861 A.U.

Fe	3.44318900	-0.69254600	-0.05678000
C	1.85709400	-1.92223700	-0.14256500
C	2.96543500	-2.59231200	0.46718800
H	2.97929300	-2.96629500	1.48509100
C	4.02792700	-2.60750300	-0.47435100
C	3.58545300	-1.94983200	-1.66162600
H	4.18636600	-1.76544800	-2.54596500
C	2.24600700	-1.52020500	-1.46271800
H	1.63352900	-0.95581100	-2.15738200
C	2.87338800	0.90841500	1.06763400
H	1.88125800	1.02239600	1.49645000
C	3.98895700	0.24939500	1.65996000
H	4.00321500	-0.22484600	2.63570000
C	5.05873400	0.26177600	0.71622100
H	6.03290500	-0.19709500	0.85031700
C	4.60080100	0.92549900	-0.46033100
H	5.16729700	1.05897400	-1.37615700
C	3.24919400	1.32434100	-0.24237400
H	2.58931100	1.81297800	-0.95254700
H	5.02295700	-3.00478700	-0.30369600
C	0.59026300	-1.64895400	0.55350600
O	0.34573400	-1.95534700	1.70346600
O	-0.29416400	-0.98910000	-0.25047600
C	-1.51431500	-0.54960400	0.37215500
C	-2.07720300	0.63400500	-0.42112300
C	-2.60284100	-1.60462100	0.16579900
H	-1.33948200	-0.33714700	1.42583900
H	-2.22760500	-2.62954000	0.26218900
C	-3.20488800	-1.26496000	-1.21351800
H	-2.92883800	-1.92013100	-2.04271000
O	-4.59520100	-1.34949100	-1.03379900
C	-4.91420400	-1.46697700	0.36274200
C	-5.82531500	-0.32187200	0.78435400
H	-5.35408400	0.63510300	0.54513500
H	-6.78030100	-0.38584200	0.25417300
H	-6.01671500	-0.36638900	1.86097700
C	-5.52773400	-2.84495100	0.60906000
H	-4.82178400	-3.63033600	0.32153200
H	-5.77568500	-2.96749700	1.66799000
H	-6.43918100	-2.96529400	0.01525600
O	-3.67256600	-1.33942000	1.06231200
O	-2.75383000	0.04147900	-1.54162300
C	-1.05927300	1.63428600	-0.96845900
H	-0.39928700	1.12216800	-1.67297400
H	-2.79477500	1.16575900	0.21952500
O	-0.27743900	2.17601700	0.10078900
C	-1.72791700	2.87295200	-1.57677800
H	-2.72849900	2.67880900	-1.96817800
H	-1.10840100	3.31174200	-2.37205500
C	-0.68373400	3.54378900	0.34263600
C	-1.07709800	3.71019200	1.80393400
H	-1.87870500	3.01074000	2.05570100
H	-0.21772000	3.51499800	2.45245700
H	-1.42904500	4.73025600	1.98660700
C	0.45582200	4.47527800	-0.07603500
H	0.18352500	5.51810100	0.11550600
H	1.36549800	4.23810800	0.48417300
H	0.67235600	4.36287200	-1.14296400
O	-1.84098900	3.74889500	-0.46011400

3c (dihedral angle = 30°)
Energy (RB+HF-LYP) = –2683.49975639 A.U.

Fe	3.54573200	-0.73233800	-0.07494500
C	1.80099100	-1.72731100	-0.10821200
C	2.83936600	-2.57378500	0.39624500
H	2.86196000	-2.99910900	1.39362800
C	3.83074200	-2.68466700	-0.61394900
C	3.41401700	-1.91119400	-1.73912300
H	3.98054400	-1.76452600	-2.65273400
C	2.16222500	-1.31345000	-1.43256900
H	1.59405000	-0.63487600	-2.05942000
C	3.27407100	0.87020200	1.15392500
H	2.33522600	1.09612300	1.65264900
C	4.32008700	0.03459100	1.64101200
H	4.32652100	-0.48774900	2.59195700

C	5.32238700	-0.04989800	0.62934300
H	6.22909400	-0.64410600	0.67785900
C	4.89187500	0.73111300	-0.48384500
H	5.41537200	0.83378300	-1.42876800
C	3.62490300	1.29906700	-0.15883500
H	2.99834800	1.91000000	-0.80129000
H	4.76887500	-3.22272600	-0.52769200
C	0.58280700	-1.38424700	0.64987400
O	0.51225500	-1.30347300	1.85914200
O	-0.45703500	-1.10482500	-0.18969800
C	-1.65917900	-0.58763800	0.41056200
C	-2.17364400	0.60460100	-0.40679200
C	-2.77953000	-1.60777800	0.20806400
H	-1.47817300	-0.36089200	1.45973300
H	-2.43863900	-2.64375800	0.32005300
C	-3.35831500	-1.27325900	-1.18084100
H	-3.08359900	-1.94166800	-1.99968000
O	-4.75051100	-1.34109700	-1.01791900
C	-5.09071900	-1.36812000	0.37777400
C	-5.92462600	-0.14444600	0.73623800
H	-5.38845600	0.76616900	0.45603800
H	-6.87834600	-0.16891700	0.20039200
H	-6.12549000	-0.12372200	1.81191700
C	-5.79951800	-2.68783600	0.67693600
H	-5.14523400	-3.53034100	0.43251200
H	-6.06531500	-2.74510900	1.73706200
H	-6.71162600	-2.77221700	0.07799500
O	-3.84939900	-1.29615900	1.08939600
O	-2.88403900	0.02439300	-1.51330300
C	-1.10996200	1.54099600	-0.98074300
H	-0.48849400	0.98120400	-1.68453400
H	-2.86256800	1.18345500	0.22437800
O	-0.28601500	2.05717800	0.06815400
C	-1.71666800	2.80328000	-1.60410700
H	-2.72928500	2.65699900	-1.98537500
H	-1.08085200	3.19606000	-2.41066900
C	-0.62143500	3.44546900	0.29678000
C	-0.99339800	3.64999400	1.75879400
H	-1.82872600	2.99714500	2.02538700
H	-0.14072300	3.41580900	2.40313800
H	-1.28897500	4.68949100	1.93188300
C	0.55964000	4.31357500	-0.14330400
H	0.33854400	5.37168600	0.02929600
H	1.45941800	4.04520600	0.41913100
H	0.76563000	4.16990200	-1.20862100
O	-1.77335900	3.70047400	-0.50039900

3c (dihedral angle = 60°)
Energy (RB+HF-LYP) = –2683.49434899 A.U.

Fe	3.72710500	-0.64268700	-0.10407100
C	1.83835400	-1.14499500	-0.56829500
C	2.71349100	-2.25266500	-0.80582700
H	2.65636800	-3.20774000	-0.29518900
C	3.67819300	-1.83946700	-1.76198300
C	3.40729900	-0.48335300	-2.11625300
H	3.99672600	0.12483000	-2.79436800
C	2.27391600	-0.04609200	-1.37970500
H	1.83421900	0.94527100	-1.38940300
C	3.72476600	-0.14880400	1.87282800
H	2.83493200	-0.16000100	2.49674000
C	4.60940500	-1.23829400	1.62772300
H	4.52010700	-2.23634600	2.04376900
C	5.58938600	-0.80544400	0.68565300
H	6.38095900	-1.41555600	0.26288900
C	5.30611400	0.55081400	0.34678800
H	5.84584400	1.15083700	-0.37856300
C	4.15256300	0.95574400	1.08079900
H	3.64390000	1.91307400	1.02301200
H	4.51006200	-2.43455200	-2.12379600
C	0.62846900	-1.17266900	0.29068300
O	0.59284000	-1.42944500	1.47574400
O	-0.46725000	-0.80789800	-0.43101200
C	-1.67530400	-0.53997400	0.30571000
C	-2.40979600	0.63615000	-0.35367900
C	-2.66140800	-1.68900200	0.10350100
H	-1.43593700	-0.37886100	1.35542700
H	-2.17499100	-2.67132100	0.08592300
C	-3.41869100	-1.32942300	-1.18636000
H	-3.12046800	-1.85814600	-2.09426500
O	-4.75292200	-1.66429900	-0.92238400
C	-4.96487400	-1.75843800	0.49498700
C	-5.85652100	-0.61833800	0.97410100
H	-5.42652900	0.34095500	0.67463800
H	-6.85331400	-0.70788600	0.53145700
H	-5.95152400	-0.64303900	2.06421100
C	-5.53637400	-3.13997900	0.80128800
H	-4.84269500	-3.91542500	0.46287400
H	-5.69536800	-3.25459300	1.87796600
H	-6.49210400	-3.27842200	0.28611000
O	-3.67145400	-1.61234900	1.10045000
O	-3.20788300	0.06149700	-1.40187400
C	-1.51180200	1.70141800	-0.98801400
H	-0.98136500	1.25471500	-1.83231600
H	-3.05960800	1.10698600	0.39718600
O	-0.55821200	2.17739600	-0.03322800
C	-2.28280200	2.96827700	-1.37499900
H	-3.33532000	2.78575700	-1.60214300
H	-1.81378500	3.47714800	-2.22923200
C	-0.92678900	3.51109700	0.38390900
C	-1.06545000	3.55445100	1.89957000
H	-1.81189100	2.82517400	2.22529400
H	-0.10839400	3.31839300	2.37432600
H	-1.38179500	4.55105600	2.22287800
C	0.11811100	4.49631000	-0.14544400
H	-0.13130900	5.51678800	0.16220400
H	1.10905200	4.24350600	0.24491400
H	0.16226500	4.46146400	-1.23828500
O	-2.20565600	3.75658000	-0.19148500

3c (dihedral angle = 90°)
Energy (RB+HF-LYP) = –2683.49074963 A.U.

Fe	3.79329000	-0.64694900	-0.13375000
C	1.83058200	-0.83522800	-0.52010700
C	2.53406600	-1.99917800	-0.96804400
H	2.37639700	-3.00256800	-0.58716000
C	3.49101700	-1.57948500	-1.92874700
C	3.38677000	-0.16356700	-2.07746600
H	4.01456900	0.45565200	-2.70963600
C	2.36568600	0.30381100	-1.20758500
H	2.06448100	1.33416700	-1.05181200
C	3.96754300	-0.44326300	1.88618200
H	3.12040400	-0.43069400	2.56688900
C	4.68163300	-1.58965800	1.43286200
H	4.48132700	-2.61743200	1.71699900
C	5.65738900	-1.15434800	0.48748300
H	6.33439200	-1.79309700	-0.07033300
C	5.54189300	0.26111700	0.35507200
H	6.11673700	0.88533900	-0.32122800
C	4.49627400	0.69982500	1.21976700
H	4.11943400	1.71216100	1.32831600
H	4.21328300	-2.21724600	-2.42738000
C	0.65521000	-0.79585900	0.39758000
O	0.67697800	-0.70811500	1.60452900
O	-0.49346800	-0.83644400	-0.33622300
C	-1.72853000	-0.56679100	0.35465500
C	-2.46342700	0.59733100	-0.33132100
C	-2.68372600	-1.73473200	0.12159300
H	-1.52459900	-0.39306300	1.40967100
H	-2.17420400	-2.70555700	0.11068500
C	-3.41735400	-1.38925800	-1.18503000
H	-3.08369900	-1.90770300	-2.08661000
O	-4.74832800	-1.76026900	-0.95574000
C	-4.99613400	-1.84878100	0.45574400
C	-5.91203400	-0.71618700	0.90683900
H	-5.48577600	0.24673200	0.61393200
H	-6.89633100	-0.81899000	0.43975200
H	-6.03423700	-0.73720700	1.99433200
C	-5.56058900	-3.23471600	0.75435400
H	-4.85089600	-4.00429700	0.43646700
H	-5.74504100	-3.34609300	1.82730100
H	-6.50195300	-3.38516400	0.21659900
O	-3.71954900	-1.68682100	1.09384800
O	-3.23782900	0.00706200	-1.38893900
C	-1.56309600	1.66331900	-0.96319600
H	-1.01815800	1.21220100	-1.79606900
H	-3.13186100	1.07057200	0.40127100
O	-0.62380400	2.15653100	-0.00418600
C	-2.33741100	2.92142900	-1.36997000
H	-3.38370700	2.72959800	-1.61728200
H	-1.85528200	3.43188600	-2.21599300
C	-1.01995700	3.48230200	0.41398300
C	-1.18821200	3.51452900	1.92683600
H	-1.93674700	2.77916700	2.23333200
H	-0.23934900	3.27792800	2.41714900
H	-1.51567900	4.50721400	2.25133200
C	0.02148600	4.48409700	-0.08985100
H	-0.24842400	5.49954600	0.21708700
H	1.00756100	4.24329900	0.31994300
H	0.08747100	4.45469700	-1.18178000
O	-2.29026700	3.71297800	-0.18679800

3c (dihedral angle = 120°)
Energy (RB+HF-LYP) = –2683.49255813 A.U.

Fe	-4.02360100	-0.13894400	-0.10529700
C	-2.08352300	-0.61895300	-0.30750700
C	-2.59937700	-0.12638400	-1.54867200
H	-2.25005500	0.76773000	-2.05336800
C	-3.66768200	-0.97712200	-1.93672400
C	-3.81772500	-1.99142200	-0.94343700
H	-4.57771400	-2.76571600	-0.93746400
C	-2.84460000	-1.77438000	0.06858000
H	-2.71690800	-2.34512700	0.98190800
C	-4.11512200	1.30712700	1.32737700
H	-3.24547100	1.69020000	1.85478600
C	-4.64560700	1.78598000	0.09492600
H	-4.25536500	2.61474500	-0.48648300
C	-5.73392900	0.94030900	-0.27333500
H	-6.32139800	1.01630500	-1.18254300
C	-5.87178600	-0.06306300	0.73102900
H	-6.58313500	-0.88237700	0.71763700
C	-4.86993600	0.16413400	1.72001700
H	-4.66759800	-0.44304800	2.59691400
H	-4.29647500	-0.84939900	-2.81156400
C	-0.95258100	-0.06076400	0.48236800

O	-1.00321800	0.35629600	1.62022900
O	0.17924700	-0.03611700	-0.27158500
C	1.37885500	0.44973700	0.36597000
C	2.59071100	-0.14324500	-0.36006000
C	1.53680200	1.94138000	0.06536500
H	1.34749600	0.23403300	1.43251500
H	0.58788200	2.48916000	0.10360100
C	2.24395700	1.97679800	-1.30540300
H	1.62695900	2.23898900	-2.16773600
O	3.23706100	2.95996800	-1.17237300
C	3.41884000	3.30839300	0.20908300
C	4.83635300	2.96824900	0.65233700
H	5.04351200	1.91248000	0.45852600
H	5.55964000	3.57491500	0.09904800
H	4.95683200	3.16481300	1.72219900
C	3.07161600	4.78536900	0.38568300
H	2.03499000	4.96638700	0.08519900
H	3.19109800	5.08146000	1.43248800
H	3.72592000	5.40580500	-0.23463700
O	2.50276900	2.49087600	0.94862200
O	2.75467500	0.67196500	-1.53218300
C	2.46163400	-1.60061100	-0.80126100
H	1.61658600	-1.69495100	-1.48817100
H	3.46641700	-0.04576200	0.29670900
O	2.23526500	-2.42012200	0.34764300
C	3.76555800	-2.15750300	-1.38882300
H	4.40484300	-1.39129100	-1.83222900
H	3.56359200	-2.93557100	-2.13861700
C	3.41169000	-3.21505700	0.60465000
C	3.85148700	-3.02182300	2.04949900
H	4.05477000	-1.96406000	2.23674100
H	3.06541800	-3.35867300	2.73192000
H	4.76093800	-3.59688900	2.24965200
C	3.10144400	-4.67628600	0.26921300
H	3.97670000	-5.30550700	0.46050100
H	2.26738600	-5.03474700	0.88049900
H	2.81963700	-4.77903800	-0.78313500
O	4.42603400	-2.69255400	-0.24690400

3c (dihedral angle = 150°)
Energy (RB+HF-LYP) = –2683.49834465 A.U.

Fe	-3.85233900	-0.40038700	-0.08509100
C	-2.05158500	-1.25252000	0.17249800
C	-2.40109200	-1.25334200	-1.21568900
H	-1.85022300	-0.73573300	-1.99338200
C	-3.60900800	-1.98658300	-1.35320600
C	-4.01036700	-2.43776800	-0.05965200
H	-4.91682900	-2.98940300	0.16656400
C	-3.05474500	-1.98471000	0.88891700
H	-3.08768100	-2.12486100	1.96385900
C	-3.69264600	1.50933000	0.60739400
H	-2.78342900	1.92156600	1.03702400
C	-4.05969700	1.50260400	-0.76915200
H	-3.47964500	1.92237100	-1.58432800
C	-5.28687800	0.78579600	-0.89336900
H	-5.80793300	0.56906900	-1.82023800
C	-5.67446600	0.34689300	0.40726400
H	-6.54220000	-0.26147400	0.64049900
C	-4.68772000	0.79412700	1.33448200
H	-4.65402800	0.59304200	2.40077900
H	-4.16082800	-2.13551700	-2.27535300
C	-0.93153200	-0.54108100	0.82087300
O	-0.92713800	-0.12727800	1.96304200
O	0.10163400	-0.35675200	-0.04794400
C	1.25032300	0.35113200	0.45682900
C	2.45927200	0.00251900	-0.41558400
C	1.09033800	1.84829400	0.17362700
H	1.38468800	0.13876900	1.51612900
H	0.05815300	2.19648600	0.29637400
C	1.66183300	2.02238700	-1.25631100
H	0.93886400	2.24182500	-2.04595600
O	2.56708900	3.09811000	-1.15698700
C	2.63255600	3.57408100	0.19530900
C	4.08772600	3.68140600	0.62651700
H	4.58182000	2.71346500	0.50851000
H	4.60839300	4.42110300	0.01119000
H	4.15055700	3.98842100	1.67493700
C	1.87661900	4.90005100	0.29965800
H	0.83075400	4.76749300	0.00416200
H	1.90334700	5.27422400	1.32790500
H	2.32788200	5.64648500	-0.36132900
O	1.99610300	2.57134100	0.99163400
O	2.28786900	0.80195200	-1.59775000
C	2.59802600	-1.45918100	-0.83645900
H	1.71540200	-1.75523400	-1.40976500
H	3.36779900	0.30954800	0.12124400
O	2.70212800	-2.27676100	0.33019500
C	3.90965700	-1.73293300	-1.58496300
H	4.30136900	-0.85887900	-2.10928800
H	3.79533500	-2.56052600	-2.29957000
C	4.05095300	-2.77702600	0.44244800
C	4.60726300	-2.43849000	1.81873000
H	4.58497000	-1.35622600	1.97170200
H	4.00723500	-2.91944500	2.59698400
H	5.64131800	-2.78637100	1.90659800
C	4.04214200	-4.28152300	0.15944900
H	5.05379800	-4.69120300	0.24393300
H	3.39098200	-4.79574800	0.87311100
H	3.66631800	-4.48189700	-0.84854200
O	4.80891700	-2.07086900	-0.53457100

3c (dihedral angle = 180°)
Energy (RB+HF-LYP) = –2683.50003854 A.U.

Fe	-3.75531700	-0.32190000	-0.10015600
C	-2.11141200	-1.09869700	0.75398300
C	-2.33295700	-1.70326200	-0.52461100
H	-1.65201700	-1.63922800	-1.36631900
C	-3.60908700	-2.32438200	-0.48987000
C	-4.17961500	-2.10669400	0.80049400
H	-5.16688400	-2.42434800	1.11917800
C	-3.26143200	-1.34666200	1.57351800
H	-3.40815900	-0.98016800	2.58365600
C	-3.41006500	1.67553900	-0.30775600
H	-2.49677800	2.16718800	0.01686700
C	-3.65062900	1.07230800	-1.57578500
H	-2.95038300	1.03033100	-2.40346600
C	-4.94488900	0.47332000	-1.53917200
H	-5.40503600	-0.10028600	-2.33715600
C	-5.50087900	0.70413900	-0.24607500
H	-6.45792500	0.33633900	0.10926300
C	-4.55083400	1.44695700	0.51488400
H	-4.63890600	1.75025500	1.55354900
H	-4.09117400	-2.83334600	-1.31786500
C	-0.93340400	-0.34252500	1.21156200
O	-0.80674600	0.14775900	2.31566000
O	0.02251000	-0.26182800	0.24185200
C	1.26126000	0.36837700	0.61730800
C	2.33753200	-0.03027500	-0.39693500
C	1.16998500	1.87945100	0.38409100
H	1.50761200	0.12233900	1.64926500
H	0.19270200	2.29575100	0.65338900
C	1.56259000	2.05562600	-1.10179400
H	0.75638500	2.31650500	-1.79165100
O	2.50987000	3.09653900	-1.10716500
C	2.82685200	3.49461300	0.23596400
C	4.33464000	3.45400300	0.44004400
H	4.71259800	2.45347300	0.21400600
H	4.82335700	4.17398800	-0.22310900
H	4.58371100	3.70367900	1.47594400
C	2.22192500	4.87394700	0.50114900
H	1.13546800	4.84408400	0.37023700
H	2.44164600	5.19632600	1.52373400
H	2.63271100	5.60866000	-0.19830200
O	2.22794900	2.51332600	1.08647400
O	2.09169100	0.81481200	-1.53321600
C	2.32790700	-1.48285300	-0.86811200
H	1.37251700	-1.69694500	-1.35496900
H	3.31975100	0.19677300	0.04099700
O	2.49190200	-2.34442600	0.25905700
C	3.53150300	-1.82088600	-1.76022400
H	3.93769600	-0.95491600	-2.28698900
H	3.27825600	-2.60074500	-2.49252200
C	3.79169200	-2.96716600	0.19798600
C	4.52078300	-2.75232400	1.51699600
H	4.61701200	-1.68186700	1.71688000
H	3.96463300	-3.21820800	2.33592800
H	5.52073800	-3.19506300	1.47420500
C	3.61390800	-4.44814000	-0.14753600
H	4.58670200	-4.94814100	-0.19378800
H	2.99819100	-4.94087800	0.61127900
H	3.11550800	-4.56144200	-1.11514200
O	4.50233300	-2.27833000	-0.82562700

3c (dihedral angle = 210°)
Energy (RB+HF-LYP) = –2683.49788006 A.U.

Fe	3.64266200	0.09413600	-0.11223300
C	2.22453400	0.59057700	1.22132800
C	2.46782100	1.68568400	0.33172300
H	1.73297100	2.10944300	-0.34421500
C	3.83427600	2.04801000	0.46095500
C	4.43908200	1.18357500	1.42264600
H	5.48605800	1.18546800	1.70731300
C	3.45141900	0.27780000	1.89414000
H	3.59533900	-0.53197300	2.60114300
C	2.93073700	-1.51397600	-1.14139100
H	1.96699600	-1.97696500	-0.94637800
C	3.19283000	-0.42740800	-2.02475900
H	2.45917400	0.08498300	-2.63823000
C	4.57337700	-0.08777500	-1.90634900
H	5.07627300	0.72582800	-2.41884200
C	5.16176300	-0.96320500	-0.94619400
H	6.19047200	-0.93048300	-0.60240700
C	4.14514800	-1.84423500	-0.47321700
H	4.24467200	-2.60414900	0.29570300
H	4.34511600	2.81614600	-0.11002900
C	0.92975700	-0.05108500	1.51580100
O	0.63995400	-0.57597200	2.57086900
O	0.05831200	0.05747200	0.47062100
C	-1.29170300	-0.37688700	0.72168400
C	-2.19521200	0.16974900	-0.38811700
C	-1.41002200	-1.88718500	0.49362600
H	-1.59613400	-0.08771500	1.72691900
H	-0.53664300	-2.44255400	0.85177900
C	-1.68944000	-2.02073500	-1.02159200

H	-0.87303200	-2.40652800	-1.63726100
O	-2.77536200	-2.91001600	-1.11533900
C	-3.27496800	-3.23298200	0.19231300
C	-4.77052200	-2.95578700	0.25274200
H	-4.96570800	-1.91375800	-0.01387900
H	-5.30237400	-3.60497600	-0.44917800
H	-5.14945000	-3.14309900	1.26211900
C	-2.92023300	-4.68532200	0.51389000
H	-1.83495600	-4.82615500	0.48799000
H	-3.28310400	-4.95430500	1.51075300
H	-3.37258100	-5.35753600	-0.22182100
O	-2.61262600	-2.34401100	1.09500200
O	-1.98623100	-0.71955200	-1.49720300
C	-1.91449300	1.59405200	-0.86331400
H	-0.90468100	1.63990300	-1.28053500
H	-3.23615700	0.10708500	-0.04092000
O	-2.01561500	2.49464400	0.24011500
C	-2.97874900	2.10602900	-1.84371500
H	-3.47300500	1.30901900	-2.40307600
H	-2.55320000	2.83160800	-2.55177500
C	-3.20647300	3.29682700	0.09324500
C	-4.05056100	3.19219600	1.35592500
H	-4.30814500	2.14652600	1.54405600
H	-3.49541000	3.58124700	2.21469700
H	-4.97411300	3.76863900	1.24370800
C	-2.79356700	4.73568800	-0.22720000
H	-3.67864600	5.37060300	-0.33679700
H	-2.16786600	5.13643900	0.57632500
H	-2.21866800	4.77424300	-1.15762200
O	-3.93483700	2.71541400	-0.98363100

3c (dihedral angle = 240°)
Energy (RB+HF-LYP) = –2683.49363759 A.U.

Fe	3.46678200	-0.43026200	-0.11946700
C	2.17499900	-0.29327300	1.41276300
C	2.61789300	1.01184100	1.02579600
H	1.97427000	1.79577400	0.64189300
C	4.02904100	1.04810100	1.17731700
C	4.46259300	-0.22598100	1.65343100
H	5.49202400	-0.52131200	1.82721600
C	3.32272500	-1.06152400	1.79774000
H	3.31300200	-2.10230600	2.10254200
C	2.45741200	-1.32168600	-1.64871300
H	1.42404400	-1.65104800	-1.57894700
C	2.91756000	-0.02999900	-2.03531100
H	2.29209700	0.80744400	-2.32627900
C	4.33798900	-0.01184500	-1.90389200
H	4.98424600	0.84128600	-2.08298300
C	4.75330200	-1.29222900	-1.43204700
H	5.77094100	-1.58127400	-1.19051900
C	3.58972700	-2.10123700	-1.27386800
H	3.54621700	-3.11547700	-0.88918500
H	4.67418200	1.88331600	0.92582100
C	0.75849000	-0.67358600	1.61655100
O	0.29447200	-1.08805900	2.65617200
O	-0.00280800	-0.38422000	0.52211300
C	-1.42928500	-0.37743800	0.71553700
C	-2.06131200	0.46070800	-0.40140500
C	-2.01744600	-1.76291300	0.43882200
H	-1.66423800	-0.02909900	1.72066600
H	-1.37967400	-2.57808900	0.79764100
C	-2.28379800	-1.76993200	-1.08310300
H	-1.61065700	-2.37625800	-1.69414700
O	-3.58575400	-2.28002000	-1.22405000
C	-4.20920000	-2.42872000	0.06214600
C	-5.53021100	-1.67217600	0.08441500
H	-5.36198800	-0.62266300	-0.17119500
H	-6.22386300	-2.10502000	-0.64259600
H	-5.98245400	-1.72894000	1.07937000
C	-4.36582000	-3.91915100	0.36462700
H	-3.38779900	-4.41076800	0.36717100
H	-4.83129500	-4.06202500	1.34476100
H	-4.98963000	-4.39674700	-0.39732600
O	-3.32086600	-1.81737300	1.00103100
O	-2.15230500	-0.42905900	-1.52580500
C	-1.27094300	1.69121200	-0.84886000
H	-0.33465900	1.35998000	-1.30527900
H	-3.06533400	0.76790300	-0.07626600
O	-0.97910800	2.52228600	0.27692000
C	-2.08258400	2.61159000	-1.76824500
H	-2.85557500	2.08892000	-2.33572200
H	-1.43029100	3.15544200	-2.46637800
C	-1.79260200	3.71487900	0.21224800
C	-2.57749200	3.86855300	1.50766500
H	-3.20117700	2.98564200	1.67122500
H	-1.89261500	3.98109000	2.35342300
H	-3.22242800	4.75136400	1.45755100
C	-0.88521800	4.91258700	-0.07862500
H	-1.47505900	5.83343300	-0.12759200
H	-0.13253100	5.01717200	0.70909600
H	-0.36507900	4.77983400	-1.03231700
O	-2.71562300	3.49551600	-0.84956100

3c (dihedral angle = 270°)
Energy (RB+HF-LYP) = –2683.4887166 A.U.

Fe	3.43345400	-0.46385100	-0.14482200
C	2.22627500	-0.37032700	1.45804100
C	2.93332500	0.86471000	1.30317600
H	2.46735900	1.82575400	1.11488800
C	4.32147500	0.57604600	1.37615700
C	4.47833800	-0.82913700	1.57312000
H	5.42277100	-1.36048200	1.62665800
C	3.18786000	-1.42128300	1.62094600
H	2.95932900	-2.47677100	1.72067100
C	2.23140200	-0.80240500	-1.75494900
H	1.15263200	-0.91707600	-1.68936600
C	2.95241700	0.41611700	-1.91303300
H	2.51719500	1.40607000	-2.00107800
C	4.34540900	0.11220100	-1.86376000
H	5.15712700	0.83067000	-1.91346300
C	4.48303800	-1.29437500	-1.67112200
H	5.41840100	-1.83078000	-1.54932000
C	3.17534500	-1.85895600	-1.60323700
H	2.92082200	-2.89796300	-1.41819000
H	5.12708100	1.29205000	1.25214900
C	0.76182700	-0.47747600	1.72312000
O	0.28544800	-0.50280000	2.83501600
O	0.01550100	-0.48191000	0.58548400
C	-1.41541800	-0.40556800	0.73711700
C	-1.98034000	0.42592500	-0.41808900
C	-2.02942700	-1.78157500	0.45902100
H	-1.66464900	-0.03085100	1.72815100
H	-1.40542400	-2.60525700	0.82521700
C	-2.26286100	-1.78751800	-1.07504500
H	-1.63684400	-2.46613700	-1.65945900
O	-3.61475600	-2.15058900	-1.23623300
C	-4.22233300	-2.39396600	0.04023300
C	-5.55589300	-1.66544600	0.11184500
H	-5.40648200	-0.59916700	-0.07696500
H	-6.24326000	-2.06462600	-0.63982300
H	-6.00418300	-1.79292600	1.10187500
C	-4.35031000	-3.90232700	0.26251100
H	-3.36542800	-4.37954600	0.22748400
H	-4.80096000	-4.10706800	1.23869900
H	-4.97530300	-4.34807500	-0.51746200
O	-3.33812400	-1.81869600	1.00542100
O	-1.98711300	-0.47896300	-1.53538300
C	-1.18168800	1.66599200	-0.81649100
H	-0.21404700	1.35358200	-1.21771800
H	-3.00773600	0.72036500	-0.16049900
O	-0.97027000	2.49227700	0.32973500
C	-1.95118100	2.58054000	-1.77765200
H	-2.68271800	2.05057500	-2.39156100
H	-1.26660900	3.13666700	-2.43377500
C	-1.79275800	3.67532900	0.22253500
C	-2.65425800	3.81326900	1.47004200
H	-3.27830900	2.92376100	1.59068800
H	-2.02157400	3.92525100	2.35552000
H	-3.30303500	4.69083600	1.38761900
C	-0.88399200	4.88499000	-0.00901700
H	-1.48076200	5.79924900	-0.08808200
H	-0.18046700	4.99343600	0.82233600
H	-0.30699200	4.76365400	-0.93100800
O	-2.64884300	3.45022600	-0.89299500

3c (dihedral angle = 300°)
Energy (RB+HF-LYP) = –2683.49019854 A.U.

Fe	3.42553500	-0.53360700	-0.14605100
C	2.07249800	-1.69097800	0.78493000
C	3.25503200	-1.57956800	1.58281700
H	3.29506400	-1.13501900	2.57142500
C	4.33787600	-2.08915800	0.81927600
C	3.83419800	-2.51321700	-0.44738200
H	4.42687100	-2.90952900	-1.26503000
C	2.43545800	-2.26645300	-0.47814600
H	1.76213900	-2.43979300	-1.31042000
C	2.55566400	1.29309600	-0.38712000
H	1.54329800	1.52594500	-0.06800100
C	3.74392200	1.40121200	0.39050600
H	3.80261600	1.74572000	1.41757100
C	4.82958800	0.91055200	-0.39442700
H	5.86135400	0.82147700	-0.07080200
C	4.30894700	0.49604400	-1.65603900
H	4.87741300	0.03689800	-2.45837800
C	2.90273000	0.73219900	-1.65068600
H	2.19596600	0.48800200	-2.43782300
H	5.37884000	-2.10633100	1.12500900
C	0.67978000	-1.39113700	1.21168100
O	0.12306500	-1.96170400	2.12689100
O	0.00616900	-0.59327600	0.33302300
C	-1.40839700	-0.44965000	0.59282500
C	-2.00342400	0.58876900	-0.36594100
C	-2.17691600	-1.71273600	0.17838300
H	-1.56543000	-0.21295600	1.64433900
H	-1.62274900	-2.63671200	0.36630200
C	-2.54855400	-1.47254900	-1.30419500
H	-2.02534100	-2.08626900	-2.04185600
O	-3.92846500	-1.74221500	-1.38499700
C	-4.44529800	-2.08399600	-0.08915200
C	-5.69379900	-1.26111500	0.19281700
H	-5.46086900	-0.19577100	0.11600600
H	-6.47663600	-1.50508300	-0.53140400
H	-6.06680000	-1.47294600	1.19947800
C	-4.69439100	-3.59218500	-0.02935400

H	-3.76368300	-4.13996500	-0.20887400
H	-5.08072500	-3.87572700	0.95462500
H	-5.41981200	-3.88683500	-0.79403500
O	-3.43260300	-1.70459100	0.84386400
O	-2.23017700	-0.12457800	-1.59098800
C	-1.14951700	1.80748600	-0.70158400
H	-0.27848800	1.47853700	-1.27442500
H	-2.95974800	0.92208700	0.06263400
O	-0.72070100	2.44561300	0.50254900
C	-1.94016200	2.90454600	-1.42855800
H	-2.80174100	2.52397600	-1.98127400
H	-1.29583100	3.47316100	-2.11369300
C	-1.39275800	3.71920300	0.63375700
C	-2.05637800	3.80034000	2.00104200
H	-2.75668100	2.96972300	2.12236000
H	-1.30193600	3.74840800	2.79166200
H	-2.60474000	4.74222700	2.10013600
C	-0.37932000	4.84074800	0.39533400
H	-0.86472700	5.81723600	0.49099900
H	0.43319000	4.77683200	1.12564200
H	0.05678700	4.76300000	-0.60510600
O	-2.41131300	3.71759600	-0.35964500

3c (dihedral angle = 330°)
Energy (RB+HF-LYP) = –2683.49980555 A.U.

Fe	3.43985700	-0.61642100	-0.11363100
C	1.97066200	-1.89063900	0.38939100
C	3.14234400	-2.16097000	1.16611600
H	3.20221100	-2.07888200	2.24586700
C	4.19047200	-2.48125000	0.26364100
C	3.67606700	-2.40907600	-1.06606500
H	4.24716700	-2.56040600	-1.97606100
C	2.30571700	-2.04088300	-0.99655800
H	1.63637300	-1.86308700	-1.83118100
C	2.74102100	1.25655100	0.28091000
H	1.74786500	1.46018300	0.67253800
C	3.91869000	0.98961500	1.03688100
H	3.98752500	0.96334300	2.11935500
C	4.97155000	0.69401100	0.12073700
H	5.98479700	0.40849700	0.38411500
C	4.44133300	0.77490700	-1.20094100
H	4.98238900	0.56171000	-2.11706100
C	3.06188700	1.12208900	-1.10086700
H	2.35200800	1.22106100	-1.91624100
H	5.21935300	-2.69416200	0.53403400
C	0.66343300	-1.52178400	0.96484300
O	0.26100700	-1.88235700	2.05196700
O	-0.10497700	-0.81564200	0.08370800
C	-1.44269500	-0.50593100	0.52065300
C	-2.01283700	0.59169200	-0.38184500
C	-2.37550300	-1.67763500	0.19843900
H	-1.44161300	-0.25587600	1.58038300
H	-1.91034400	-2.65465700	0.36786600
C	-2.81895200	-1.41743800	-1.25949600
H	-2.39137500	-2.07098600	-2.02337800
O	-4.21415400	-1.59172100	-1.25306800
C	-4.68962700	-1.79115000	0.08818100
C	-5.78787700	-0.78364800	0.39806200
H	-5.41321600	0.23198900	0.24542400
H	-6.64508600	-0.94623500	-0.26208000
H	-6.11764400	-0.88975700	1.43613600
C	-5.14505300	-3.24279600	0.24058700
H	-4.31328400	-3.92484200	0.03765000
H	-5.50498800	-3.42452900	1.25806200
H	-5.95143200	-3.46292300	-0.46584100
O	-3.57516900	-1.52313400	0.94272600
O	-2.42029500	-0.09368600	-1.57615400
C	-1.05708900	1.71309800	-0.77951800
H	-0.22378300	1.29098200	-1.34737800
H	-2.88476400	1.02948100	0.12457300
O	-0.55738300	2.34644500	0.40166900
C	-1.76140000	2.85394100	-1.52712400
H	-2.66030500	2.53385800	-2.05789200
H	-1.08092400	3.34696700	-2.23587500
C	-1.11508600	3.67713300	0.50308300
C	-1.74497000	3.85827000	1.87673600
H	-2.51567100	3.09943900	2.03538500
H	-0.98439500	3.76148100	2.65722600
H	-2.20327900	4.84901500	1.95456700
C	-0.01349000	4.69987900	0.21467400
H	-0.41286600	5.71660600	0.28621200
H	0.80352600	4.58970800	0.93431700
H	0.39737200	4.55543400	-0.78908200
O	-2.14571300	3.73329700	-0.47589200

3c (to give the major diastereomer of **4c**)
Energy (RB+HF-LYP) = –1543.29573099 A.U.

Fe	3.49085300	-0.67803200	-0.09296800
C	1.87476500	-1.92680000	0.22088000
C	3.01386400	-2.41531700	0.94392900
H	3.06465700	-2.52080000	2.01834700
C	4.04010600	-2.69424500	0.00161800
C	3.54727700	-2.38043200	-1.30429000
H	4.10607400	-2.45684500	-2.22776600
C	2.21347400	-1.90310000	-1.17543800
H	1.56822000	-1.56444800	-1.97328700
C	2.94353800	1.28105600	0.35439000
H	1.93043600	1.58118600	0.59168600
C	3.93081100	0.81937800	1.27797400
H	3.79987200	0.71614300	2.34705300
C	5.10192600	0.47160800	0.53780100
H	6.01427100	0.05821800	0.94753400
C	4.83887400	0.71426800	-0.84426400
H	5.51768900	0.52020400	-1.66441000
C	3.50535800	1.21436400	-0.95619000
H	2.99738800	1.46573400	-1.87801200
H	5.03632000	-3.04641900	0.23463600
C	0.62511100	-1.49512600	0.86611700
O	0.40185600	-1.55894600	2.05790300
O	-0.27539100	-1.02336100	-0.04691800
C	-1.53935200	-0.56811100	0.46655100
C	-2.05234400	0.58172600	-0.40610300
C	-2.59347700	-1.64573200	0.19660100
H	-1.44709000	-0.32341600	1.52329500
H	-2.20784300	-2.66200500	0.33918300
C	-3.08419300	-1.34053700	-1.23868500
H	-2.76077100	-2.03035300	-2.02160400
O	-4.48793700	-1.37894800	-1.15868600
C	-4.90941400	-1.55209100	0.20284000
C	-5.90160400	-0.45873600	0.57502100
H	-5.45072200	0.52327000	0.40881600
H	-6.80197500	-0.54212800	-0.04101200
H	-6.18580400	-0.54702300	1.62819400
C	-5.47885100	-2.96188400	0.37100400
H	-4.72038800	-3.71027200	0.11966000
H	-5.79900300	-3.12284500	1.40524000
H	-6.33724700	-3.10575700	-0.29259900
O	-3.73444400	-1.38869700	1.00019800
O	-2.57883300	-0.06092000	-1.57759500
C	-1.01880800	1.61304100	-0.85430500
H	-0.24176800	1.11431600	-1.43925400
H	-2.85653400	1.09401900	0.14077300
O	-0.42357000	2.22571700	0.29367300
C	-1.65411900	2.79653000	-1.59516900
H	-2.58378400	2.53965500	-2.10668100
H	-0.95346500	3.23747600	-2.31873900
C	-0.91077500	3.58223400	0.41815800
C	-1.50430200	3.78441500	1.80588200
H	-2.31116800	3.06604400	1.97348600
H	-0.73558400	3.63969600	2.57089400
H	-1.90823900	4.79723500	1.90064400
C	0.23719200	4.54881500	0.11613500
H	-0.10618900	5.58424900	0.20775900
H	1.06436400	4.38833200	0.81466400
H	0.61471100	4.39486900	-0.89941300
O	-1.95405000	3.70372600	-0.54040600

3c (to give the minor diastereomer of **4c**)
Energy (RB+HF-LYP) = –1543.29229946 A.U.

Fe	-3.72188500	-0.26956500	-0.11450500
C	-1.96150700	-1.20512900	0.43616400
C	-2.21738800	-1.42703000	-0.95953500
H	-1.58151100	-1.10885600	-1.77313500
C	-3.45989300	-2.11045500	-1.06786800
C	-3.97826000	-2.31105800	0.25038000
H	-4.92500200	-2.77428200	0.49486500
C	-3.06029000	-1.75126400	1.18001700
H	-3.15763900	-1.71468000	2.25577200
C	-3.58259500	1.76159600	0.30525500
H	-2.71755800	2.22566600	0.76097500
C	-3.79427700	1.56341600	-1.09319000
H	-3.12167000	1.85811800	-1.88783400
C	-5.03268000	0.87064900	-1.25582300
H	-5.46026200	0.54488600	-2.19495500
C	-5.58371700	0.64071300	0.04092100
H	-6.50146400	0.10923800	0.25585600
C	-4.68690500	1.19098900	1.00678200
H	-4.80416500	1.15193300	2.08152900
H	-3.94692600	-2.39653500	-1.99080000
C	-0.81996700	-0.50967900	1.05248200
O	-0.68056500	-0.32282600	2.24348800
O	0.08268300	-0.10533800	0.10967300
C	1.27969900	0.53402900	0.58233800
C	2.46687700	0.09127300	-0.28286400
C	1.20592200	2.02898300	0.25492900
H	1.40821200	0.34254200	1.64659600
H	0.19224200	2.43439800	0.35923300
C	1.79118000	2.13372600	-1.17596200
H	1.08374800	2.36906100	-1.97488200
O	2.75173000	3.16112400	-1.10134500
C	2.84362300	3.66567300	0.23824600
C	4.30223900	3.69421500	0.67253800
H	4.73403600	2.69370300	0.58487900
H	4.87028500	4.38120000	0.03820600
H	4.38175200	4.02666900	1.71210300
C	2.17097300	5.03851800	0.30598200
H	1.11939300	4.96256000	0.01047300
H	2.21900500	5.43713000	1.32424500
H	2.66833500	5.73826000	-0.37285800
O	2.14529000	2.72537600	1.05719100
O	2.35315300	0.87292000	-1.48104700
C	2.51141600	-1.37513400	-0.68023900

H	1.58729300	-1.63944900	-1.20939000
H	3.39131000	0.34407700	0.25578900
O	2.65605700	-2.15564300	0.50393600
O	3.90102100	-3.14946700	-1.14788100
C	3.73795100	-1.78174900	-1.49956000
H	4.61977000	-1.18395300	-1.22051600
H	3.59034500	-1.71484600	-2.57934300
C	3.46814600	-3.30626700	0.20502000
C	2.62713900	-4.57581200	0.28908600
H	2.26201600	-4.72278000	1.31021500
H	1.77016900	-4.49705100	-0.38594700
H	3.22353600	-5.44657700	-0.00182300
C	4.65957800	-3.30962500	1.16243900
H	4.31340000	-3.33957900	2.20051300
H	5.29468600	-4.18147000	0.97604400
H	5.25714800	-2.40334500	1.02398100

3c (to give the major diastereomer of **4c**)
Energy (RM06) = –1542.42061652 A.U.

Fe	3.30260800	-0.68762500	-0.05534300
C	1.80783200	-2.02428100	-0.17447700
C	2.94777000	-2.61743700	0.45633700
H	2.96742000	-2.99238000	1.47379200
C	4.02719200	-2.55617000	-0.46383100
C	3.56368300	-1.92752900	-1.65878200
H	4.16772800	-1.69939200	-2.53069500
C	2.19393800	-1.59253900	-1.48604500
H	1.55759400	-1.07012700	-2.19200500
C	2.60074400	0.86675800	1.05970700
H	1.59479100	0.91035400	1.46879700
C	3.74746700	0.28518100	1.67325800
H	3.77532100	-0.18963300	2.64842600
C	4.83228200	0.37446500	0.75107400
H	5.83314400	-0.01599700	0.90394400
C	4.35272200	1.00804000	-0.43345600
H	4.92660200	1.18308800	-1.33760800
C	2.97261000	1.31142200	-0.24195900
H	2.29455800	1.75501000	-0.96447800
H	5.04385200	-2.88384600	-0.27390700
C	0.56810700	-1.71147200	0.53870800
O	0.32836400	-2.00596700	1.68761800
O	-0.28711300	-1.01281600	-0.24698100
C	-1.45993300	-0.51401200	0.39213100
C	-2.00595300	0.62940600	-0.44470100
C	-2.57055900	-1.53557700	0.25335600
H	-1.24762900	-0.24645700	1.43289100
H	-2.24027200	-2.56706000	0.45026800
C	-3.11232600	-1.29275700	-1.15687800
H	-2.77500200	-1.98318400	-1.93813300
O	-4.48839200	-1.42496100	-1.02860200
C	-4.86177600	-1.29349900	0.34095900
C	-5.69062800	-0.04551300	0.53553400
H	-5.14284600	0.82550200	0.15715400
H	-6.63545900	-0.13105300	-0.01393200
H	-5.91104600	0.10260700	1.59941300
C	-5.57596900	-2.56024700	0.76028000
H	-4.91023100	-3.42252500	0.63087700
H	-5.87374000	-2.49850400	1.81369800
H	-6.47036100	-2.71448900	0.14495700
O	-3.64999300	-1.14838100	1.06899800
O	-2.70017300	0.00974300	-1.51957300
C	-0.96273600	1.56631800	-1.02175400
H	-0.35568400	1.02357400	-1.75991300
H	-2.70523100	1.21406800	0.18168900
O	-0.12777000	2.04170300	0.01804600
C	-1.58411300	2.84134000	-1.56956200
H	-2.59476100	2.69495400	-1.96673200
H	-0.95305900	3.29742600	-2.35088000
C	-0.50015300	3.38651000	0.34050300
C	-0.84912000	3.47050300	1.80709600
H	-1.65724500	2.76668200	2.03901000
H	0.02873800	3.21779200	2.41471500
H	-1.17709200	4.48430000	2.06556100
C	0.63983900	4.31023900	-0.04342900
H	0.38939300	5.34845300	0.20587800
H	1.55350000	4.02489200	0.49343600
H	0.84222800	4.24683000	-1.12016500
O	-1.65974200	3.65598700	-0.41970000

3c (to give the minor diastereomer of **4c**)
Energy (RM06) = –1542.41325353 A.U.

Fe	-3.50965800	-0.45660400	-0.16130700
C	-2.05206800	-1.28302000	0.95157300
C	-2.17184500	-1.96813400	-0.30120300
H	-1.39988000	-2.03633200	-1.05988100
C	-3.49216900	-2.48684000	-0.37873900
C	-4.18945400	-2.12116500	0.81210200
H	-5.23173800	-2.33266100	1.02622700
C	-3.30437400	-1.37840300	1.63695600
H	-3.52330500	-0.91703900	2.59371200
C	-3.00258600	1.48993000	-0.44262200
H	-2.10709800	1.94996000	-0.03320700
C	-3.09776700	0.81218000	-1.69274000
H	-2.29059400	0.66892600	-2.40411300
C	-4.42250700	0.29797000	-1.81097600
H	-4.80144700	-0.30377300	-2.63039000
C	-5.14197700	0.65697400	-0.63373200
H	-6.16376100	0.37552700	-0.40159300
C	-4.26379100	1.39398700	0.21357800
H	-4.49639300	1.77250200	1.20316000
H	-3.91423400	-3.02460200	-1.22122800
C	-0.94240900	-0.44571000	1.41522700
O	-0.89032500	0.11269300	2.48706100
O	0.02859400	-0.35245600	0.47583700
C	1.18262800	0.40497100	0.83424100
C	2.25804100	0.14467000	-0.20729000
C	0.90706400	1.87750100	0.59500300
H	1.49073200	0.18144300	1.86081000
H	-0.07459300	2.20522300	0.97157700
C	1.10912500	2.04210900	-0.91215900
H	0.20302000	2.06508700	-1.53004600
O	1.75191200	3.26503400	-1.04495700
C	2.33990100	3.63916600	0.19910800
C	3.84592300	3.64463000	0.08036100
H	4.19151700	2.67075500	-0.28597600
H	4.16549000	4.41816300	-0.62772000
H	4.30352600	3.84560300	1.05632200
C	1.76505400	4.97701200	0.61103100
H	0.67610000	4.89728700	0.71749200
H	2.19145600	5.29547300	1.56958300
H	1.98658000	5.73643300	-0.14820100
O	1.96420700	2.63429400	1.13176900
O	1.89188100	0.94143700	-1.32679300
C	2.40924000	-1.28273900	-0.67319600
H	1.45320800	-1.63885400	-1.08996100
H	3.22450000	0.47937200	0.21476500
O	2.79474500	-2.07954700	0.42761700
O	4.00580900	-2.76983400	-1.36416500
C	3.54437500	-1.47613900	-1.66946200
H	4.33228200	-0.71295000	-1.52597300
H	3.22376100	-1.44872000	-2.71535900
C	3.87512900	-2.92821500	0.03399500
C	3.51510400	-4.36669700	0.31645000
H	3.36149800	-4.51414900	1.39175400
H	2.59174300	-4.62222900	-0.21490400
H	4.31735200	-5.03309700	-0.02222200
C	5.13320900	-2.48077300	0.75490000
H	4.98527200	-2.53272200	1.84023200
H	5.97954900	-3.12191500	0.48000700
H	5.37890300	-1.44355900	0.49372000

<SCRF Method (PCM, solvent = THF)>

3c (dihedral angle = 0°)
Energy (RB+HF-LYP) = –2683.51374466 A.U.

Fe	3.45968300	-0.70652400	-0.07364600
C	1.85552800	-1.90940700	0.04865300
C	2.96605500	-2.50109100	0.73119200
H	2.99427700	-2.72227200	1.79254300
C	4.01001100	-2.67128200	-0.21580600
C	3.55393600	-2.18727600	-1.47900400
H	4.14027200	-2.14414300	-2.39086900
C	2.22456100	-1.71130400	-1.32257300
H	1.60668500	-1.24469000	-2.08199900
C	2.93352100	1.05085000	0.81339700
H	1.95144200	1.24257500	1.23761200
C	4.05109100	0.46743300	1.47695800
H	4.07753200	0.14091000	2.51129800
C	5.10266600	0.32407100	0.52361900
H	6.07284600	-0.12611900	0.70701900
C	4.63142500	0.81588600	-0.72960000
H	5.18205300	0.80462100	-1.66456100
C	3.28983500	1.26439500	-0.54960800
H	2.62323100	1.65458400	-1.31246500
H	5.00258700	-3.05554700	-0.00562900
C	0.59524100	-1.54300100	0.71059200
O	0.36035900	-1.70015700	1.89554200
O	-0.29614400	-0.99822900	-0.16328800
C	-1.54605400	-0.54021100	0.38509200
C	-2.06568700	0.62431000	-0.46265800
C	-2.62317300	-1.60504000	0.14875700
H	-1.42459700	-0.30097800	1.43985100
H	-2.23649400	-2.62645800	0.23157600
C	-3.20017200	-1.25372500	-1.24555300
H	-2.97944500	-1.95702100	-2.05136000
O	-4.59700200	-1.18390200	-1.05561000
C	-4.93067600	-1.49609800	0.30784700
C	-5.91648800	-0.46516600	0.83504100
H	-5.49364500	0.53842700	0.73757800
H	-6.85102100	-0.51452300	0.26858500
H	-6.13752800	-0.65892200	1.88894200
C	-5.45818900	-2.92920900	0.38699500
H	-4.70766400	-3.63592300	0.01843700
H	-5.70333900	-3.18704400	1.42197600

H	-6.35991100	-3.03360300	-0.22423500
O	-3.70602900	-1.36843800	1.03735300
O	-2.64306400	-0.00697200	-1.61927600
C	-1.02817700	1.63929900	-0.93986100
H	-0.31339700	1.14147800	-1.60004900
H	-2.84350800	1.14496400	0.11342500
O	-0.33405500	2.17904000	0.18959300
C	-1.66460900	2.87488300	-1.58864700
H	-2.63869400	2.67719000	-2.04049600
H	-0.99984500	3.31653900	-2.34292200
C	-0.74189400	3.55355400	0.39164800
C	-1.21581600	3.73695900	1.82614700
H	-2.03674600	3.04659200	2.03847800
H	-0.39549700	3.54044300	2.52282500
H	-1.56489400	4.76256500	1.98122200
C	0.42385200	4.47393600	0.02588800
H	0.14432400	5.52051900	0.18342000
H	1.29497800	4.24603500	0.64767200
H	0.70781600	4.34102600	-1.02252200
O	-1.85210400	3.75138500	-0.47951900

3c (dihedral angle = 30°)
Energy (RB+HF-LYP) = –2683.51060073 A.U.

Fe	3.65842100	-0.64224800	-0.06142000
C	1.88457700	-1.54433800	-0.33511500
C	2.88611200	-2.51669200	-0.01782600
H	2.87603700	-3.15214300	0.86097100
C	3.89305900	-2.43617600	-1.01541800
C	3.52258000	-1.41952700	-1.94660500
H	4.11108700	-1.09457300	-2.79820000
C	2.28423600	-0.86119600	-1.53063900
H	1.74975000	-0.04177000	-1.99871400
C	3.41280700	0.65803500	1.48809400
H	2.47189800	0.80069800	2.01300800
C	4.42265500	-0.30016200	1.79094000
H	4.39432000	-1.01937100	2.60279700
C	5.44136700	-0.19397200	0.79788000
H	6.32805000	-0.81526200	0.72475800
C	5.05711100	0.82785700	-0.12011800
H	5.60186000	1.11832400	-1.01250200
C	3.80231200	1.35360300	0.30707100
H	3.20768700	2.11256100	-0.19189000
H	4.81215600	-3.01215200	-1.03893600
C	0.64329400	-1.35895500	0.43733300
O	0.51682300	-1.57037000	1.62992200
O	-0.35790400	-0.87751500	-0.34679400
C	-1.59113500	-0.52547100	0.30976400
C	-2.26249600	0.60677100	-0.47348500
C	-2.60050600	-1.66614000	0.14192700
H	-1.40218500	-0.29038000	1.35552300
H	-2.13416300	-2.65648100	0.17810400
C	-3.31364500	-1.34667800	-1.19492300
H	-3.09927100	-2.01727000	-2.02973200
O	-4.69148300	-1.40313200	-0.89689000
C	-4.89068900	-1.73155800	0.48922300
C	-5.89889300	-0.76899100	1.09771100
H	-5.55364000	0.26084900	0.97197100
H	-6.86982200	-0.88139900	0.60638600
H	-6.02271200	-0.97647600	2.16485800
C	-5.31005400	-3.19714500	0.60737800
H	-4.54394000	-3.85125200	0.17880000
H	-5.45328000	-3.46732000	1.65822600
H	-6.24838700	-3.36612000	0.07011700
O	-3.62256500	-1.51832600	1.11772800
O	-2.89451100	-0.05144300	-1.58494100
C	-1.33748600	1.69071600	-1.02556900
H	-0.66522200	1.24528600	-1.76333000
H	-3.01949800	1.06857400	0.17567300
O	-0.56746700	2.25154500	0.04134000
C	-2.10213200	2.89656000	-1.58470100
H	-3.10229500	2.64984900	-1.94697600
H	-1.53881500	3.38827200	-2.38904400
C	-1.03747400	3.59152100	0.31881300
C	-1.39096600	3.71281800	1.79430500
H	-2.15196300	2.97290400	2.05716500
H	-0.50290200	3.54447900	2.41068200
H	-1.77917100	4.71314100	2.00993900
C	0.03491400	4.58977900	-0.12145800
H	-0.29402600	5.61411000	0.08054300
H	0.96642100	4.40786300	0.42382300
H	0.23901900	4.49124400	-1.19200900
O	-2.23204700	3.74277900	-0.44443900

3c (dihedral angle = 60°)
Energy (RB+HF-LYP) = –2683.50524486 A.U.

Fe	3.81469800	-0.57285700	-0.09297800
C	1.91627700	-1.10146300	-0.48255500
C	2.77612300	-2.24036300	-0.59565800
H	2.71187600	-3.12879800	0.02300000
C	3.73766500	-1.95350900	-1.60003200
C	3.48001900	-0.64440500	-2.10777600
H	4.07097500	-0.12677400	-2.85609300
C	2.35812500	-0.10999900	-1.41928300
H	1.93022200	0.87907100	-1.54120300
C	3.83476500	0.14745600	1.81301300
H	2.95010300	0.22026500	2.44012500
C	4.70426500	-0.97439100	1.69020900
H	4.60654500	-1.91609000	2.22014200
C	5.68143700	-0.66657800	0.69743300
H	6.46211600	-1.33179300	0.34305500
C	5.41154500	0.64461700	0.20505900
H	5.95231700	1.14929100	-0.58888200
C	4.26907800	1.14687700	0.89493200
H	3.77140800	2.09744400	0.72968600
H	4.55932400	-2.59723200	-1.89590000
C	0.69768100	-1.04437500	0.36124900
O	0.64982300	-1.19202300	1.56695900
O	-0.38866400	-0.75382600	-0.40129200
C	-1.63632300	-0.52011700	0.28280500
C	-2.40997600	0.57275400	-0.46270300
C	-2.54996900	-1.73753500	0.10529500
H	-1.44667500	-0.29379000	1.33023000
H	-1.99792600	-2.68338900	0.08501800
C	-3.33795000	-1.43409500	-1.19496100
H	-3.11843900	-2.07407200	-2.05235200
O	-4.69741100	-1.57460200	-0.83860000
C	-4.81041700	-2.00666700	0.52736300
C	-5.87350500	-1.17799900	1.23096000
H	-5.62211200	-0.11605600	1.16350800
H	-6.84903800	-1.34365000	0.76448200
H	-5.93857800	-1.46340800	2.28519600
C	-5.09237100	-3.50909000	0.56667400
H	-4.29281600	-4.06309100	0.06423200
H	-5.16065000	-3.85577500	1.60250000
H	-6.03641600	-3.72994800	0.05910900
O	-3.54107100	-1.71715700	1.12266700
O	-3.01597400	-0.11044700	-1.57343900
C	-1.57529400	1.72892500	-1.01314300
H	-0.89897000	1.34589500	-1.78148600
H	-3.18489900	0.96571000	0.21025800
O	-0.80772200	2.31042600	0.04453900
C	-2.43105900	2.89733500	-1.51459200
H	-3.42307800	2.59671000	-1.85828200
H	-1.92323000	3.44805300	-2.31768000
C	-1.36083300	3.60415500	0.38233300
C	-1.68216600	3.65031600	1.86952300
H	-2.38583500	2.85291700	2.12413200
H	-0.76872800	3.52006800	2.45736400
H	-2.12936900	4.61449300	2.13075600
C	-0.37061900	4.68815100	-0.04742200
H	-0.76278300	5.67986600	0.19940100
H	0.58515100	4.55187200	0.46819300
H	-0.18852100	4.64049400	-1.12538600
O	-2.58312300	3.69963000	-0.34558700

3c (dihedral angle = 90°)
Energy (RB+HF-LYP) = –2683.50147000 A.U.

Fe	3.88366600	-0.54920400	-0.11963000
C	1.92058700	-0.72912900	-0.50707000
C	2.61352300	-1.91189200	-0.92023500
H	2.44502600	-2.90263400	-0.51217600
C	3.57749500	-1.52817600	-1.88911700
C	3.48766400	-0.11594000	-2.07722100
H	4.12334000	0.47936900	-2.72428900
C	2.46865300	0.38532800	-1.22382700
H	2.17701200	1.42239900	-1.09772600
C	4.05395500	-0.29137900	1.89445500
H	3.20497300	-0.25172700	2.57182900
C	4.75808900	-1.45678700	1.47533300
H	4.54686800	-2.47430100	1.78715900
C	5.74083900	-1.05734700	0.52142900
H	6.41319200	-1.71786000	-0.01633300
C	5.63963300	0.35497500	0.34951300
H	6.22257300	0.95457500	-0.34195600
C	4.59583100	0.82762000	1.19836400
H	4.22862400	1.84617500	1.27765100
H	4.29495500	-2.18650200	-2.36755800
C	0.72837500	-0.67298800	0.38739700
O	0.72557300	-0.57398800	1.59626900
O	-0.40141800	-0.72505900	-0.36688400
C	-1.66726600	-0.54004800	0.30000800
C	-2.47684100	0.53398300	-0.43863900
C	-2.52426900	-1.79208800	0.09038900
H	-1.49890800	-0.31982500	1.35212700
H	-1.92832100	-2.71033700	0.05082000
C	-3.32192600	-1.49749100	-1.20603800
H	-3.07544600	-2.11367300	-2.07357400
O	-4.67562700	-1.69724100	-0.85449300
C	-4.77097000	-2.17257600	0.49795400
C	-5.87356800	-1.41491700	1.22028900
H	-5.67481600	-0.34063000	1.17891800
H	-6.83973500	-1.61710800	0.74875100
H	-5.92435000	-1.72912900	2.26705900
C	-4.98196600	-3.68727900	0.49582300
H	-4.15551000	-4.18984200	-0.01708700
H	-5.03787300	-4.06430400	1.52176900
H	-5.91272900	-3.93843100	-0.02204900
O	-3.51773200	-1.84005100	1.10492900
O	-3.05278300	-0.15670800	-1.56089600
C	-1.67769400	1.72137100	-0.97660900
H	-0.99036300	1.36611000	-1.74877700
H	-3.26843500	0.89423100	0.23325300
O	-0.92590200	2.31559700	0.08484400
C	-2.56760900	2.86895700	-1.46587700

H	-3.55017900	2.54301200	-1.81359000
H	-2.07561500	3.44306900	-2.26237300
C	-1.51978000	3.58621700	0.44037300
C	-1.84375400	3.60127800	1.92765100
H	-2.52366000	2.77973300	2.16975100
H	-0.92726500	3.48922500	2.51441000
H	-2.31961500	4.54787100	2.20234200
C	-0.56336400	4.70626000	0.02711800
H	-0.98517900	5.68165800	0.28963300
H	0.39653000	4.59076500	0.54012800
H	-0.38117500	4.68090800	-1.05157400
O	-2.74374200	3.65354600	-0.28813800

3c (dihedral angle = 120°)
Energy (RB+HF-LYP) = –2683.50376149 A.U.

Fe	-4.02126800	-0.16186700	-0.09776200
C	-2.08771000	-0.64327900	-0.35230800
C	-2.61607500	-0.07954800	-1.55740400
H	-2.26664400	0.83860300	-2.01683800
C	-3.69580500	-0.90027700	-1.97716800
C	-3.84047400	-1.96671500	-1.03923600
H	-4.60616800	-2.73493900	-1.06557600
C	-2.85251900	-1.81243400	-0.03007700
H	-2.71717200	-2.43350000	0.84866400
C	-4.08299300	1.20366000	1.41339100
H	-3.20360800	1.55112600	1.94925300
C	-4.62597600	1.75331500	0.21643700
H	-4.23713300	2.61016500	-0.32373400
C	-5.72542300	0.93669300	-0.18301700
H	-6.32419300	1.06669200	-1.07863400
C	-5.85767900	-0.11952800	0.76641000
H	-6.57533400	-0.93196900	0.71760200
C	-4.84122900	0.04596400	1.75274700
H	-4.63199700	-0.60998400	2.59210000
H	-4.33505100	-0.72024000	-2.83506800
C	-0.94147100	-0.13359000	0.44648600
O	-0.97007700	0.22481300	1.60715500
O	0.17715900	-0.07293800	-0.32246700
C	1.37785000	0.42994600	0.30106900
C	2.59001700	-0.15148600	-0.43107500
C	1.51380700	1.92732700	-0.00077100
H	1.35985500	0.21923300	1.36858000
H	0.54780500	2.44297600	-0.03143600
C	2.30067600	1.96956000	-1.33730000
H	1.75355200	2.33644700	-2.20852600
O	3.40410100	2.81365500	-1.08209500
C	3.31435300	3.36103800	0.24331400
C	4.67362300	3.26858400	0.91824000
H	5.01366500	2.22951200	0.93012800
H	5.40410800	3.87635500	0.37635600
H	4.61004300	3.63534800	1.94701800
C	2.77235300	4.78940500	0.17329100
H	1.78526400	4.80342200	-0.30017000
H	2.68369900	5.21159800	1.17907900
H	3.44582300	5.42041800	-0.41474100
O	2.39981800	2.50982500	0.94311000
O	2.69545200	0.64311700	-1.62545600
C	2.50197700	-1.62299300	-0.83299900
H	1.66491900	-1.76121800	-1.52238400
H	3.47522300	-0.00212700	0.20262300
O	2.28941000	-2.41729400	0.33686100
C	3.82220400	-2.16321300	-1.39633800
H	4.44047000	-1.39824900	-1.87037600
H	3.64570100	-2.97870500	-2.11023800
C	3.49477900	-3.15714800	0.63812300
C	3.91195500	-2.88731200	2.07693700
H	4.06671300	-1.81503900	2.22495000
H	3.13581000	-3.23325800	2.76604800
H	4.84241500	-3.41536300	2.30775400
C	3.24444000	-4.64052500	0.35888600
H	4.14116000	-5.22630600	0.58505000
H	2.42080500	-5.00724700	0.97933300
H	2.97775900	-4.79722800	-0.69074600
O	4.49556100	-2.62775700	-0.22836900

3c (dihedral angle = 150°)
Energy (RB+HF-LYP) = –2683.50986291 A.U.

Fe	-3.84884600	-0.41095000	-0.08354600
C	-2.04674300	-1.25357400	0.19503100
C	-2.39088200	-1.27843100	-1.19427400
H	-1.83845100	-0.77224100	-1.97835000
C	-3.59621900	-2.01728000	-1.32420200
C	-4.00131800	-2.44806800	-0.02487300
H	-4.90711200	-2.99844300	0.20701400
C	-3.05062700	-1.97661600	0.91967900
H	-3.08732600	-2.09899700	1.99666800
C	-3.69712900	1.51044400	0.57772700
H	-2.79072500	1.93233500	1.00391700
C	-4.05884000	1.47982800	-0.79990800
H	-3.47681100	1.88765100	-1.61972500
C	-5.28353900	0.75757600	-0.91688400
H	-5.80040600	0.52401600	-1.84200700
C	-5.67492800	0.33922500	0.38937100
H	-6.54186500	-0.26764800	0.62936700
C	-4.69301600	0.80458700	1.31279200
H	-4.66288400	0.62132700	2.38240300
H	-4.14405700	-2.18306600	-2.24584600
C	-0.92592100	-0.53567400	0.83069400
O	-0.91898700	-0.09708400	1.96673300
O	0.11167300	-0.37727400	-0.03444300
C	1.25925000	0.34715100	0.45106300
C	2.46096600	0.00350800	-0.43317200
C	1.08181600	1.84357700	0.16731300
H	1.41170600	0.14008300	1.50894000
H	0.04574200	2.18007100	0.27939100
C	1.65951700	2.02549300	-1.25947800
H	0.94061900	2.26758700	-2.04532700
O	2.59550600	3.07584100	-1.14189000
C	2.60576700	3.58563100	0.20243300
C	4.04361000	3.73923300	0.67262600
H	4.56500000	2.78127700	0.59586000
H	4.56349500	4.47809300	0.05579500
H	4.06655100	4.07634500	1.71320000
C	1.81076300	4.89070000	0.25915800
H	0.77860100	4.72634400	-0.06679100
H	1.79652200	5.28245300	1.28096300
H	2.26500100	5.63877300	-0.39783000
O	1.97245400	2.57606000	0.99576600
O	2.26631700	0.79853800	-1.61668400
C	2.60921000	-1.45873400	-0.85095600
H	1.73234000	-1.76198100	-1.42905000
H	3.37191300	0.32323800	0.09136100
O	2.71169600	-2.27477600	0.31853900
C	3.92425300	-1.73016700	-1.59285400
H	4.31408600	-0.85884000	-2.12288000
H	3.81819400	-2.56452000	-2.29899500
C	4.06620800	-2.76491100	0.44299200
C	4.60961400	-2.41624500	1.82151000
H	4.57425500	-1.33399400	1.97351400
H	4.01156100	-2.90411000	2.59691900
H	5.64604600	-2.75461900	1.91758400
C	4.07318300	-4.26933600	0.16401700
H	5.08827400	-4.66811900	0.25782900
H	3.42562700	-4.78804900	0.87774900
H	3.70542700	-4.47754100	-0.84529700
O	4.82243100	-2.05258500	-0.53339900

3c (dihedral angle = 180°)
Energy (RB+HF-LYP) = –2683.51180465 A.U.

Fe	-3.75428600	-0.31925100	-0.09372500
C	-2.10568900	-1.07612500	0.76921200
C	-2.32871500	-1.70330800	-0.49817900
H	-1.65021400	-1.65166700	-1.34270300
C	-3.60279100	-2.32768600	-0.44930500
C	-4.17058500	-2.08957500	0.83865500
H	-5.15600100	-2.40475100	1.16542600
C	-3.25275300	-1.31350100	1.59599700
H	-3.39795500	-0.93012500	2.60007300
C	-3.41586700	1.67537600	-0.33661000
H	-2.50327300	2.17537000	-0.02296600
C	-3.65788900	1.04965400	-1.59341300
H	-2.95970800	0.99560000	-2.42213800
C	-4.95015700	0.44737900	-1.54299800
H	-5.41060900	-0.14130800	-2.32974600
C	-5.50344500	0.69871000	-0.25256900
H	-6.45838600	0.33412000	0.11163100
C	-4.55373000	1.45746200	0.49292100
H	-4.64000400	1.77832900	1.52644600
H	-4.08546600	-2.85232400	-1.26711300
C	-0.92579800	-0.31525400	1.20623700
O	-0.79177600	0.19827000	2.30273800
O	0.02922100	-0.25998600	0.23785000
C	1.27132500	0.37723900	0.59113000
C	2.33723600	-0.04013200	-0.42678100
C	1.18117400	1.88886300	0.34635500
H	1.52985500	0.14297400	1.62282200
H	0.19157500	2.29975600	0.57095700
C	1.62440700	2.05811500	-1.12956500
H	0.85373600	2.38370900	-1.83175800
O	2.66154600	3.01608800	-1.09075200
C	2.83485800	3.50477200	0.24991400
C	4.31778800	3.54303300	0.58294600
H	4.75391700	2.54873600	0.45382000
H	4.83306900	4.24674600	-0.07731900
H	4.46425500	3.86569600	1.61810000
C	2.14908900	4.86423200	0.39180300
H	1.08242200	4.78236800	0.15879200
H	2.25559800	5.23832700	1.41476700
H	2.59781200	5.58769400	-0.29581600
O	2.20435000	2.53307700	1.09101800
O	2.07787600	0.79351800	-1.57049200
C	2.31933800	-1.49878700	-0.87992800
H	1.36399200	-1.71490000	-1.36564800
H	3.32360100	0.19447500	-0.00309200
O	2.47692100	-2.34605200	0.26070000
C	3.51931100	-1.85931000	-1.76727100
H	3.93430500	-1.00516500	-2.30616100
H	3.25974800	-2.64714100	-2.48688300
C	3.77151000	-2.98611400	0.20690300
C	4.50160200	-2.76587000	1.52400900
H	4.60802400	-1.69465500	1.71565200
H	3.94172400	-3.22106300	2.34635500
H	5.49632100	-3.22066500	1.48671800
C	3.57806400	-4.46725000	-0.12606700

H	4.54593600	-4.97699700	-0.16715700
H	2.96130800	-4.94786600	0.63969600
H	3.07726700	-4.58508000	-1.09184500
O	4.48797300	-2.31131800	-0.82411700

3c (dihedral angle = 210°)
Energy (RB+HF-LYP) = –2683.50985869 A.U.

Fe	-3.65672300	-0.12807900	-0.10570100
C	-2.21179700	-0.66604000	1.18206000
C	-2.45635600	-1.72337400	0.24843000
H	-1.72762800	-2.10737100	-0.45717600
C	-3.81637000	-2.10782300	0.38247500
C	-4.41574500	-1.29445200	1.39100800
H	-5.45791300	-1.32193200	1.69150400
C	-3.43124000	-0.39843600	1.88712000
H	-3.57313200	0.37709800	2.63191200
C	-2.98007400	1.53289100	-1.07286000
H	-2.01876300	1.99856500	-0.87230100
C	-3.24365200	0.48359000	-1.99975800
H	-2.51401600	0.00808700	-2.64682200
C	-4.61807200	0.12206300	-1.87528100
H	-5.11964500	-0.67405800	-2.41579500
C	-5.20114400	0.94654900	-0.86793500
H	-6.22375200	0.88587300	-0.51008000
C	-4.18737600	1.81810000	-0.37184100
H	-4.28336500	2.54173500	0.43172200
H	-4.32733400	-2.85598900	-0.21432200
C	-0.91971000	-0.02878700	1.48852300
O	-0.62260900	0.45292700	2.56614800
O	-0.05490300	-0.08956800	0.43890900
C	1.28729200	0.37337800	0.68535500
C	2.19821600	-0.15353100	-0.42697000
C	1.36980200	1.88902000	0.46233000
H	1.60218400	0.08788600	1.68811100
H	0.46610400	2.41681600	0.78294000
C	1.69275800	2.02954800	-1.04738100
H	0.90663700	2.45801800	-1.67315200
O	2.83687600	2.85554100	-1.09994700
C	3.19857200	3.28725400	0.22265600
C	4.69922300	3.13009700	0.41008800
H	4.99046300	2.09226600	0.22679200
H	5.23524800	3.77925200	-0.28842200
H	4.98357700	3.40582100	1.42995300
C	2.71036600	4.71938200	0.44415400
H	1.62396500	4.77863100	0.32228800
H	2.96784700	5.05656800	1.45304300
H	3.17606000	5.39347800	-0.28132600
O	2.53228200	2.38447400	1.11115700
O	1.94632200	0.72672600	-1.53664700
C	1.96438900	-1.59054300	-0.88988600
H	0.95953700	-1.67635400	-1.31223800
H	3.23877400	-0.04879800	-0.08977300
O	2.08873200	-2.47362000	0.22714100
C	3.04886300	-2.08176800	-1.85792700
H	3.52087700	-1.27859300	-2.42745400
H	2.65179100	-2.83200800	-2.55478200
C	3.30636700	-3.24201500	0.09742000
C	4.13678300	-3.09765800	1.36478200
H	4.35904600	-2.04254400	1.54636900
H	3.58862900	-3.49859700	2.22252600
H	5.07824500	-3.64701500	1.26618100
C	2.94126800	-4.69509400	-0.21305400
H	3.84708900	-5.30195900	-0.31084500
H	2.32720600	-5.10966700	0.59241800
H	2.37244900	-4.76077600	-1.14560100
O	4.02210500	-2.64504000	-0.98157000

3c (dihedral angle = 240°)
Energy (RB+HF-LYP) = –2683.50525912 A.U.

Fe	3.49903400	-0.39441500	-0.10478600
C	2.17430500	-0.27861300	1.40083000
C	2.61961600	1.03225400	1.03676400
H	1.98088900	1.81741600	0.64723600
C	4.02704300	1.07283000	1.21874800
C	4.45593400	-0.20427600	1.69096700
H	5.48271300	-0.49709100	1.88366800
C	3.31692400	-1.04600400	1.80235700
H	3.30527300	-2.08990500	2.09623100
C	2.52640100	-1.27422400	-1.66426600
H	1.49323500	-1.60859000	-1.61995200
C	2.98901300	0.02328700	-2.02773100
H	2.36622700	0.86107100	-2.32341700
C	4.40622600	0.04600300	-1.86583200
H	5.05240500	0.90362000	-2.02235600
C	4.81700100	-1.23743600	-1.39833400
H	5.83052000	-1.52471300	-1.13809600
C	3.65387900	-2.05287300	-1.27331300
H	3.60663000	-3.07119800	-0.90003100
H	4.67372700	1.91327500	0.98963300
C	0.75732900	-0.66343400	1.58157100
O	0.28633400	-1.09324500	2.61650400
O	0.00380700	-0.36166900	0.49206600
C	-1.42643800	-0.39131500	0.66516700
C	-2.06180500	0.44945800	-0.44727100
C	-1.98069100	-1.79166300	0.37109500
H	-1.68227300	-0.05916000	1.67045700
H	-1.28619300	-2.58917800	0.65367400
C	-2.32622000	-1.75324300	-1.14102000
H	-1.73985700	-2.41117000	-1.78662700
O	-3.69206000	-2.11045600	-1.21105100
C	-4.16345400	-2.50619100	0.08637300
C	-5.53497500	-1.89665900	0.32799400
H	-5.48068000	-0.80915300	0.22923500
H	-6.25309600	-2.28569700	-0.39972200
H	-5.88712600	-2.14732900	1.33302900
C	-4.15394300	-4.03177100	0.19676400
H	-3.14404800	-4.42320400	0.03658300
H	-4.49518400	-4.34250600	1.18904900
H	-4.81672400	-4.46916100	-0.55621400
O	-3.23933000	-1.92896400	1.01477900
O	-2.09912400	-0.43195600	-1.58392900
C	-1.30949800	1.71477700	-0.86111100
H	-0.35449200	1.42974300	-1.30976600
H	-3.08285100	0.71290500	-0.13791100
O	-1.06794800	2.53133500	0.28754500
C	-2.13724600	2.62412700	-1.77735900
H	-2.88590900	2.08841600	-2.36477300
H	-1.49261500	3.19980100	-2.45482200
C	-1.90953000	3.70645700	0.22580400
C	-2.71447200	3.82415300	1.51225600
H	-3.31535000	2.92258100	1.66027200
H	-2.04330600	3.94877600	2.36719000
H	-3.38094600	4.69093000	1.46404200
C	-1.02988400	4.92953800	-0.04047600
H	-1.64297100	5.83534100	-0.08403500
H	-0.29182500	5.04472500	0.75943100
H	-0.49400800	4.82259700	-0.98862300
O	-2.81294800	3.47252600	-0.85201200

3c (dihedral angle = 270°)
Energy (RB+HF-LYP) = –2683.50053322 A.U.

Fe	3.47701300	-0.38705200	-0.13793300
C	2.24780000	-0.30433000	1.44869500
C	2.96452300	0.92793500	1.31811100
H	2.50716800	1.89398400	1.13437800
C	4.34970500	0.62973600	1.40734900
C	4.49515200	-0.77857100	1.59025800
H	5.43546000	-1.31642000	1.65098600
C	3.20052500	-1.36310500	1.61300900
H	2.96414600	-2.41821100	1.69729500
C	2.29588700	-0.69956100	-1.76868100
H	1.21561300	-0.80819500	-1.71966800
C	3.02651800	0.51614000	-1.90247700
H	2.59865700	1.50975200	-1.98521400
C	4.41678400	0.20293200	-1.83705000
H	5.23350800	0.91680800	-1.86698000
C	4.54305300	-1.20659800	-1.65875300
H	5.47329200	-1.75023100	-1.52996000
C	3.23109700	-1.76369200	-1.61587100
H	2.96761800	-2.80313200	-1.44645500
H	5.16135700	1.34203800	1.30301100
C	0.78223300	-0.41595000	1.69937200
O	0.30395100	-0.45860500	2.81450800
O	0.03971100	-0.41218500	0.56681300
C	-1.39628600	-0.41448100	0.71346500
C	-2.00506600	0.39537500	-0.43399300
C	-1.92925300	-1.82450000	0.42688900
H	-1.66837400	-0.05918900	1.70522900
H	-1.23974900	-2.61049100	0.75347300
C	-2.20409200	-1.81625600	-1.10217000
H	-1.58770500	-2.48478900	-1.70715600
O	-3.56578000	-2.17300500	-1.22644300
C	-4.09032500	-2.56055300	0.05288100
C	-5.47753700	-1.96383100	0.22613100
H	-5.43122700	-0.87699300	0.11685200
H	-6.15826700	-2.36978300	-0.52776400
H	-5.87074900	-2.20711000	1.21758600
C	-4.06935200	-4.08446200	0.18206700
H	-3.04900300	-4.46655600	0.07415500
H	-4.45351200	-4.38725300	1.16102200
H	-4.69165500	-4.53775000	-0.59559800
O	-3.21384200	-1.96239500	1.01477400
O	-1.95662100	-0.50206700	-1.55835400
C	-1.28683800	1.68818100	-0.81709400
H	-0.29619400	1.44839100	-1.21214200
H	-3.04882900	0.62204900	-0.17531600
O	-1.14641000	2.51329000	0.34201800
C	-2.10419700	2.55889200	-1.77978700
H	-2.79782400	1.98964200	-2.40220700
H	-1.45061600	3.15978800	-2.42606500
C	-2.02746800	3.65476000	0.22716500
C	-2.90263100	3.74840600	1.46876600
H	-3.47766000	2.82630300	1.59006000
H	-2.28200700	3.89994900	2.35685600
H	-3.59614400	4.59053400	1.38121400
C	-1.18232500	4.90950000	-0.00175700
H	-1.82661300	5.79050000	-0.08523100
H	-0.49348000	5.05785800	0.83566100
H	-0.59226300	4.81808800	-0.91884700
O	-2.86284800	3.37971300	-0.89482600

3c (dihedral angle = 300°)

Energy (RB+HF-LYP) = –2683.50178647 A.U.

Fe	3.43526400	-0.52971200	-0.14370400
C	2.07307300	-1.65493000	0.81462700
C	3.24939800	-1.51740400	1.61748600
H	3.28183200	-1.04029200	2.59107800
C	4.33784800	-2.05300900	0.88020200
C	3.84412000	-2.51835600	-0.37581700
H	4.44292100	-2.94245700	-1.17483200
C	2.44616800	-2.27125200	-0.42622300
H	1.77919100	-2.47210600	-1.25772200
C	2.56942000	1.28828900	-0.45263400
H	1.55493500	1.53378400	-0.14999600
C	3.75149200	1.42145300	0.33093900
H	3.80225100	1.80002500	1.34638400
C	4.84297600	0.90420200	-0.42835900
H	5.87203500	0.82502400	-0.09352100
C	4.33222800	0.44841300	-1.67976000
H	4.90674400	-0.03758300	-2.46170800
C	2.92628000	0.68579000	-1.69379600
H	2.22572700	0.41629900	-2.47817300
H	5.37620200	-2.06109600	1.19497800
C	0.67731500	-1.35068800	1.22301500
O	0.11937900	-1.90508200	2.15201600
O	0.00494100	-0.57356200	0.33253700
C	-1.41527900	-0.44060000	0.57414100
C	-2.00806400	0.59245700	-0.39104200
C	-2.16501600	-1.71539800	0.15567200
H	-1.58568100	-0.20032300	1.62246200
H	-1.58683600	-2.62916000	0.31724100
C	-2.55817100	-1.46580000	-1.32137800
H	-2.06450700	-2.09602500	-2.06461700
O	-3.95251400	-1.68339200	-1.37112200
C	-4.43067500	-2.11967700	-0.08737200
C	-5.70131700	-1.36050700	0.26067700
H	-5.50842000	-0.28437200	0.24476100
H	-6.48785600	-1.59232500	-0.46339900
H	-6.05058300	-1.64623200	1.25737400
C	-4.61985400	-3.63711600	-0.10087900
H	-3.67571100	-4.13960300	-0.33448800
H	-4.96842800	-3.98510700	0.87637800
H	-5.35762700	-3.91919400	-0.85834400
O	-3.40907700	-1.74739400	0.84278100
O	-2.21097500	-0.12830900	-1.61833200
C	-1.16467100	1.82256400	-0.71498200
H	-0.29049900	1.50893800	-1.29129000
H	-2.97448300	0.91117300	0.02481600
O	-0.74221000	2.45120800	0.49698700
C	-1.96168300	2.92141700	-1.43127500
H	-2.81842900	2.54258400	-1.99244900
H	-1.31940100	3.50460100	-2.10418600
C	-1.42652400	3.71867600	0.64458100
C	-2.09088800	3.77673000	2.01232100
H	-2.78034600	2.93584500	2.12680800
H	-1.33529000	3.72857200	2.80197000
H	-2.64908500	4.71164600	2.12193800
C	-0.42446800	4.85188300	0.41843100
H	-0.91861100	5.82223900	0.52984500
H	0.38833400	4.78679600	1.14831600
H	0.01007200	4.79171100	-0.58388500
O	-2.44548800	3.71607000	-0.35122800

3c (dihedral angle = 330°)
Energy (RB+HF-LYP) = –2683.51093439 A.U.

Fe	3.44666800	-0.61705800	-0.11143800
C	1.97115900	-1.86692300	0.43253700
C	3.13919500	-2.11281200	1.22275900
H	3.19567200	-1.99157300	2.29899900
C	4.18923200	-2.46948400	0.33629200
C	3.67963600	-2.44410200	-0.99697600
H	4.25328700	-2.63054400	-1.89881400
C	2.31039800	-2.06883100	-0.94581000
H	1.64455700	-1.91928300	-1.78873200
C	2.75327700	1.27149800	0.21201200
H	1.75953300	1.49276000	0.59242500
C	3.92738300	1.02822300	0.98139000
H	3.99242600	1.04124400	2.06433800
C	4.98228800	0.69569500	0.08038000
H	5.99358900	0.41644700	0.35759200
C	4.45688300	0.73014200	-1.24524000
H	5.00028800	0.48175500	-2.15104600
C	3.07837000	1.08556400	-1.16279300
H	2.37164200	1.15718500	-1.98374600
H	5.21640600	-2.67597800	0.61792000
C	0.66176900	-1.47914300	0.98616800
O	0.25391500	-1.80656000	2.08580900
O	-0.10107700	-0.79933100	0.08620600
C	-1.44950300	-0.49375400	0.49529300
C	-2.00607600	0.59934100	-0.42022600
C	-2.36990100	-1.67575900	0.16419400
H	-1.46977500	-0.23714200	1.55291800
H	-1.88109200	-2.64645100	0.29589600
C	-2.83988800	-1.39072900	-1.28538700
H	-2.47317000	-2.07323300	-2.05516000
O	-4.24938600	-1.45450000	-1.23046000
C	-4.67732900	-1.82805500	0.09022400
C	-5.82684200	-0.93024400	0.51915400
H	-5.51709100	0.11737600	0.47520100
H	-6.68520700	-1.07622000	-0.14311700
H	-6.13159800	-1.17022100	1.54216300
C	-5.03443000	-3.31493000	0.11110800
H	-4.17158600	-3.92234100	-0.18071300
H	-5.34971000	-3.61534100	1.11514900
H	-5.85093400	-3.51679400	-0.58895700
O	-3.55514200	-1.56709300	0.93940600
O	-2.37351200	-0.09826700	-1.62290700
C	-1.05388900	1.73345000	-0.79140100
H	-0.20809700	1.32744400	-1.35195900
H	-2.89857500	1.02267100	0.06132300
O	-0.57836800	2.35428500	0.40704200
C	-1.75259200	2.87945500	-1.53509400
H	-2.63795000	2.56282700	-2.09008400
H	-1.06173100	3.39049100	-2.21875200
C	-1.15229500	3.67893100	0.52213600
C	-1.80669500	3.82941700	1.88771200
H	-2.57052300	3.05877600	2.02262400
H	-1.05713100	3.73053100	2.67839300
H	-2.27628200	4.81403000	1.97552700
C	-0.05859600	4.71782600	0.26751500
H	-0.47067600	5.72852600	0.35070200
H	0.74593900	4.60646500	1.00092700
H	0.36990800	4.59447700	-0.73163900
O	-2.16828200	3.73733700	-0.47480300

3c (to give the major diastereomer of **4c**)
Energy (RB+HF-LYP) = –1543.30649183 A.U.

Fe	3.48445200	-0.68988000	-0.09589800
C	1.86804200	-1.90670400	0.32100000
C	3.01381400	-2.34532300	1.06835000
H	3.08000600	-2.37609500	2.14680200
C	4.02932800	-2.69811500	0.13915300
C	3.52526100	-2.47859900	-1.18178400
H	4.07510400	-2.62513800	-2.10215700
C	2.19495600	-1.98674700	-1.07722000
H	1.54515300	-1.70632900	-1.89390600
C	2.96904300	1.29705000	0.25366400
H	1.97106100	1.62130500	0.52153700
C	3.99854900	0.88711300	1.15615300
H	3.92237800	0.85563000	2.23516500
C	5.13064100	0.48513200	0.38242500
H	6.06050700	0.09176600	0.77219200
C	4.80082900	0.64303300	-0.99799300
H	5.43744400	0.39215800	-1.83646700
C	3.46515900	1.14492300	-1.07685700
H	2.91385600	1.34276000	-1.98689700
H	5.02596600	-3.03763600	0.38855300
C	0.62200800	-1.42951100	0.93649000
O	0.40587400	-1.40015400	2.13457200
O	-0.28413000	-1.03626500	-0.00187900
C	-1.56085900	-0.56568200	0.46728200
C	-2.03664500	0.58132000	-0.42990900
C	-2.61355200	-1.64217600	0.17747800
H	-1.49894800	-0.30998300	1.52328600
H	-2.22507400	-2.65874400	0.30246700
C	-3.09550800	-1.31699300	-1.25975600
H	-2.81863600	-2.03318700	-2.03638200
O	-4.50171000	-1.24738200	-1.16485000
C	-4.92577900	-1.54901400	0.17477700
C	-5.95572700	-0.52249100	0.62083400
H	-5.53465500	0.48395900	0.54716900
H	-6.84568200	-0.58339100	-0.01248000
H	-6.25211000	-0.71059600	1.65716600
C	-5.44401400	-2.98698500	0.23407500
H	-4.66226000	-3.68942300	-0.07286400
H	-5.75765700	-3.23604500	1.25266600
H	-6.29999500	-3.10844600	-0.43696700
O	-3.75605700	-1.40203300	0.98531800
O	-2.51771400	-0.07540700	-1.61548100
C	-0.98477300	1.60967500	-0.84171700
H	-0.18945200	1.11219200	-1.40257300
H	-2.86339100	1.09443300	0.08071600
O	-0.42779300	2.21309800	0.33077700
C	-1.58542700	2.79996700	-1.59924300
H	-2.49657800	2.55307300	-2.14755800
H	-0.85532700	3.24137500	-2.29083400
C	-0.91159100	3.57356700	0.44654600
C	-1.55168400	3.77113800	1.81377300
H	-2.36702900	3.05562300	1.95142100
H	-0.80938900	3.62106800	2.60334200
H	-1.95207300	4.78605600	1.90083000
C	0.24972000	4.53544000	0.18802300
H	-0.09213300	5.57184000	0.27398100
H	1.04924000	4.36928400	0.91671100
H	0.66227800	4.38404300	-0.81415100
O	-1.92210800	3.70254700	-0.54854300

3c (to give the minor diastereomer of **4c**)
Energy (RB+HF-LYP) = –1542.43100702 A.U.

Fe	-3.71128600	-0.25901300	-0.10772100
C	-1.95394900	-1.22938800	0.38214200
C	-2.22521800	-1.38594500	-1.02117200

H	-1.59593200	-1.03781400	-1.82772900
C	-3.47132800	-2.05907400	-1.14744700
C	-3.97890900	-2.31661100	0.16518600
H	-4.92599100	-2.78541800	0.39741100
C	-3.05021500	-1.80428800	1.11120200
H	-3.14312200	-1.82090900	2.18796900
C	-3.55748200	1.75792400	0.37864400
H	-2.68293500	2.20833900	0.83011500
C	-3.79754100	1.60776700	-1.02154700
H	-3.14005500	1.92907800	-1.81868700
C	-5.04113600	0.92288600	-1.18280200
H	-5.48779600	0.62905300	-2.12370100
C	-5.56708700	0.64975000	0.11648600
H	-6.48146800	0.11233900	0.33148600
C	-4.64944800	1.16533700	1.08277600
H	-4.74781700	1.09178400	2.15780800
H	-3.96830000	-2.30084300	-2.07770800
C	-0.80324200	-0.56766600	1.01231000
O	-0.63253100	-0.46041800	2.21283900
O	0.07187600	-0.09457200	0.08012900
C	1.27129200	0.54100000	0.55404100
C	2.46047000	0.08916300	-0.30396800
C	1.20187100	2.03691200	0.22509200
H	1.39664200	0.35033300	1.61849000
H	0.18591600	2.43982800	0.30085200
C	1.82232200	2.14218200	-1.19211000
H	1.13943900	2.41429400	-1.99990300
O	2.82973300	3.12353800	-1.07633400
C	2.83567500	3.67526500	0.25043000
C	4.26754800	3.75225300	0.75745700
H	4.72572600	2.75980500	0.72951000
H	4.85220300	4.43243200	0.13110000
H	4.28454700	4.12442900	1.78624100
C	2.12449200	5.02950300	0.24372300
H	1.09336100	4.91947700	-0.10790900
H	2.10658400	5.45436200	1.25221000
H	2.64335300	5.72592800	-0.42219800
O	2.11833500	2.73435200	1.05487700
O	2.34785400	0.86730500	-1.50661200
C	2.49970300	-1.37988000	-0.69450300
H	1.58186200	-1.64057400	-1.23571000
H	3.38424200	0.34489300	0.23352400
O	2.61732100	-2.15848900	0.49623500
O	3.88207100	-3.16806600	-1.13040300
C	3.73451900	-1.79930800	-1.49446600
H	4.61743300	-1.20876800	-1.20723200
H	3.60055100	-1.74094000	-2.57633500
C	3.45187000	-3.30365500	0.22670700
C	2.63087500	-4.58326900	0.33873700
H	2.26593900	-4.71129500	1.36239500
H	1.77495700	-4.53566100	-0.34086800
H	3.24285400	-5.45185100	0.07498400
C	4.64207800	-3.26586400	1.18453800
H	4.29509400	-3.28182000	2.22261800
H	5.29039800	-4.13216000	1.01879100
H	5.22551600	-2.35315400	1.02862400

3c (to give the major diastereomer of **4c**)
Energy (RM06) = –1543.30392014 A.U.

Fe	3.29799700	-0.68972200	-0.05147000
C	1.80474500	-2.02760000	-0.16024300
C	2.94714700	-2.61612800	0.47380300
H	2.97525000	-2.98825300	1.49228400
C	4.02454700	-2.56216500	-0.44943800
C	3.55898700	-1.94241500	-1.64823600
H	4.16168900	-1.72106200	-2.52282600
C	2.18989000	-1.60492200	-1.47633400
H	1.55421000	-1.08888100	-2.18780300
C	2.61081100	0.87656100	1.05756400
H	1.61010800	0.92996400	1.47882600
C	3.76420700	0.29921300	1.66390600
H	3.80569300	-0.16329400	2.64468700
C	4.83859100	0.37837500	0.72806900
H	5.84066000	-0.01218400	0.87303600
C	4.34596400	1.00171900	-0.45698600
H	4.90965400	1.16714700	-1.36942100
C	2.96803300	1.30865600	-0.25284300
H	2.28414400	1.74933000	-0.97188700
H	5.04134700	-2.88901200	-0.25878600
C	0.56477600	-1.70732500	0.54584800
O	0.31811100	-1.99904300	1.69757200
O	-0.28422200	-1.01044100	-0.24159800
C	-1.46363500	-0.50826600	0.38438900
C	-2.00213500	0.63016100	-0.46381500
C	-2.57322200	-1.53239200	0.24621400
H	-1.25900000	-0.22942600	1.42350700
H	-2.24444300	-2.56443500	0.43992600
C	-3.11548500	-1.29218200	-1.16442200
H	-2.79278200	-1.99739000	-1.93806200
O	-4.49589100	-1.38923700	-1.03169600
C	-4.86601200	-1.29087000	0.34485000
C	-5.70615800	-0.05610700	0.56603400
H	-5.16447600	0.82885800	0.21099400
H	-6.65017800	-0.13810900	0.01488200
H	-5.93164600	0.06449400	1.63213400
C	-5.56202000	-2.57358000	0.74363400
H	-4.88867900	-3.42663600	0.59302600
H	-5.85495400	-2.53442700	1.79943000
H	-6.46056400	-2.72431100	0.13358200
O	-3.64964500	-1.14348400	1.06628300
O	-2.67918300	-0.00201900	-1.54468800
C	-0.95364200	1.56988500	-1.02787800
H	-0.33786500	1.03254300	-1.76273000
H	-2.71306700	1.21241500	0.15104700
O	-0.13314900	2.03801600	0.02645100
C	-1.56547800	2.84783700	-1.57878500
H	-2.57127300	2.70746900	-1.98995100
H	-0.92289100	3.30536500	-2.34810700
C	-0.50123500	3.38510800	0.34765600
C	-0.86277800	3.46785400	1.81088400
H	-1.67807100	2.76926000	2.03437200
H	0.00813700	3.20697300	2.42478300
H	-1.18221500	4.48400200	2.07088900
C	0.64435300	4.30475400	-0.02684000
H	0.39611300	5.34356500	0.22221800
H	1.55069100	4.01682500	0.52079400
H	0.85799000	4.23989400	-1.10120200
O	-1.65514700	3.65809400	-0.42402700

3c (to give the minor diastereomer of **4c**)
Energy (RM06) = –1542.42457291 A.U.

Fe	-3.51683400	-0.45831700	-0.15352600
C	-2.03984400	-1.30002700	0.92058100
C	-2.16374800	-1.95090000	-0.35142900
H	-1.39912300	-1.99212100	-1.11962000
C	-3.47806400	-2.48353000	-0.43085700
C	-4.16898400	-2.16068600	0.77601300
H	-5.20682500	-2.39050500	0.99281900
C	-3.28668200	-1.42923700	1.61406700
H	-3.50931800	-1.00146200	2.58559600
C	-3.06978400	1.51374500	-0.36988800
H	-2.19614300	1.99821900	0.05803500
C	-3.13293100	0.87204300	-1.64145600
H	-2.31705000	0.78001500	-2.35139100
C	-4.43975300	0.31933200	-1.78704300
H	-4.79233500	-0.26992300	-2.62715700
C	-5.17997700	0.61844700	-0.60531900
H	-6.19348600	0.29604200	-0.39037500
C	-4.33258100	1.35701100	0.27208200
H	-4.58696900	1.69917000	1.26967900
H	-3.90147500	-3.00164700	-1.28488600
C	-0.93140900	-0.47054500	1.39355100
O	-0.87031700	0.06448300	2.48033800
O	0.03469500	-0.35639100	0.45443700
C	1.18684300	0.40475200	0.81141500
C	2.26564100	0.14324100	-0.22668700
C	0.90719700	1.87684700	0.57105200
H	1.49584900	0.18344100	1.83814100
H	-0.08080200	2.20227000	0.93159800
C	1.12510900	2.04608800	-0.93349000
H	0.22407700	2.08304300	-1.55698600
O	1.79469100	3.25685900	-1.05691300
C	2.33414400	3.65103100	0.20684600
C	3.84128400	3.69169900	0.13332700
H	4.22112400	2.72071900	-0.20678900
H	4.16399500	4.46509800	-0.57327400
H	4.26418600	3.91805500	1.11914000
C	1.71169600	4.97272300	0.59912500
H	0.62188600	4.86704400	0.66986300
H	2.10012700	5.30212200	1.56998900
H	1.94132500	5.73863000	-0.15103900
O	1.95534300	2.63351600	1.12600200
O	1.89511000	0.93517700	-1.34967100
C	2.41840300	-1.28638300	-0.68822900
H	1.46528100	-1.64154300	-1.11141100
H	3.22971400	0.48469300	0.19397500
O	2.79036200	-2.08555100	0.41774700
O	4.02792000	-2.77380200	-1.35457600
C	3.56031700	-1.48374200	-1.67677000
H	4.34473100	-0.71747900	-1.53844000
H	3.24330900	-1.47142400	-2.72390600
C	3.89845000	-2.91221900	0.04724700
C	3.57404600	-4.35347600	0.35511300
H	3.41891800	-4.48409300	1.43231700
H	2.66166000	-4.64613100	-0.17654200
H	4.39744300	-5.00459900	0.03846000
C	5.14151900	-2.42049300	0.76436700
H	4.99087800	-2.46034500	1.84976800
H	6.00350300	-3.04730100	0.50544200
H	5.36543700	-1.38240000	0.48807700

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