Electronic Supplementary Information (Esi)

Iron catalyzed diastereoselective hydrogenation of chiral imines

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General Information

NMR spectra

^{1}H-NMR and ^{13}C-NMR spectra were recorded with instruments at 300 MHz (Bruker AMX 300 and Brucker F300). The chemical shifts are reported in ppm (δ), with the solvent reference relative to tetramethylsilane (TMS).

TLC

Reactions and chromatographic purifications were monitored by analytical thin-layer chromatography (TLC) using silica gel 60 F254 pre-coated glass plates and visualized using UV light, phosphomolybdic acid or ninhydrin.

Chromatographic purification

Purification of the products was performed by column chromatography with flash technique (according to the Still method) using as stationary phase silica gel 230-400 mesh (SIGMA ALDRICH).

Dry solvents

Dichloromethane (DCM) was dried by distillation under nitrogen atmosphere on CaH_2. The other dry solvents used are commercially available and they are stored under nitrogen over molecular sieves (bottles with crown cap).

Reactions work-up

The organic phases, if necessary, were dried over Na_2SO_4. The solvents were removed under reduced pressure and then at high vacuum pump (0.1-0.005 mmHg).

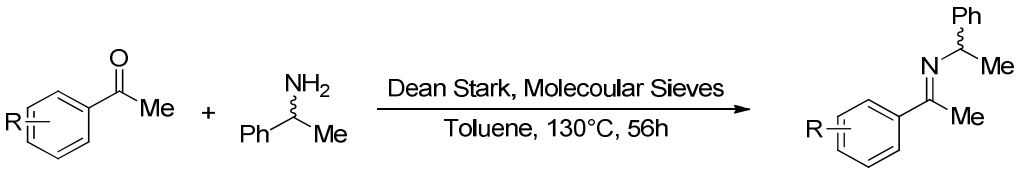
Batch hydrogenations:

The hydrogenations were run in a 450 mL Parr autoclave equipped with a removable aluminum block that can accommodate up to 4 magnetically stirred 20 mL-glass vials, fitted with a Teflon septum.

Gas chromatography with mass-selective detector (GC-MS): Agilent 6890N Network GC-System, mass detector 5975 MS. Column: HP-5MS (30m × 0.25 mm × 0.25 µm, 5% phenylmethylsiloxane, carrier gas: H_2. Standard heating procedure: 50 ℃ (2 min), 25 ℃/ min -> 300 ℃ (5 min)

The iron complexes Cat **A,**[1] Cat **B**[2] and Cat **C**[3] were prepared following literature procedures.

Synthesis of Imines

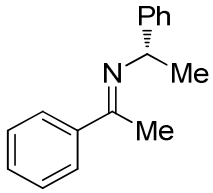


General procedure (A): Toluene (8 mL), 4 Å molecular sieves, amine (6.6 mmol, 1.5 eq.) and ketone (4.4 mmol, 1 eq.) were introduced in a one necks 25 mL round-bottomed flask provided with a condenser and a Dean-Stark apparatus. The reaction mixture was heated to 130 ℃ and stirred at this temperature for 56 h. After cooling to room temperature, molecular sieves were removed filtering over Na_2SO_4 pad and washed with DCM. The solvent was removed under reduced pressure. The residual starting materials were removed by fractional distillation at P = 3 x 10^{-2} mbar at 150 ℃ with Glass Oven B-585 Kugelrohr (only terminal round flask inserted). in order to remove the excess of amine.

General procedure (B): Toluene (6 mL), molecular sieves (350 mg), amine (1.5 eq, 6.6 mmol) and ketone (1 eq, 4.4 mmol) were introduced in a 25 mL vial without inert atmosphere. The stirred mixture was subjected to 200 W microwave irradiation and heated to 130 ℃ for 6 h 30 min. Constant microwave irradiation as well as simultaneous air-cooling (2 bar) were used during the entire reaction time. After cooling to room temperature, the reaction mixture was filtered on Na_2SO_4 , and washed with DCM, the solvent was removed under reduced pressure. The residual starting materials were removed by fractional distillation at P = 3 x 10^{-2} mbar at 150 ℃ with Glass Oven B-585 Kugelrohr (only terminal round flask inserted).

General procedure (C): The selected ketone was charged in a two round bottomed flask, posed under nitrogen and dissolved in dry Toluene (0.1M). At this solution was added Ti(*i*PrOH)$_4$ (2 eq.), after 5 minutes of mixing the (*R*)-(+)-2-Methyl-2-propanesulfinamide was added. The reaction mixture was stirred for 18 hours at 110 °C, then p oured into a same volume solution of brine. The resulting slurry was filtered over celite and the cake was washed with AcOEt. The two phases were separated and the organic phase was further washed with brine. The organic layer was dried with Na_2SO_4 pad, and the solvent was removed under reduced pressure. The desired imines were obtained pure after chromatographic purification.

N-(1-(*S*)-phenylethyl)-ethan-1-(phenyl)-1-imine **(1a)**



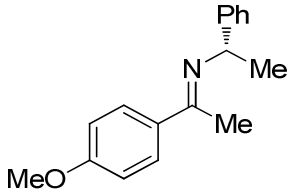
Synthetized according to general procedure A starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 60% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine is a 92:8 mixture of the *E* and the *Z* isomers.

Major isomer:

^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.87 (m, 1H), 7.57 – 7.21 (m, 9 H), 4.87 (q, J = 6.5 Hz, 1 H), 2.29 (s, 3 H), 1.57 (d, J = 6.5 Hz, 3H).

Compound **1a** is known and all analytical data are in agreement with literature[4]

N-(1-(*S*)-phenylethyl)-ethan-1-(4-(methoxy)phenyl)-1-imine **(1b)**



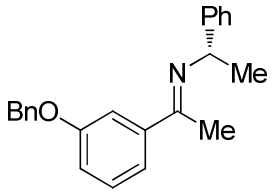
Synthetized according to general procedure B starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 50% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine is a 95:5 mixture of the *E* and the *Z* isomers.

Major isomer:

1H NMR (300 MHz, $CDCl_3$), E isomer: δ 7.2-8.0 (m, 9H), 4.90 (q, J=6.50 Hz, 1H), 3.86 (s, 3H), 2.29 (s, 3H), 1.62 (d, J=6.50 Hz, 3H)

Compound **1b** is known and all analytical data are in agreement with literature[5]

N-(1-(*S*)-phenylethyl)-ethan-1-(3-(benzyloxy)phenyl)-1-imine **(1c)**



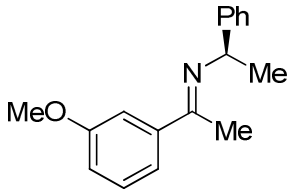
Synthetized according to general procedure A and B starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 45% (Procedure A) and 25% (Procedure B) yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine is a 91:9 mixture of the *E* and the *Z* isomers.

Major isomer:

^{1}H NMR (300 MHz, $CDCl_3$) *E* δ: 7.99-7.94 (m, 1H), 7.58-7.31 (m, 12H), 5.19 (s, 2H), 4.94 (q, 1H, *J* = 9.0 Hz), 2.25 (s, 3H), 1.66 (d, 3H, *J* = 9.0 Hz).

Compound **1c** is known and all analytical data are in agreement with literature.[4]

N-(1-(*R*)-phenylethyl)-ethan-1-(3-(methoxy)phenyl)-1-imine **(1d)**



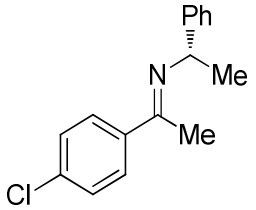
Prepared according to general procedure A and B starting from the corresponding ketone and (*R*)-phenylethylamine. The pure product was obtained in 50% (Procedure A) and 35% (Procedure B) yield after purification by fractional distillation yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 ℃. The imine was a 90:10 mixture of the *E* and the *Z* isomers as reported in literature.

Major isomer:

^{1}H NMR (300 MHz, $CDCl_3$) *E* δ 7.55–7.20 (m, 9H), 4.86 (q, *J* = 6.6 Hz, 1H), 3.88 (s, 3H), 2.28 (s, 3H), 1.56 (d, *J* = 6.6 Hz, 3H).

Compound **1d** is known and all analytical data are in agreement with literature.[6]

N-(1-(*S*)-phenylethyl)-ethan-1-(4-(chloro)phenyl)-1-imine **(1e)**



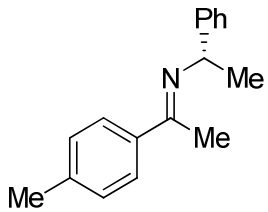
Synthetized according to general procedure B starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 30 % yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 ℃. The imine is a 93:7 mixture of the *E* and the *Z* isomers.

Major isomer:

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (d, J = 8.6 Hz, 2H), 7.44 – 7.31 (m, 7H), 4.85 (q, J = 6.5 Hz, 1H), 2.27 (s, 3H), 1.55 (d, J = 6.5 Hz, 3H).

Compound **1e** is known and all analytical data are in agreement with literature.[5]

N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Methyl)phenyl)-1-imine **(1f)**

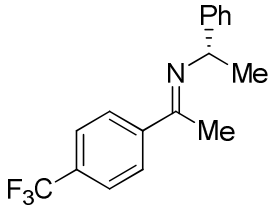


Synthetized according to general procedure B starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 40% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 ℃. The imine is a 92:8 mixture of the *E* and the *Z* isomers.

Major isomer:

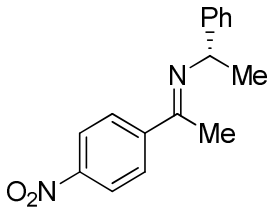
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (d, J = 8.2 Hz, 2H), 7.47-7.20 (m,7H), 4.84 (q, J = 6.6 Hz, 1H), 2.38 (s, 3H), 2.25 (s, 3H), 1.55 (d, J = 6.6 Hz, 3H).
Compound **1f** is known and all analytical data are in agreement with literature.[7]

N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Trifluoromethyl)phenyl)-1-imine **(1g)**



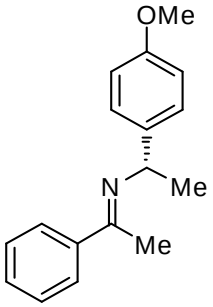
Synthetized according to general procedure B starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 25% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine is a 93:7 mixture of the *E* and the *Z* isomers.
Major isomer:
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 8.3 Hz, 2H), 7.71 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 7.3 Hz, 2H), 7.42 (t, J = 7.5 Hz, 2H), 7.33 (d, J = 7.3 Hz, 1H), 4.94 (q, J = 6.5 Hz, 1H), 2.34 (s, 3H), 1.64 (d, J = 6.5 Hz, 3H).
^{19}F NMR (282 MHz, $CDCl_3$) δ -62.99 (s).
Compound **1g** is known and all analytical data are in agreement with literature.[8]

N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Nitro)phenyl)-1-imine **(1h)**



Synthetized according to general procedure B starting from the corresponding ketone and (*S*)-phenylethylamine. The pure product was obtained in 50% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine is a 95:5 mixture of the *E* and the *Z* isomers.
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 – 8.23 (d, J = 8.89 Hz, 2H), 8.08 (d, J = 8.89 2H), 7.61 – 7.50 (m, 2H), 7.43 (t, J = 7.5 Hz, 2H), 7.38 – 7.25 (m, 1H), 4.95 (q, J = 6.5 Hz, 1H), 2.38 (s, 3H), 1.64 (d, J = 6.5 Hz, 3H).
Compound **1h** is known and all analytical data are in agreement with literature.[9]

N-(α-Methylbenzyliden)-α-(4-methoxyphenyl)aethylamine **(1i)**



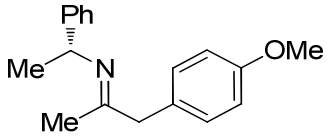
Synthetized according to general procedure B starting from the corresponding ketone and (*R*)-4-Methoxy-α-methylbenzylamine. The pure product was obtained in 50% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine is a 95:5 mixture of the *E* and the *Z* isomers.

Major isomer:

1H NMR (300 MHz, CDCl3), E isomer: δ 7.2-8.0 (m, 9H), 4.90 (q, J=6.50 Hz, 1H), 3.86 (s, 3H), 2.29 (s, 3H), 1.62 (d, J=6.50 Hz, 3H)

Compound **1i** is known and all analytical data are in agreement with literature.[5]

N-(1-(*R*)-phenylethyl)-propan-1-(4-methoxyphenyl)-1-imine **(1j)**



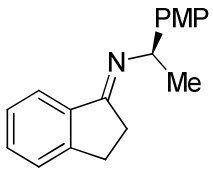
Synthetized according to general procedure B starting from 4-methoxyphenylacetone and (*R*)-phenylethylamine. The pure product was obtained in 85% yield after purification by fractional distillation at P = 3 x 10^{-2} mbar with Glass Oven B-585 Kugelrohr set to 95 °C. The imine was obtained as yellow oil a 7:3 E/Z mixture.

Major isomer: (*E*)

^{1}H NMR (300 MHz, $CDCl_3$) *E:* δ: 7.45 – 7.11 (m, 7H), 6.86-6.84 (m, 2H), 4.63 (q, 1H, J = 6.6 Hz), 3.90 (s, 3H), 3.56 (s, 2H),1,77 (s, 3H), 1.53 (d, 3H, *J* = 6.6 Hz).

Compound **1j** is known and all analytical data are in agreement with literature.[10]

(*R*)-*N*-(4-methoxyphenylethyl)indanimine **(1k)**



Synthetized according to general procedure A starting from 1-indanone and (*R*)-4-Methoxy-α-methylbenzylamine . The pure product was obtained in 60% yield after purification by crystallization in Et_2O. The imine was a pure *E* isomer.

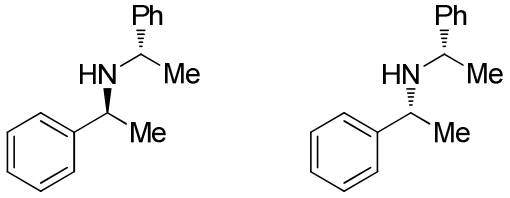
^{1}H NMR (300 MHz, $CDCl_3$)*:* δ: 7.99 (d, 1H, J = 6.5 Hz), 7.41-7.31 (m, 5H), 6.91 - 6.88 (m, 2H), 4.66 (q, 1H, J = 6.6 Hz), 3.81 (s, 3H), 3.11-3.05 (m, 2H), 2.90-2.83 (m, 1H), 2.72-2.57 (m, 1H), 1.50 (d, 3H, *J* = 6.6 Hz).

Compound **1k** is known and all analytical data are in agreement with literature.[10]

Imines Reductions

General procedures Iron catalyzed imine hydrogenation: The selected pre-catalyst (0.1 eq.) was dissolved into degassed ethanol (0.1M solution). The imine (1 eq.), and the trimethylamine N-oxide (0.4 equivalent) were charged into a 20 mL-glass vial, equipped with a rubber septum. The mixture was posed under nitrogen atmosphere. The vial was located in the removable aluminum block of a 450 mL Parr autoclave. The solution of the catalyst was added to the vial, the rubber septum was pierced with a nail. The reaction set up was set at the desired hydrogen pressure and the system was purged 3 times. The reaction temperature was then set. After 18 hours the heating system was shut down and the pressure was released. The crude mixture was analyzed by NMR in order to evaluate the dr. For removing the iron particles the crude where filtered over HPLC-filter (CPS-F-NY2545/100), and the solvent was removed under reducing pressure. The desired amine were obtained as pure compounds after chromatographic purification using (hexanes/AcOEt) as eluent.

N-(1-phenylethyl)-(S)-α-methylbenzylamine **(2a, 2a')**

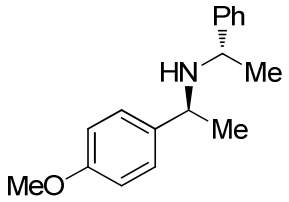


Diasteroisomer A Diasteroisomer B

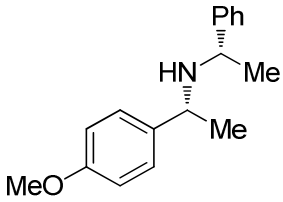
^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 3.77 (m, 2H, diast. B), 3.49 (m, 2H diast. A). The major diasteroisomer A was obtained pure after flash column chromatography on silica gel with a 90:10 hexane/ethyl acetate mixture as eluent. Rf = 0.18.

^{1}H NMR (300 MHz, $CDCl_3$) Diast. A δ 7.46 – 7.12 (m, 10H), 3.50 (m, 2H), 1.57 (s, 1H), 1.28 (2d, J = 6.6 Hz, 6H).
^{1}H NMR (300 MHz, $CDCl_3$) Diast. B δ 7.46 – 7.12 (m, 10H), 3.78 (m, 2H), 1.57 (s, 1H), 1.37 (2d, J = 6.6 Hz, 6H).
Compound **2a** is known and all analytical data are in agreement with literature.[11]

N-(1-(4-methoxyphenyl)ethyl)-(S)-α-methylbenzylamine **(2b, 2b')**



Diasteroisomer A

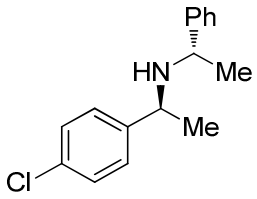


Diasteroisomer B

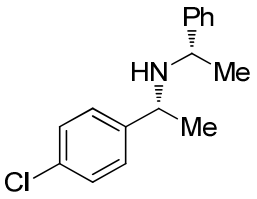
^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 1.37 (t, J = 6 Hz (2d collapsed) , 6H, diast. B), 1.29 (t, J = 6 Hz (2d collapsed), 6H diast. A).

^{1}H NMR (300 MHz, $CDCl_3$) Diast. A δ 7.47 – 7.07 (m, 7H), 6.96 – 6.79 (m, 2H), 3.84 (s, 3H), 3.51 (m, 2H), 1.29 (t, J = 6 Hz (2d collapsed), 6H diast. A).
^{1}H NMR (300 MHz, $CDCl_3$) Diast. B δ 7.47 – 7.07 (m, 7H), 6.96 – 6.79 (m, 2H), 3.84 (s, 3H), 3.81 – 3.70 (m, 2H), (t, J = 6 Hz (2d collapsed) , 6H,).
Compound **2b** is known and all analytical data are in agreement with literature.[11]

N-(1-(4-chlorophenyl)ethyl)-(S)-α-methylbenzylamine **(2e, 2e')**



Diasteroisomer A

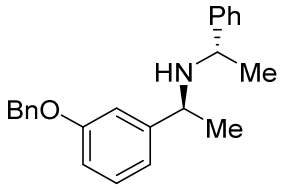


Diasteroisomer B

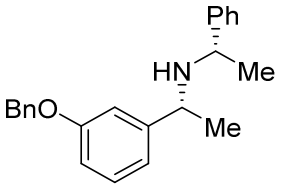
^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 3.76 (m, 2H, diast. B), 3.51 (m, 2H diast. A).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30-7.18 (m, 9H), 3.55 – 3.42 (m, 2H), 1.57 (s, 1H), 1.26 (2d, J = 6.7 Hz, 6H).
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30-7.18 (m, 9H), 3.75 (q, J = 6.8 Hz, 2H), 1.57 (s, 1H), 1.35 (2d, J = 6.8 Hz, 6H).
Compound **2e** is known and all analytical data are in agreement with literature.[11]

N-(1-(3-benzyloxyphenyl)ethyl)-(S)-α-methylbenzylamine **(2c, 2c')**



Diastereoisomer A

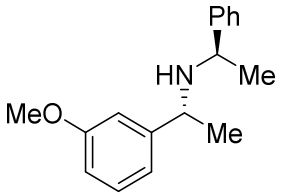


Diastereoisomer B

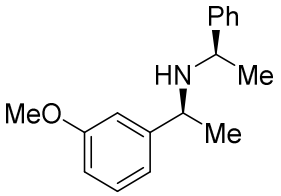
^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 3.77 (m, 2H, diast. B), 3.49 (m, 2H diast. A). The major diasteroisomer A was obtained pure after flash column chromatography on silica gel with a 90:10 hexane/ethyl acetate mixture as eluent. Rf = 0.18.

^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.47-7.20 (m, 11H), 6.89-6.87 (m, 2H), 6.81 (d, 1H, *J* = 7.5 Hz), 5.08 (s, 2H), 3.49 (m, 2H), 1.26 (d, 6H, J=6.3 Hz).
Compound **2c** is known and all analytical data are in agreement with literature.[11]

N-(1-(3-methoxyphenyl)ethyl)-(S)-α-methylbenzylamine **(2d, 2d')**



Diastereoisomer A



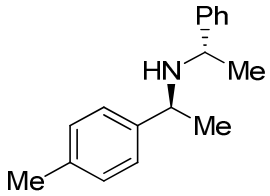
Diastereoisomer B

^{1}H NMR (300 MHz, $CDCl_3$): Selected signals for the evaluation of the diasteroisomeric ratio: 3.79 (m, 2H, diast. B), 3.50 (m, 2H, diast. A).

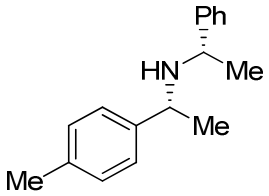
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39–7.05 (m, 6H), 6.81 (m, 3H), 3.82 (s, 3H), 3.50 (m, 2H), 1.54 (br, 1H), 1.28 (dd, 6H, J=6.5 Hz).

Compound **2d/2d'** is known and all analytical data are in agreement with literature.[12]

N-(1-(4-methylphenyl)ethyl)-(S)-α-methylbenzylamine **(2f, 2f')**



Diasteroisomer A

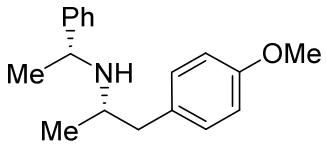


Diasteroisomer B

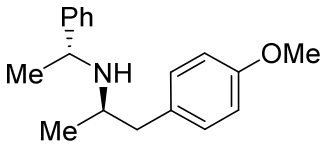
^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 3.76 (m, 2H, diast. B), 3.51 (m, 2H diast. A).
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38-7.11 (m, 9H), 3.55 – 3.42 (m, 2H), 2.38 (s, 3H), 1.57 (s, 1H), 1.26 (2d, J = 6.7 Hz, 6H).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30-7.18 (m, 9H), 3.75 (q, J = 6.8 Hz, 2H), 2.36 (s, 3H), 1.57 (s, 1H), 1.35 (2d, J = 6.8 Hz, 6H).
Compound **2f** is known and all analytical data are in agreement with literature.[11]

(*R*)-1-(4-methoxyphenyl)-*N*-((*R*)-1-phenylethyl)propan-2-amine **(2j, 2j')**



Diastereoisomer A

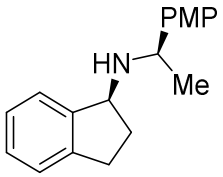


Diastereoisomer B

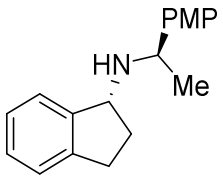
The mixtures of the two diasteroisomers is a light yellow oil. The reaction leaded to a mixture of the two diasteroisomers. Major (B) Minor (A).
^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 1.07 (d, 3H, diast. A), 0.95 (d, 3H, diast. B).
After chromatographic purification on silica gel, using a mixture of 9:1 ETP:AcOEt as eluent, a diasteroisomeric mixture (9:1) of amines was obtained in 60% yield.

Major isomer:
^{1}H NMR (300 MHz, CDCl3) δ 7.42 – 7.22 (m, 5H), 7.02 (d, J = 8.6 Hz, 2H), 6.82 (d, J = 8.6 Hz, 2H), 3.98 (m, 1H), 3.80 (s, 3H), 2.93 – 2.73 (m, 2H), 2.54-2.47 (m, 1H), 1.37 (d, J = 6.6 Hz, 3H), 0.97 (d, J = 6.2 Hz, 3H).
Compound **2j** is known and all analytical data are in agreement with literature.[10]

(*R, R*)-*N*-1-indan-(1-*p*-methoxyphenylethyl)amine **(2k, 2k')**



Diastereoisomer A



Diastereoisomer B

The mixtures of the two diasteroisomers is a transparent oil. The reaction leaded to a mixture of the two diasteroisomers. Major (B) Minor (A).

^{1}H NMR (300 MHz, $CDCl_3$) δ: Selected signals for the evaluation of the diasteroisomeric ratio: 2.45 (m, 1H, diast. A), 2.20 (m, 1H, diast. B).

After chromatographic purification on silica gel ,using a mixture of 8:2 (ETP:AcOEt) as eluent, a diasteroisomeric pure amine was obtained with a 55 % of isolated yield.

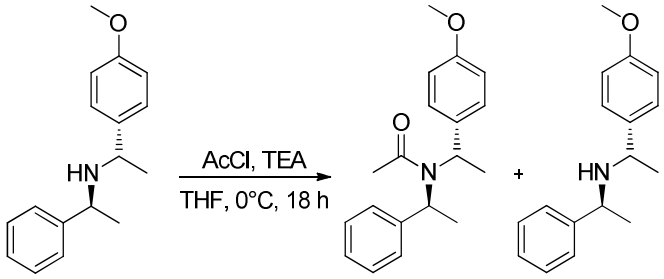
Major isomer:

^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.38 (d, 2H, J = 8.6 Hz), 7.25-7.19 (m, 4H), 6.92 (d, 2H. J = 8.6 Hz) 4.15-4.22 (m, 2H), 3.84 (s, 3H), 2.98-3.05 (m, 1H), 2.75-2.82 (m, 1H), 2.28-2.22 (m, 1H), 1.74-1.82 (m, 1H), 1.40 (d, 3H, J = 6.5 Hz).

Compound **2k** is known and all analytical data are in agreement with literature.[10]

.

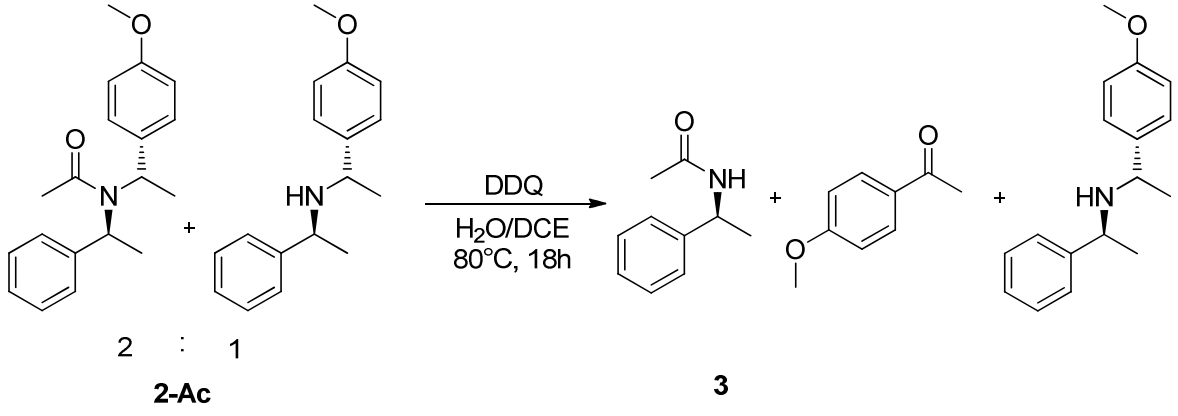
General procedure for metal-free deprotection



Amine **2b** (150 mg, 0.68 mmol, 1 eq) was dissolved in 1 mL of dry THF and the solution was cooled down to 0 ℃. Triethyl amine (0.141mL, 1,02 mmol, 1 .5 eq) was added to the solution, then AcCl (0.048mL, 0.68mmol, 1 eq), was slowly added to the reaction mixture. The solution was stirred at room temperature for 14 hours. 2 mL of NH_4Cl (sat. sol.) were added, the organic phase was collected and the aqueous one was further extracted with AcOEt (3 * 5mL). The collected organic phase was dried over Na_2SO_4 the solvent was removed under reduced pressure. The crude product was purified using column chromatography (from 9:1 to 7:3 Hexanes/AcOEt), giving the desired compound **2-Ac** in a 75% yield. The acetylated compound was not separable from the starting material. The mixture was used without further purification.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 – 6.47 (m, 9H), 3.74 (s, *3*H), 3.42 – 3.20 (m, 2H), 2.23 – 2.01 (m, 3H), 1.72 (m, *6*H).

GC-MS: t_R = 11.419 min and 11.460, (EI, 70 eV): *m/z* = 297 $[M]^+$, 192, 150, 135, 120, 105, 91. 77
Compound **2-Ac** is known and all analytical data are in agreement with literature.[13]



The procedure for the amide deprotection was known in literature[13], and was followed with slightly modification, regarding the purification. Amide **2-Ac** (50 mg, 0.16 mmol, 1 eq) was dissolved in 1 mL of DCE, DDQ (138,5 mg, 0.50mmol, 3 eq), was dissolved in 1 mL of H_2O and slowly added to the reaction mixture. The solution was stirred at 70 ℃ for 14 hours. The reaction was cooled down to

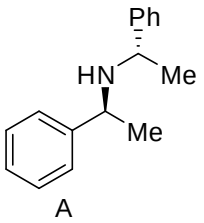
room temperature and 1 mL of a saturated solution of $NaHCO_3$ was added, 5 mL of DCM were added. The organic phase was collected and further washed with a saturated solution of $NaHCO_3$ (3 * 2 mL). The organic phase was dried over Na_2SO_4 the solvent was removed under reduced pressure. The crude product **3** was purified using column chromatography (9:1 pentane/AcOEt), giving the desired compound in a 87% yield. The not acetylated compound was recovered unreacted.

^{1}H NMR (300 MHz, CDCl3) δ 7.42 - 7.18 (m, 5 H), 5.99 (br. s., 1 H), 5.09 (m, 1 H), 1.93 (s, 3 H), 1.44 (d, J = 7.1 Hz, 3 H).

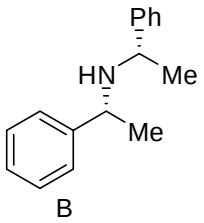
GC-MS: t_R = 6.54 min, (EI, 70 eV): *m/z* = 163 $[M]^+$, 148, 120, 106, 77.
$[\alpha]^{25}_D$ = 106.3° (c: 1g/100mL $CHCl_3$); lit. 115° (c: 1g/100mL $CHCl_3$).[14c]

Compound **3** is known and all analytical data are in agreement with literature.[14]

^{1}H NMR Spectra

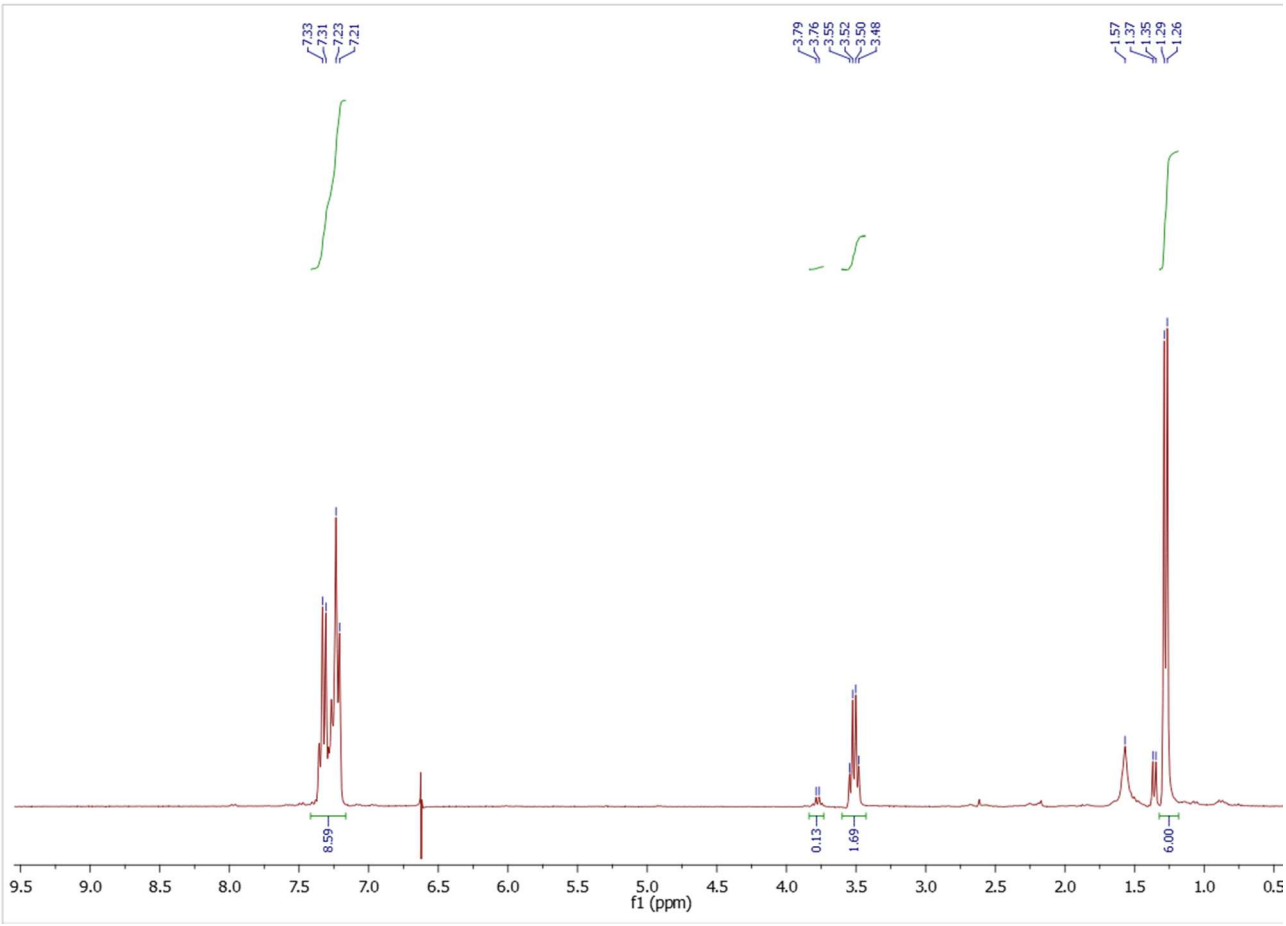


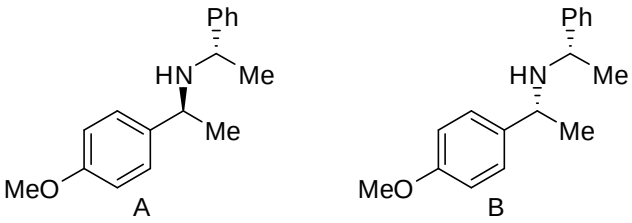
A



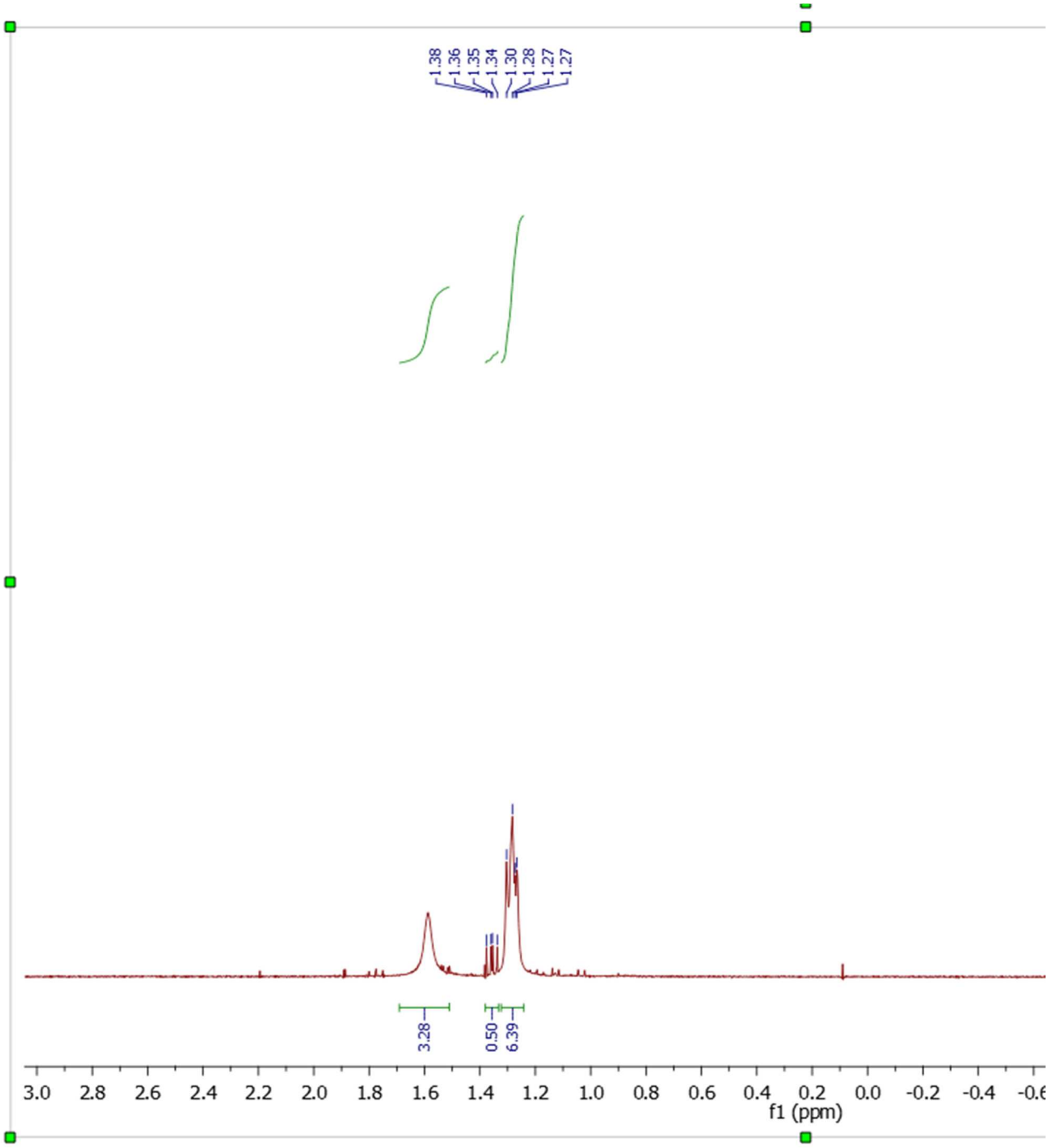
B

93:7 Ratio




Ph
HN
Me
Me
MeO
A
Ph
HN
Me
Me
MeO
B

93:7 Ratio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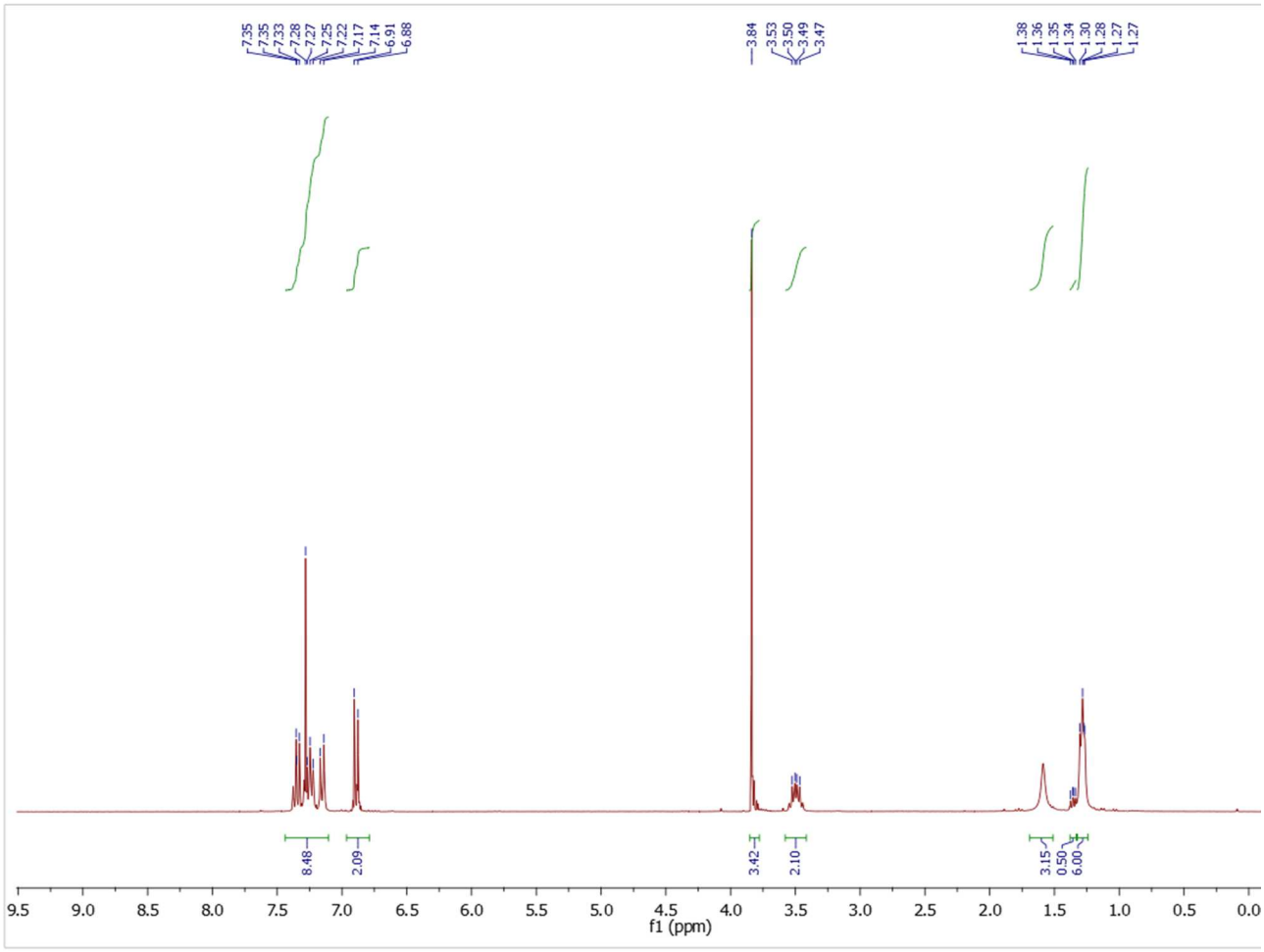
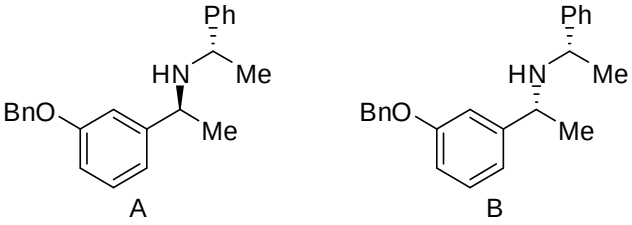
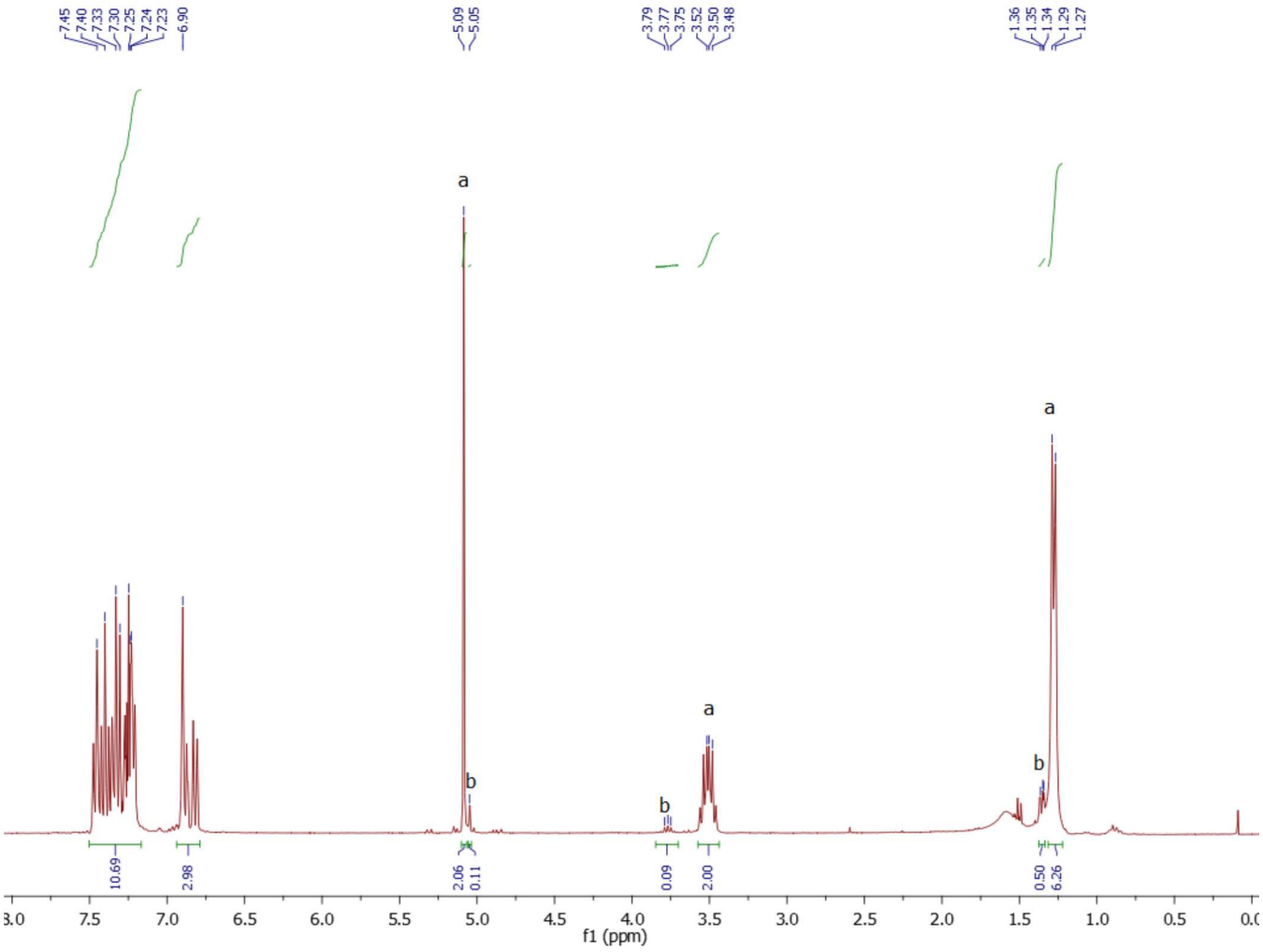
1.34
1.30
1.28
1.27
1.27
3.28
0.50
6.39
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
f1 (ppm)


7.35
7.35
7.33
7.28
7.27
7.25
7.22
7.17
7.14
6.91
6.88
3.84
3.53
3.50
3.49
3.47
1.38
1.36
1.35
1.34
1.30
1.28
1.27
1.27
8.48
2.09
3.42
2.10
3.15
0.50
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Ph
HN
Me
BnO
Me
A
Ph
HN
Me
BnO
Me
B

93:7 Ratio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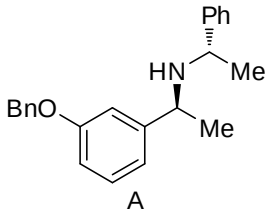
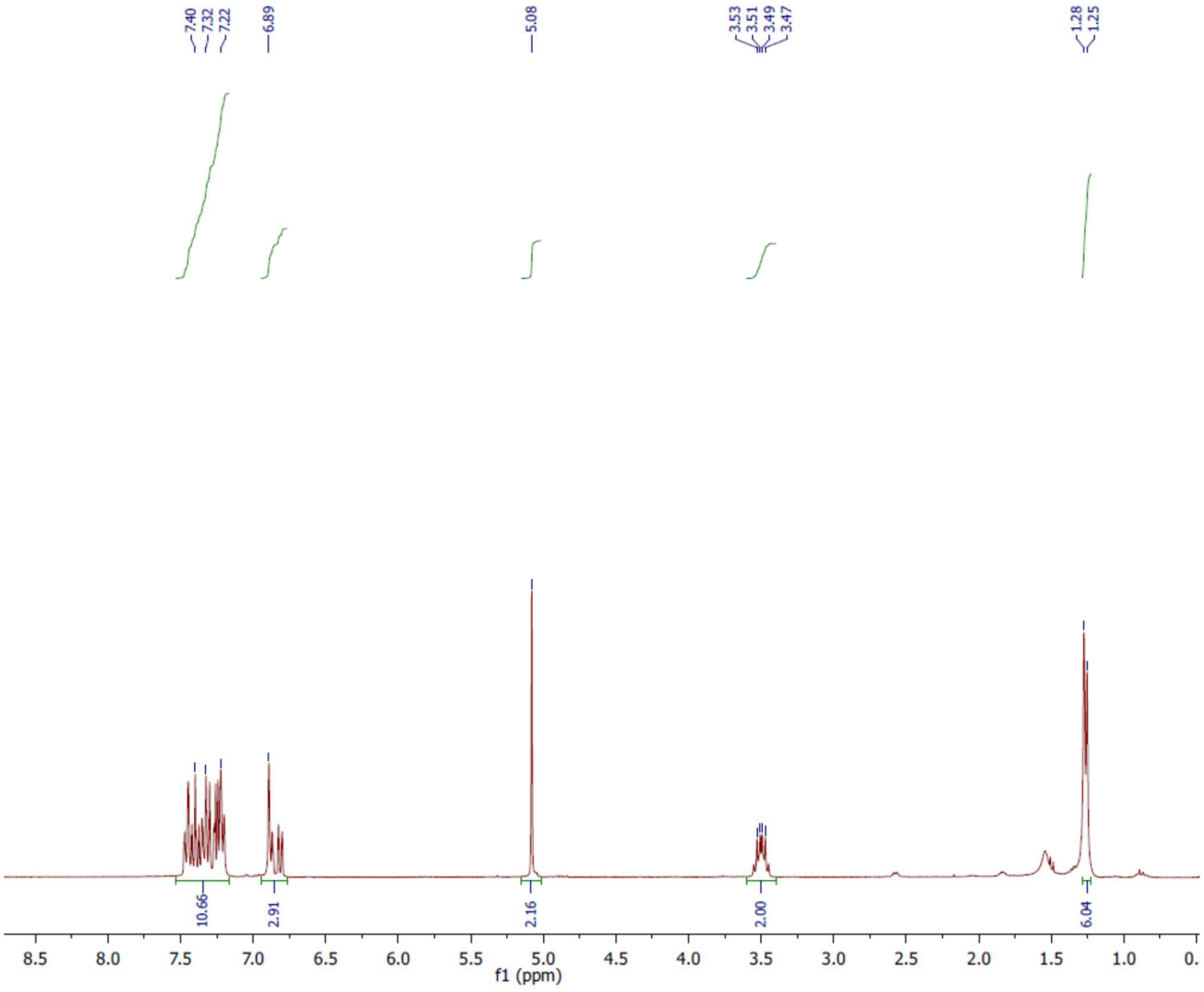
7.24
7.23
6.90
5.09
5.05
3.79
3.77
3.75
3.52
3.50
3.48
1.36
1.35
1.34
1.29
1.27
a
b
a
b
a
b
10.69
2.98
2.06
0.11
0.09
2.00
0.50
6.26
f1 (ppm)


Ph
HN
Me
BnO
Me
A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7.22
6.89
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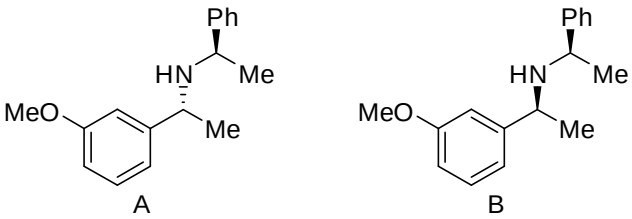
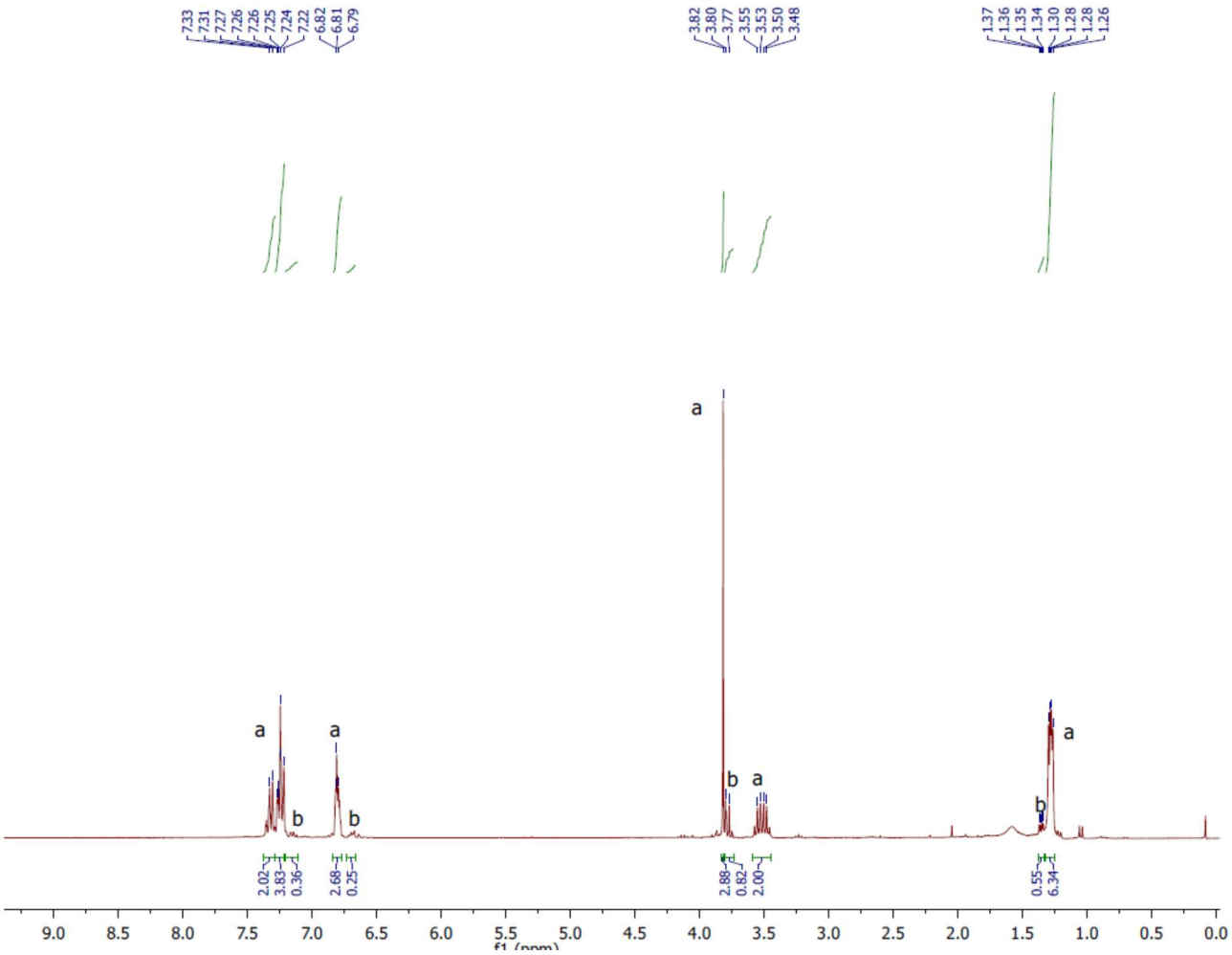
3.53
3.51
3.49
3.47
1.28
1.25
10.66
2.91
2.16
2.00
6.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.
f1 (ppm)


Ph
HN
Me
MeO
Me
A
Ph
HN
Me
MeO
Me
B

92:8 ratio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6.79
3.82
3.80
3.77
3.55
3.53
3.50
3.48
1.37
1.36
1.35
1.34
1.30
1.28
1.28
1.26
a
a
b
b
a
b a
b
a
2.02
3.83
0.36
2.68
0.25
2.88
0.82
2.00
0.55
6.34
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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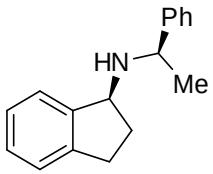
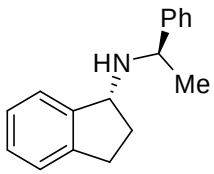
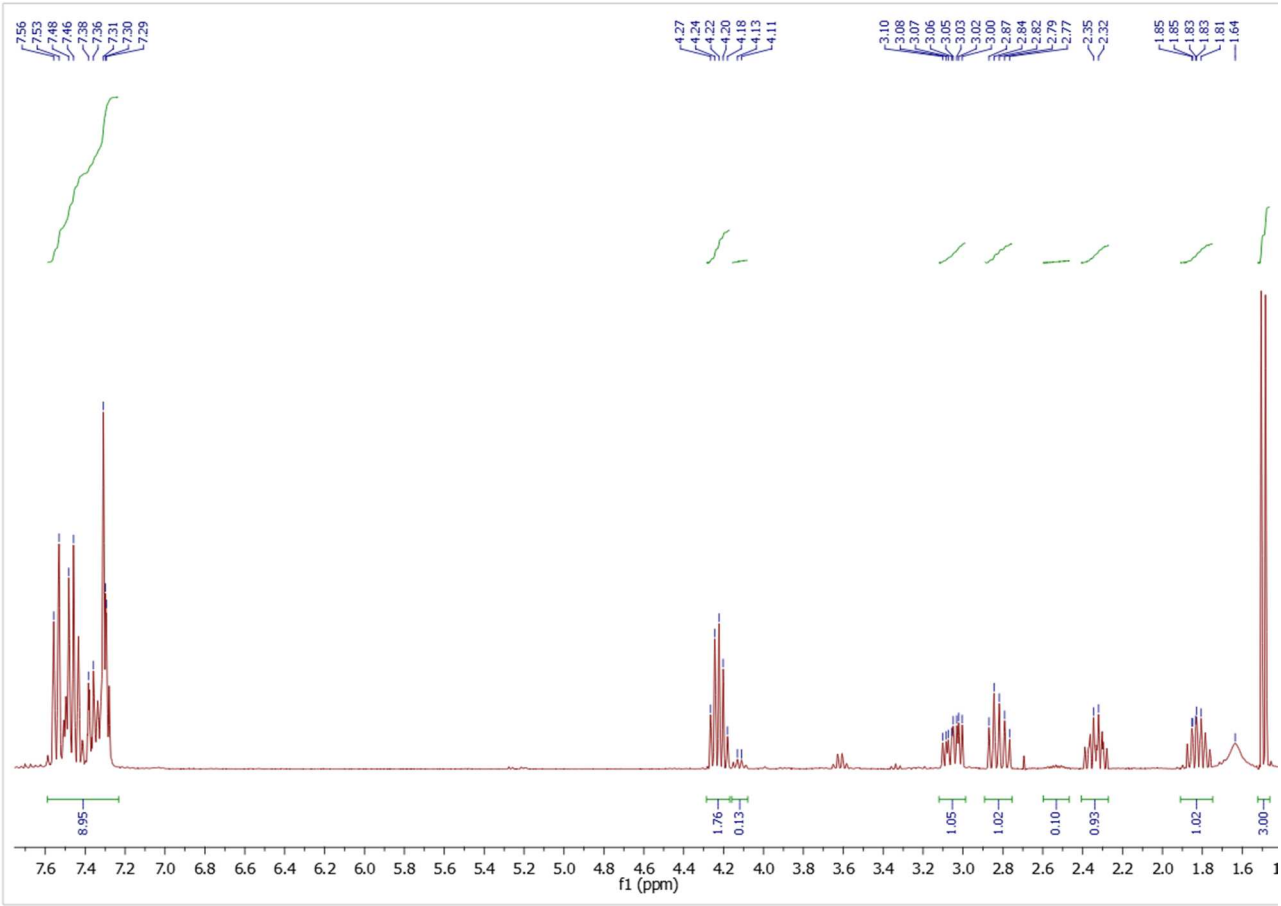
1.5
1.0
0.5
0.0
f1 (ppm)


Ph
HN
Me

A


Ph
HN
Me

B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4.24
4.22
4.20
4.18
4.13
4.11
3.10
3.08
3.07
3.06
3.05
3.03
3.02
3.00
2.87
2.84
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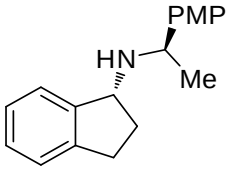
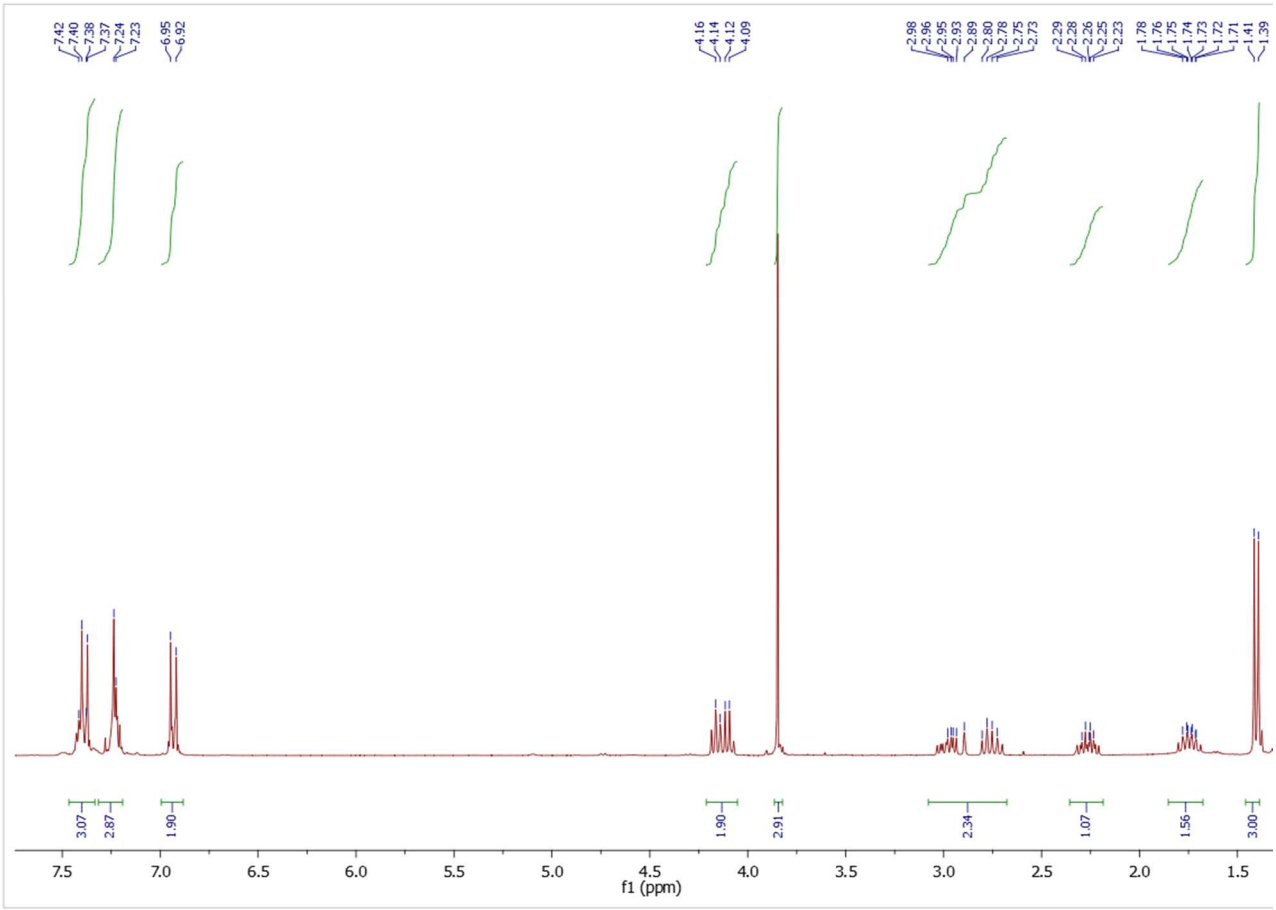
2.32
1.85
1.85
1.83
1.83
1.81
1.64
8.95
1.76
0.13
1.05
1.02
0.10
0.93
1.02
3.00
7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6
f1 (ppm)


PMP
HN
Me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6.95
6.92
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4.14
4.12
4.09
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2.96
2.95
2.93
2.89
2.80
2.78
2.75
2.73
2.29
2.28
2.26
2.25
2.23
1.78
1.76
1.75
1.74
1.73
1.72
1.71
1.41
1.39
3.07
2.87
1.90
1.90
2.91
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1.07
1.56
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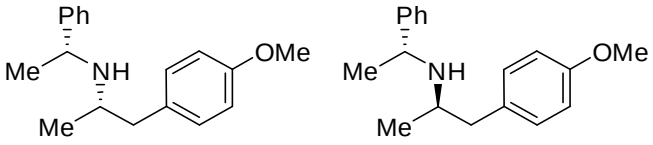
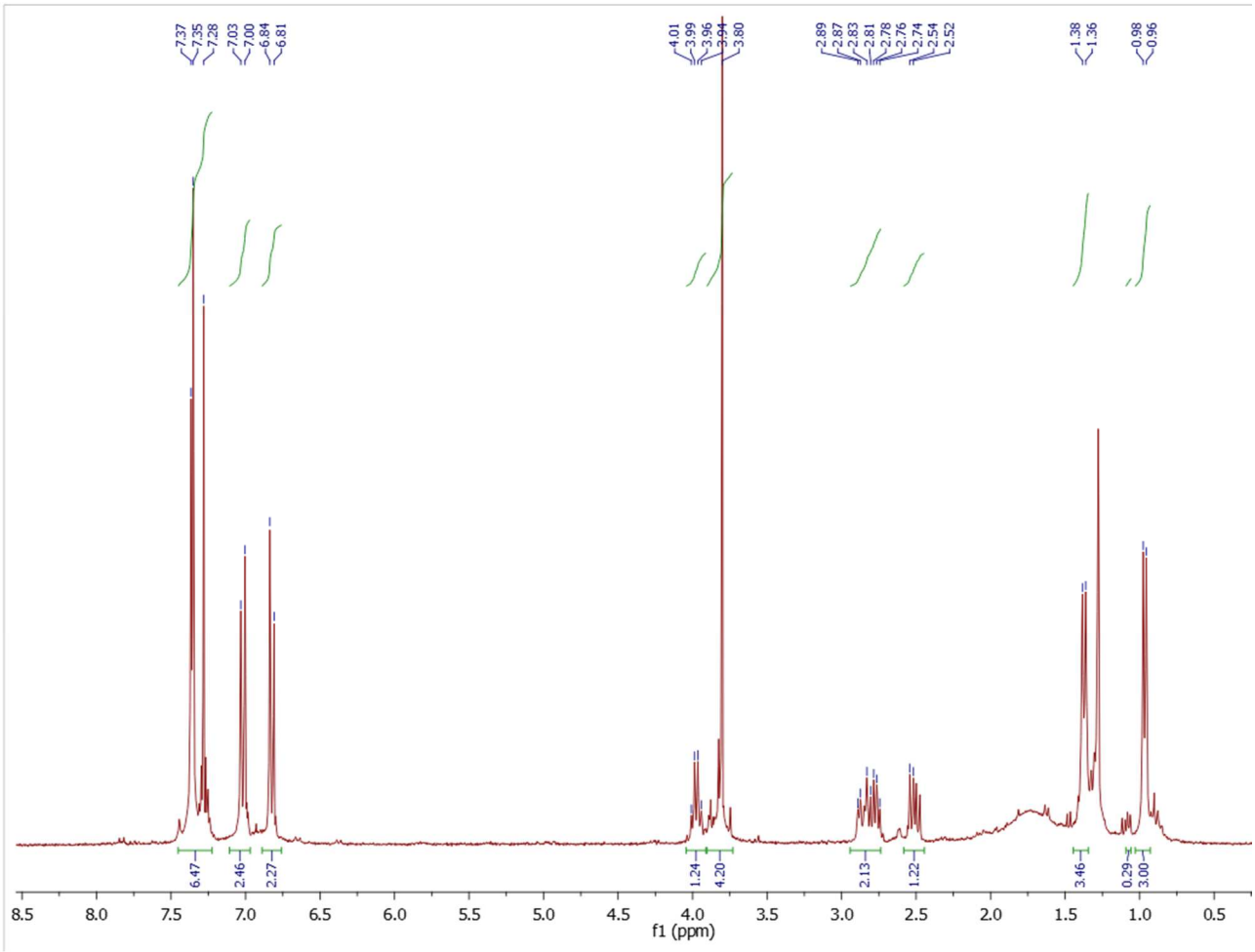
1.5
f1 (ppm)


Ph
Me
NH
Me
OMe
Ph
Me
NH
Me
OMe

A **B**

9:1 ratio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6.84
6.81
4.01
3.99
3.96
3.94
3.80
2.89
2.87
2.83
2.81
2.78
2.76
2.74
2.54
2.52
1.38
1.36
0.98
0.96
6.47
2.46
2.27
1.24
4.20
2.13
1.22
3.46
0.29
3.00
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
3.5
3.0
2.5
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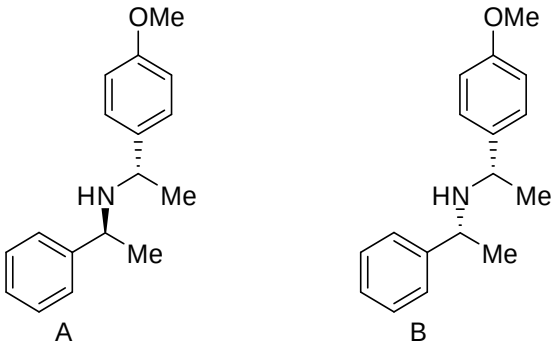
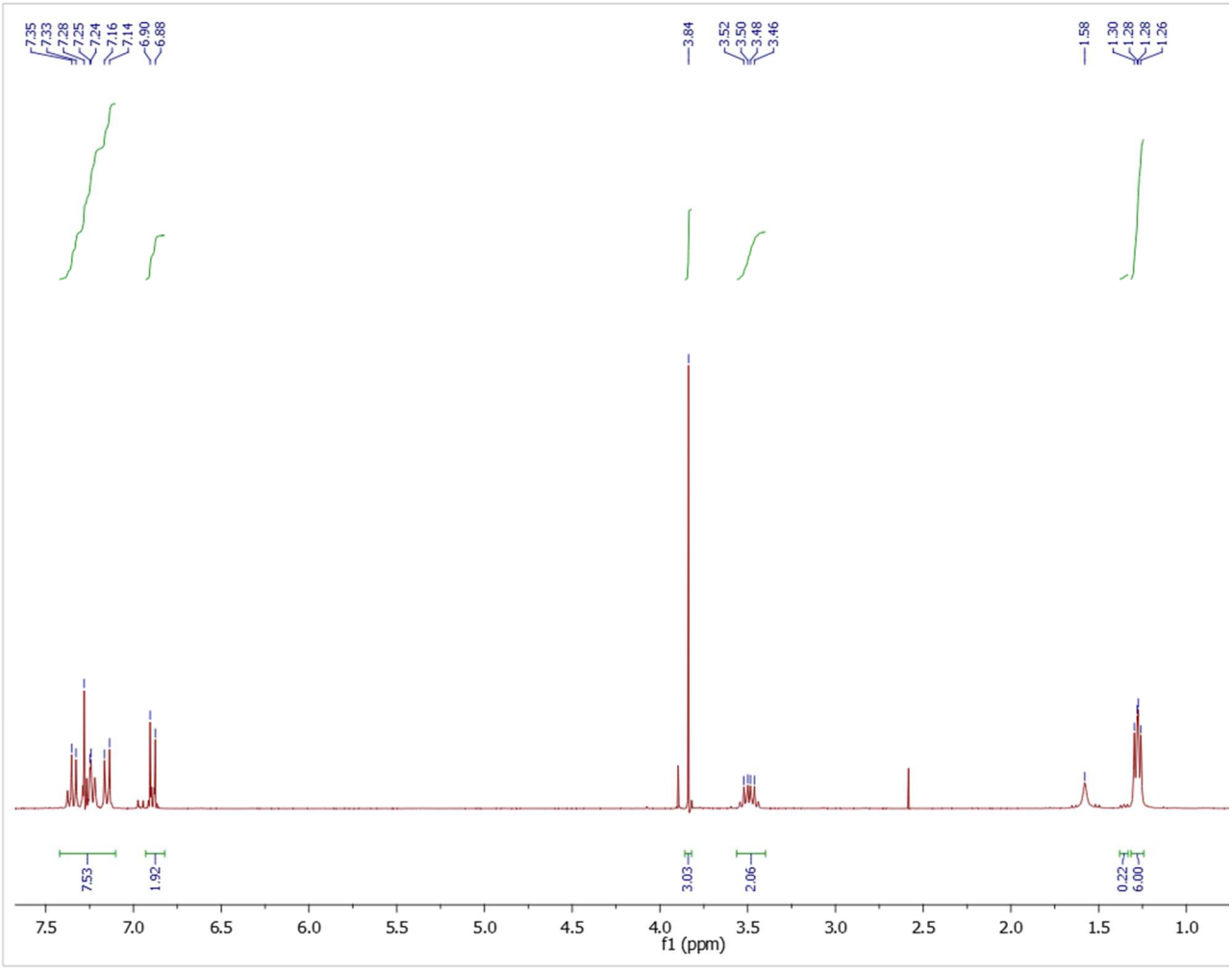
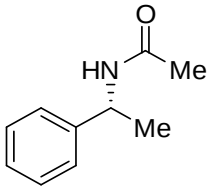
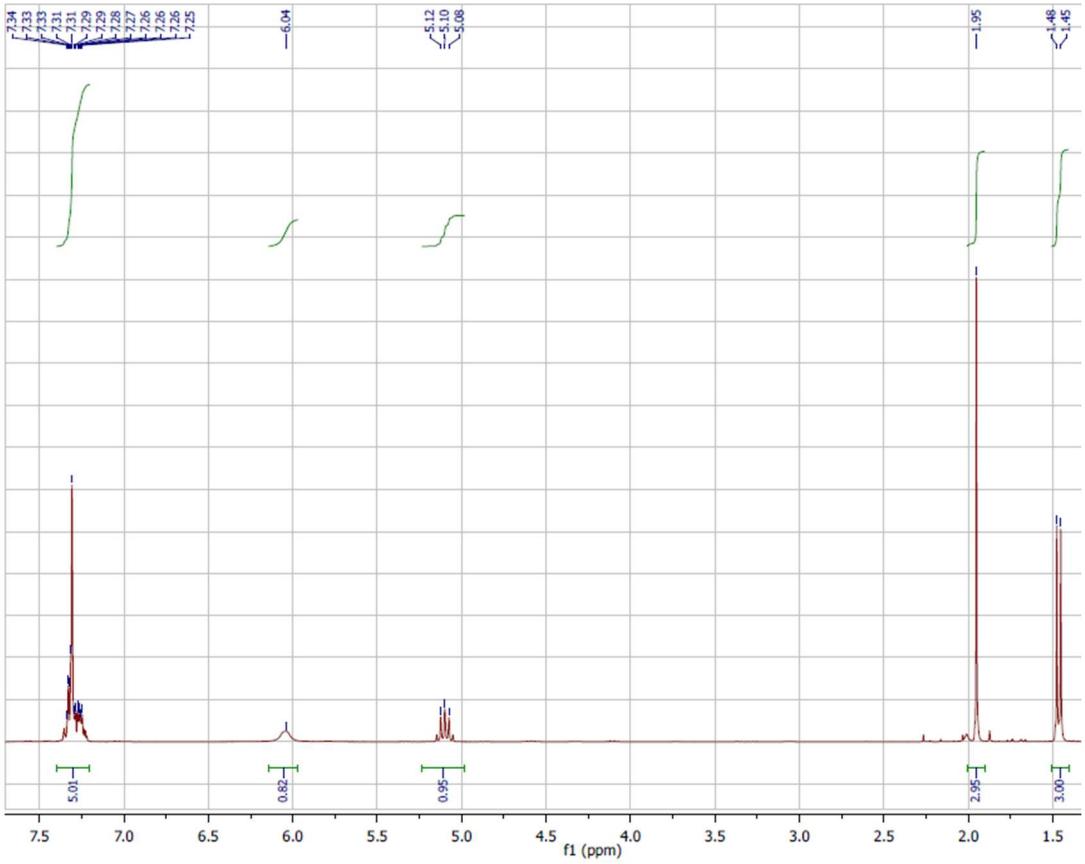
1.5
1.0
0.5
f1 (ppm)


OMe
HN
Me
Me
A
OMe
HN
Me
Me
B

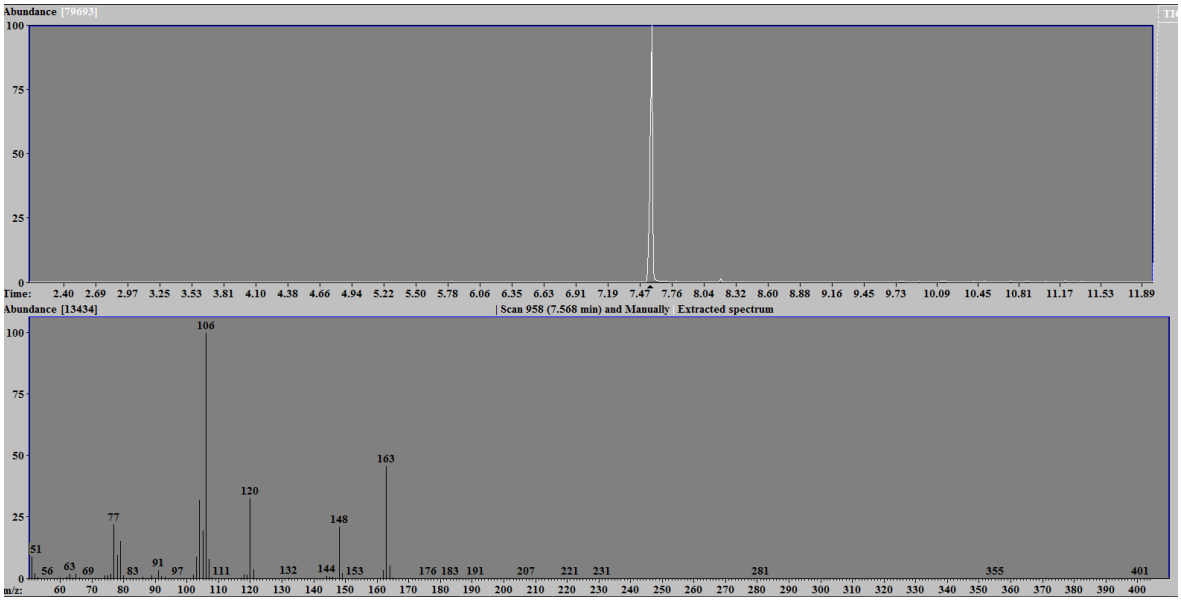
96:4 Ratio


7.35
7.33
7.28
7.25
7.24
7.16
7.14
6.90
6.88
3.84
3.52
3.50
3.48
3.46
1.58
1.30
1.28
1.28
1.26
7.53
1.92
3.03
2.06
0.22
6.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


O
HN
Me
Me


7.34
7.33
7.33
7.31
7.31
7.29
7.29
7.28
7.27
7.26
7.26
7.26
7.25
6.04
5.12
5.10
5.08
1.95
1.48
1.45
5.01
0.82
0.95
2.95
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

GC-MS:


Abundance [79693]
100
75
50
25
0
Time: 2.40 2.69 2.97 3.25 3.53 3.81 4.10 4.38 4.66 4.94 5.22 5.50 5.78 6.06 6.35 6.63 6.91 7.19 7.47 7.76 8.04 8.32 8.60 8.88 9.16 9.45 9.73 10.09 10.45 10.81 11.17 11.53 11.89
Abundance [13434]
Scan 958 (7.568 min) and Manually Extracted spectrum
106
163
120
148
77
51
91
m/z: 56 63 69 83 97 111 132 144 153 176 183 191 207 221 231 281 355 401
60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400

DFT data

Calculations were performed with the GAUSSIAN09[15] within the framework of density functional theory (DFT) by using the hybrid B3LYP functional for all atoms except for iron. The SDD-functional with default parameters was used for iron to account for the influence of d-orbitals. The geometry of intermediate complexes and transition states was optimized in the gas phase without geometry constraints using the 6-31G(d,p) basis set for all atoms except for iron, which was described by the SDD basis set. The stationary points localized thereby were verified using frequency-calculations with the same basis set as before.

The free energies in the energy profiles representing two molecules were calculated by summing up the free energies of the two structures derived from separate calculations without taking into account Basis Set Superposition Errors (BSSE) and additional degrees of freedom of translation and rotation.

*DFT studies on pre-catalyst **B** → catalyst **B** activation*

The energy profiles for oxidative removal of one CO followed by hydrogen coordination and activation (intermediate I to VII, figure S1) was reproduced using the functional described above. As reported in literature, it was found that the step from V to VII, (corresponding to hydrogen activation and cleavage) is the rate-determining step, with an energy barrier of 22.24 kcal/mol. This value match with those reported by Renaud and co. workers[2] demonstrating that B3LYP-631g(d,p) Fe(SDD) functional could be used instead of more time consuming M06 functional with the TZVP basis set on main-group atoms including solvent effects (EtOH with PCM model).

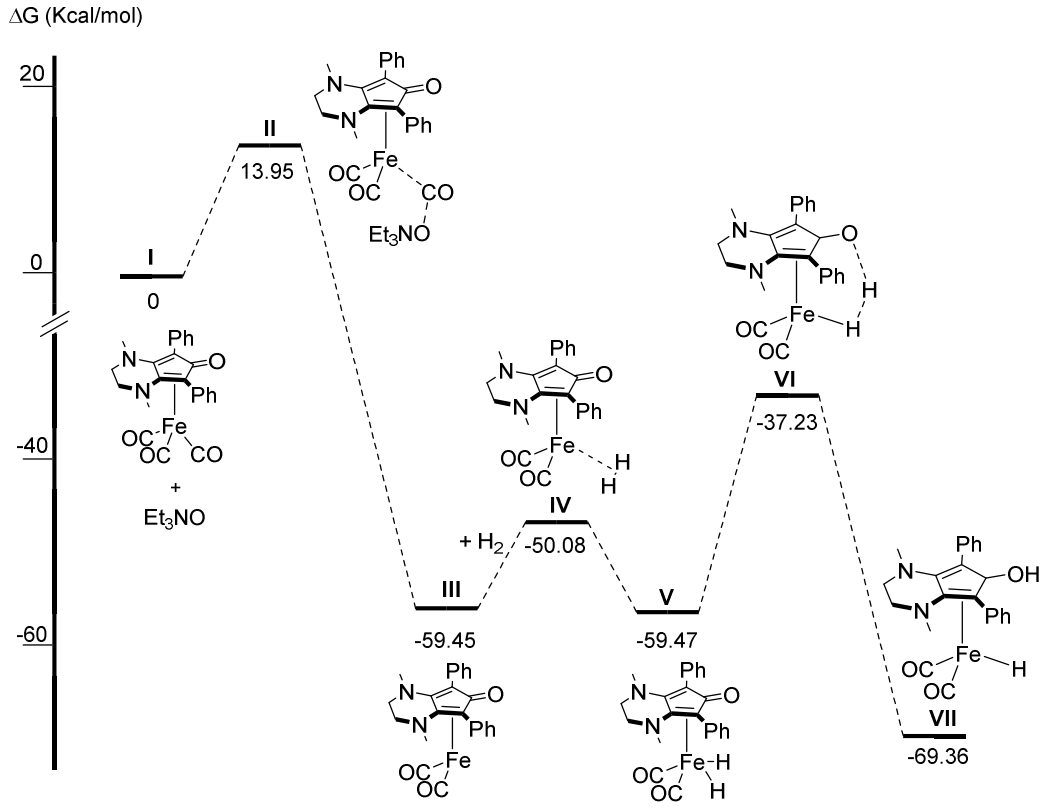


Figure S1

DFT studies on imines reduction

The reduction of *N*-(1-(S)-phenylethyl)-ethan-1-(phenyl)-1-imine (**1a**), *N*-(1-(*S*)-phenylethyl)-ethan-1-(4-(methoxy)phenyl)-1-imine (**1b**), *N*-(1-(*S*)-phenylethyl)-ethan-1-(4-(Methyl)phenyl)-1-imine (**1f**) and *N*-(1-(*S*)-phenylethyl)-ethan-1-(4-(Trifluoromethyl)phenyl)-1-imine (**1g**) promoted by precatalyst **B**, was studied and the two lowest energy transition states (TSs) leading to the formation of (1R,1'S) and (1S,1'S) amines were located. In order to simplify the problem, we adopted a stepwise procedure for the location of the TS structures. First of all, a conformational analysis with Monte Carlo techniques was performed with OPLS_2005 force field[16] on a simple model of the complexes and TSs using the imine in both its conformations (E and *Z*). In this way, the best arrangement for the different substituents around a model of the reaction moiety was obtained. Subsequently, the two lowest energy structures leading to the formation of (1*R*,1'*S*) and (1*S*,1'*S*) diastereoisomers, were fully optimized to the relative TSs with DFT calculations performed with GAUSSIAN 09 program as previously described.

*Energy profile for (E) and (Z) N-(1-(S)-phenylethyl)-ethan-1-(phenyl)-1-imine **(1a)** reduction*

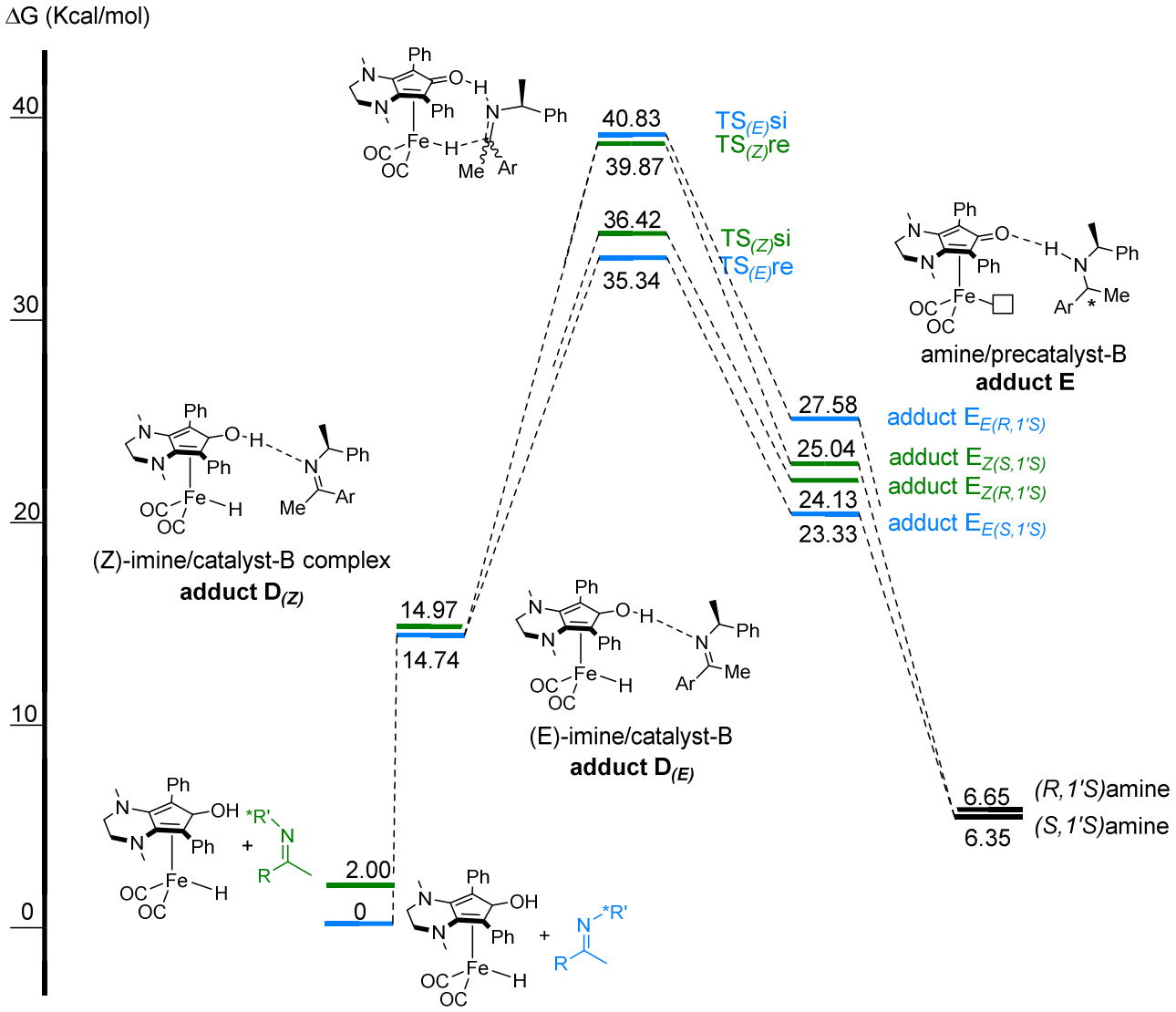


Figure S2

Energy profile for (E) and (Z) N-(1-(S)-phenylethyl)-ethan-1-(4-(methoxy)phenyl)-1-imine ***(1b)*** *reduction*

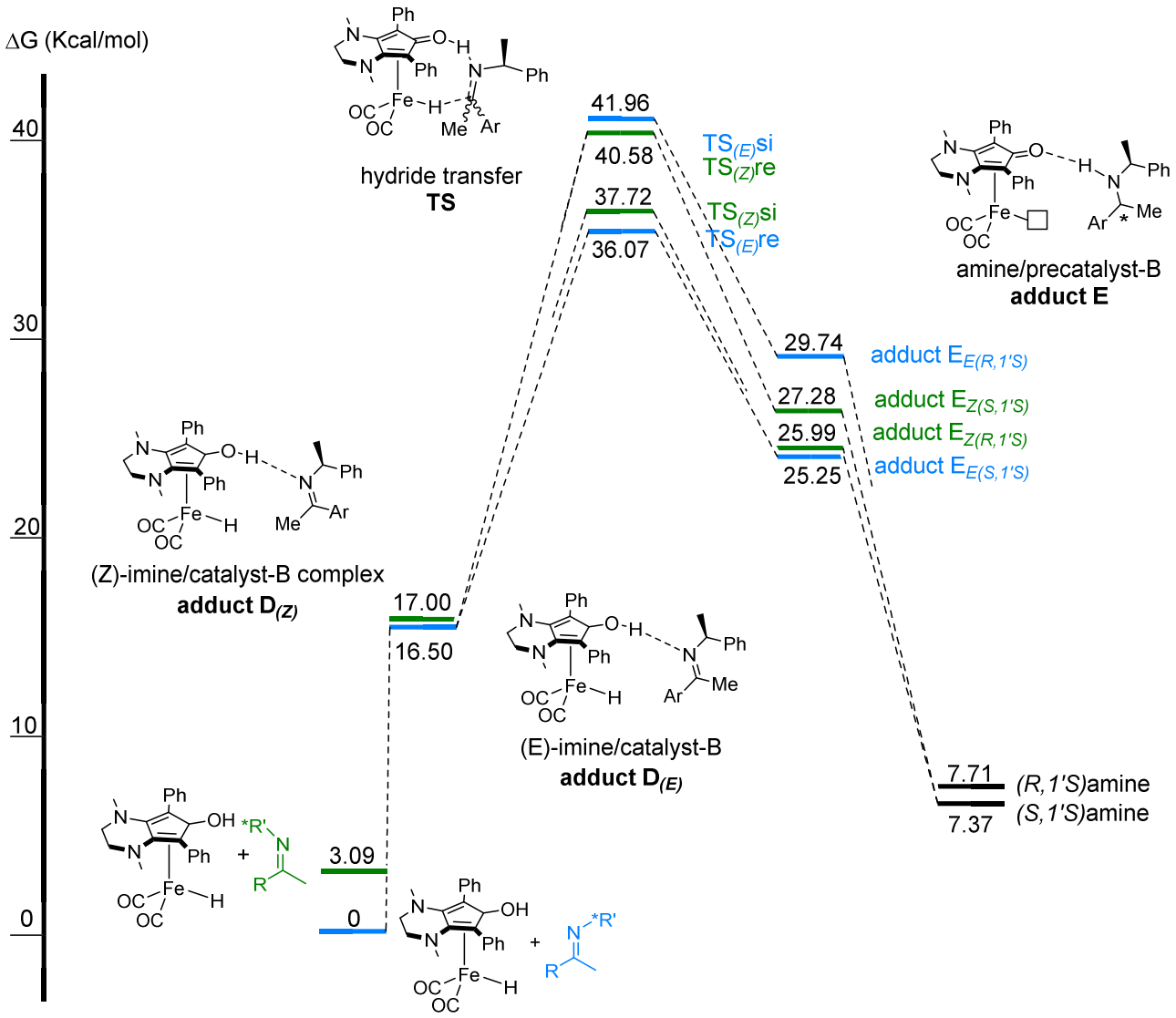


Figure S3

*Energy profile for (E) and (Z) N-(1-(S)-phenylethyl)-ethan-1-(4-(Methyl)phenyl)-1-imine **(1f)** reduction*

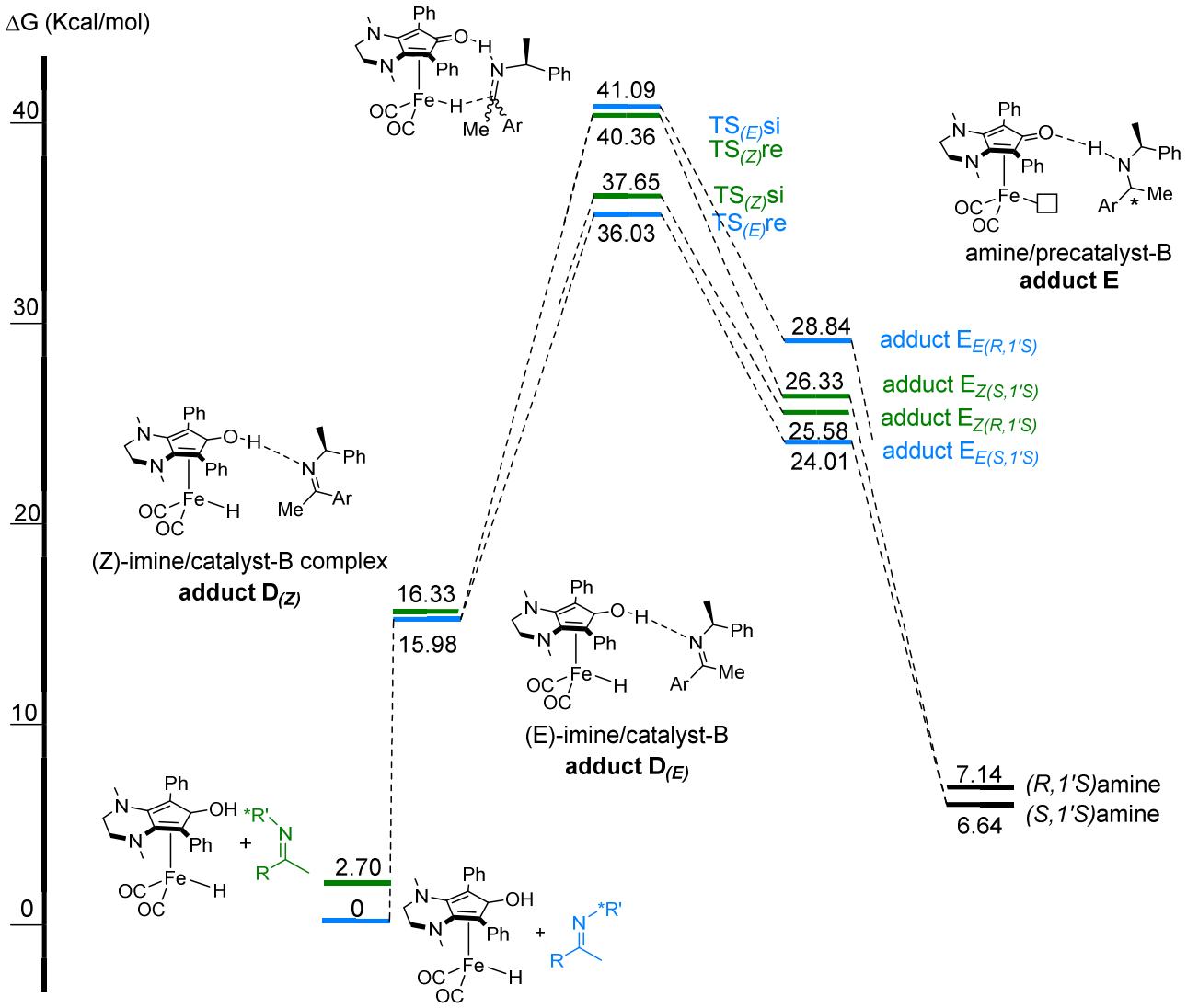


Figure S4

Energy profile for (E) and (Z) N-(1-(S)-phenylethyl)-ethan-1-(4-(Trifluoromethyl)phenyl)-1-imine ***(1g)*** *reduction*

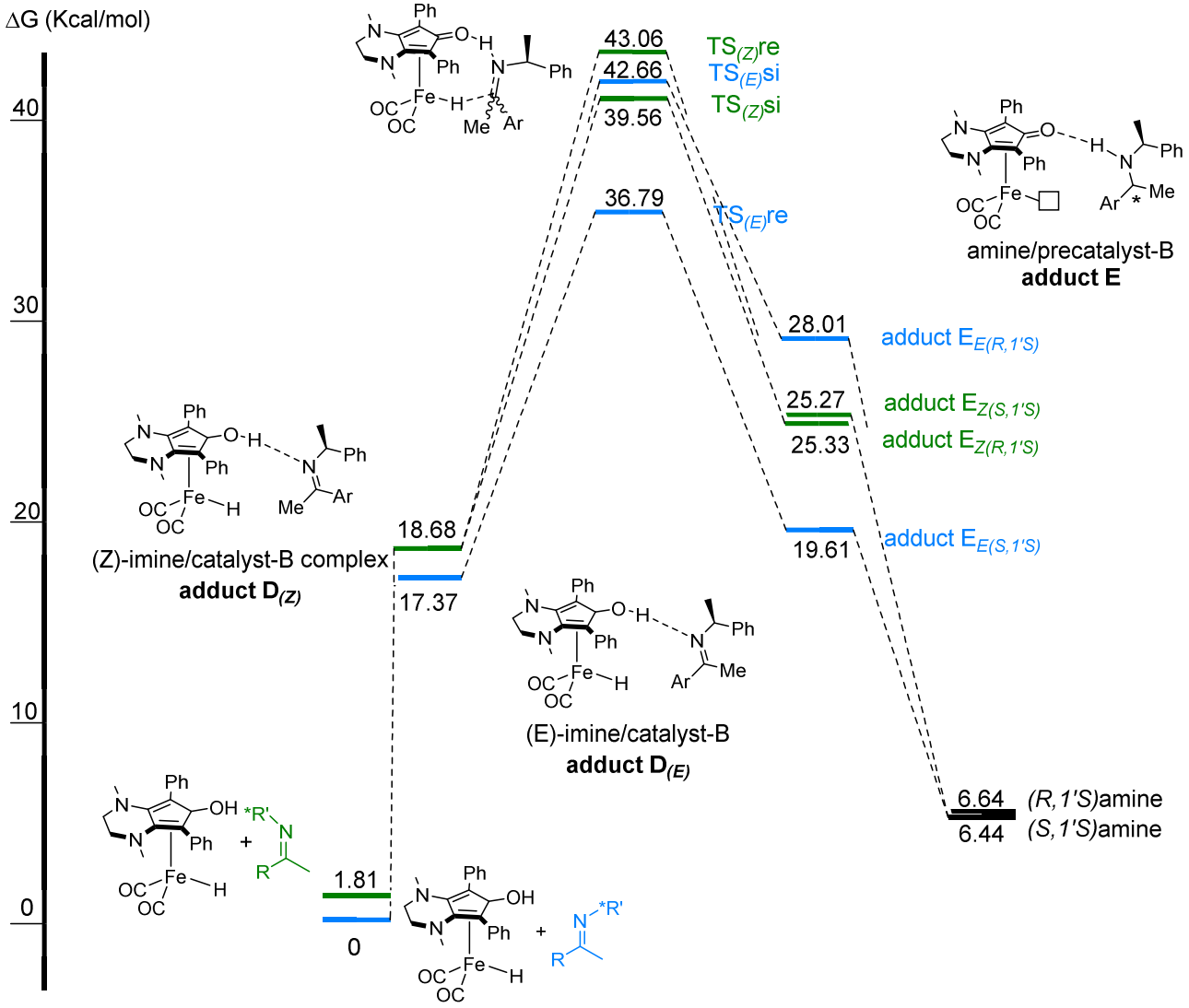


Figure S5

Catalyst B – structure I

C	0.75017	0.95713	-0.72235	H	0.61712	2.91629	-2.80261
C	-1.16818	-0.36965	-0.50850	H	1.31598	4.07059	-1.65988
C	0.01031	-1.28764	-0.68267	C	3.48390	-0.45307	-1.50681
C	-0.63550	3.33010	-1.10996	H	3.19345	0.36553	-2.15765
H	-0.54216	3.65375	-0.05973	C	2.56735	-0.93645	-0.55695
H	-1.18578	4.10476	-1.65205	C	5.12549	-2.08891	-0.80973
C	-0.70120	0.95760	-0.82083	H	6.11362	-2.53036	-0.90275
C	-2.54994	-0.92021	-0.57102	C	-3.50542	-0.71056	0.43564
C	-2.83621	2.18729	-1.11117	H	-3.24531	-0.11550	1.30484
H	-3.18106	2.33750	-0.07833	C	2.61647	2.50044	-0.24746
H	-3.30958	1.29195	-1.50868	H	3.26853	3.16706	-0.81912
H	-3.15439	3.04402	-1.71086	H	3.21080	1.64321	0.06608
C	1.18962	-0.39822	-0.47097	H	2.26498	3.03271	0.65112
C	0.74557	3.14188	-1.73635	C	-2.90154	-1.72524	-1.66854
H	-2.16209	-1.92937	-2.43526	H	-6.12042	-2.47332	-0.84688
C	-4.17925	-2.27551	-1.76820	O	-0.00569	-2.50032	-0.83598
H	-4.43076	-2.89493	-2.62443	N	-1.38530	2.08096	-1.20704
C	4.21641	-2.58973	0.12520	N	1.51107	2.06840	-1.09691
H	4.49325	-3.42654	0.76005	Fe	0.00846	0.26984	1.18032
C	-4.78405	-1.25902	0.33379	C	-0.34090	-1.22781	2.12503
H	-5.50848	-1.08211	1.12377	O	-0.57929	-2.15843	2.75839
C	2.94998	-2.02253	0.24828	C	-1.10169	1.42888	1.97210
H	2.24474	-2.42211	0.96878	O	-1.80982	2.17502	2.50087
C	4.75263	-1.02145	-1.62721	C	1.42428	0.76336	2.15941
H	5.44721	-0.63216	-2.36662	O	2.33998	1.00627	2.81761
C	-5.12683	-2.04114	-0.77034				

Zero-point correction= 0.390811 (Hartree/Particle)
Thermal correction to Energy= 0.419291
Thermal correction to Enthalpy= 0.420235
Thermal correction to Gibbs Free Energy= 0.331747
Sum of electronic and zero-point Energies= -1460.573723
Sum of electronic and thermal Energies= -1460.545243
Sum of electronic and thermal Enthalpies= -1460.544299
Sum of electronic and thermal Free Energies= -1460.632787

Catalyst B – structure II

C	-0.92663	-1.70100	-0.34944	H	-3.36986	-1.77462	0.72776
C	1.08193	-0.58645	-0.74363	H	-2.45976	-2.88430	1.77906
C	-0.02905	0.30759	-1.19465	C	2.82794	0.07601	-2.39304
C	0.21407	-4.16331	0.17594	H	2.05008	0.06253	-3.14879
H	0.14803	-4.04444	1.27095	C	4.13454	0.42098	-2.74041
H	0.66096	-5.14151	-0.02823	H	4.37035	0.65848	-3.77432
C	0.49733	-1.88248	-0.48044	C	-4.35942	1.87187	-0.72992
C	2.49387	-0.24152	-1.06389	H	-4.71466	2.79828	-0.28525
C	2.50156	-3.33124	-0.25454	C	4.81380	0.16557	-0.44061
H	2.85277	-3.09058	0.75990	H	5.58057	0.20535	0.32838
H	3.05072	-2.71781	-0.96613	C	-3.09147	1.39055	-0.40181
H	2.72871	-4.38157	-0.45757	H	-2.45567	1.93160	0.28928
C	-1.24865	-0.31801	-0.66597	C	-4.71265	-0.02518	-2.17445
C	-1.17945	-4.08768	-0.45254	H	-5.33815	-0.58220	-2.86709
H	-1.08341	-4.29231	-1.52692	C	5.13445	0.46242	-1.76676
H	-1.82187	-4.86125	-0.02391	H	6.15215	0.72993	-2.03747
C	-3.44421	-0.50640	-1.84973	O	0.08735	1.38979	-1.79398
H	-3.09074	-1.43688	-2.28247	N	1.06765	-3.13757	-0.41649
C	-2.61373	0.19203	-0.95491	N	-1.81792	-2.78521	-0.25849
C	-5.17640	1.16742	-1.61622	Fe	-0.02148	-0.42742	1.10172
H	-6.16509	1.54180	-1.86715	C	0.78169	1.24774	1.58116
C	3.50593	-0.17342	-0.09174	O	1.70440	1.70613	2.16010
H	3.26255	-0.38230	0.94411	C	0.94269	-1.35814	2.26397
C	-2.85918	-2.73699	0.76143	O	1.54277	-1.98595	3.03166
H	-3.60012	-3.51541	0.55524	C	-1.40909	-0.21698	2.19163

O	-2.30764	-0.01954	2.89297	H	1.45214	2.79466	-1.01217
O	-0.24197	2.51127	0.91087	H	1.94730	4.49640	-0.64985
N	0.32280	3.74297	0.47806	H	2.36755	3.17682	0.48658
C	-0.67376	4.28140	-0.50210	C	0.47804	4.63947	1.66401
H	-1.61437	4.42884	0.02690	H	0.84999	5.61586	1.34238
H	-0.30629	5.22692	-0.90936	H	-0.49980	4.73384	2.13486
H	-0.78330	3.51723	-1.27292	H	1.17682	4.16127	2.34756
C	1.63648	3.53630	-0.23178				

Zero-point correction= 0.518755 (Hartree/Particle)
Thermal correction to Energy= 0.553422
Thermal correction to Enthalpy= 0.554366
Thermal correction to Gibbs Free Energy= 0.453420
Sum of electronic and zero-point Energies= -1710.075697
Sum of electronic and thermal Energies= -1710.041030
Sum of electronic and thermal Enthalpies= -1710.040085
Sum of electronic and thermal Free Energies= -1710.141031
Imaginary frequency -109.52

Catalyst B – structure III

C	-0.72288	0.91394	-0.69052	H	-2.94976	-0.12138	-2.44439
C	0.73773	0.87423	-0.71742	C	-4.34097	-2.40086	0.35744
C	0.70937	3.05820	-1.70810	H	-2.48760	-2.01627	1.38351
C	-0.60112	3.29742	-0.97091	C	-5.10710	-2.16155	-0.78481
C	-1.20830	-0.40105	-0.39738	H	-5.18366	-1.15298	-2.69072
C	-0.03032	-1.29079	-0.25952	H	-4.72064	-3.05081	1.14064
C	1.17862	-0.44962	-0.40711	H	-6.08566	-2.62024	-0.89345
H	1.31437	3.96753	-1.69680	C	2.54007	-1.02065	-0.48603
H	-0.39921	3.62965	0.06205	C	3.42489	-0.62568	-1.50625
N	-1.41232	2.07913	-0.97100	C	2.94945	-2.03422	0.39918
N	1.48285	1.97337	-1.09951	C	4.68773	-1.20594	-1.62116
C	-2.74721	2.30080	-0.41549	H	3.11422	0.13457	-2.21658
H	-3.36695	1.41462	-0.52133	C	4.21265	-2.61141	0.27995
H	-2.69872	2.57265	0.64893	H	2.26288	-2.37851	1.16327
H	-3.21833	3.12141	-0.96393	C	5.08929	-2.19831	-0.72549
C	2.67504	2.36390	-0.34957	H	5.35528	-0.88597	-2.41655
H	3.22912	1.48197	-0.03376	H	4.51137	-3.39057	0.97554
H	3.32742	2.96171	-0.99253	H	6.07333	-2.64972	-0.81380
H	2.41684	2.95311	0.54300	O	-0.05968	-2.44366	0.21494
H	-1.17322	4.08690	-1.46933	Fe	0.00187	0.14017	1.24792
H	0.49525	2.81221	-2.75599	C	-1.27092	0.76732	2.31144
C	-2.57431	-0.96415	-0.49328	C	1.32665	0.71527	2.28146
C	-3.34534	-0.74877	-1.64994	O	2.19705	1.11308	2.93109
C	-3.08480	-1.81264	0.50217	O	-2.10369	1.19758	2.99049
C	-4.60289	-1.33506	-1.79074				

Zero-point correction= 0.381982 (Hartree/Particle)
Thermal correction to Energy= 0.408400
Thermal correction to Enthalpy= 0.409344
Thermal correction to Gibbs Free Energy= 0.324904
Sum of electronic and zero-point Energies= -1347.218410
Sum of electronic and thermal Energies= -1347.191992
Sum of electronic and thermal Enthalpies= -1347.191048
Sum of electronic and thermal Free Energies= -1347.275488

Catalyst B – structure IV

C	-0.69017	1.02076	-0.66153	H	-0.73519	3.58358	0.35726
C	0.75321	1.06646	-0.66451	N	-1.44628	2.13843	-1.02904
C	0.63971	3.39204	-1.30146	N	1.42939	2.26854	-0.79060
C	-0.77219	3.39546	-0.73123	C	-2.87969	2.15815	-0.76067
C	-1.08934	-0.34909	-0.40398	H	-3.35779	1.27971	-1.18978
C	0.12630	-1.19474	-0.62717	H	-3.11313	2.19336	0.31474
C	1.26616	-0.25268	-0.38433	H	-3.30269	3.04787	-1.23560
H	1.14797	4.32023	-1.01911	C	2.83251	2.31688	-1.19431

H	3.42808	1.60668	-0.62739	C	3.54838	-0.47036	0.69528
H	2.95887	2.10232	-2.26621	C	4.41431	-2.09760	-1.39038
H	3.21109	3.32396	-0.99814	H	2.43412	-1.84912	-2.19996
H	-1.33637	4.21241	-1.19139	C	4.84956	-0.97332	0.69904
H	0.59000	3.36016	-2.40157	H	3.20653	0.14657	1.52243
C	-2.43723	-0.97033	-0.51788	C	5.28791	-1.78817	-0.34677
C	-2.81277	-1.53070	-1.75146	H	4.74189	-2.74232	-2.20110
C	-3.32873	-1.07166	0.55925	H	5.51560	-0.73837	1.52458
C	-4.05521	-2.14302	-1.90917	H	6.29829	-2.18690	-0.34207
H	-2.11988	-1.48919	-2.58628	O	0.17855	-2.40228	-0.81333
C	-4.57250	-1.68557	0.40182	H	1.74207	1.77066	3.46434
H	-3.04594	-0.67185	1.52643	Fe	0.01258	0.32057	1.21279
C	-4.94210	-2.21915	-0.83305	H	1.90897	2.41846	3.13813
H	-4.32695	-2.56811	-2.87131	C	0.33158	-1.06106	2.31217
H	-5.24901	-1.75159	1.24929	C	-1.23838	1.12964	2.19564
H	-5.90893	-2.69928	-0.95436	O	-2.01118	1.65979	2.87664
C	2.66572	-0.75541	-0.36014	O	0.46114	-1.98539	2.99019
C	3.11554	-1.58817	-1.39782				

Zero-point correction= 0.392142 (Hartree/Particle)
Thermal correction to Energy= 0.421819
Thermal correction to Enthalpy= 0.422763
Thermal correction to Gibbs Free Energy= 0.330035
Sum of electronic and zero-point Energies= -1348.377226
Sum of electronic and thermal Energies= -1348.347549
Sum of electronic and thermal Enthalpies= -1348.346605
Sum of electronic and thermal Free Energies= -1348.439333
Imaginary frequency -66.10

Catalyst B – structure V

C	-0.68790	0.79785	-0.66124	C	-4.32223	-2.38761	0.70066
C	0.76168	0.72244	-0.82268	H	-2.49207	-1.88422	1.71589
C	0.67690	2.69079	-2.20333	C	-5.06606	-2.27211	-0.47492
C	-0.60052	3.05059	-1.46319	H	-5.10640	-1.47030	-2.47719
C	-1.15798	-0.49696	-0.20692	H	-4.71834	-2.94765	1.54301
C	0.00687	-1.42175	-0.22131	H	-6.04453	-2.73757	-0.55124
C	1.20174	-0.51499	-0.24397	C	2.57249	-1.08477	-0.14555
H	1.28293	3.59294	-2.33311	C	2.89241	-2.22331	-0.90568
H	-0.34769	3.56532	-0.51926	C	3.55541	-0.56072	0.71170
N	-1.41362	1.86473	-1.21075	C	4.16153	-2.79730	-0.83050
N	1.46170	1.71924	-1.44120	H	2.13341	-2.66509	-1.54062
C	-2.70009	2.22307	-0.61542	C	4.82611	-1.13282	0.78197
H	-3.30894	1.33947	-0.44159	H	3.32366	0.29977	1.33098
H	-2.57036	2.75832	0.33804	C	5.13515	-2.25312	0.00852
H	-3.23460	2.87844	-1.30974	H	4.38702	-3.67657	-1.42744
C	2.85283	1.57151	-1.85514	H	5.56999	-0.70746	1.44985
H	3.45541	1.14045	-1.05923	H	6.12207	-2.70310	0.06710
H	2.95399	0.93876	-2.74819	O	0.00437	-2.64106	-0.09593
H	3.24762	2.56390	-2.08850	H	-0.07546	-0.91010	2.28360
H	-1.18713	3.74502	-2.07323	Fe	-0.01250	0.43545	1.29139
H	0.43555	2.30224	-3.20505	H	0.66919	-0.60286	2.40640
C	-2.53350	-1.05342	-0.26851	C	-1.40366	1.08495	2.19534
C	-3.28400	-0.96159	-1.45393	C	1.10473	1.71116	1.85261
C	-3.06797	-1.78634	0.80145	O	1.81264	2.56349	2.18658
C	-4.54097	-1.55797	-1.55350	O	-2.30816	1.46518	2.80535
H	-2.87545	-0.41572	-2.29984				

Zero-point correction= 0.398270 (Hartree/Particle)
Thermal correction to Energy= 0.425687
Thermal correction to Enthalpy= 0.426631
Thermal correction to Gibbs Free Energy= 0.339731
Sum of electronic and zero-point Energies= -1348.395747
Sum of electronic and thermal Energies= -1348.368330
Sum of electronic and thermal Enthalpies= -1348.367386
Sum of electronic and thermal Free Energies= -1348.454286

Catalyst B – structure VI

C	-0.72497	0.90232	-0.69801	C	-4.44396	-2.24878	0.43745
C	0.71607	0.87650	-0.68817	H	-2.66932	-1.74554	1.54767
C	0.68806	2.98384	-1.81594	C	-5.11455	-2.15587	-0.78295
C	-0.63519	3.25946	-1.10756	H	-5.02114	-1.41575	-2.80764
C	-1.20137	-0.42711	-0.35656	H	-4.90168	-2.77295	1.27153
C	-0.03090	-1.29253	-0.24197	H	-6.09651	-2.60431	-0.90310
C	1.16140	-0.47909	-0.39127	C	2.53236	-1.02961	-0.49626
H	1.27814	3.90113	-1.87722	C	3.42046	-0.54422	-1.47339
H	-0.44661	3.65119	-0.09198	C	2.95267	-2.09848	0.31634
N	-1.43416	2.03655	-1.04742	C	4.69439	-1.09432	-1.61778
N	1.47959	1.96011	-1.12833	H	3.10321	0.26243	-2.12596
C	-2.78098	2.26473	-0.52969	C	4.22549	-2.64521	0.16642
H	-3.37389	1.35509	-0.57344	H	2.26680	-2.51015	1.04570
H	-2.75726	2.62328	0.51018	C	5.10494	-2.14436	-0.79607
H	-3.26680	3.02597	-1.14688	H	5.36349	-0.70348	-2.37955
C	2.56632	2.45161	-0.28521	H	4.53045	-3.46901	0.80565
H	2.19501	3.00694	0.59138	H	6.09748	-2.57158	-0.90700
H	3.17547	1.61837	0.06457	O	-0.06598	-2.49546	0.25974
H	3.20848	3.11133	-0.87573	H	-0.10396	-1.83942	1.48905
H	-1.20845	4.01593	-1.65387	Fe	0.00748	0.16918	1.28228
H	0.48006	2.65153	-2.84060	H	-0.11942	-1.24441	2.22110
C	-2.57323	-0.98585	-0.46413	C	-1.23560	1.01184	2.26264
C	-3.25094	-0.91326	-1.69407	C	1.41445	0.71820	2.24838
C	-3.18447	-1.66992	0.59661	O	2.32849	1.01088	2.88691
C	-4.51283	-1.48594	-1.85004	O	-2.03641	1.50440	2.93158
H	-2.78076	-0.40423	-2.53127				

Zero-point correction= 0.395780 (Hartree/Particle)
Thermal correction to Energy= 0.422122
Thermal correction to Enthalpy= 0.423067
Thermal correction to Gibbs Free Energy= 0.339054
Sum of electronic and zero-point Energies= -1348.362122
Sum of electronic and thermal Energies= -1348.335779
Sum of electronic and thermal Enthalpies= -1348.334835
Sum of electronic and thermal Free Energies= -1348.418848
Imaginary frequency -1583.59

Catalyst B – structure VII

C	-0.70960	0.92747	-0.72884	H	-2.87697	-0.37732	-2.48778
C	0.71746	0.87353	-0.73584	C	-4.37169	-2.29301	0.53186
C	0.72418	2.94500	-1.90220	H	-2.58921	-1.68919	1.59281
C	-0.58617	3.26653	-1.18149	C	-5.08575	-2.21911	-0.66403
C	-1.20696	-0.38981	-0.35934	H	-5.09539	-1.46011	-2.68357
C	-0.05280	-1.23803	-0.25066	H	-4.78585	-2.82683	1.38242
C	1.14209	-0.48336	-0.40976	H	-6.05589	-2.69916	-0.75208
H	1.32565	3.85103	-2.00936	C	2.50725	-1.05371	-0.47608
H	-0.37154	3.65990	-0.17121	C	3.40184	-0.63653	-1.47642
N	-1.42080	2.06742	-1.10592	C	2.91799	-2.05749	0.41806
N	1.51905	1.93467	-1.19714	C	4.67394	-1.20182	-1.57243
C	-2.72304	2.33092	-0.50180	H	3.09358	0.13531	-2.17388
H	-3.35950	1.44947	-0.54652	C	4.18747	-2.62211	0.31527
H	-2.63307	2.64540	0.54933	H	2.23568	-2.38884	1.19314
H	-3.21058	3.13345	-1.06317	C	5.07236	-2.19604	-0.67837
C	2.54023	2.46053	-0.29284	H	5.35247	-0.86572	-2.35174
H	3.15693	1.64414	0.08480	H	4.48840	-3.39445	1.01752
H	3.19096	3.14261	-0.84833	H	6.06318	-2.63499	-0.75337
H	2.11023	2.99711	0.56893	O	-0.06957	-2.58247	-0.10578
H	-1.14255	4.03651	-1.72714	H	-0.98510	-2.85901	0.05427
H	0.49077	2.57749	-2.90920	Fe	0.00560	0.26978	1.25598
C	-2.57419	-0.96322	-0.43471	H	-0.14711	-0.87177	2.21405
C	-3.29965	-0.90747	-1.63907	C	-1.17882	1.07738	2.27865
C	-3.12828	-1.66611	0.64965	C	1.38354	0.70122	2.26704
C	-4.54695	-1.51990	-1.74775	O	2.28760	0.91624	2.95593

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O      -1.95741     1.53588     3.00393

Zero-point correction=                  0.402224 (Hartree/Particle)
 Thermal correction to Energy=              0.428824
 Thermal correction to Enthalpy=            0.429768
 Thermal correction to Gibbs Free Energy=      0.345737
 Sum of electronic and zero-point Energies=       -1348.413569
 Sum of electronic and thermal Energies=          -1348.386969
 Sum of electronic and thermal Enthalpies=        -1348.386025
 Sum of electronic and thermal Free Energies=     -1348.470056
```

(E)-*N*-(1-(*S*)-phenylethyl)-ethan-1-(phenyl)-1-imine (1a)

```
Zero-point correction=                  0.287833 (Hartree/Particle)
 Thermal correction to Energy=              0.303214
 Thermal correction to Enthalpy=            0.304158
 Thermal correction to Gibbs Free Energy=      0.241740
 Sum of electronic and zero-point Energies=        -674.425729
 Sum of electronic and thermal Energies=          -674.410348
 Sum of electronic and thermal Enthalpies=         -674.409404
 Sum of electronic and thermal Free Energies=      -674.471821
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(Z)-*N*-(1-(*S*)-phenylethyl)-ethan-1-(phenyl)-1-imine (1a)

```
Zero-point correction=                  0.287342 (Hartree/Particle)
 Thermal correction to Energy=              0.302847
 Thermal correction to Enthalpy=            0.303792
 Thermal correction to Gibbs Free Energy=      0.242060
 Sum of electronic and zero-point Energies=        -674.423344
 Sum of electronic and thermal Energies=          -674.407839
 Sum of electronic and thermal Enthalpies=         -674.406895
 Sum of electronic and thermal Free Energies=      -674.468627
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(1a) Adduct $D_{(E)}$

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C      -2.66982    -0.54270    -1.17294          C       4.23899     1.54996    -1.15545
C      -2.95303     0.76727    -0.68419          C       5.55370     1.91860    -1.46781
C      -4.96326     0.74309    -1.95171          C       3.41764     2.47548    -0.49283
C      -4.97279    -0.77308    -1.75509          C       6.04392     3.18223    -1.12884
C      -1.26699    -0.83806    -0.89873          C       3.90812     3.73575    -0.15241
C      -0.70651     0.35850    -0.33157          C       5.22160     4.09412    -0.46762
C      -1.73571     1.32654    -0.11619          H      -5.98416     1.13225    -1.92328
N      -3.61383    -1.30246    -1.87035          H      -5.40731    -1.01968    -0.76903
N      -4.16861     1.43430    -0.93220          H      -2.58107    -3.14172    -1.94628
C      -3.58325    -2.75853    -1.76883          H      -3.92417    -3.10900    -0.78224
C      -4.92171     1.92740     0.21908          H      -4.24881    -3.17283    -2.53216
C      -0.45050    -1.96674    -1.41777          H      -4.27186     2.52703     0.85753
C      -0.33567    -2.15488    -2.80752          H      -5.73219     2.57228    -0.13437
C       0.24723    -2.83377    -0.56422          H      -5.34986     1.11372     0.82760
C       0.44060    -3.19094    -3.32593          H      -5.59251    -1.25297    -2.52072
C       1.03323    -3.86391    -1.08488          H      -4.54746     0.96696    -2.94209
C       1.12973    -4.04914    -2.46433          H      -0.87149    -1.48890    -3.47809
C      -1.50076     2.71907     0.33093          H       0.16414    -2.70024     0.50905
C      -0.65236     3.00336     1.41504          H       0.50917    -3.32663    -4.40178
C      -2.08296     3.79337    -0.36376          H       1.56421    -4.52390    -0.40519
C      -0.39486     4.32055     1.79051          H       1.73330    -4.85755    -2.86741
C      -1.82743     5.11085     0.01879          H      -0.20153     2.18248     1.96100
C      -0.98192     5.38095     1.09542          H      -2.74136     3.58582    -1.20086
O       0.57895     0.64393    -0.07475          H       0.25972     4.51893     2.63486
O      -3.38275     0.86474     3.29658          H      -2.28838     5.92748    -0.53027
O      -2.97476    -3.13612     1.83414          H      -0.78450     6.40691     1.39314
C       3.80510    -1.24517     0.36102          H       1.25032    -0.06629    -0.24498
N       3.08849    -0.50469    -0.40818          H       4.56283    -0.40669    -1.93598
C       3.71103     0.17613    -1.56338          H       1.83027     0.88213    -2.40722
C       2.68807     0.27420    -2.70478          H       3.15080     0.73813    -3.58125
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H	2.32734	-0.72071	-2.98215	H	1.43610	-3.54367	4.62399
H	6.19832	1.21415	-1.98924	H	3.21205	-4.76078	3.37662
H	2.39432	2.21099	-0.24632	H	4.31260	-3.70519	1.44180
H	7.06629	3.45023	-1.38098	H	1.85463	-0.20919	1.94337
H	3.25769	4.44064	0.35807	H	0.76662	-1.25911	3.89766
H	5.59949	5.07715	-0.20099	C	-2.96060	0.33838	2.35525
H	-1.07092	-0.67936	1.91752	C	-2.71244	-2.07223	1.45496
C	1.91693	-3.08020	3.76751	Fe	-2.21093	-0.45557	0.97576
C	2.91614	-3.76171	3.06963	C	5.28991	-1.50250	0.15495
C	3.54049	-3.16043	1.97720	H	5.82141	-0.55225	0.04951
C	3.15941	-1.87702	1.54910	H	5.72329	-2.03912	0.99845
C	2.15265	-1.20243	2.25821	H	5.47428	-2.08433	-0.75579
C	1.54121	-1.79784	3.36087				

Zero-point correction= 0.691227 (Hartree/Particle)
Thermal correction to Energy= 0.734936
Thermal correction to Enthalpy= 0.735880
Thermal correction to Gibbs Free Energy= 0.610193
Sum of electronic and zero-point Energies= -2022.837345
Sum of electronic and thermal Energies= -2022.793636
Sum of electronic and thermal Enthalpies= -2022.792692
Sum of electronic and thermal Free Energies= -2022.918380

(1a) Adduct $D_{(Z)}$

C	2.96900	-1.15500	0.77900				
C	3.47300	0.14700	0.47500	H	6.48300	1.44800	-0.24700
C	5.58800	-0.53200	1.33100	H	5.63600	0.33400	-1.36300
C	5.21300	-1.94800	0.89000	H	5.81000	-2.68500	1.43700
C	1.51500	-1.11700	0.67200	H	5.39600	-0.43900	2.40700
C	1.16300	0.25700	0.42300	H	0.79800	-1.68300	3.19300
C	2.34700	1.03200	0.22600	H	0.06500	-2.87300	-0.86200
N	3.80200	-2.19600	1.18200	H	-0.79900	-3.39900	3.99400
N	4.83000	0.50000	0.61700	H	-1.53900	-4.59400	-0.07200
C	3.39900	-3.58100	0.96900	H	-1.97700	-4.86400	2.36300
C	5.50300	1.06800	-0.55100	H	0.79500	2.57600	-1.39900
C	0.54100	-2.15700	1.10600	H	3.95200	2.78300	1.50400
C	0.28200	-2.31900	2.47900	H	0.80000	5.04200	-1.58600
C	-0.13500	-2.98500	0.19800	H	3.95900	5.25400	1.32400
C	-0.61700	-3.28600	2.92900	H	2.38300	6.39700	-0.22500
C	-1.03700	-3.95200	0.64700	H	-0.84300	0.26000	0.25500
C	-1.28100	-4.10700	2.01300	H	-4.39900	-0.13700	1.18300
C	2.37300	2.50500	0.06600	H	-1.74100	0.60400	2.51900
C	1.48600	3.16300	-0.80300	H	-3.30800	0.44100	3.33700
C	3.26100	3.28100	0.83100	H	-2.53400	-0.98000	2.59800
C	1.48900	4.55300	-0.90400	H	-5.86100	1.62000	1.32100
C	3.26400	4.67200	0.72500	H	-1.69700	2.49700	0.69900
C	2.37900	5.31400	-0.14100	H	-6.39600	4.03100	1.15900
O	-0.04700	0.83000	0.45000	H	-2.23000	4.89700	0.52600
O	3.29000	1.05800	-3.44600	H	-4.58100	5.68500	0.75500
O	2.58000	-3.08100	-2.64200	H	0.99800	-0.43800	-1.98400
C	-3.12400	-0.71900	-0.93100	C	-7.25300	-1.87000	-1.37600
N	-2.60800	-0.07100	0.04500	C	-6.86700	-0.55200	-1.62500
C	-3.44100	0.39600	1.17300	C	-5.53500	-0.16700	-1.46400
C	-2.70800	0.09500	2.49000	C	-4.57400	-1.10300	-1.05500
C	-3.74400	1.88500	1.02600	C	-4.96700	-2.42700	-0.81500
C	-5.06300	2.33800	1.15100	C	-6.30100	-2.80600	-0.96700
C	-2.72600	2.82500	0.80000	H	-8.29100	-2.16700	-1.50000
C	-5.36600	3.69900	1.05700	H	-7.60300	0.18000	-1.94400
C	-3.03000	4.18300	0.70200	H	-5.23900	0.86100	-1.64900
C	-4.34900	4.62600	0.83100	H	-4.22700	-3.15700	-0.49700
H	6.65500	-0.35900	1.16700	H	-6.59600	-3.83300	-0.77000
H	5.42200	-2.07600	-0.18800	C	2.93500	0.41000	-2.55500
H	2.40800	-3.76400	1.38000	C	2.50100	-2.08500	-2.05100
H	3.39500	-3.85700	-0.09700	Fe	2.28700	-0.54600	-1.22600
H	4.11000	-4.22900	1.49100	C	-2.25500	-1.14300	-2.08900
H	4.92500	1.90700	-0.93900	H	-2.29700	-2.23000	-2.22100

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H      -2.64100    -0.70300    -3.01600              H      -1.21800    -0.83300    -1.95000

Zero-point correction=                  0.690790 (Hartree/Particle)
 Thermal correction to Energy=             0.734607
 Thermal correction to Enthalpy=           0.735551
 Thermal correction to Gibbs Free Energy=      0.608725
 Sum of electronic and zero-point Energies=       -2022.835964
 Sum of electronic and thermal Energies=          -2022.792147
 Sum of electronic and thermal Enthalpies=        -2022.791202
 Sum of electronic and thermal Free Energies=     -2022.918028
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(1a) TS*(E)re*

```
Fe      1.04842    -0.48790    -1.08751              C      -0.18837    -3.30322     2.29864
C       0.82220    -0.48058     1.19257              C      -1.22790    -3.35592     0.12827
C       0.75774    -1.80180     0.56692              C      -1.08440    -4.26917     2.75575
C       2.05707    -2.07073    -0.01861              H       0.56100    -2.89843     2.97204
C       2.85848    -0.88025     0.08131              C      -2.12344    -4.32809     0.58209
C       2.05178     0.15442     0.69881              H      -1.29520    -3.00634    -0.89612
C       0.20139    -1.40514    -2.32081              C      -2.05597    -4.78834     1.89754
C       1.77537     0.59397    -2.26382              H      -1.02323    -4.61633     3.78356
O      -0.04725     0.05619     1.94200              H      -2.87449    -4.72438    -0.09623
O      -0.41913    -1.94921    -3.14094              H      -2.75315    -5.54288     2.25078
O       2.19744     1.32898    -3.06099              N       2.59176    -3.31122    -0.38784
H      -0.60582     5.33216     1.67061              N       4.20201    -0.88555    -0.27365
C      -0.53360     4.77645     0.74064              C       4.05178    -3.30695    -0.50862
C       0.08109     5.34802    -0.37296              H       4.50173    -3.43192     0.48465
C      -1.07220     3.49348     0.66429              H       4.35511    -4.16033    -1.12033
C       0.16795     4.61943    -1.56236              C       4.58003    -2.01127    -1.12202
H       0.48968     6.35280    -0.31672              H       5.67268    -2.04425    -1.18300
C      -0.99700     2.75176    -0.52761              H       4.18556    -1.88800    -2.14695
H      -1.58072     3.07472     1.52471              C       4.90322     0.35427    -0.57723
C      -0.36193     3.33501    -1.63867              H       5.96911     0.12949    -0.67487
H       0.65363     5.05013    -2.43300              H       4.55741     0.81456    -1.51630
C      -1.68559     1.43111    -0.62993              H       4.77767     1.07394     0.22827
H      -0.25740     2.77731    -2.56191              C       1.88739    -4.12426    -1.37294
H      -0.20440     0.45183    -1.02865              H       1.96755    -3.71226    -2.39307
N      -2.10184     0.87875     0.51344              H       2.30498    -5.13538    -1.36585
H      -1.36419     0.83352     1.25921              H       0.83280    -4.19970    -1.11438
C      -2.39168     1.10872    -1.92410              C      -4.46151     0.15236     0.13124
H      -1.78309     1.39905    -2.77869              C      -5.02860     1.39394     0.44816
H      -2.61914     0.04688    -2.00951              C      -5.23308    -0.77771    -0.57549
H      -3.33298     1.66844    -1.96942              C      -6.33363     1.69959     0.05998
C      -3.06805    -0.23283     0.61386              H      -4.44034     2.12594     0.99422
C       2.48711     1.47177     1.24288              C      -6.54122    -0.47724    -0.95898
C       2.69900     2.61455     0.45795              H      -4.80531    -1.74553    -0.82681
C       2.68995     1.57488     2.63061              C      -7.09539     0.76437    -0.64413
C       3.13799     3.80796     1.03379              H      -6.75629     2.66895     0.30929
H       2.52541     2.56849    -0.61067              H      -7.12401    -1.21111    -1.50858
C       3.11990     2.76869     3.20856              H      -8.11117     1.00244    -0.94614
H       2.50399     0.70714     3.25542              H      -2.70108    -1.07297     0.00993
C       3.35318     3.89014     2.41007              C      -3.12652    -0.69065     2.08104
H       3.30225     4.67714     0.40322              H      -2.12793    -0.95038     2.43589
H       3.27427     2.82159     4.28294              H      -3.53669     0.10541     2.71126
H       3.69352     4.82019     2.85721              H      -3.78037    -1.56196     2.16288
C      -0.23958    -2.83012     0.97535

Zero-point correction=                  0.690151 (Hartree/Particle)
 Thermal correction to Energy=             0.732727
 Thermal correction to Enthalpy=           0.733671
 Thermal correction to Gibbs Free Energy=      0.613338
 Sum of electronic and zero-point Energies=       -2022.808743
 Sum of electronic and thermal Energies=          -2022.766168
 Sum of electronic and thermal Enthalpies=        -2022.765223
 Sum of electronic and thermal Free Energies=     -2022.885556
Imaginary  frequency -231.85
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(1a) TS*(E)si*

Fe	1.30181	0.58938	-0.94882	C	2.77376	-0.81123	3.07978
C	0.09135	0.47786	0.95009	C	1.57244	-2.31148	1.62507
C	1.51156	0.15765	1.14596	C	3.16471	-1.89114	3.87102
C	2.27652	1.34629	0.85144	H	3.09037	0.19366	3.34035
C	1.38985	2.35542	0.34014	C	1.96104	-3.39015	2.41797
C	0.05667	1.79335	0.28100	H	0.95992	-2.47869	0.74919
C	2.59278	-0.46911	-1.50784	C	2.76062	-3.18694	3.54419
C	1.12967	1.39521	-2.49689	H	3.78267	-1.71794	4.74821
O	-0.89971	-0.25366	1.22985	H	1.64037	-4.39291	2.14877
O	3.41269	-1.19504	-1.89203	H	3.06584	-4.02821	4.16038
O	0.98356	1.86234	-3.55306	N	3.61157	1.61506	1.17666
H	-0.17738	-5.89155	-0.07004	N	1.83449	3.64705	0.08085
C	0.12404	-5.10664	-0.75770	C	3.95419	3.03774	1.12417
C	1.22298	-5.29194	-1.59700	H	3.63819	3.52522	2.05552
C	-0.60618	-3.91973	-0.80815	H	5.04038	3.13387	1.05022
C	1.58543	-4.27989	-2.48960	C	3.28549	3.75195	-0.04884
H	1.79096	-6.21680	-1.55983	H	3.55546	4.81307	-0.04374
C	-0.24485	-2.88841	-1.69450	H	3.63063	3.31693	-1.00408
H	-1.47587	-3.79447	-0.17384	C	1.09584	4.51975	-0.82235
C	0.85870	-3.09446	-2.54056	H	1.54388	5.51637	-0.77736
H	2.44324	-4.40900	-3.14234	H	1.12903	4.16984	-1.86607
C	-1.10164	-1.66837	-1.80255	H	0.05538	4.60023	-0.51583
H	1.17190	-2.31371	-3.22309	C	4.65303	0.69969	0.72018
H	0.23405	-0.45837	-1.45784	H	4.87660	0.82301	-0.35165
N	-1.97331	-1.46067	-0.80687	H	5.56665	0.88031	1.29493
H	-1.53682	-1.39012	0.14352	H	4.34840	-0.33182	0.89291
C	-1.37014	-1.14604	-3.19451	C	-3.89472	-0.73513	0.51572
H	-2.01374	-1.84583	-3.74030	C	-4.09362	-1.95633	1.17287
H	-1.84395	-0.16447	-3.17246	C	-4.39545	0.43299	1.09773
H	-0.43871	-1.05739	-3.75203	C	-4.76525	-2.00617	2.39429
C	-3.23266	-0.68355	-0.85778	H	-3.71983	-2.87539	0.72950
C	-1.21040	2.54951	0.07345	C	-5.07594	0.38391	2.31506
C	-1.81804	2.71928	-1.18048	H	-4.24267	1.38732	0.60394
C	-1.81871	3.15135	1.18909	C	-5.26087	-0.83465	2.96917
C	-2.97863	3.48497	-1.32052	H	-4.90282	-2.96022	2.89557
H	-1.35811	2.27285	-2.05537	H	-5.45252	1.30239	2.75667
C	-2.97612	3.91818	1.05235	H	-5.78429	-0.87198	3.92034
H	-1.36983	3.01795	2.16883	H	-3.00741	0.36288	-1.09270
C	-3.55985	4.09154	-0.20534	C	-4.22882	-1.24218	-1.89475
H	-3.42350	3.61257	-2.30379	H	-3.90688	-1.10238	-2.92720
H	-3.42223	4.38049	1.92868	H	-4.40170	-2.30896	-1.72344
H	-4.45806	4.69276	-0.31464	H	-5.18400	-0.72473	-1.77238
C	1.97585	-1.00473	1.93682				

Zero-point correction= 0.689716 (Hartree/Particle)
 Thermal correction to Energy= 0.732301
 Thermal correction to Enthalpy= 0.733245
 Thermal correction to Gibbs Free Energy= 0.612837
 Sum of electronic and zero-point Energies= -2022.799929
 Sum of electronic and thermal Energies= -2022.757345
 Sum of electronic and thermal Enthalpies= -2022.756400
 Sum of electronic and thermal Free Energies= -2022.876808
Imaginary frequency -249.41

(1a) $TS_{(Z)re}$

Fe	1.34758	-0.43829	-0.86137	C	2.22886	0.59505	3.48167
C	0.60947	0.90624	0.84737	C	2.92721	-1.49559	2.51513
C	1.95230	0.34938	1.03083	C	2.62287	0.14693	4.74170
C	2.80346	0.90826	-0.00169	H	1.78395	1.57851	3.37200
C	1.97754	1.64861	-0.91946	C	3.32759	-1.94426	3.77553
C	0.59798	1.52141	-0.48959	H	3.02339	-2.15948	1.66335
C	2.24720	-1.94884	-0.83971	C	3.18047	-1.12400	4.89422
C	0.96376	-0.60267	-2.56773	H	2.49231	0.79237	5.60609
O	-0.36835	0.78746	1.63904	H	3.74711	-2.94122	3.88069
O	2.77306	-2.98540	-0.82035	H	3.48964	-1.47371	5.87526
O	0.68371	-0.75450	-3.68639	N	4.20323	0.99351	-0.01836
H	-2.58813	-2.92604	-3.99489	N	2.53128	2.42169	-1.93232
C	-2.34278	-3.33568	-3.01967	C	4.70734	2.03857	-0.91238
C	-2.38221	-4.71713	-2.80741	H	4.63409	3.01271	-0.41246
C	-1.97135	-2.47880	-1.98832	H	5.76407	1.84691	-1.11431
C	-2.03685	-5.23180	-1.55863	C	3.92618	2.10679	-2.22348
H	-2.66919	-5.38534	-3.61391	H	4.33132	2.89865	-2.86207
C	-1.63263	-2.98414	-0.72147	H	4.01620	1.15069	-2.77012
H	-1.91137	-1.41182	-2.16799	C	1.74687	2.81498	-3.09474
C	-1.65597	-4.37379	-0.52538	H	2.33691	3.52636	-3.67938
H	-2.05667	-6.30359	-1.38473	H	1.49206	1.96104	-3.74166
C	-1.23551	-2.08398	0.40402	H	0.82566	3.30686	-2.79017
H	-1.38853	-4.79131	0.43911	C	4.99642	-0.23096	0.00411
H	0.05113	-1.26693	-0.49060	H	4.94697	-0.78354	-0.94945
N	-2.02752	-1.10706	0.85687	H	6.03999	0.02522	0.20967
H	-1.49937	-0.40175	1.42862	H	4.65487	-0.88640	0.80203
C	-0.29402	-2.62780	1.45832	C	-3.79851	0.51534	1.25921
H	0.53560	-3.17730	1.01614	C	-3.88265	0.29800	2.64132
H	0.09114	-1.81213	2.07043	C	-4.25344	1.72965	0.73825
H	-0.86081	-3.30025	2.11639	C	-4.40696	1.27776	3.48336
C	-3.30447	-0.58362	0.32363	H	-3.52699	-0.63838	3.06243
C	-0.58030	2.28826	-0.98642	C	-4.78624	2.70870	1.57893
C	-1.35144	1.90383	-2.09535	H	-4.17591	1.91957	-0.32791
C	-0.93068	3.47554	-0.32015	C	-4.86514	2.48602	2.95358
C	-2.40528	2.70032	-2.55049	H	-4.45798	1.09730	4.55342
H	-1.10073	0.99293	-2.62723	H	-5.12945	3.64928	1.15741
C	-1.98493	4.27042	-0.76937	H	-5.27494	3.24917	3.60920
H	-0.36210	3.77512	0.55477	H	-3.14027	-0.13896	-0.66473
C	-2.72169	3.89128	-1.89378	C	-4.38773	-1.67619	0.22436
H	-2.97368	2.39147	-3.42391	H	-4.14002	-2.45501	-0.49622
H	-2.22877	5.18842	-0.24187	H	-4.54643	-2.13900	1.20285
H	-3.53568	4.51524	-2.25244	H	-5.32781	-1.20987	-0.08329
C	2.38610	-0.21170	2.34023				

Zero-point correction= 0.689866 (Hartree/Particle)
Thermal correction to Energy= 0.732576
Thermal correction to Enthalpy= 0.733520
Thermal correction to Gibbs Free Energy= 0.612281
Sum of electronic and zero-point Energies= -2022.800751
Sum of electronic and thermal Energies= -2022.758041
Sum of electronic and thermal Enthalpies= -2022.757097
Sum of electronic and thermal Free Energies= -2022.878336
Imaginary frequency -325.23

(1a) $TS_{(Z)si}$

Fe	1.26700	-0.03400	1.00200	C	0.92900	3.27500	-2.12900
C	1.32400	0.22000	-1.28300	C	-0.35000	3.25200	-0.09000
C	1.42100	1.45900	-0.51000	C	0.24000	4.41100	-2.55300
C	2.67600	1.41900	0.21600	H	1.69000	2.83400	-2.76600
C	3.24000	0.10100	0.08000	C	-1.03800	4.39300	-0.50900
C	2.34100	-0.69200	-0.74000	H	-0.58400	2.80900	0.87200
C	0.58800	0.93200	2.30200	C	-0.74700	4.97700	-1.74200
C	1.57200	-1.40100	2.06300	H	0.47300	4.85400	-3.51700
O	0.47000	-0.05700	-2.17500	H	-1.80400	4.82400	0.13100
O	0.08600	1.53700	3.15900	H	-1.28300	5.86300	-2.07000
O	1.71500	-2.31800	2.76400	N	3.38700	2.48600	0.76400
H	-4.33900	-3.55400	3.02500	N	4.51200	-0.18500	0.56800
C	-3.87800	-2.61300	2.74200	C	4.78700	2.18400	1.07500
C	-4.08700	-1.46900	3.51100	H	5.40200	2.31800	0.17500
C	-3.06900	-2.55800	1.60600	H	5.13900	2.89400	1.82700
C	-3.48100	-0.26700	3.13600	C	4.97000	0.75700	1.58400
H	-4.70800	-1.51400	4.40000	H	6.03000	0.56500	1.77900
C	-2.47100	-1.35100	1.20900	H	4.41900	0.61900	2.53200
H	-2.91600	-3.45900	1.02300	C	4.93400	-1.55800	0.80100
C	-2.68400	-0.20800	1.99600	H	6.00200	-1.55200	1.03900
H	-3.61700	0.62500	3.74000	H	4.39500	-2.03000	1.63900
C	-1.62100	-1.33000	-0.02200	H	4.78800	-2.16300	-0.09100
H	-2.18800	0.71900	1.74000	C	2.72700	3.41600	1.67200
H	-0.18500	-0.60400	0.72000	H	2.58600	2.98900	2.67900
N	-1.89800	-0.53500	-1.05900	H	3.33100	4.32400	1.75600
H	-1.10300	-0.47100	-1.73500	H	1.75300	3.70000	1.27900
C	-0.89300	-2.59800	-0.41100	C	-4.29000	0.17000	-0.99600
H	-1.62100	-3.30400	-0.83100	C	-4.77000	-0.96900	-1.65500
H	-0.15500	-2.38100	-1.18300	C	-5.19400	0.96600	-0.28400
H	-0.40200	-3.05800	0.44600	C	-6.12300	-1.30500	-1.59800
C	-2.83500	0.60400	-1.12700	H	-4.07800	-1.59500	-2.21200
C	2.57400	-2.01600	-1.38700	C	-6.54900	0.63500	-0.23000
C	2.55000	-3.24500	-0.70700	H	-4.83400	1.85200	0.23400
C	2.79700	-2.03900	-2.77600	C	-7.01700	-0.50400	-0.88600
C	2.77100	-4.44600	-1.38200	H	-6.47900	-2.19400	-2.11300
H	2.35700	-3.26200	0.35900	H	-7.23500	1.26300	0.33000
C	3.01300	-3.23900	-3.45300	H	-8.07100	-0.76600	-0.84300
H	2.78700	-1.10300	-3.32500	H	-2.60400	1.32100	-0.33300
C	3.00600	-4.44900	-2.75800	C	-2.60200	1.30900	-2.47500
H	2.75300	-5.38200	-0.82900	H	-1.55700	1.60600	-2.57800
H	3.18500	-3.22700	-4.52600	H	-2.86300	0.64200	-3.30300
H	3.17400	-5.38500	-3.28300	H	-3.23700	2.19600	-2.53800
C	0.65200	2.67600	-0.88800				

Zero-point correction= 0.690187 (Hartree/Particle)
 Thermal correction to Energy= 0.732881
 Thermal correction to Enthalpy= 0.733825
 Thermal correction to Gibbs Free Energy= 0.612505
 Sum of electronic and zero-point Energies= -2022.806154
 Sum of electronic and thermal Energies= -2022.763461
 Sum of electronic and thermal Enthalpies= -2022.762516
 Sum of electronic and thermal Free Energies= -2022.883836
Imaginary frequency -322.10

(1a) adduct $E_{E(S,1'S)}$

Fe	1.07224	-0.33545	-1.01051	C	-0.33166	-3.22844	2.18231
C	0.97501	-0.55803	1.25452	C	-1.11337	-3.34409	-0.09356
C	0.85937	-1.83511	0.50686	C	-1.30115	-4.15522	2.56478
C	2.12423	-2.06703	-0.13854	H	0.33743	-2.80801	2.92618
C	2.92138	-0.85202	-0.03175	C	-2.07967	-4.27802	0.28662
C	2.18399	0.11464	0.73777	H	-1.06137	-3.02691	-1.12914
C	0.38807	-1.23925	-2.37091	C	-2.17646	-4.68888	1.61696
C	1.78683	0.87718	-2.07897	H	-1.37305	-4.45878	3.60538
O	0.13366	-0.07554	2.03147	H	-2.76008	-4.67916	-0.45952
O	0.00177	-1.86074	-3.27019	H	-2.93085	-5.41197	1.91327
O	2.30138	1.62253	-2.80244	N	2.64142	-3.20088	-0.71684
H	-1.37038	5.71994	1.23293	N	4.23257	-0.82054	-0.47494
C	-1.11286	5.06743	0.40293	C	4.08902	-3.22881	-0.90925
C	-0.39538	5.56801	-0.68329	H	4.61247	-3.49692	0.02274
C	-1.51075	3.72833	0.43259	H	4.32204	-3.99581	-1.65408
C	-0.08031	4.71554	-1.74451	C	4.58825	-1.88275	-1.40979
H	-0.08919	6.61016	-0.70770	H	5.67893	-1.91144	-1.49693
C	-1.19460	2.86145	-0.62108	H	4.17377	-1.68123	-2.41211
H	-2.07866	3.34594	1.27221	C	4.90603	0.44532	-0.75893
C	-0.47810	3.37950	-1.71158	H	5.98505	0.26542	-0.77433
H	0.47540	5.08927	-2.60002	H	4.60617	0.85728	-1.73284
C	-1.63722	1.39154	-0.61217	H	4.68967	1.17755	0.01414
H	-0.22428	2.73657	-2.54801	C	1.97353	-4.49430	-0.65452
H	-0.67682	0.76724	-0.75563	H	0.94348	-4.41867	-0.99887
N	-2.26291	1.05824	0.64816	H	2.50506	-5.18272	-1.31622
H	-1.54286	1.04196	1.37063	H	1.96635	-4.92026	0.35811
C	-2.50259	1.08139	-1.84311	C	-4.50150	0.01131	0.25992
H	-1.95524	1.33107	-2.75470	C	-5.20080	1.21439	0.41946
H	-2.77063	0.02396	-1.89254	C	-5.16512	-1.07607	-0.32170
H	-3.42300	1.66920	-1.82173	C	-6.52811	1.32706	0.00339
C	-3.07656	-0.15845	0.78222	H	-4.68589	2.06352	0.85777
C	2.68468	1.36770	1.36705	C	-6.49376	-0.96822	-0.73657
C	2.19521	2.63207	1.01463	H	-4.63309	-2.01666	-0.44935
C	3.62989	1.28005	2.40498	C	-7.18060	0.23636	-0.57627
C	2.65009	3.77963	1.66724	H	-7.05429	2.26968	0.13000
H	1.45354	2.72034	0.22936	H	-6.98980	-1.82253	-1.18972
C	4.08814	2.42619	3.05341	H	-8.21306	0.32575	-0.90255
H	4.00727	0.30436	2.70000	H	-2.61734	-1.00475	0.24683
C	3.59971	3.68193	2.68444	C	-3.12948	-0.53272	2.27551
H	2.25327	4.74763	1.37636	H	-2.12218	-0.72445	2.65175
H	4.82107	2.33789	3.85071	H	-3.58019	0.28368	2.85011
H	3.95383	4.57556	3.19070	H	-3.74061	-1.42773	2.41728
C	-0.21041	-2.81662	0.84349				

Zero-point correction= 0.694122 (Hartree/Particle)
Thermal correction to Energy= 0.737985
Thermal correction to Enthalpy= 0.738929
Thermal correction to Gibbs Free Energy= 0.613423
Sum of electronic and zero-point Energies= -2022.824006
Sum of electronic and thermal Energies= -2022.780143
Sum of electronic and thermal Enthalpies= -2022.779199
Sum of electronic and thermal Free Energies= -2022.904705

(1a) adduct $E_{E(R,1'S)}$

Fe	-1.22974	-0.62318	-0.93684	C	-1.95053	0.82362	3.35724
C	-0.04016	-0.63302	1.00327	C	-2.05376	2.21231	1.38804
C	-1.46465	-0.24430	1.15775	C	-2.27643	1.92099	4.15307
C	-2.25967	-1.39770	0.86313	H	-1.76661	-0.14325	3.81843
C	-1.39965	-2.40069	0.24708	C	-2.37721	3.31286	2.18489
C	-0.04544	-1.90606	0.24587	H	-1.95744	2.33680	0.31550
C	-2.69924	0.20795	-1.47251	C	-2.49436	3.17039	3.56756
C	-0.97732	-1.37708	-2.51342	H	-2.35282	1.80209	5.23039
O	0.94536	0.05919	1.29283	H	-2.52921	4.28106	1.71724
O	-3.72570	0.65046	-1.78028	H	-2.74528	4.02701	4.18683
O	-0.84257	-1.87679	-3.55219	N	-3.58504	-1.64022	1.07920
H	0.04761	6.15496	-0.29704	N	-1.89506	-3.66134	-0.04609
C	-0.30634	5.29844	-0.86473	C	-4.04675	-3.01774	0.94849
C	-1.52626	5.36235	-1.53774	H	-3.88070	-3.58327	1.87818
C	0.47196	4.13891	-0.91665	H	-5.12416	-3.00356	0.75740
C	-1.96128	4.25414	-2.26951	C	-3.34516	-3.71398	-0.21186
H	-2.13006	6.26477	-1.49870	H	-3.65013	-4.76443	-0.23825
C	0.04225	3.01861	-1.63679	H	-3.64892	-3.24687	-1.16423
H	1.42496	4.09043	-0.40391	C	-1.16615	-4.55286	-0.94326
C	-1.18257	3.09836	-2.31755	H	-1.62142	-5.54524	-0.88518
H	-2.90716	4.28776	-2.80310	H	-1.20228	-4.21158	-1.98883
C	0.89514	1.74286	-1.72424	H	-0.12568	-4.63371	-0.63817
H	-1.53665	2.24859	-2.89310	C	-4.51759	-0.64822	1.59574
H	0.19790	0.87664	-1.43968	H	-5.51559	-0.87279	1.20704
N	2.00825	1.81405	-0.79839	H	-4.56213	-0.64209	2.69259
H	1.64385	1.65747	0.14194	H	-4.23609	0.34898	1.26124
C	1.27951	1.47149	-3.18673	C	3.92262	0.88297	0.40080
H	1.86745	2.29902	-3.59225	C	4.18404	2.03473	1.15588
H	1.84842	0.54409	-3.29006	C	4.37823	-0.34959	0.88032
H	0.37632	1.37461	-3.79319	C	4.87786	1.95402	2.36362
C	3.21798	0.97907	-0.94941	H	3.83427	2.99810	0.79673
C	1.21194	-2.67679	0.02631	C	5.07967	-0.43193	2.08409
C	1.87566	-2.74828	-1.20732	H	4.17380	-1.25306	0.31367
C	1.77482	-3.35367	1.12243	C	5.33147	0.71933	2.83148
C	3.04822	-3.49415	-1.34920	H	5.06591	2.85695	2.93859
H	1.46609	-2.22800	-2.06542	H	5.42056	-1.39991	2.44175
C	2.94653	-4.09703	0.98401	H	5.87329	0.65539	3.77123
H	1.28491	-3.29205	2.08987	H	2.96247	-0.04549	-1.26186
C	3.58638	-4.17374	-0.25539	C	4.21717	1.57227	-1.96644
H	3.54093	-3.54059	-2.31634	H	3.83212	1.58298	-2.98681
H	3.36103	-4.61399	1.84496	H	4.46848	2.59932	-1.68530
H	4.49802	-4.75389	-0.36596	H	5.13898	0.98179	-1.96143
C	-1.84686	0.95066	1.96121				

Zero-point correction= 0.693777 (Hartree/Particle)
Thermal correction to Energy= 0.737822
Thermal correction to Enthalpy= 0.738766
Thermal correction to Gibbs Free Energy= 0.612493
Sum of electronic and zero-point Energies= -2022.816644
Sum of electronic and thermal Energies= -2022.772599
Sum of electronic and thermal Enthalpies= -2022.771654
Sum of electronic and thermal Free Energies= -2022.897928

(1a) adduct $E_{Z(S,1'S)}$

Fe	-1.30273	0.25887	-0.85786	C	-1.67326	0.71999	3.57316
C	-0.77409	-0.83633	1.09777	C	-2.69089	2.30877	2.06987
C	-1.98778	0.02322	1.20040	C	-1.78774	1.63911	4.61665
C	-2.99713	-0.58044	0.38144	H	-1.20779	-0.24263	3.74778
C	-2.34903	-1.54310	-0.50193	C	-2.81050	3.22302	3.11536
C	-0.96655	-1.67680	-0.10593	H	-3.02503	2.59287	1.07836
C	-2.20800	1.72382	-1.27074	C	-2.36040	2.89225	4.39517
C	-0.87605	-0.03281	-2.54279	H	-1.42506	1.37272	5.60546
O	0.26055	-0.73023	1.77146	H	-3.24509	4.20045	2.92509
O	-2.87813	2.62512	-1.56200	H	-2.44700	3.60743	5.20812
O	-0.64539	-0.22649	-3.66357	N	-4.34743	-0.42209	0.37121
H	1.20724	3.95195	-4.34165	N	-3.13532	-2.32391	-1.34138
C	1.75321	3.84796	-3.40795	C	-5.15702	-1.15503	-0.60186
C	2.92295	4.57665	-3.19449	H	-5.63227	-2.01744	-0.11173
C	1.28053	2.97605	-2.42350	H	-5.95687	-0.49451	-0.95949
C	3.61497	4.42671	-1.98964	C	-4.33428	-1.62401	-1.79347
H	3.29448	5.25291	-3.95927	H	-4.94083	-2.31347	-2.38668
C	1.96739	2.81524	-1.21609	H	-4.06919	-0.76689	-2.43516
H	0.37225	2.40914	-2.60205	C	-2.51747	-3.17358	-2.35505
C	3.14092	3.55556	-1.01016	H	-3.29649	-3.80405	-2.79198
H	4.52839	4.98880	-1.81390	H	-2.04371	-2.59417	-3.16139
C	1.42233	1.93587	-0.09191	H	-1.76758	-3.81835	-1.90265
H	3.68175	3.42711	-0.07791	C	-5.10074	0.32229	1.37194
H	0.61528	1.26725	-0.54460	H	-5.32082	1.34718	1.04645
N	2.44127	1.15577	0.58165	H	-6.04924	-0.19667	1.54278
H	2.06004	0.85749	1.47696	H	-4.56039	0.36471	2.31463
C	0.73777	2.82811	0.95858	C	3.89712	-0.75780	0.94219
H	-0.05810	3.42235	0.50348	C	4.86353	-0.03611	1.65732
H	0.30571	2.22219	1.75841	C	3.81077	-2.14088	1.13900
H	1.47336	3.51161	1.39323	C	5.72687	-0.68332	2.54168
C	2.98421	-0.05837	-0.05901	H	4.92253	1.03974	1.52423
C	-0.02095	-2.78663	-0.42261	C	4.67692	-2.79103	2.02037
C	0.78688	-2.83010	-1.56912	H	3.05595	-2.71077	0.60593
C	0.07734	-3.84583	0.49690	C	5.63861	-2.06521	2.72453
C	1.63913	-3.91054	-1.80579	H	6.46861	-0.10819	3.08988
H	0.74750	-2.01864	-2.28599	H	4.59244	-3.86521	2.16271
C	0.93212	-4.92332	0.26525	H	6.30992	-2.56994	3.41410
H	-0.52212	-3.81747	1.40200	H	2.16308	-0.75086	-0.29999
C	1.71339	-4.96267	-0.89185	C	3.75112	0.21924	-1.36285
H	2.25120	-3.92313	-2.70313	H	3.10760	0.64302	-2.13745
H	0.98902	-5.73032	0.99032	H	4.58088	0.91140	-1.19359
H	2.37931	-5.80101	-1.07488	H	4.16254	-0.72279	-1.73877
C	-2.13226	1.03504	2.28072				

Zero-point correction= 0.694248 (Hartree/Particle)
Thermal correction to Energy= 0.738255
Thermal correction to Enthalpy= 0.739199
Thermal correction to Gibbs Free Energy= 0.613036
Sum of electronic and zero-point Energies= -2022.820757
Sum of electronic and thermal Energies= -2022.776749
Sum of electronic and thermal Enthalpies= -2022.775805
Sum of electronic and thermal Free Energies= -2022.901969

(1a) adduct $E_{Z(R,1'S)}$

Fe	-1.30273	0.25887	-0.85786	C	-1.67326	0.71999	3.57316
C	-0.77409	-0.83633	1.09777	C	-2.69089	2.30877	2.06987
C	-1.98778	0.02322	1.20040	C	-1.78774	1.63911	4.61665
C	-2.99713	-0.58044	0.38144	H	-1.20779	-0.24263	3.74778
C	-2.34903	-1.54310	-0.50193	C	-2.81050	3.22302	3.11536
C	-0.96655	-1.67680	-0.10593	H	-3.02503	2.59287	1.07836
C	-2.20800	1.72382	-1.27074	C	-2.36040	2.89225	4.39517
C	-0.87605	-0.03281	-2.54279	H	-1.42506	1.37272	5.60546
O	0.26055	-0.73023	1.77146	H	-3.24509	4.20045	2.92509
O	-2.87813	2.62512	-1.56200	H	-2.44700	3.60743	5.20812
O	-0.64539	-0.22649	-3.66357	N	-4.34743	-0.42209	0.37121
H	1.20724	3.95195	-4.34165	N	-3.13532	-2.32391	-1.34138
C	1.75321	3.84796	-3.40795	C	-5.15702	-1.15503	-0.60186
C	2.92295	4.57665	-3.19449	H	-5.63227	-2.01744	-0.11173
C	1.28053	2.97605	-2.42350	H	-5.95687	-0.49451	-0.95949
C	3.61497	4.42671	-1.98964	C	-4.33428	-1.62401	-1.79347
H	3.29448	5.25291	-3.95927	H	-4.94083	-2.31347	-2.38668
C	1.96739	2.81524	-1.21609	H	-4.06919	-0.76689	-2.43516
H	0.37225	2.40914	-2.60205	C	-2.51747	-3.17358	-2.35505
C	3.14092	3.55556	-1.01016	H	-3.29649	-3.80405	-2.79198
H	4.52839	4.98880	-1.81390	H	-2.04371	-2.59417	-3.16139
C	1.42233	1.93587	-0.09191	H	-1.76758	-3.81835	-1.90265
H	3.68175	3.42711	-0.07791	C	-5.10074	0.32229	1.37194
H	0.61528	1.26725	-0.54460	H	-5.32082	1.34718	1.04645
N	2.44127	1.15577	0.58165	H	-6.04924	-0.19667	1.54278
H	2.06004	0.85749	1.47696	H	-4.56039	0.36471	2.31463
C	0.73777	2.82811	0.95858	C	3.89712	-0.75780	0.94219
H	-0.05810	3.42235	0.50348	C	4.86353	-0.03611	1.65732
H	0.30571	2.22219	1.75841	C	3.81077	-2.14088	1.13900
H	1.47336	3.51161	1.39323	C	5.72687	-0.68332	2.54168
C	2.98421	-0.05837	-0.05901	H	4.92253	1.03974	1.52423
C	-0.02095	-2.78663	-0.42261	C	4.67692	-2.79103	2.02037
C	0.78688	-2.83010	-1.56912	H	3.05595	-2.71077	0.60593
C	0.07734	-3.84583	0.49690	C	5.63861	-2.06521	2.72453
C	1.63913	-3.91054	-1.80579	H	6.46861	-0.10819	3.08988
H	0.74750	-2.01864	-2.28599	H	4.59244	-3.86521	2.16271
C	0.93212	-4.92332	0.26525	H	6.30992	-2.56994	3.41410
H	-0.52212	-3.81747	1.40200	H	2.16308	-0.75086	-0.29999
C	1.71339	-4.96267	-0.89185	C	3.75112	0.21924	-1.36285
H	2.25120	-3.92313	-2.70313	H	3.10760	0.64302	-2.13745
H	0.98902	-5.73032	0.99032	H	4.58088	0.91140	-1.19359
H	2.37931	-5.80101	-1.07488	H	4.16254	-0.72279	-1.73877
C	-2.13226	1.03504	2.28072				

Zero-point correction= 0.693972 (Hartree/Particle)
Thermal correction to Energy= 0.737963
Thermal correction to Enthalpy= 0.738907
Thermal correction to Gibbs Free Energy= 0.613231
Sum of electronic and zero-point Energies= -2022.822687
Sum of electronic and thermal Energies= -2022.778695
Sum of electronic and thermal Enthalpies= -2022.777751
Sum of electronic and thermal Free Energies= -2022.903427

(S,1'S)-N-(1-phenylethyl)-α-methylbenzylamine

Zero-point correction= 0.312012 (Hartree/Particle)
Thermal correction to Energy= 0.327592
Thermal correction to Enthalpy= 0.328536
Thermal correction to Gibbs Free Energy= 0.266882
Sum of electronic and zero-point Energies= -675.612222
Sum of electronic and thermal Energies= -675.596642
Sum of electronic and thermal Enthalpies= -675.595698
Sum of electronic and thermal Free Energies= -675.657352

(R,1'S)-N-(1-phenylethyl)-α-methylbenzylamine

```
Zero-point correction=                 0.311969 (Hartree/Particle)
 Thermal correction to Energy=             0.327583
 Thermal correction to Enthalpy=           0.328527
 Thermal correction to Gibbs Free Energy=      0.266978
 Sum of electronic and zero-point Energies=        -675.611874
 Sum of electronic and thermal Energies=        -675.596261
 Sum of electronic and thermal Enthalpies=         -675.595316
 Sum of electronic and thermal Free Energies=      -675.656865
```

(E)-N-(1-(*S*)-phenylethyl)-ethan-1-(4-(methoxy)phenyl)-1-imine (1b)

```
Zero-point correction=                 0.320391 (Hartree/Particle)
 Thermal correction to Energy=             0.338394
 Thermal correction to Enthalpy=           0.339338
 Thermal correction to Gibbs Free Energy=      0.270632
 Sum of electronic and zero-point Energies=        -788.919295
 Sum of electronic and thermal Energies=        -788.901292
 Sum of electronic and thermal Enthalpies=         -788.900348
 Sum of electronic and thermal Free Energies=      -788.969055
```

(Z)-N-(1-(*S*)-phenylethyl)-ethan-1-(4-(methoxy)phenyl)-1-imine (1b)

```
Zero-point correction=                 0.320063 (Hartree/Particle)
 Thermal correction to Energy=             0.338095
 Thermal correction to Enthalpy=           0.339039
 Thermal correction to Gibbs Free Energy=      0.271968
 Sum of electronic and zero-point Energies=        -788.916031
 Sum of electronic and thermal Energies=        -788.897999
 Sum of electronic and thermal Enthalpies=         -788.897054
 Sum of electronic and thermal Free Energies=      -788.964126
```

(1b) Adduct $D_{(E)}$

C	2.77800	-0.29700	1.33600	O	2.45500	-3.65700	-0.78700
C	3.17600	0.77000	0.47800	C	-3.80800	-0.55700	0.35500
C	5.26700	0.82000	1.60500	N	-2.96400	0.29600	0.82200
C	5.07500	-0.67600	1.85500	C	-3.42000	1.35800	1.74200
C	1.33000	-0.45400	1.22500	C	-2.30100	1.68100	2.74300
C	0.87400	0.59900	0.35900	C	-3.85100	2.59600	0.95800
C	1.99400	1.31000	-0.17500	C	-5.10100	3.18200	1.19700
N	3.67700	-0.95400	2.18200	C	-3.00100	3.18400	0.00800
N	4.48000	1.30200	0.46600	C	-5.49900	4.33000	0.50800
C	3.46100	-2.36200	2.50400	C	-3.40000	4.32900	-0.68200
C	5.18800	1.33600	-0.81200	C	-4.64900	4.90600	-0.43600
C	0.43100	-1.26900	2.08400	H	6.32200	1.03800	1.41900
C	0.39600	-1.03200	3.47000	H	5.39100	-1.24600	0.96200
C	-0.41900	-2.24800	1.55000	H	2.43700	-2.53700	2.82200
C	-0.45300	-1.76400	4.29800	H	3.67900	-3.01700	1.64600
C	-1.27800	-2.97300	2.37900	H	4.12800	-2.63600	3.32700
C	-1.29600	-2.73800	3.75400	H	4.56600	1.81800	-1.56700
C	1.89500	2.53800	-0.99800	H	6.10000	1.92900	-0.69900
C	1.00500	2.61900	-2.08300	H	5.45600	0.33000	-1.17600
C	2.65600	3.67300	-0.67000	H	5.69500	-1.00500	2.69700
C	0.88100	3.79900	-2.81500	H	4.96600	1.37000	2.50600
C	2.53400	4.85100	-1.40800	H	1.05100	-0.27600	3.89500
C	1.64500	4.92000	-2.48200	H	-0.39800	-2.44000	0.48300
O	-0.38200	0.97900	0.08500	H	-0.46000	-1.57300	5.36800
O	3.29700	-0.34600	-3.37000	H	-1.92800	-3.72600	1.94300

H	-1.95700	-3.31000	4.39900	C	-3.33800	-1.56700	-0.63000
H	0.41600	1.74800	-2.34800	C	-2.30400	-1.26200	-1.53800
H	3.34800	3.62100	0.16500	C	-1.85200	-2.20100	-2.45200
H	0.19200	3.83900	-3.65300	H	-3.88500	-4.80100	-1.58300
H	3.13200	5.71700	-1.13900	H	-4.68800	-3.13200	0.00500
H	1.55100	5.83700	-3.05700	H	-1.85900	-0.27500	-1.52400
H	-1.12700	0.44500	0.47200	H	-1.05900	-1.96200	-3.15200
H	-4.28800	1.01800	2.32200	C	2.88800	-0.51200	-2.29900
H	-1.41800	2.06700	2.22800	C	2.38200	-2.50100	-0.72700
H	-2.64400	2.43900	3.45400	Fe	2.15400	-0.75700	-0.71900
H	-2.01300	0.78300	3.29800	C	-5.28300	-0.57400	0.72800
H	-5.76600	2.74100	1.93700	H	-5.72000	0.41400	0.55500
H	-2.02700	2.74800	-0.18900	H	-5.84100	-1.29400	0.13000
H	-6.47200	4.77100	0.70900	H	-5.42900	-0.81500	1.78700
H	-2.72800	4.77200	-1.41100	O	-1.89600	-4.33700	-3.41100
H	-4.95500	5.79700	-0.97600	C	-2.40300	-5.66200	-3.47400
H	0.92200	-1.06200	-1.50900	H	-3.47200	-5.67500	-3.72000
C	-2.41100	-3.48900	-2.48100	H	-1.84500	-6.15900	-4.26800
C	-3.43800	-3.81500	-1.58600	H	-2.24400	-6.20000	-2.53100
C	-3.89600	-2.85300	-0.68400				

Zero-point correction= 0.723926 (Hartree/Particle)
Thermal correction to Energy= 0.770193
Thermal correction to Enthalpy= 0.771137
Thermal correction to Gibbs Free Energy= 0.640017
Sum of electronic and zero-point Energies= -2137.328904
Sum of electronic and thermal Energies= -2137.282637
Sum of electronic and thermal Enthalpies= -2137.281693
Sum of electronic and thermal Free Energies= -2137.412813

(1b) Adduct $D_{(Z)}$

C	-3.23109	-1.41265	-0.75529	C	3.25163	5.29230	-0.72441
C	-3.88209	-0.18907	-0.40805	H	-6.99925	-1.07349	-1.00737
C	-5.92612	-1.11044	-1.21109	H	-5.51140	-2.64363	0.27119
C	-5.36135	-2.47580	-0.81076	H	-2.38454	-3.91601	-1.49062
C	-1.78981	-1.19944	-0.68540	H	-3.25514	-4.16912	0.03947
C	-1.60104	0.20338	-0.41879	H	-4.01970	-4.58542	-1.51341
C	-2.86553	0.82294	-0.17087	H	-5.48779	1.35398	1.08520
N	-3.94343	-2.53935	-1.15865	H	-7.00196	0.73176	0.42332
N	-5.27618	-0.00305	-0.50385	H	-6.00186	-0.29860	1.49079
C	-3.36186	-3.86818	-1.01439	H	-5.88320	-3.27311	-1.35042
C	-5.97619	0.46162	0.69245	H	-5.78584	-0.97942	-2.29131
C	-0.70983	-2.10407	-1.17164	H	-1.01455	-1.53652	-3.22849
C	-0.43622	-2.15689	-2.54962	H	-0.16018	-2.88137	0.75368
C	0.04753	-2.91068	-0.30995	H	0.74907	-3.02953	-4.11975
C	0.55722	-2.99888	-3.05083	H	1.60798	-4.38157	-0.12715
C	1.04267	-3.75307	-0.81026	H	2.07076	-4.46040	-2.57119
C	1.30073	-3.80071	-2.18132	H	-1.47091	2.50350	1.45709
C	-3.06465	2.27801	0.02608	H	-4.70152	2.39737	-1.36808
C	-2.24049	3.01739	0.89215	H	-1.76525	4.94679	1.70868
C	-4.05748	2.95867	-0.69900	H	-4.99833	4.84499	-1.12559
C	-2.40772	4.39413	1.02857	H	-3.53185	6.13344	0.41732
C	-4.22391	4.33707	-0.55715	H	0.39708	0.45561	-0.31687
C	-3.40042	5.06083	0.30574	H	3.91748	0.60639	-1.39293
O	-0.47392	0.92299	-0.46696	H	1.12655	1.07805	-2.57109
O	-3.71380	0.66381	3.51788	H	2.66316	1.16962	-3.45593
O	-2.51483	-3.33688	2.61305	H	2.10888	-0.38275	-2.78753
C	2.82330	-0.30464	0.71131	H	5.11451	2.56407	-1.53226
N	2.18981	0.35668	-0.18592	H	0.93103	2.80847	-0.56480
C	2.89949	1.00488	-1.30653	H	5.32845	5.01134	-1.23523
C	2.14996	0.69651	-2.61328	H	1.14556	5.24327	-0.25710
C	3.01041	2.50998	-1.07114	H	3.34312	6.36642	-0.58918
C	4.24221	3.15142	-1.25536	H	-1.28716	-0.50233	1.97147
C	1.89598	3.28243	-0.71022	C	7.08402	-0.98010	0.93477
C	4.36432	4.53263	-1.08638	C	6.56407	0.30739	1.13821
C	2.01951	4.66137	-0.53707	C	5.19697	0.53338	1.04768

C	4.31003	-0.51874	0.76013	C	2.05412	-0.91789	1.85576
C	4.83935	-1.80018	0.57415	H	2.23771	-1.99672	1.91073
C	6.21380	-2.03862	0.64706	H	2.41240	-0.49433	2.80171
H	7.25321	1.11410	1.36554	H	0.98168	-0.73704	1.76725
H	4.81075	1.53612	1.20079	O	8.43789	-1.09467	1.03923
H	4.17270	-2.62870	0.34993	C	9.02348	-2.37286	0.84400
H	6.58829	-3.04204	0.48322	H	8.82651	-2.75860	-0.16450
C	-3.30040	0.08221	2.60629	H	10.09805	-2.23412	0.97107
C	-2.57238	-2.32783	2.04249	H	8.66408	-3.10027	1.58312
Fe	-2.57139	-0.76111	1.24363				

Zero-point correction= 0.723443 (Hartree/Particle)
Thermal correction to Energy= 0.769843
Thermal correction to Enthalpy= 0.770788
Thermal correction to Gibbs Free Energy= 0.638559
Sum of electronic and zero-point Energies= -2137.327130
Sum of electronic and thermal Energies= -2137.280729
Sum of electronic and thermal Enthalpies= -2137.279785
Sum of electronic and thermal Free Energies= -2137.412013

(1b) TS*(E)re*

Fe	0.24308	-1.24921	-1.08519	H	-1.50603	-2.70848	3.07039
C	0.15194	-1.08194	1.20298	C	-4.57416	-2.25584	0.75898
C	-0.74913	-2.07305	0.61161	H	-3.15407	-1.79295	-0.78549
C	0.07251	-3.10231	0.00360	C	-4.76411	-2.60393	2.09673
C	1.44720	-2.67977	0.05548	H	-3.78646	-3.03349	3.97090
C	1.49004	-1.36173	0.65916	H	-5.43050	-2.12454	0.10277
C	-1.03444	-1.43989	-2.27349	H	-5.76706	-2.74534	2.48951
C	1.44717	-0.88458	-2.31051	N	-0.30202	-4.40860	-0.33832
O	-0.16170	-0.11396	1.95455	N	2.47568	-3.53329	-0.32302
O	-1.88609	-1.48059	-3.06510	C	0.83210	-5.32459	-0.47881
O	2.21046	-0.59733	-3.14035	H	1.13526	-5.68675	0.51198
H	2.70570	4.21018	1.64419	H	0.51337	-6.18967	-1.06576
C	2.40747	3.75914	0.70593	C	2.03717	-4.65911	-1.14122
C	3.24522	3.79576	-0.41408	H	2.86436	-5.37241	-1.21593
C	1.16721	3.13101	0.61892	H	1.77662	-4.33208	-2.16413
C	2.81788	3.20659	-1.61612	C	3.79616	-3.02217	-0.66231
C	0.72792	2.52588	-0.56859	H	4.47328	-3.87362	-0.77505
H	0.52087	3.13601	1.48859	H	3.79849	-2.45009	-1.60348
C	1.58528	2.58164	-1.68676	H	4.17813	-2.38480	0.13169
H	3.47985	3.23996	-2.47502	C	-1.38836	-4.61312	-1.29004
C	-0.63345	1.93290	-0.65625	H	-1.09899	-4.35374	-2.32250
H	1.30189	2.10424	-2.61741	H	-1.69340	-5.66340	-1.26205
H	-0.14334	0.27813	-1.02140	H	-2.25165	-4.01126	-1.01240
N	-1.30422	1.80250	0.49967	C	-3.61483	2.66799	0.09575
H	-0.75334	1.32550	1.24823	C	-3.29773	4.00674	0.36205
C	-1.39763	2.11732	-1.94618	C	-4.79832	2.38266	-0.59536
H	-0.75036	1.95086	-2.80548	C	-4.14086	5.03485	-0.06124
H	-2.24463	1.43616	-2.01928	H	-2.38020	4.24140	0.89410
H	-1.77547	3.14469	-1.99592	C	-5.64720	3.40877	-1.01391
C	-2.74790	1.52662	0.61468	H	-5.05622	1.34761	-0.80741
C	2.67376	-0.60038	1.14949	C	-5.31953	4.73949	-0.75003
C	3.54717	0.11552	0.31742	H	-3.87742	6.06800	0.14799
C	2.92793	-0.59661	2.53310	H	-6.56014	3.16807	-1.55140
C	4.66159	0.77316	0.84179	H	-5.97532	5.54005	-1.07992
H	3.35705	0.15650	-0.74844	H	-2.97996	0.61595	0.04646
C	4.03455	0.06773	3.06037	C	-3.06681	1.25758	2.09557
H	2.24485	-1.11938	3.19461	H	-2.43537	0.45436	2.47909
C	4.91292	0.74855	2.21465	H	-2.89923	2.16197	2.68994
H	5.32591	1.31492	0.17412	H	-4.11650	0.97220	2.19595
H	4.21258	0.04933	4.13227	O	4.47805	4.36846	-0.44191
H	5.78343	1.25594	2.62238	C	4.98654	4.93026	0.76102
C	-2.15543	-2.24051	1.07232	H	5.05471	4.17705	1.55518
C	-2.36598	-2.58778	2.41880	H	5.98531	5.29786	0.52147
C	-3.28400	-2.07114	0.25472	H	4.36815	5.76769	1.10786
C	-3.65253	-2.76674	2.92609				

```
Zero-point correction=                  0.723007 (Hartree/Particle)
 Thermal correction to Energy=              0.768160
 Thermal correction to Enthalpy=            0.769104
 Thermal correction to Gibbs Free Energy=      0.643311
 Sum of electronic and zero-point Energies=       -2137.301937
 Sum of electronic and thermal Energies=          -2137.256785
 Sum of electronic and thermal Enthalpies=        -2137.255841
 Sum of electronic and thermal Free Energies=     -2137.381634
Imaginary frequency                                 -298.29
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(1b) TS*(E)si*

Fe	0.36100	-1.45600	-0.93700	H	-0.45000	-3.08200	3.35200
C	0.79500	-0.31600	0.96600	C	-3.38500	-0.65700	2.66900
C	-0.00700	-1.53000	1.18000	H	-2.25900	-0.02200	0.95300
C	0.80900	-2.66600	0.82200	C	-3.43700	-1.50900	3.77400
C	2.04000	-2.19300	0.25200	H	-2.40000	-3.04900	4.87200
C	1.99500	-0.74600	0.22100	H	-4.20400	0.02800	2.46800
C	-1.10400	-2.29200	-1.44400	H	-4.29500	-1.49400	4.44100
C	1.09900	-1.55200	-2.52500	N	0.59500	-4.01400	1.13600
O	0.48700	0.86500	1.28400	N	3.07100	-3.06900	-0.07600
O	-2.08300	-2.80500	-1.79700	C	1.79500	-4.84400	1.00900
O	1.53700	-1.56400	-3.60400	H	2.41000	-4.73900	1.91200
H	-5.07800	2.31400	0.31600	H	1.49000	-5.89100	0.93400
C	-4.52100	1.72700	-0.40500	C	2.64100	-4.45800	-0.20300
C	-5.15600	0.77000	-1.20600	H	3.53300	-5.09100	-0.25300
C	-3.15200	1.95100	-0.55100	H	2.06300	-4.61100	-1.13300
C	-4.40100	0.04900	-2.14600	C	4.09900	-2.68000	-1.03300
C	-2.38000	1.23300	-1.47800	H	4.87100	-3.45500	-1.03800
H	-2.67900	2.71600	0.05400	H	3.70300	-2.57600	-2.05600
C	-3.04300	0.28000	-2.27800	H	4.56100	-1.74000	-0.74200
H	-4.90300	-0.69600	-2.75300	C	-0.65400	-4.64900	0.72500
C	-0.94300	1.57100	-1.67800	H	-0.66700	-4.89100	-0.34900
H	-2.48500	-0.31000	-2.99500	H	-0.79300	-5.57200	1.29700
H	-0.28100	-0.07200	-1.38000	H	-1.49700	-3.99300	0.94100
N	-0.37100	2.32300	-0.72200	C	1.06500	3.87000	0.50100
H	-0.40300	1.89800	0.23200	C	0.03700	4.52800	1.19000
C	-0.45300	1.63000	-3.10700	C	2.35700	3.89600	1.03400
H	-0.89600	2.49100	-3.62000	C	0.29300	5.18500	2.39300
H	0.63400	1.69900	-3.16000	H	-0.97200	4.52500	0.78500
H	-0.76000	0.73500	-3.64800	C	2.61700	4.56100	2.23300
C	0.80500	3.21400	-0.85200	H	3.16100	3.38500	0.51500
C	3.14500	0.16700	-0.03000	C	1.58600	5.20500	2.91800
C	3.46200	0.68900	-1.29400	H	-0.51700	5.68300	2.91900
C	3.97800	0.50400	1.05100	H	3.62500	4.56500	2.63600
C	4.58500	1.50000	-1.47800	H	1.78700	5.71700	3.85500
H	2.83900	0.43200	-2.14400	H	1.68700	2.62300	-1.12200
C	5.10100	1.31200	0.87100	C	0.59400	4.32700	-1.89800
H	3.73900	0.12100	2.03900	H	0.56300	3.95900	-2.92400
C	5.41200	1.81200	-0.39700	H	-0.33200	4.87500	-1.69600
H	4.81600	1.88200	-2.46800	H	1.42400	5.03500	-1.82500
H	5.73400	1.55200	1.72100	O	-6.48100	0.47400	-1.16000
H	6.28900	2.43700	-0.54000	C	-7.29300	1.14600	-0.20700
C	-1.21400	-1.55500	2.03600	H	-8.29800	0.74300	-0.33200
C	-1.27400	-2.40300	3.15700	H	-6.95100	0.95600	0.81800
C	-2.28700	-0.67900	1.81200	H	-7.31200	2.22900	-0.38500
C	-2.37500	-2.38300	4.01300				

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Zero-point correction=                  0.722368 (Hartree/Particle)
 Thermal correction to Energy=              0.767609
 Thermal correction to Enthalpy=            0.768553
 Thermal correction to Gibbs Free Energy=      0.642430
 Sum of electronic and zero-point Energies=       -2137.292313
 Sum of electronic and thermal Energies=          -2137.247072
 Sum of electronic and thermal Enthalpies=        -2137.246128
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 Sum of electronic and thermal Free Energies=     -2137.372251
Imaginary frequency                                -298.20
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(1b) $TS_{(Z)re}$

Fe	0.95200	-1.15800	-0.61300	H	3.47000	1.50000	2.35200
C	1.46700	0.83500	0.40800	C	3.03900	-1.88600	4.16800
C	2.34600	-0.28700	0.75400	H	2.11700	-2.57400	2.35600
C	3.05700	-0.67200	-0.45000	C	3.63700	-0.81800	4.83600
C	2.49600	0.05200	-1.56000	H	4.24600	1.24600	4.68500
C	1.40900	0.87400	-1.06100	H	2.90100	-2.83800	4.67400
C	0.95500	-2.80800	-0.00600	H	3.97300	-0.93200	5.86200
C	0.08600	-1.61500	-2.07200	N	4.24900	-1.39900	-0.55800
O	0.81300	1.55200	1.21500	N	3.06900	-0.00300	-2.82500
O	0.88200	-3.88800	0.42000	C	4.93700	-1.21100	-1.83700
O	-0.52800	-1.93100	-3.00800	H	5.51900	-0.28000	-1.80600
H	-4.39800	-1.87000	-2.27400	H	5.63900	-2.03600	-1.98200
C	-4.10100	-2.00500	-1.23900	C	3.96700	-1.13700	-3.01400
C	-4.72100	-3.02000	-0.48900	H	4.52100	-0.98600	-3.94700
C	-3.11800	-1.21600	-0.66700	H	3.40300	-2.08400	-3.10300
C	-4.32600	-3.23400	0.83600	C	2.30600	0.36100	-4.01100
C	-2.71600	-1.40400	0.67100	H	2.98900	0.37600	-4.86500
H	-2.62800	-0.46200	-1.27100	H	1.49500	-0.35200	-4.22700
C	-3.32600	-2.43500	1.39600	H	1.87600	1.35400	-3.90200
H	-4.77800	-4.01300	1.43700	C	4.32700	-2.74500	-0.00100
C	-1.66000	-0.56600	1.30600	H	3.74800	-3.47900	-0.58600
H	-3.03600	-2.62100	2.42400	H	5.37400	-3.05900	0.02400
H	-0.42700	-0.93400	0.13500	H	3.95800	-2.75000	1.02200
N	-1.72400	0.77300	1.34400	C	-2.29500	3.12800	1.09100
H	-0.79500	1.20700	1.55500	C	-2.06600	3.46200	2.43300
C	-0.88300	-1.15100	2.46700	C	-2.26300	4.14300	0.13000
H	-0.57700	-2.17800	2.27300	C	-1.80400	4.78100	2.80300
H	-0.00200	-0.54200	2.67300	H	-2.08300	2.68400	3.19200
H	-1.52100	-1.12700	3.36100	C	-2.00900	5.46500	0.49900
C	-2.66700	1.70500	0.69000	H	-2.41900	3.89700	-0.91600
C	0.68800	1.96300	-1.78100	C	-1.77900	5.78800	1.83600
C	-0.42300	1.74900	-2.61100	H	-1.62100	5.02100	3.84600
C	1.15900	3.28000	-1.63600	H	-1.98100	6.23900	-0.26300
C	-1.01600	2.80500	-3.30800	H	-1.57600	6.81600	2.12400
H	-0.80300	0.74200	-2.74200	H	-2.57800	1.62600	-0.40000
C	0.56600	4.33700	-2.32600	C	-4.12900	1.44100	1.10800
H	2.00100	3.46800	-0.97800	H	-4.49400	0.46700	0.78400
C	-0.51900	4.10300	-3.17400	H	-4.22500	1.51000	2.19600
H	-1.86200	2.60900	-3.96100	H	-4.76500	2.21200	0.66400
H	0.95400	5.34400	-2.20300	O	-5.67500	-3.73600	-1.14100
H	-0.97500	4.92300	-3.72100	C	-6.31200	-4.80000	-0.44800
C	2.77000	-0.52600	2.16200	H	-6.85600	-4.43900	0.43400
C	3.36000	0.54600	2.85600	H	-7.02200	-5.23500	-1.15400
C	2.60300	-1.73900	2.84900	H	-5.59200	-5.56800	-0.13900
C	3.79100	0.40200	4.17400				

```
Zero-point correction=                 0.722493 (Hartree/Particle)
 Thermal correction to Energy=             0.767866
 Thermal correction to Enthalpy=           0.768810
 Thermal correction to Gibbs Free Energy=      0.641098
 Sum of electronic and zero-point Energies=       -2137.293046
 Sum of electronic and thermal Energies=          -2137.247673
 Sum of electronic and thermal Enthalpies=        -2137.246729
 Sum of electronic and thermal Free Energies=     -2137.374441
Imaginary frequency                                   -350.79
```

(1b) $TS_{(Z)si}$

Fe	-1.34512	-0.36375	-0.93351	H	-2.63902	3.40330	1.66819
C	-1.80924	0.53396	1.13401	C	0.28039	4.56601	-0.58874
C	-1.88753	1.46742	0.00797	H	0.19589	2.59820	-1.45095
C	-2.99358	1.04665	-0.82813	C	-0.25699	5.44551	0.35188
C	-3.44525	-0.24176	-0.37255	H	-1.73561	5.69450	1.90247
C	-2.63015	-0.63030	0.76604	H	1.10112	4.88426	-1.22613
C	-0.55903	0.26357	-2.37471	H	0.14199	6.45087	0.45300
C	-1.32169	-2.01461	-1.53856	N	-3.70016	1.80028	-1.76471
O	-1.09597	0.65040	2.17129	N	-4.58690	-0.83083	-0.91289
O	0.01368	0.65370	-3.30852	C	-4.99263	1.22967	-2.15095
O	-1.24254	-3.10854	-1.92448	H	-5.76028	1.52847	-1.42528
H	4.69372	-3.60182	-1.10616	H	-5.27849	1.63711	-3.12406
C	4.15443	-2.66525	-1.17972	C	-4.95281	-0.29480	-2.21977
C	4.42153	-1.75516	-2.20796	H	-5.94248	-0.68021	-2.48504
C	3.17243	-2.36880	-0.23305	H	-4.24003	-0.62067	-2.99907
C	3.69296	-0.55566	-2.27317	C	-4.82539	-2.26050	-0.77607
C	2.45628	-1.16468	-0.26646	H	-5.82810	-2.47723	-1.15523
H	2.98192	-3.09194	0.55191	H	-4.10151	-2.86590	-1.34521
C	2.73396	-0.26923	-1.31767	H	-4.78513	-2.56010	0.26857
H	3.88986	0.12722	-3.09264	C	-2.98975	2.51946	-2.81511
C	1.42642	-0.88928	0.77595	H	-2.63835	1.84945	-3.61702
H	2.15683	0.64176	-1.41298	H	-3.65764	3.26879	-3.25018
H	0.09499	-0.60592	-0.30159	H	-2.12938	3.04182	-2.40137
N	1.46993	0.20617	1.54828	C	3.77640	1.15015	1.57624
H	0.57635	0.36305	2.06296	C	4.23330	0.31498	2.60412
C	0.76873	-2.07026	1.45943	C	4.71772	1.81179	0.78021
H	1.48436	-2.50803	2.16797	C	5.59943	0.14259	2.82599
H	-0.09937	-1.73578	2.02737	H	3.51197	-0.20390	3.22908
H	0.46421	-2.83130	0.74219	C	6.08568	1.64546	1.00277
C	2.28832	1.42084	1.38385	H	4.37750	2.46051	-0.02334
C	-2.84918	-1.72732	1.75220	C	6.53122	0.80851	2.02648
C	-2.60568	-3.08651	1.49284	H	5.93697	-0.51049	3.62617
C	-3.29964	-1.37504	3.03732	H	6.80170	2.16491	0.37204
C	-2.83466	-4.05857	2.46778	H	7.59524	0.67466	2.19957
H	-2.23622	-3.38769	0.51943	H	2.12978	1.84709	0.38732
C	-3.52349	-2.34454	4.01469	C	1.79166	2.45039	2.41391
H	-3.46263	-0.32773	3.26776	H	0.72195	2.63217	2.29012
C	-3.29643	-3.69261	3.73317	H	1.97187	2.08804	3.43111
H	-2.64433	-5.10342	2.23736	H	2.33369	3.39004	2.28489
H	-3.87436	-2.04417	4.99826	O	5.34652	-1.93865	-3.18754
H	-3.47132	-4.44921	4.49300	C	6.09891	-3.14332	-3.18923
C	-1.29702	2.83213	0.08507	H	6.76605	-3.07960	-4.04991
C	-1.82369	3.73025	1.03011	H	6.69723	-3.24662	-2.27517
C	-0.23050	3.27179	-0.71545	H	5.45183	-4.02276	-3.29772
C	-1.31100	5.02061	1.16338				

Zero-point correction= 0.723075 (Hartree/Particle)
 Thermal correction to Energy= 0.768327
 Thermal correction to Enthalpy= 0.769271
 Thermal correction to Gibbs Free Energy= 0.642384
 Sum of electronic and zero-point Energies= -2137.298301
 Sum of electronic and thermal Energies= -2137.253050
 Sum of electronic and thermal Enthalpies= -2137.252106
 Sum of electronic and thermal Free Energies= -2137.378993
Imaginary frequency -359.52

(1b) adduct $E_{E(S,1'S)}$

Fe	1.00800	-0.69200	-0.98600	H	-0.02600	-3.36600	2.75800
C	0.85700	-1.05600	1.25000	C	-2.57900	-4.32800	0.01400
C	0.61700	-2.26400	0.42200	H	-1.41300	-3.09200	-1.29800
C	1.85900	-2.59200	-0.22300	C	-2.73100	-4.83200	1.30600
C	2.77400	-1.47100	-0.05000	H	-1.92000	-4.85900	3.30500
C	2.14200	-0.48900	0.79400	H	-3.29600	-4.58600	-0.76100
C	0.29000	-1.43700	-2.42400	H	-3.56600	-5.48500	1.54500
C	1.83600	0.54400	-1.94000	N	2.25900	-3.73700	-0.86500
O	0.05800	-0.53700	2.04900	N	4.08700	-1.54800	-0.49400
O	-0.11600	-1.96300	-3.37400	C	3.69800	-3.91000	-1.04100
O	2.41600	1.31000	-2.58800	H	4.17400	-4.27700	-0.11800
H	-0.82100	5.41800	1.58700	H	3.86200	-4.66000	-1.82100
C	-0.64600	4.77900	0.72700	C	4.34300	-2.60100	-1.47100
C	0.11600	5.28200	-0.33600	H	5.42600	-2.73900	-1.54900
C	-1.17000	3.49200	0.67000	H	3.96700	-2.31300	-2.46800
C	0.34000	4.47400	-1.45700	C	4.85900	-0.33600	-0.76700
C	-0.94900	2.66100	-0.43900	H	5.92300	-0.59100	-0.74800
H	-1.76900	3.12000	1.49300	H	4.61800	0.08200	-1.75500
C	-0.19300	3.18400	-1.49500	H	4.67200	0.42100	-0.01100
H	0.92200	4.83100	-2.29800	C	1.45100	-4.94900	-0.89800
C	-1.53500	1.24600	-0.51800	H	0.43800	-4.73200	-1.23100
H	-0.00600	2.58300	-2.37800	H	1.90500	-5.64100	-1.61200
H	-0.64300	0.53100	-0.69700	H	1.39300	-5.44600	0.08000
N	-2.19800	0.90600	0.72200	C	-4.54600	0.16400	0.29600
H	-1.48700	0.76500	1.44000	C	-5.08800	1.43400	0.53000
C	-2.42000	1.09100	-1.76400	C	-5.34600	-0.79800	-0.33400
H	-1.84300	1.33200	-2.66000	C	-6.39300	1.73600	0.13900
H	-2.79300	0.07000	-1.87200	H	-4.46700	2.18700	1.00600
H	-3.27600	1.76800	-1.71300	C	-6.65300	-0.50100	-0.72300
C	-3.15000	-0.21100	0.78900	H	-4.93800	-1.78900	-0.51900
C	2.77100	0.64100	1.52500	C	-7.18200	0.76900	-0.48900
C	2.25200	1.94200	1.46300	H	-6.79500	2.72800	0.32400
C	3.85300	0.39300	2.38900	H	-7.25600	-1.26000	-1.21500
C	2.81100	2.96900	2.22500	H	-8.19700	1.00500	-0.79500
H	1.40900	2.15300	0.81600	H	-2.79900	-1.07100	0.19700
C	4.41500	1.42000	3.14600	C	-3.24100	-0.66900	2.25700
H	4.25400	-0.61500	2.46200	H	-2.26000	-0.99400	2.61200
C	3.89500	2.71400	3.06600	H	-3.59600	0.15500	2.88500
H	2.39200	3.96900	2.15900	H	-3.94800	-1.49800	2.34900
H	5.25300	1.20700	3.80400	O	0.58800	6.55600	-0.18600
H	4.33000	3.51500	3.65700	C	1.36100	7.11000	-1.23700
C	-0.55800	-3.14300	0.68400	H	0.79100	7.17100	-2.17300
C	-0.73400	-3.64500	1.98500	H	1.63000	8.11800	-0.91600
C	-1.50900	-3.48500	-0.29100	H	2.27800	6.53300	-1.41600
C	-1.80600	-4.48300	2.29200				

Zero-point correction= 0.726664 (Hartree/Particle)
Thermal correction to Energy= 0.773086
Thermal correction to Enthalpy= 0.774030
Thermal correction to Gibbs Free Energy= 0.642551
Sum of electronic and zero-point Energies= -2137.314764
Sum of electronic and thermal Energies= -2137.268343
Sum of electronic and thermal Enthalpies= -2137.267399
Sum of electronic and thermal Free Energies= -2137.398878

(1b) adduct $E_{E(R,1'S)}$

Fe	0.14100	-1.39400	-0.88900	C	0.73300	-1.52600	-2.54600
C	0.96300	-0.42700	0.99300	O	0.89100	0.76600	1.31900
C	-0.06100	-1.47300	1.24400	O	-2.32300	-2.85600	-1.48600
C	0.49500	-2.72800	0.84000	O	1.11000	-1.64300	-3.63800
C	1.71900	-2.46900	0.09200	H	-4.97400	3.16300	0.30100
C	1.97100	-1.05000	0.10200	C	-4.45700	2.43400	-0.31400
C	-1.38100	-2.21400	-1.27100	C	-5.21000	1.42700	-0.93200

C	-3.07900	2.49600	-0.49800	N	0.06300	-4.00300	1.06500
C	-4.55900	0.48500	-1.73900	N	2.51800	-3.51900	-0.33000
C	-2.40600	1.55600	-1.29200	C	0.99800	-5.08900	0.79000
H	-2.50400	3.28400	-0.02800	H	1.67100	-5.25700	1.64400
C	-3.17500	0.56300	-1.90800	H	0.42500	-6.00700	0.63400
H	-5.11000	-0.30700	-2.23300	C	1.81600	-4.79400	-0.46200
C	-0.88800	1.62900	-1.51900	H	2.56100	-5.58300	-0.60100
H	-2.69500	-0.17900	-2.54000	H	1.15500	-4.78900	-1.34500
H	-0.47700	0.58300	-1.27300	C	3.55100	-3.30600	-1.34000
N	-0.29700	2.61500	-0.63700	H	4.17100	-4.20500	-1.39000
H	-0.26700	2.22000	0.30300	H	3.12700	-3.11600	-2.33700
C	-0.58600	1.82400	-3.01200	H	4.18500	-2.46600	-1.06500
H	-1.02100	2.75800	-3.37500	C	-1.24000	-4.34000	1.62200
H	0.48800	1.82600	-3.21200	H	-1.60400	-5.25300	1.13900
H	-1.02800	1.00500	-3.58500	H	-1.20200	-4.50900	2.70600
C	1.02100	3.23000	-0.89800	H	-1.95400	-3.54200	1.42800
C	3.23600	-0.34000	-0.24200	C	1.56500	3.79600	0.41100
C	3.49800	0.22000	-1.50100	C	0.77100	4.62200	1.21800
C	4.21300	-0.20400	0.76000	C	2.88700	3.55300	0.79700
C	4.70600	0.87200	-1.76000	C	1.28700	5.18800	2.38500
H	2.75700	0.13500	-2.28800	H	-0.25800	4.81800	0.93200
C	5.41900	0.44700	0.50500	C	3.40800	4.12400	1.95900
H	4.01700	-0.61400	1.74700	H	3.51100	2.90300	0.18900
C	5.67200	0.98600	-0.75900	C	2.61000	4.94300	2.75800
H	4.88900	1.29300	-2.74400	H	0.65500	5.82200	3.00100
H	6.16000	0.53700	1.29500	H	4.43700	3.91900	2.24400
H	6.61200	1.49300	-0.96000	H	3.01300	5.38400	3.66600
C	-1.17700	-1.23400	2.19800	H	1.74700	2.48700	-1.26300
C	-1.03200	-1.63400	3.53800	C	0.94000	4.38600	-1.91900
C	-2.34400	-0.55300	1.82600	H	0.67400	4.05300	-2.92200
C	-2.03700	-1.38500	4.47200	H	0.19500	5.11900	-1.59300
H	-0.12000	-2.13800	3.84800	H	1.91000	4.88900	-1.97800
C	-3.34900	-0.29800	2.76200	O	-6.55500	1.44900	-0.69100
H	-2.46900	-0.22000	0.80200	C	-7.36100	0.45600	-1.30300
C	-3.20200	-0.71700	4.08500	H	-8.38500	0.66200	-0.98700
H	-1.90700	-1.70300	5.50200	H	-7.30600	0.50500	-2.39800
H	-4.24300	0.23300	2.45100	H	-7.08000	-0.55400	-0.97700
H	-3.98400	-0.51800	4.81200				

Zero-point correction= 0.726377 (Hartree/Particle)
Thermal correction to Energy= 0.773028
Thermal correction to Enthalpy= 0.773972
Thermal correction to Gibbs Free Energy= 0.641895
Sum of electronic and zero-point Energies= -2137.307241
Sum of electronic and thermal Energies= -2137.260590
Sum of electronic and thermal Enthalpies= -2137.259646
Sum of electronic and thermal Free Energies= -2137.391722

(1b) adduct $E_{Z(S,1'S)}$

Fe	1.07700	-0.87900	-0.68700	H	-1.65500	-2.42700	-1.33100
C	1.57300	0.86400	0.73800	C	-4.16500	-1.54600	0.76500
C	2.29700	-0.39900	1.05800	H	-6.17500	-2.33600	0.67500
C	3.22200	-0.63200	-0.01300	C	-1.76500	-0.73200	0.85900
C	2.83400	0.20800	-1.13800	H	-4.36800	-0.89100	1.60600
C	1.78500	1.10400	-0.70800	H	-0.88400	-0.71000	0.12500
C	1.15600	-2.64400	-0.57800	N	-2.17700	0.60400	1.23200
C	0.40200	-0.93500	-2.31500	H	-1.50700	0.95800	1.91300
O	0.80200	1.48000	1.48900	C	-1.27900	-1.44800	2.13200
O	1.29400	-3.79600	-0.55100	H	-0.93000	-2.45700	1.90100
O	-0.00100	-0.99700	-3.40100	H	-0.46100	-0.89500	2.60100
H	-3.42100	-3.84500	-2.26100	H	-2.10600	-1.52300	2.84400
C	-3.64700	-3.21000	-1.41200	C	-2.31500	1.65600	0.20600
C	-4.92500	-3.18500	-0.84700	C	1.35000	2.38400	-1.33900
C	-2.64000	-2.39800	-0.87700	C	0.40500	2.47500	-2.37200
C	-5.17700	-2.34400	0.24900	C	1.91700	3.57600	-0.85500
C	-2.87400	-1.55400	0.20800	C	0.06200	3.71000	-2.92500

H	-0.06400	1.57500	-2.75400	H	2.33300	0.45100	-3.95900
C	1.57300	4.81200	-1.40300	H	2.94800	1.95700	-3.24400
H	2.63200	3.52700	-0.03900	C	4.94000	-2.08900	1.06400
C	0.64700	4.88300	-2.44500	H	4.64700	-3.14600	1.12200
H	-0.67000	3.75400	-3.72600	H	6.02800	-2.03800	0.95400
H	2.02700	5.71800	-1.01200	H	4.66700	-1.60100	1.99600
H	0.37700	5.84400	-2.87300	C	-2.61900	2.97100	0.91600
C	2.28200	-0.97600	2.42900	C	-3.63700	3.04600	1.87800
C	2.34400	-0.10500	3.53200	C	-1.91000	4.13500	0.59900
C	2.19300	-2.35700	2.68100	C	-3.94300	4.25600	2.50000
C	2.33500	-0.60100	4.83600	H	-4.17800	2.14300	2.14400
H	2.37800	0.96400	3.36000	C	-2.21700	5.34900	1.21800
C	2.19100	-2.85100	3.98400	H	-1.10700	4.09000	-0.13000
H	2.11500	-3.05200	1.85200	C	-3.23500	5.41400	2.17000
C	2.26300	-1.97500	5.06900	H	-4.73400	4.29500	3.24500
H	2.38300	0.09100	5.67200	H	-1.65300	6.24100	0.96000
H	2.12000	-3.92200	4.15000	H	-3.47200	6.35700	2.65500
H	2.25400	-2.36000	6.08500	H	-1.36200	1.77800	-0.33000
N	4.33300	-1.41500	-0.07600	C	-3.40000	1.36200	-0.84300
N	3.63400	0.22300	-2.27500	H	-3.16700	0.47600	-1.43800
C	5.09700	-1.49100	-1.32000	H	-4.37500	1.20800	-0.37100
H	5.99500	-0.86000	-1.24200	H	-3.47800	2.21800	-1.52000
H	5.43200	-2.52600	-1.46300	O	-5.98700	-3.92800	-1.28300
C	4.27000	-1.06700	-2.52500	C	-5.78700	-4.79400	-2.38600
H	4.93400	-0.97000	-3.38900	H	-6.74600	-5.28400	-2.56500
H	3.51700	-1.83800	-2.76000	H	-5.49200	-4.24100	-3.28900
C	3.20100	0.92600	-3.47900	H	-5.02700	-5.55700	-2.17300
H	4.03300	0.92900	-4.18900				

Zero-point correction= 0.726864 (Hartree/Particle)
Thermal correction to Energy= 0.773440
Thermal correction to Enthalpy= 0.774384
Thermal correction to Gibbs Free Energy= 0.642610
Sum of electronic and zero-point Energies= -2137.311381
Sum of electronic and thermal Energies= -2137.264805
Sum of electronic and thermal Enthalpies= -2137.263860
Sum of electronic and thermal Free Energies= -2137.395635

(1b) adduct $E_{Z(R,1'S)}$

Fe	-1.27700	-0.34800	-0.84600	H	-0.19400	-1.87400	2.21100
C	-1.95300	0.59100	1.15700	H	0.35400	-2.96500	0.92000
C	-1.91500	1.52300	0.00300	C	2.19600	1.28100	1.41400
C	-2.95200	1.11100	-0.90400	C	-3.03400	-1.68700	1.67100
C	-3.38300	-0.22700	-0.52300	C	-2.78400	-3.04900	1.43800
C	-2.71600	-0.59500	0.70600	C	-3.59500	-1.32200	2.90800
C	-0.60100	0.29000	-2.34700	C	-3.11200	-4.01400	2.39200
C	-1.23100	-2.01100	-1.44700	H	-2.32800	-3.36200	0.50600
O	-1.32300	0.71000	2.22100	C	-3.91700	-2.28500	3.86400
O	-0.25200	0.71700	-3.37000	H	-3.76500	-0.27200	3.12100
O	-1.22800	-3.08800	-1.87700	C	-3.68200	-3.63600	3.60800
H	5.53800	-2.99100	0.37500	H	-2.91000	-5.06100	2.18500
C	4.68000	-2.52100	-0.09500	H	-4.35000	-1.97500	4.81100
C	4.67900	-2.37100	-1.49100	H	-3.93100	-4.38700	4.35300
C	3.60700	-2.06700	0.65700	C	-1.27000	2.86000	0.12300
C	3.59100	-1.75600	-2.11300	C	-1.69800	3.71600	1.15400
C	2.49800	-1.45000	0.05000	C	-0.25100	3.31000	-0.73100
H	3.63200	-2.17400	1.73600	C	-1.14600	4.98800	1.30700
C	2.51800	-1.30400	-1.33600	H	-2.46400	3.37200	1.84100
H	3.56100	-1.61900	-3.18800	C	0.29900	4.58400	-0.58100
C	1.31100	-1.00900	0.90000	H	0.11200	2.66300	-1.52100
H	1.68400	-0.82200	-1.83400	C	-0.14800	5.42900	0.43600
H	0.52200	-0.61200	0.15700	H	-1.49400	5.63200	2.10900
N	1.63900	0.00100	1.88000	H	1.08400	4.91300	-1.25700
H	0.80000	0.18400	2.42900	H	0.28300	6.41900	0.55400
C	0.67300	-2.20000	1.63100	N	-3.55400	1.78500	-1.92100
H	1.39800	-2.64600	2.31800	N	-4.45000	-0.80600	-1.19700

C	-4.61100	1.13100	-2.69200	H	4.00700	0.31500	3.21300
H	-5.59600	1.47900	-2.34800	C	5.75600	1.91900	0.15400
H	-4.50700	1.41800	-3.74500	H	3.76700	2.23000	-0.61300
C	-4.53400	-0.38700	-2.59200	C	6.52700	1.42200	1.20500
H	-5.44000	-0.81400	-3.03200	H	6.48600	0.45500	3.13300
H	-3.66900	-0.76100	-3.16500	H	6.23900	2.36100	-0.71400
C	-4.83100	-2.19300	-0.95900	H	7.61100	1.47500	1.16300
H	-5.79400	-2.37000	-1.44600	H	1.79100	1.53100	0.41900
H	-4.10000	-2.91000	-1.36300	C	1.75500	2.38600	2.39000
H	-4.94700	-2.37700	0.10600	H	0.66500	2.43800	2.44200
C	-3.16100	3.11900	-2.35900	H	2.14600	2.18100	3.39200
H	-2.28100	3.09300	-3.01500	H	2.14200	3.35600	2.06700
H	-3.99500	3.55600	-2.91300	O	5.78000	-2.85400	-2.14100
H	-2.94200	3.76400	-1.50900	C	5.83200	-2.72200	-3.55000
C	3.71800	1.27200	1.31300	H	5.80900	-1.67000	-3.86200
C	4.50200	0.77500	2.36300	H	6.77900	-3.16700	-3.86200
C	4.36300	1.84400	0.21100	H	5.00600	-3.25600	-4.03900
C	5.89300	0.84800	2.31100				

Zero-point correction= 0.726500 (Hartree/Particle)
Thermal correction to Energy= 0.773066
Thermal correction to Enthalpy= 0.774010
Thermal correction to Gibbs Free Energy= 0.642449
Sum of electronic and zero-point Energies= -2137.313640
Sum of electronic and thermal Energies= -2137.267074
Sum of electronic and thermal Enthalpies= -2137.266130
Sum of electronic and thermal Free Energies= -2137.397690

(S,1'S)-N-(1-(4-methoxyphenyl)ethyl)-(S)-α-methylbenzylamine

Zero-point correction= 0.344646 (Hartree/Particle)
Thermal correction to Energy= 0.362807
Thermal correction to Enthalpy= 0.363751
Thermal correction to Gibbs Free Energy= 0.296168
Sum of electronic and zero-point Energies= -790.104476
Sum of electronic and thermal Energies= -790.086315
Sum of electronic and thermal Enthalpies= -790.085371
Sum of electronic and thermal Free Energies= -790.152954

(R,1'S)-N-(1-(4-methoxyphenyl)ethyl)-(S)-α-methylbenzylamine

Zero-point correction= 0.344524 (Hartree/Particle)
Thermal correction to Energy= 0.362730
Thermal correction to Enthalpy= 0.363674
Thermal correction to Gibbs Free Energy= 0.296343
Sum of electronic and zero-point Energies= -790.104237
Sum of electronic and thermal Energies= -790.086031
Sum of electronic and thermal Enthalpies= -790.085087
Sum of electronic and thermal Free Energies= -790.152418

(E)-N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Methyl)phenyl)-1-imine (1f)

Zero-point correction= 0.315142 (Hartree/Particle)
Thermal correction to Energy= 0.332459
Thermal correction to Enthalpy= 0.333403
Thermal correction to Gibbs Free Energy= 0.265810
Sum of electronic and zero-point Energies= -713.719401
Sum of electronic and thermal Energies= -713.702084
Sum of electronic and thermal Enthalpies= -713.701140
Sum of electronic and thermal Free Energies= -713.768733

(Z)-N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Methyl)phenyl)-1-imine (1f)

```
Zero-point correction=                 0.314890 (Hartree/Particle)
 Thermal correction to Energy=             0.332220
 Thermal correction to Enthalpy=           0.333164
 Thermal correction to Gibbs Free Energy=      0.267076
 Sum of electronic and zero-point Energies=        -713.716616
 Sum of electronic and thermal Energies=        -713.699287
 Sum of electronic and thermal Enthalpies=         -713.698343
 Sum of electronic and thermal Free Energies=      -713.764430
```

(1f) Adduct D*(E)*

C	-2.70481	-0.36819	-1.29669	H	-5.62501	-1.00811	-2.68465
C	-3.02664	0.85009	-0.62972	H	-4.66928	1.28904	-2.80908
C	-5.06031	0.91481	-1.85471	H	-0.94405	-0.89922	-3.75366
C	-5.01042	-0.61325	-1.86790	H	0.26283	-2.61171	-0.00557
C	-1.28313	-0.63365	-1.09964	H	0.48219	-2.52390	-4.96257
C	-0.75543	0.49825	-0.38626	H	1.70565	-4.22570	-1.20415
C	-1.81828	1.38025	-0.01664	H	1.81445	-4.19935	-3.69208
N	-3.63493	-1.07009	-2.07029	H	-0.27179	2.01170	2.13376
N	-4.27487	1.49046	-0.75898	H	-2.94373	3.71880	-0.75954
C	-3.54761	-2.52553	-2.14529	H	0.09627	4.25005	3.12151
C	-5.02365	1.77544	0.46308	H	-2.58136	5.96293	0.22495
C	-0.43989	-1.64271	-1.79276	H	-1.05909	6.24061	2.17355
C	-0.36129	-1.62826	-3.19772	H	1.22054	0.14656	-0.38370
C	0.31736	-2.58997	-1.08865	H	4.47774	0.10350	-2.16438
C	0.44096	-2.54457	-3.87699	H	1.73118	1.43250	-2.35604
C	1.12806	-3.50047	-1.76975	H	3.02258	1.48883	-3.57001
C	1.19061	-3.48404	-3.16342	H	2.22019	-0.05310	-3.19358
C	-1.63214	2.70676	0.61591	H	6.11689	1.71074	-1.98935
C	-0.77262	2.87745	1.71526	H	2.34421	2.42691	-0.05209
C	-2.27686	3.83856	0.08789	H	6.99732	3.83166	-1.06636
C	-0.56745	4.14014	2.26817	H	3.22027	4.54258	0.86642
C	-2.07236	5.10063	0.64712	H	5.55162	5.26016	0.36939
C	-1.21672	5.25794	1.73794	H	-1.01508	-0.83245	1.71093
O	0.52307	0.80368	-0.12094	C	1.98587	-3.38334	3.19947
O	-3.36637	0.37782	3.33006	C	2.97960	-3.93699	2.38345
O	-2.76059	-3.36456	1.34986	C	3.57409	-3.19290	1.36461
C	3.78242	-1.07883	0.00458	C	3.17437	-1.87142	1.11082
N	3.04564	-0.23445	-0.62769	C	2.17619	-1.31435	1.92806
C	3.63576	0.61652	-1.68255	C	1.60037	-2.05618	2.95440
C	2.58347	0.88713	-2.76832	H	3.29545	-4.96413	2.54794
C	4.17258	1.91408	-1.08190	H	4.33827	-3.65971	0.74995
C	5.48200	2.32787	-1.35708	H	1.85596	-0.29345	1.75496
C	3.36341	2.72778	-0.27339	H	0.83223	-1.59777	3.57144
C	5.97910	3.52710	-0.84029	C	-2.94292	0.00697	2.31772
C	3.86069	3.92328	0.24443	C	-2.57942	-2.24572	1.10376
C	5.16880	4.32763	-0.03568	Fe	-2.18908	-0.55246	0.83030
H	-6.09451	1.25595	-1.76170	C	5.25907	-1.30107	-0.28420
H	-5.42076	-1.00757	-0.92006	H	5.79175	-0.34611	-0.25250
H	-2.53865	-2.84389	-2.39725	H	5.71547	-1.96420	0.44988
H	-3.84013	-3.00361	-1.19712	H	5.41353	-1.72992	-1.28112
H	-4.22365	-2.87316	-2.93223	C	1.34603	-4.17910	4.31127
H	-4.38418	2.29637	1.17662	H	1.74526	-5.19594	4.35802
H	-5.86380	2.43412	0.22211	H	1.51556	-3.70668	5.28577
H	-5.41047	0.86350	0.94737	H	0.26118	-4.24865	4.17325

```
Zero-point correction=                 0.718872 (Hartree/Particle)
 Thermal correction to Energy=             0.764310
 Thermal correction to Enthalpy=           0.765254
 Thermal correction to Gibbs Free Energy=      0.635853
 Sum of electronic and zero-point Energies=       -2062.130307
 Sum of electronic and thermal Energies=          -2062.084868
 Sum of electronic and thermal Enthalpies=        -2062.083924
```

Sum of electronic and thermal Free Energies= -2062.213325

(1f) Adduct $D_{(Z)}$

C	-3.09668	-1.30294	-0.75680	H	-5.83636	-3.03247	-1.34921
C	-3.68639	-0.04040	-0.44104	H	-5.60747	-0.76601	-2.33373
C	-5.76650	-0.86812	-1.25301	H	-0.85180	-1.57773	-3.19801
C	-5.27887	-2.25282	-0.81945	H	-0.13339	-2.91367	0.81447
C	-1.64697	-1.16413	-0.67289	H	0.83908	-3.17859	-4.04191
C	-1.38801	0.23094	-0.42743	H	1.56021	-4.52176	-0.01925
C	-2.62080	0.92055	-0.20661	H	2.05472	-4.65984	-2.45422
N	-3.86258	-2.39820	-1.14897	H	-1.17326	2.55231	1.42593
N	-5.06697	0.21741	-0.55914	H	-4.34299	2.57035	-1.46981
C	-3.35518	-3.75239	-0.96540	H	-1.34108	5.01155	1.63122
C	-5.75604	0.74303	0.61815	H	-4.51334	5.03365	-1.27262
C	-0.61021	-2.13271	-1.12941	H	-3.01339	6.26841	0.28199
C	-0.31919	-2.21977	-2.50208	H	0.61609	0.37340	-0.30005
C	0.08803	-2.96816	-0.24539	H	4.16290	0.29522	-1.32002
C	0.63328	-3.12243	-2.97664	H	1.42413	0.92405	-2.54634
C	1.04170	-3.87177	-0.71913	H	2.97660	0.91923	-3.40808
C	1.31742	-3.95250	-2.08523	H	2.32235	-0.59313	-2.73887
C	-2.74526	2.38743	-0.03732	H	5.48797	2.16537	-1.41920
C	-1.90145	3.09658	0.83503	H	1.30117	2.68964	-0.58899
C	-3.68423	3.10753	-0.79525	H	5.85206	4.59665	-1.13196
C	-1.99751	4.48241	0.94576	H	1.66412	5.10884	-0.29185
C	-3.77963	4.49502	-0.67902	H	3.93953	6.08364	-0.56054
C	-2.93726	5.18858	0.19042	H	-1.14023	-0.44170	1.97719
O	-0.22275	0.88793	-0.47193	C	7.19696	-1.49049	1.05768
O	-3.52139	0.86945	3.47432	C	6.74592	-0.18528	1.29318
O	-2.50886	-3.19928	2.65623	C	5.39520	0.14507	1.18352
C	2.98171	-0.51726	0.77691	C	4.45109	-0.83222	0.84116
N	2.40314	0.16794	-0.13814	C	4.89330	-2.14387	0.61816
C	3.17019	0.75644	-1.25458	C	6.24651	-2.46250	0.71737
C	2.42396	0.48302	-2.57050	H	7.46129	0.58599	1.56801
C	3.37139	2.25330	-1.02752	H	5.07213	1.16549	1.36558
C	4.64777	2.81119	-1.17504	H	4.17492	-2.91593	0.35506
C	2.29872	3.09936	-0.70774	H	6.56933	-3.48438	0.53320
C	4.85443	4.18298	-1.01151	C	-3.12853	0.25187	2.57744
C	2.50648	4.46877	-0.53981	C	-2.51279	-2.20011	2.06578
C	3.78259	5.01657	-0.69135	Fe	-2.42725	-0.65075	1.23839
H	-6.83840	-0.77095	-1.06312	C	2.16704	-1.05816	1.92583
H	-5.44871	-2.39054	0.26392	H	2.27818	-2.14568	1.99951
H	-2.37199	-3.86158	-1.41869	H	2.54734	-0.64325	2.86710
H	-3.28651	-4.03507	0.09671	H	1.10980	-0.80677	1.82630
H	-4.03957	-4.44491	-1.46369	C	8.66495	-1.83549	1.14368
H	-5.22372	1.61399	1.00161	H	8.81520	-2.86918	1.46959
H	-6.76133	1.06485	0.32925	H	9.15442	-1.72872	0.16738
H	-5.83549	0.00053	1.42965	H	9.19037	-1.17921	1.84368

Zero-point correction= 0.718317 (Hartree/Particle)
Thermal correction to Energy= 0.763971
Thermal correction to Enthalpy= 0.764915
Thermal correction to Gibbs Free Energy= 0.634146
Sum of electronic and zero-point Energies= -2062.128587
Sum of electronic and thermal Energies= -2062.082933
Sum of electronic and thermal Enthalpies= -2062.081989
Sum of electronic and thermal Free Energies= -2062.212758

(1f) $TS_{(E)re}$

Fe	0.95281	-0.73906	-1.08658	C	-1.52174	-4.30440	2.75551
C	0.74173	-0.71633	1.19795	H	0.24704	-3.09713	2.97234
C	0.54566	-2.02242	0.56726	C	-2.56424	-4.25997	0.58303
C	1.80847	-2.41377	-0.02819	H	-1.61615	-3.01672	-0.89216
C	2.72306	-1.30772	0.07227	C	-2.53913	-4.72738	1.89744
C	2.02363	-0.20053	0.69586	H	-1.49308	-4.65772	3.78266
C	0.01355	-1.56710	-2.31604	H	-3.35097	-4.58056	-0.09482
C	1.77649	0.26733	-2.26598	H	-3.30452	-5.41286	2.25026
O	-0.06760	-0.10251	1.95423	N	2.21786	-3.69998	-0.40330
O	-0.66270	-2.04507	-3.13322	N	4.05867	-1.44530	-0.28563
O	2.26722	0.95589	-3.06534	C	3.67098	-3.84011	-0.52055
H	-0.11928	5.16735	1.74358	H	4.10372	-4.00793	0.47405
C	-0.09330	4.62206	0.80360	H	3.89012	-4.71960	-1.13122
C	0.58999	5.16562	-0.29221	C	4.32650	-2.60332	-1.13247
C	-0.75228	3.40133	0.70982	H	5.41079	-2.74428	-1.18886
C	0.59839	4.43170	-1.48600	H	3.95092	-2.44297	-2.15923
C	-0.74873	2.66844	-0.49074	C	4.88336	-0.28276	-0.58315
H	-1.30084	3.02597	1.56577	H	5.92095	-0.61503	-0.67943
C	-0.05404	3.20698	-1.58630	H	4.58948	0.21381	-1.52142
H	1.12760	4.82276	-2.35112	H	4.83094	0.44326	0.22470
C	-1.56218	1.42455	-0.61397	C	1.43816	-4.43649	-1.39183
H	0.00325	2.66007	-2.52025	H	1.55696	-4.03097	-2.41097
H	-0.21683	0.31054	-1.02157	H	1.75627	-5.48324	-1.38902
N	-2.04472	0.90809	0.52276	H	0.38137	-4.41146	-1.13238
H	-1.32028	0.78205	1.27077	C	-4.46407	0.43438	0.12357
C	-2.29611	1.19636	-1.91361	C	-4.89966	1.72482	0.45388
H	-1.66128	1.44228	-2.76309	C	-5.32462	-0.40092	-0.59857
H	-2.62530	0.16324	-2.01893	C	-6.16318	2.16978	0.06347
H	-3.17842	1.84572	-1.94651	H	-4.24035	2.38488	1.01037
C	-3.11960	-0.09875	0.60508	C	-6.59197	0.03923	-0.98432
C	2.58853	1.06717	1.23801	H	-4.99859	-1.40485	-0.86063
C	2.92028	2.17860	0.44952	C	-7.01449	1.32820	-0.65619
C	2.79953	1.15358	2.62573	H	-6.48386	3.17500	0.32276
C	3.48648	3.31938	1.02120	H	-7.24509	-0.62269	-1.54605
H	2.73978	2.14826	-0.61835	H	-7.99781	1.67551	-0.95985
C	3.35388	2.29683	3.19982	H	-2.84060	-0.96531	-0.00877
H	2.52148	0.31298	3.25332	C	-3.23067	-0.56643	2.06609
C	3.70888	3.38304	2.39745	H	-2.26495	-0.92875	2.42202
H	3.75033	4.16086	0.38644	H	-3.56214	0.25897	2.70475
H	3.51189	2.33701	4.27421	H	-3.96792	-1.36961	2.13533
H	4.14997	4.27133	2.84158	C	1.30310	6.49037	-0.17767
C	-0.54557	-2.94962	0.97669	H	2.15803	6.41537	0.50488
C	-0.53819	-3.42747	2.29921	H	1.67743	6.83071	-1.14695
C	-1.58068	-3.37657	0.13021	H	0.64159	7.26722	0.22130

Zero-point correction= 0.717536 (Hartree/Particle)
Thermal correction to Energy= 0.761967
Thermal correction to Enthalpy= 0.762912
Thermal correction to Gibbs Free Energy= 0.638194
Sum of electronic and zero-point Energies= -2062.102025
Sum of electronic and thermal Energies= -2062.057594
Sum of electronic and thermal Enthalpies= -2062.056650
Sum of electronic and thermal Free Energies= -2062.181367
Imaginary frequency -260.13

(1f) $TS_{(E)si}$

Fe	0.37657	1.38623	-0.94963	C	3.23402	1.11078	4.02547
C	-0.45975	0.49908	0.95320	H	1.70324	2.48850	3.39977
C	0.75588	1.29789	1.16562	C	3.56748	-0.80737	2.60541
C	0.45126	2.66586	0.82117	H	2.31111	-0.91767	0.86531
C	-0.86756	2.71875	0.25300	C	3.90989	-0.07849	3.74575
C	-1.39776	1.37098	0.21924	H	3.48686	1.68567	4.91256
C	2.04596	1.59084	-1.46630	H	4.08419	-1.73467	2.37300
C	-0.27828	1.75344	-2.53405	H	4.69396	-0.43257	4.40947
O	-0.63987	-0.70991	1.26783	N	1.17866	3.81713	1.13927
O	3.14600	1.68375	-1.82568	N	-1.46885	3.93214	-0.06797
O	-0.68526	1.92583	-3.61106	C	0.41296	5.05803	1.00405
H	3.92707	-4.20720	0.29940	H	-0.18967	5.21845	1.90750
C	3.62799	-3.44720	-0.41813	H	1.11285	5.89326	0.91860
C	4.60186	-2.81162	-1.19689	C	-0.51978	5.03363	-0.20557
C	2.27584	-3.13897	-0.55732	H	-1.08465	5.96990	-0.26020
C	4.16984	-1.85704	-2.13095	H	0.06948	4.93595	-1.13531
C	1.84648	-2.17237	-1.48311	C	-2.57087	3.98236	-1.02021
H	1.54179	-3.66782	0.03969	H	-2.96555	5.00221	-1.03287
C	2.82416	-1.54470	-2.27521	H	-2.25617	3.71784	-2.04206
H	4.90140	-1.34414	-2.74970	H	-3.37213	3.31124	-0.71886
C	0.38800	-1.93215	-1.68889	C	2.58741	3.90149	0.76660
H	2.53721	-0.78523	-2.99271	H	2.72318	4.13326	-0.30197
H	0.43254	-0.12988	-1.39688	H	3.07060	4.68321	1.36105
N	-0.43221	-2.38378	-0.72945	H	3.08954	2.95937	0.98225
H	-0.23129	-2.00270	0.22443	C	-2.38076	-3.20514	0.49474
C	-0.08353	-1.80022	-3.11851	C	-1.69938	-4.18911	1.22296
H	-0.01079	-2.76849	-3.62737	C	-3.59669	-2.72264	0.98744
H	-1.11103	-1.44038	-3.17434	C	-2.21588	-4.67003	2.42607
H	0.54923	-1.09916	-3.66084	H	-0.75719	-4.58213	0.85052
C	-1.86417	-2.73497	-0.86147	C	-4.11928	-3.20892	2.18649
C	-2.81837	0.99154	-0.02198	H	-4.13280	-1.95590	0.43761
C	-3.32698	0.63894	-1.28169	C	-3.43033	-4.18192	2.91136
C	-3.70917	1.01849	1.06564	H	-1.67040	-5.42684	2.98293
C	-4.68277	0.34809	-1.45551	H	-5.06226	-2.81780	2.55833
H	-2.65923	0.62309	-2.13600	H	-3.83417	-4.55535	3.84817
C	-5.06364	0.73097	0.89524	H	-2.43275	-1.84597	-1.15747
H	-3.32973	1.27504	2.05024	C	-2.10312	-3.86286	-1.88643
C	-5.55778	0.39773	-0.36865	H	-1.91624	-3.56044	-2.91724
H	-5.05501	0.09001	-2.44335	H	-1.47462	-4.72863	-1.65684
H	-5.73335	0.76747	1.75013	H	-3.14720	-4.17952	-1.81779
H	-6.61323	0.17924	-0.50462	C	6.06870	-3.12340	-1.03065
C	1.87780	0.84223	2.01808	H	6.58110	-3.16467	-1.99719
C	2.22627	1.56433	3.17465	H	6.56781	-2.34997	-0.43387
C	2.56318	-0.35207	1.75234	H	6.22071	-4.07992	-0.52280

Zero-point correction= 0.716891 (Hartree/Particle)
 Thermal correction to Energy= 0.761477
 Thermal correction to Enthalpy= 0.762421
 Thermal correction to Gibbs Free Energy= 0.636967
 Sum of electronic and zero-point Energies= -2062.093380
 Sum of electronic and thermal Energies= -2062.048795
 Sum of electronic and thermal Enthalpies= -2062.047850
 Sum of electronic and thermal Free Energies= -2062.173304
Imaginary frequency -256.03

(1f) $TS_{(Z)re}$

Fe	-1.21898	0.86910	-0.65462	C	-3.29029	-1.38158	4.24879
C	-0.97124	-1.12438	0.45909	H	-2.57686	-2.37607	2.47961
C	-2.19622	-0.38439	0.77492	C	-3.43954	1.01932	4.11759
C	-3.00229	-0.33817	-0.42889	H	-2.82779	1.90373	2.26158
C	-2.22296	-0.86513	-1.51822	C	-3.60288	-0.15895	4.84629
C	-0.90987	-1.21097	-1.00869	H	-3.40248	-2.30633	4.80833
C	-1.81774	2.43145	-0.11458	H	-3.66598	1.97934	4.57374
C	-0.59013	1.54086	-2.15107	H	-3.96245	-0.12479	5.87094
O	-0.09668	-1.51684	1.28188	N	-4.37868	-0.09662	-0.54075
O	-2.14122	3.48163	0.26497	N	-2.78188	-1.08504	-2.77150
O	-0.14054	2.01660	-3.11256	C	-4.95707	-0.61473	-1.78275
H	3.52031	3.32891	-2.43885	H	-5.13656	-1.69243	-1.67916
C	3.22339	3.42578	-1.39761	H	-5.92326	-0.13154	-1.94788
C	3.50170	4.61653	-0.70648	C	-4.04599	-0.38832	-2.98768
C	2.55866	2.37360	-0.78121	H	-4.51135	-0.79442	-3.89191
C	3.08142	4.71112	0.62361	H	-3.88599	0.69348	-3.14597
C	2.14571	2.46662	0.55944	C	-1.94436	-1.18899	-3.95864
H	2.32806	1.47976	-1.34891	H	-2.57690	-1.49393	-4.79704
C	2.40532	3.66104	1.24653	H	-1.46028	-0.23442	-4.21752
H	3.27976	5.62077	1.18452	H	-1.17294	-1.94364	-3.82195
C	1.44056	1.34582	1.25047	C	-4.92027	1.18163	-0.09212
H	2.09685	3.77389	2.28019	H	-4.63867	2.01632	-0.75633
H	0.15370	1.19946	0.06547	H	-6.01139	1.11225	-0.05494
N	1.97017	0.12102	1.35172	H	-4.57003	1.40644	0.91290
H	1.25027	-0.60469	1.59029	C	3.33152	-1.89592	1.16111
C	0.49683	1.68639	2.38519	C	3.18604	-2.27054	2.50377
H	-0.14654	2.52910	2.13646	C	3.70588	-2.86648	0.22733
H	-0.11603	0.82058	2.63628	C	3.40205	-3.58988	2.89968
H	1.09573	1.93978	3.27042	H	2.89217	-1.53000	3.24238
C	3.18737	-0.44035	0.72906	C	3.93047	-4.18609	0.62319
C	0.15329	-1.99477	-1.69984	H	3.80436	-2.59423	-0.81929
C	1.12261	-1.42256	-2.53927	C	3.77932	-4.55207	1.96068
C	0.17985	-3.38825	-1.51660	H	3.27596	-3.86622	3.94273
C	2.05723	-2.21804	-3.20663	H	4.21369	-4.92844	-0.11764
H	1.12063	-0.35024	-2.69895	H	3.94855	-5.57975	2.26960
C	1.11528	-4.18433	-2.17708	H	3.09333	-0.41983	-0.36257
H	-0.54694	-3.84507	-0.85204	C	4.45583	0.32962	1.15027
C	2.05326	-3.60343	-3.03335	H	4.45214	1.36600	0.81283
H	2.78390	-1.75313	-3.86789	H	4.55941	0.31334	2.23924
H	1.10907	-5.25999	-2.02443	H	5.32947	-0.16927	0.72151
H	2.77526	-4.22343	-3.55766	C	4.20415	5.76199	-1.39364
C	-2.67715	-0.24721	2.17779	H	3.53792	6.25943	-2.10888
C	-2.83075	-1.42374	2.93332	H	4.53987	6.51502	-0.67554
C	-2.97433	0.97515	2.80152	H	5.07753	5.41500	-1.95594

Zero-point correction= 0.717162 (Hartree/Particle)
Thermal correction to Energy= 0.761802
Thermal correction to Enthalpy= 0.762746
Thermal correction to Gibbs Free Energy= 0.636781
Sum of electronic and zero-point Energies= -2062.094093
Sum of electronic and thermal Energies= -2062.049453
Sum of electronic and thermal Enthalpies= -2062.048509
Sum of electronic and thermal Free Energies= -2062.174474
Imaginary frequency -338.49

(1f) $TS_{(Z)si}$

Fe	1.48366	-0.04386	0.99156	C	-0.06451	3.27287	-0.09425
C	1.50394	0.19084	-1.29699	C	0.51925	4.40779	-2.56962
C	1.65149	1.43126	-0.53362	H	1.92379	2.79230	-2.79873
C	2.91835	1.35980	0.16770	C	-0.72827	4.43081	-0.50743
C	3.44091	0.02552	0.03159	H	-0.29628	2.83901	0.87221
C	2.50379	-0.74746	-0.76493	C	-0.43960	5.00267	-1.74704
C	0.85386	0.95034	2.29595	H	0.75017	4.84112	-3.53893
C	1.77103	-1.40990	2.06056	H	-1.47271	4.88392	0.14189
O	0.62698	-0.06724	-2.17144	H	-0.95713	5.90163	-2.06980
O	0.38376	1.57489	3.15708	N	3.67287	2.41005	0.69040
O	1.90321	-2.32287	2.76807	N	4.71468	-0.29344	0.49497
H	-4.15419	-3.38643	3.17154	C	5.06830	2.06958	0.97762
C	-3.68009	-2.45903	2.86396	H	5.67025	2.17841	0.06607
C	-3.84785	-1.30007	3.62060	H	5.45554	2.77446	1.71788
C	-2.89541	-2.43756	1.71078	C	5.21991	0.64105	1.49492
C	-3.22497	-0.11710	3.21564	H	6.27776	0.42003	1.66954
H	-4.44998	-1.31908	4.52427	H	4.68481	0.52646	2.45505
C	-2.28045	-1.24951	1.28302	C	5.10406	-1.67701	0.72560
H	-2.77389	-3.34959	1.13729	H	6.17611	-1.69890	0.94107
C	-2.45241	-0.09153	2.05826	H	4.57064	-2.13114	1.57618
H	-3.32965	0.78640	3.80879	H	4.92300	-2.28030	-0.16099
C	-1.45505	-1.26358	0.03544	C	3.05915	3.37076	1.59888
H	-1.94316	0.82154	1.77751	H	2.92708	2.96111	2.61392
H	0.00994	-0.57398	0.73718	H	3.69155	4.26147	1.65857
N	-1.73299	-0.47292	-1.00568	H	2.08580	3.67899	1.22233
H	-0.95112	-0.43817	-1.69767	C	-4.10273	0.29476	-0.90507
C	-0.77310	-2.55701	-0.35548	C	-4.63025	-0.83335	-1.54548
H	-1.53036	-3.24530	-0.75394	C	-4.97712	1.11596	-0.18694
H	-0.04450	-2.37050	-1.14444	C	-5.98922	-1.13007	-1.46205
H	-0.27895	-3.02393	0.49547	H	-3.97071	-1.48324	-2.11404
C	-2.64049	0.68942	-1.06876	C	-6.33816	0.82016	-0.10965
C	2.68294	-2.08369	-1.40278	H	-4.59159	1.99957	0.31636
C	2.64082	-3.30445	-0.70851	C	-6.86917	-0.31039	-0.74192
C	2.86967	-2.12735	-2.79631	H	-6.37531	-2.01139	-1.96923
C	2.81069	-4.51879	-1.37500	H	-6.99656	1.47633	0.45476
H	2.47340	-3.30506	0.36227	H	-2.37579	1.40796	-0.28597
C	3.03380	-3.34041	-3.46488	C	-2.41357	1.37555	-2.42721
H	2.87261	-1.19774	-3.35512	H	-1.36268	1.64487	-2.55242
C	3.00978	-4.54274	-2.75647	H	-2.70624	0.70808	-3.24417
H	2.77956	-5.44773	-0.81192	H	-3.02688	2.27749	-2.48778
H	3.17867	-3.34442	-4.54178	C	-8.33627	-0.65265	-0.62965
H	3.13811	-5.48851	-3.27550	H	-8.69965	-1.15750	-1.53016
C	0.90917	2.66780	-0.90460	H	-8.52434	-1.32516	0.21699
C	1.18448	3.25514	-2.15223	H	-8.94598	0.24256	-0.47442

Zero-point correction= 0.717621 (Hartree/Particle)
Thermal correction to Energy= 0.762152
Thermal correction to Enthalpy= 0.763096
Thermal correction to Gibbs Free Energy= 0.637466
Sum of electronic and zero-point Energies= -2062.098629
Sum of electronic and thermal Energies= -2062.054098
Sum of electronic and thermal Enthalpies= -2062.053154
Sum of electronic and thermal Free Energies= -2062.178784
Imaginary frequency -329.39

(1f) adduct $E_{E(S,1'S)}$

Fe	1.10100	-0.43600	-1.00600	C	-1.13600	-4.42400	2.47300
C	1.01400	-0.71100	1.24800	H	0.46500	-3.04000	2.86700
C	0.93800	-1.97500	0.47500	C	-1.93000	-4.49500	0.19800
C	2.20900	-2.15700	-0.17100	H	-0.96100	-3.16600	-1.18300
C	2.96500	-0.91800	-0.05000	C	-2.00200	-4.95300	1.51400
C	2.20600	0.00700	0.75100	H	-1.19000	-4.76400	3.50300
C	0.46100	-1.33100	-2.39300	H	-2.60400	-4.89100	-0.55600
C	1.75600	0.84800	-2.03000	H	-2.73200	-5.70800	1.79200
O	0.15600	-0.27100	2.03200	N	2.76200	-3.26300	-0.76700
O	0.10500	-1.94600	-3.31000	N	4.27400	-0.83200	-0.50000
O	2.23000	1.64700	-2.72300	C	4.21400	-3.24800	-0.93000
H	-1.61800	5.47800	1.34000	H	4.72600	-3.50000	0.01300
C	-1.32800	4.85500	0.49700	H	4.48500	-4.00700	-1.66900
C	-0.63200	5.42700	-0.57300	C	4.67900	-1.88700	-1.42300
C	-1.66500	3.49900	0.50500	H	5.77200	-1.88100	-1.49100
C	-0.28000	4.58800	-1.64100	H	4.27700	-1.70300	-2.43400
C	-1.31100	2.66200	-0.55900	C	4.87500	0.46000	-0.82800
H	-2.21500	3.08200	1.34000	H	5.96400	0.35400	-0.79900
C	-0.61500	3.23600	-1.63400	H	4.58300	0.79700	-1.83300
H	0.26400	4.99700	-2.48800	H	4.58300	1.21700	-0.10500
C	-1.69100	1.17500	-0.57800	C	2.12200	-4.57200	-0.75600
H	-0.32500	2.62400	-2.48200	H	1.09800	-4.50700	-1.12200
H	-0.70800	0.59200	-0.73800	H	2.68300	-5.23000	-1.42300
N	-2.29800	0.79200	0.67700	H	2.10000	-5.02600	0.24400
H	-1.57500	0.78300	1.39700	C	-4.50900	-0.30900	0.28300
C	-2.54700	0.85500	-1.81300	C	-5.23700	0.87300	0.46900
H	-2.01200	1.14300	-2.72100	C	-5.15100	-1.40300	-0.31000
H	-2.77600	-0.21100	-1.88200	C	-6.57100	0.95800	0.06800
H	-3.48900	1.40800	-1.77900	H	-4.73900	1.72800	0.91600
C	-3.07500	-0.45000	0.78800	C	-6.48600	-1.32300	-0.70900
C	2.67400	1.24900	1.42100	H	-4.59600	-2.32800	-0.45900
C	1.99800	2.46800	1.27500	C	-7.20200	-0.13900	-0.52200
C	3.76500	1.18900	2.30600	H	-7.12000	1.88500	0.21600
C	2.41300	3.60000	1.97900	H	-6.96500	-2.18200	-1.17200
H	1.14500	2.53200	0.61000	H	-8.24000	-0.07100	-0.83700
C	4.18300	2.32200	3.00300	H	-2.59800	-1.27100	0.22800
H	4.28900	0.24600	2.44200	C	-3.10200	-0.86300	2.27200
C	3.50700	3.53300	2.84100	H	-2.08600	-1.03400	2.63500
H	1.87200	4.53300	1.84800	H	-3.57200	-0.07500	2.87100
H	5.03200	2.25600	3.67900	H	-3.68500	-1.78000	2.39700
H	3.83000	4.41600	3.38700	C	-0.29200	6.89900	-0.59700
C	-0.10100	-2.99700	0.78900	H	0.73200	7.06900	-0.94800
C	-0.19800	-3.45600	2.11400	H	-0.95800	7.45000	-1.27300
C	-0.99500	-3.52000	-0.15800	H	-0.38800	7.34800	0.39500

Zero-point correction= 0.721393 (Hartree/Particle)
Thermal correction to Energy= 0.767209
Thermal correction to Enthalpy= 0.768154
Thermal correction to Gibbs Free Energy= 0.637418
Sum of electronic and zero-point Energies= -2062.116549
Sum of electronic and thermal Energies= -2062.070733
Sum of electronic and thermal Enthalpies= -2062.069789
Sum of electronic and thermal Free Energies= -2062.200524

(1f) adduct $E_{E(R,1'S)}$

Fe	-0.03585	-1.39433	-0.91614	C	-2.46732	-1.20483	4.33007
C	0.73634	-0.45031	0.99434	H	-0.54330	-2.02534	3.82289
C	-0.34390	-1.44708	1.20498	C	-3.66651	-0.14059	2.52735
C	0.17477	-2.72986	0.83983	H	-2.69193	-0.14638	0.61098
C	1.44104	-2.53148	0.14490	C	-3.59400	-0.52072	3.86767
C	1.75706	-1.12521	0.15966	H	-2.39517	-1.49447	5.37486
C	-1.56838	-2.15845	-1.36674	H	-4.53023	0.40289	2.15591
C	0.62788	-1.54957	-2.54443	H	-4.40455	-0.28012	4.54983
O	0.69948	0.74862	1.30407	N	-0.32391	-3.98197	1.05346
O	-2.52049	-2.76869	-1.62193	N	2.21114	-3.62026	-0.23305
O	1.05132	-1.67907	-3.61725	C	0.57661	-5.10877	0.83677
H	-4.98955	3.41207	-0.01082	H	1.20314	-5.29195	1.72272
C	-4.49846	2.64320	-0.60335	H	-0.02682	-6.00543	0.66660
C	-5.27362	1.67117	-1.24398	C	1.46198	-4.86560	-0.38010
C	-3.10546	2.65273	-0.71135	H	2.17756	-5.68784	-0.47591
C	-4.60087	0.69950	-1.99964	H	0.84121	-4.84553	-1.29229
C	-2.43565	1.67929	-1.45911	C	3.28795	-3.46246	-1.20594
H	-2.52246	3.42054	-0.21700	H	3.87866	-4.38248	-1.21611
C	-3.21232	0.70583	-2.10642	H	2.90718	-3.27968	-2.22208
H	-5.17100	-0.07393	-2.50929	H	3.93939	-2.63878	-0.92414
C	-0.90658	1.68372	-1.60794	C	-1.65797	-4.25362	1.57003
H	-2.72964	-0.06339	-2.70160	H	-2.03700	-5.16763	1.10130
H	-0.55990	0.62139	-1.34230	H	-1.66779	-4.38913	2.65932
N	-0.31565	2.64557	-0.69879	H	-2.33471	-3.43720	1.32403
H	-0.35699	2.25392	0.24214	C	1.54416	3.73695	0.44528
C	-0.52499	1.86278	-3.08495	C	0.74907	4.60755	1.20362
H	-0.89265	2.81919	-3.46574	C	2.82967	3.43220	0.90509
H	0.55665	1.81043	-3.23238	C	1.22656	5.15545	2.39461
H	-0.97948	1.06826	-3.68094	H	-0.25175	4.85092	0.85933
C	1.04513	3.18947	-0.88902	C	3.31257	3.98534	2.09201
C	3.06967	-0.47710	-0.12299	H	3.45346	2.74930	0.33625
C	3.41467	0.07554	-1.36522	C	2.51271	4.84831	2.84240
C	4.00533	-0.39348	0.92291	H	0.59387	5.82439	2.97212
C	4.66293	0.67046	-1.56398	H	4.31239	3.73240	2.43477
H	2.70727	0.03024	-2.18539	H	2.88617	5.27532	3.76923
C	5.25131	0.20173	0.72761	H	1.75071	2.40728	-1.20900
H	3.74672	-0.79869	1.89693	C	1.08337	4.34041	-1.91821
C	5.58675	0.73357	-0.51977	H	0.85991	4.01382	-2.93456
H	4.90991	1.08705	-2.53646	H	0.36077	5.11355	-1.64050
H	5.95856	0.25275	1.55072	H	2.08065	4.79170	-1.92335
H	6.55706	1.19658	-0.67466	C	-6.78167	1.67836	-1.15201
C	-1.49571	-1.14725	2.09756	H	-7.18261	0.66484	-1.04653
C	-1.42581	-1.50854	3.45437	H	-7.12762	2.26927	-0.29879
C	-2.62565	-0.45007	1.64957	H	-7.23363	2.11069	-2.05373

Zero-point correction= 0.721157 (Hartree/Particle)
Thermal correction to Energy= 0.767115
Thermal correction to Enthalpy= 0.768059
Thermal correction to Gibbs Free Energy= 0.637351
Sum of electronic and zero-point Energies= -2062.109022
Sum of electronic and thermal Energies= -2062.063065
Sum of electronic and thermal Enthalpies= -2062.062120
Sum of electronic and thermal Free Energies= -2062.192828

(1f) adduct $E_{Z(S,1'S)}$

Fe	-1.23430	0.60194	-0.77317	C	-2.00507	0.79854	4.83465
C	-1.15340	-0.98955	0.88781	H	-1.71659	-0.91818	3.56926
C	-2.17104	0.07348	1.12375	C	-2.54532	2.85966	3.70862
C	-3.18837	-0.09341	0.12650	H	-2.67640	2.76394	1.57188
C	-2.65803	-0.95742	-0.92123	C	-2.29790	2.16159	4.89255
C	-1.38208	-1.47957	-0.49010	H	-1.80262	0.24532	5.74747
C	-1.77072	2.28714	-0.86524	H	-2.76199	3.92393	3.73725
C	-0.70671	0.60278	-2.45494	H	-2.32543	2.67704	5.84828
O	-0.19682	-1.26826	1.62546	N	-4.47003	0.35985	0.07425
O	-2.20533	3.35848	-0.96173	N	-3.49148	-1.33905	-1.96653
O	-0.41002	0.61315	-3.57696	C	-5.30067	0.05649	-1.09038
H	2.32253	4.29884	-3.15515	H	-5.98863	-0.76709	-0.84856
C	2.73444	3.87865	-2.24060	H	-5.90952	0.93899	-1.32448
C	4.00127	4.28030	-1.80789	C	-4.46532	-0.30688	-2.30939
C	1.98854	2.94105	-1.52061	H	-5.13015	-0.69457	-3.08577
C	4.49743	3.71022	-0.62479	H	-3.96283	0.59029	-2.70856
C	2.48672	2.37236	-0.34693	C	-2.95886	-2.07195	-3.11065
H	1.01010	2.64627	-1.88677	H	-3.79977	-2.39060	-3.73239
C	3.75661	2.77621	0.09290	H	-2.28020	-1.46301	-3.72618
H	5.48120	4.00232	-0.26306	H	-2.42473	-2.95848	-2.77627
C	1.65682	1.41377	0.50406	C	-5.16990	1.00829	1.17473
H	4.16053	2.33625	0.99936	H	-5.20711	2.09873	1.05205
H	0.78076	1.06299	-0.14230	H	-6.19734	0.62979	1.20101
N	2.41252	0.29377	1.02606	H	-4.69727	0.78037	2.12613
H	1.87973	-0.10755	1.79525	C	3.42482	-1.91491	1.00118
C	1.06416	2.18053	1.69956	C	4.43730	-1.59005	1.91528
H	0.46534	3.02848	1.35885	C	3.05083	-3.25640	0.86290
H	0.43097	1.52649	2.30378	C	5.06524	-2.58370	2.66657
H	1.87618	2.56153	2.32621	H	4.71814	-0.54899	2.04165
C	2.77345	-0.83420	0.14483	C	3.68128	-4.25300	1.61088
C	-0.65147	-2.67504	-1.00376	H	2.25632	-3.52149	0.17211
C	0.21583	-2.65711	-2.10707	C	4.69132	-3.92089	2.51466
C	-0.83379	-3.89300	-0.32528	H	5.84666	-2.31405	3.37240
C	0.85293	-3.82248	-2.53770	H	3.37491	-5.28903	1.49230
H	0.39104	-1.72982	-2.63925	H	5.17942	-4.69546	3.10009
C	-0.19404	-5.05715	-0.75058	H	1.86308	-1.26398	-0.30118
H	-1.48124	-3.92041	0.54598	C	3.71291	-0.44521	-1.00900
C	0.64900	-5.02745	-1.86368	H	3.24624	0.26102	-1.69961
H	1.51638	-3.78363	-3.39700	H	4.63502	0.00628	-0.63208
H	-0.35268	-5.98615	-0.21020	H	3.97682	-1.34760	-1.56940
H	1.14834	-5.93260	-2.19711	C	4.81671	5.28832	-2.58362
C	-2.22341	0.82303	2.40717	H	5.06632	6.16052	-1.96807
C	-1.96700	0.13512	3.60776	H	5.76472	4.85768	-2.92722
C	-2.50117	2.20024	2.48134	H	4.27574	5.64597	-3.46427

Zero-point correction= 0.721534 (Hartree/Particle)
Thermal correction to Energy= 0.767410
Thermal correction to Enthalpy= 0.768354
Thermal correction to Gibbs Free Energy= 0.637778
Sum of electronic and zero-point Energies= -2062.113075
Sum of electronic and thermal Energies= -2062.067199
Sum of electronic and thermal Enthalpies= -2062.066255
Sum of electronic and thermal Free Energies= -2062.196830

(1f) adduct $E_{Z(R,1'S)}$

Fe	-1.24274	-0.22976	-0.89935	C	-0.61121	4.78522	1.85898
C	-1.70433	0.48013	1.25388	H	-2.01489	3.21040	2.28612
C	-1.68955	1.54946	0.22498	C	0.70347	4.50804	-0.14370
C	-2.81789	1.32033	-0.63506	H	0.32968	2.72356	-1.27971
C	-3.30348	-0.03205	-0.39253	C	0.37087	5.25733	0.98571
C	-2.57467	-0.59230	0.72205	H	-0.87067	5.35447	2.74716
C	-0.64724	0.55452	-2.36517	H	1.47368	4.86012	-0.82420
C	-1.34720	-1.80382	-1.69860	H	0.87731	6.19673	1.18785
O	-0.99225	0.42370	2.26984	N	-3.45315	2.15383	-1.50258
O	-0.35579	1.08679	-3.35543	N	-4.45461	-0.45980	-1.04205
O	-1.44418	-2.81707	-2.25376	C	-4.60739	1.66508	-2.25762
H	5.49473	-3.29937	-0.49787	H	-5.53634	2.01976	-1.78860
C	4.64010	-2.74071	-0.87292	H	-4.56541	2.08319	-3.27013
C	4.56704	-2.42807	-2.23959	C	-4.62390	0.14562	-2.35913
C	3.64369	-2.34455	0.01187	H	-5.58893	-0.16803	-2.76614
C	3.45745	-1.70422	-2.68179	H	-3.83670	-0.19605	-3.05226
C	2.52909	-1.61717	-0.43436	C	-4.89691	-1.84656	-0.95534
H	3.73455	-2.58417	1.06629	H	-5.90068	-1.91095	-1.38394
C	2.45578	-1.30416	-1.79232	H	-4.23932	-2.53756	-1.50455
H	3.37098	-1.44453	-3.73433	H	-4.94607	-2.16440	0.08342
C	1.42421	-1.24039	0.54794	C	-3.00916	3.50634	-1.81666
H	1.60969	-0.73703	-2.16593	H	-2.25402	3.51424	-2.61460
H	0.61774	-0.69877	-0.07332	H	-3.87563	4.08236	-2.15246
N	1.87522	-0.40246	1.63606	H	-2.59509	3.99593	-0.93842
H	1.08344	-0.25563	2.26107	C	3.99548	0.82609	1.13091
C	0.76389	-2.49168	1.14578	C	4.80006	0.15782	2.06387
H	1.50226	-3.06634	1.71155	C	4.61690	1.49880	0.07430
H	-0.04698	-2.21088	1.82184	C	6.18848	0.16124	1.94072
H	0.35869	-3.13050	0.35740	H	4.32183	-0.37933	2.87788
C	2.48278	0.90016	1.31816	C	6.00793	1.50519	-0.05411
C	-2.89984	-1.77659	1.56854	H	4.00498	2.01863	-0.65953
C	-2.73542	-3.11128	1.16446	C	6.79917	0.83644	0.87992
C	-3.37723	-1.53586	2.86934	H	6.79711	-0.36447	2.67209
C	-3.06610	-4.16567	2.01644	H	6.47119	2.02833	-0.88657
H	-2.34436	-3.33186	0.17839	H	7.88136	0.83761	0.78218
C	-3.70273	-2.58866	3.72373	H	2.04748	1.30670	0.38992
H	-3.48198	-0.51179	3.21186	C	2.15446	1.88150	2.45734
C	-3.55284	-3.90968	3.29911	H	1.07255	1.97600	2.57817
H	-2.93195	-5.18919	1.67769	H	2.58509	1.52403	3.39902
H	-4.07024	-2.37463	4.72342	H	2.57628	2.86697	2.24413
H	-3.80433	-4.73136	3.96361	C	5.66544	-2.84653	-3.18834
C	-0.94677	2.82075	0.45564	H	5.91069	-3.90842	-3.07483
C	-1.26014	3.57866	1.59832	H	5.37980	-2.67740	-4.23056
C	0.05634	3.29821	-0.40197	H	6.58770	-2.28265	-3.00187

Zero-point correction= 0.721556 (Hartree/Particle)
Thermal correction to Energy= 0.767316
Thermal correction to Enthalpy= 0.768260
Thermal correction to Gibbs Free Energy= 0.638673
Sum of electronic and zero-point Energies= -2062.115137
Sum of electronic and thermal Energies= -2062.069377
Sum of electronic and thermal Enthalpies= -2062.068433
Sum of electronic and thermal Free Energies= -2062.198020

(S,1'S)-N-(1-(4-methylphenyl)ethyl)-(S)-α-methylbenzylamine

Zero-point correction= 0.339456 (Hartree/Particle)
Thermal correction to Energy= 0.356935
Thermal correction to Enthalpy= 0.357879
Thermal correction to Gibbs Free Energy= 0.290977
Sum of electronic and zero-point Energies= -714.905313
Sum of electronic and thermal Energies= -714.887834
Sum of electronic and thermal Enthalpies= -714.886889

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 Sum of electronic and thermal Free Energies=      -714.953792
```

(R,1'S)-N-(1-(4-methylphenyl)ethyl)-(S)-α-methylbenzylamine

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Zero-point correction=                0.339366 (Hartree/Particle)
 Thermal correction to Energy=            0.356877
 Thermal correction to Enthalpy=          0.357821
 Thermal correction to Gibbs Free Energy=      0.291406
 Sum of electronic and zero-point Energies=        -714.905045
 Sum of electronic and thermal Energies=         -714.887534
 Sum of electronic and thermal Enthalpies=         -714.886590
 Sum of electronic and thermal Free Energies=      -714.953005
```

(E)-N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Trifluoromethyl)phenyl)-1-imine (1g)

```
Zero-point correction=                0.292496 (Hartree/Particle)
 Thermal correction to Energy=            0.311563
 Thermal correction to Enthalpy=          0.312507
 Thermal correction to Gibbs Free Energy=      0.240280
 Sum of electronic and zero-point Energies=       -1011.457198
 Sum of electronic and thermal Energies=          -1011.438132
 Sum of electronic and thermal Enthalpies=        -1011.437187
 Sum of electronic and thermal Free Energies=     -1011.509414
```

(Z)-N-(1-(*S*)-phenylethyl)-ethan-1-(4-(Trifluoromethyl)phenyl)-1-imine (1g)

```
Zero-point correction=                0.292029 (Hartree/Particle)
 Thermal correction to Energy=            0.311229
 Thermal correction to Enthalpy=          0.312173
 Thermal correction to Gibbs Free Energy=      0.239690
 Sum of electronic and zero-point Energies=       -1011.454197
 Sum of electronic and thermal Energies=          -1011.434997
 Sum of electronic and thermal Enthalpies=        -1011.434053
 Sum of electronic and thermal Free Energies=     -1011.506536
```

(1g) Adduct D*(E)*

C	2.80796	0.30964	1.47195	C	-3.51352	1.75835	1.61006
C	3.17116	1.13729	0.36835	C	-2.42355	2.32550	2.53118
C	5.28051	1.49400	1.40332	C	-3.99865	2.79371	0.59822
C	5.12198	0.10421	2.02059	C	-5.28350	3.33909	0.71145
C	1.36373	0.10484	1.43122	C	-3.16531	3.23530	-0.44159
C	0.87278	0.90806	0.34381	C	-5.73291	4.30708	-0.19028
C	1.96698	1.48564	-0.37012	C	-3.61574	4.19901	-1.34326
N	3.73396	-0.10632	2.43299	C	-4.89946	4.73804	-1.22208
N	4.46475	1.66746	0.19760	H	6.32756	1.67371	1.14663
C	3.54929	-1.38962	3.10429	H	5.43761	-0.66610	1.29329
C	5.14937	1.39490	-1.06454	H	2.53845	-1.48522	3.49367
C	0.49119	-0.48768	2.47843	H	3.74897	-2.23865	2.43246
C	0.47122	0.07752	3.76681	H	4.24644	-1.44286	3.94593
C	-0.34987	-1.57796	2.21198	H	4.50243	1.66072	-1.90133
C	-0.35328	-0.44526	4.76274	H	6.04817	2.01625	-1.12473
C	-1.18331	-2.09333	3.20680	H	5.43680	0.33592	-1.17216
C	-1.18544	-1.53346	4.48483	H	5.75979	0.00573	2.90601
C	1.83188	2.47165	-1.46742	H	4.98470	2.24537	2.14612
C	0.92724	2.26868	-2.52396	H	1.11756	0.92314	3.98447
C	2.57515	3.66426	-1.44175	H	-0.33676	-2.02322	1.22278
C	0.77172	3.22895	-3.52180	H	-0.34744	-0.00223	5.75481
C	2.42067	4.62126	-2.44560	H	-1.82270	-2.94174	2.98049
C	1.51797	4.40960	-3.48827	H	-1.82522	-1.94320	5.26138
O	-0.39858	1.19652	0.01926	H	0.35303	1.34957	-2.55796
O	3.21325	-0.86004	-3.10716	H	3.27894	3.83076	-0.63288
O	2.60636	-3.46124	0.24018	H	0.07134	3.05061	-4.33322
C	-3.76100	-0.41221	0.62461	H	3.00587	5.53612	-2.40876
N	-2.98654	0.57380	0.90221	H	1.39931	5.15457	-4.27002

H	-1.11058	0.72465	0.51852	C	-1.70258	-2.34625	-1.90609
H	-4.36971	1.48409	2.23927	H	-3.26047	-4.95434	-0.37593
H	-1.55280	2.64321	1.95224	H	-4.27763	-3.09501	0.89008
H	-2.81081	3.19221	3.07534	H	-1.97664	-0.27553	-1.40411
H	-2.10096	1.57150	3.25491	H	-0.98936	-2.14060	-2.69649
H	-5.93585	3.01133	1.51809	C	2.83749	-0.77587	-2.01513
H	-2.16481	2.82646	-0.54415	C	2.46930	-2.33285	0.01515
H	-6.73223	4.72038	-0.08529	Fe	2.15677	-0.65012	-0.39762
H	-2.95841	4.53158	-2.14183	C	-5.22900	-0.49243	1.00988
H	-5.24563	5.48910	-1.92647	H	-5.75581	0.39896	0.65623
H	0.91560	-1.18024	-1.04034	H	-5.71156	-1.36511	0.57001
C	-2.05581	-3.66576	-1.60906	H	-5.35572	-0.53856	2.09757
C	-2.98448	-3.93006	-0.60031	C	-1.38162	-4.79195	-2.34546
C	-3.55728	-2.87554	0.10793	F	-1.24017	-4.51501	-3.66038
C	-3.18946	-1.54724	-0.16023	F	-2.07208	-5.94987	-2.24520
C	-2.26095	-1.29726	-1.18292	F	-0.14175	-5.02600	-1.85849

Zero-point correction= 0.696065 (Hartree/Particle)
Thermal correction to Energy= 0.743401
Thermal correction to Enthalpy= 0.744345
Thermal correction to Gibbs Free Energy= 0.609586
Sum of electronic and zero-point Energies= -2359.865313
Sum of electronic and thermal Energies= -2359.817977
Sum of electronic and thermal Enthalpies= -2359.817033
Sum of electronic and thermal Free Energies= -2359.951792

(1g) Adduct D*(Z)*

C	-3.60143	-1.47959	-0.70162	H	-3.52762	-4.21775	0.15152
C	-4.28145	-0.26818	-0.36545	H	-4.30645	-4.68938	-1.37817
C	-6.31051	-1.26359	-1.11504	H	-5.90698	1.24683	1.13806
C	-5.70194	-2.60620	-0.70207	H	-7.41250	0.56325	0.51843
C	-2.16675	-1.22288	-0.66401	H	-6.35568	-0.41525	1.57995
C	-2.01564	0.19074	-0.43181	H	-6.20657	-3.42584	-1.22446
C	-3.29184	0.78010	-0.17621	H	-6.18913	-1.14543	-2.19902
N	-4.28653	-2.63479	-1.06590	H	-1.43365	-1.60488	-3.21441
N	-5.68262	-0.12711	-0.43481	H	-0.44754	-2.80216	0.78421
C	-3.66233	-3.94234	-0.90591	H	0.36976	-3.05202	-4.10171
C	-6.37270	0.33223	0.76947	H	1.36114	-4.25759	-0.09256
C	-1.06568	-2.10215	-1.14959	H	1.77648	-4.38810	-2.54312
C	-0.81751	-2.18268	-2.53124	H	-1.89428	2.55526	1.34743
C	-0.25952	-2.85360	-0.28233	H	-5.22401	2.25510	-1.34542
C	0.19880	-2.99821	-3.03021	H	-2.26375	4.99359	1.53968
C	0.75862	-3.66999	-0.78023	H	-5.59647	4.69766	-1.16222
C	0.99100	-3.74579	-2.15489	H	-4.11818	6.08054	0.28456
C	-3.53270	2.23304	-0.01292	H	-0.03154	0.48897	-0.36452
C	-2.70234	3.02541	0.79868	H	3.48332	0.67192	-1.49599
C	-4.57538	2.85780	-0.71828	H	0.67101	1.11891	-2.63202
C	-2.91197	4.39923	0.90150	H	2.19480	1.23062	-3.53640
C	-4.78398	4.23341	-0.60987	H	1.66545	-0.32930	-2.86635
C	-3.95398	5.01008	0.19900	H	4.70111	2.60581	-1.43696
O	-0.90748	0.93875	-0.51908	H	0.45905	2.86533	-0.77072
O	-4.03687	0.70191	3.53271	H	4.90923	5.04463	-1.07308
O	-2.80894	-3.30657	2.69294	H	0.66702	5.29300	-0.40220
C	2.44055	-0.20004	0.65121	H	2.89097	6.40282	-0.54907
N	1.77696	0.41013	-0.25621	H	-1.62353	-0.46855	1.96375
C	2.46315	1.06070	-1.39370	C	6.70240	-0.81586	0.69442
C	1.69809	0.74971	-2.68852	C	6.16003	0.33151	1.27860
C	2.56791	2.56204	-1.13559	C	4.78227	0.53993	1.25467
C	3.81499	3.19450	-1.21219	C	3.93474	-0.39426	0.64429
C	1.43459	3.33541	-0.84099	C	4.48733	-1.54566	0.06623
C	3.93360	4.57104	-1.00584	C	5.86478	-1.75459	0.08690
C	1.55457	4.70905	-0.62997	H	6.81280	1.05436	1.75600
C	2.80225	5.33242	-0.71238	H	4.36383	1.43491	1.70463
H	-7.38129	-1.25396	-0.89655	H	3.83484	-2.27613	-0.40367
H	-5.83619	-2.76333	0.38340	H	6.28887	-2.64787	-0.35892
H	-2.69252	-3.97015	-1.39897	C	-3.63279	0.10407	2.62777

C	-2.88720	-2.31061	2.10271	H	0.65512	-0.60268	1.80360
Fe	-2.92043	-0.76153	1.26997	C	8.19455	-1.01136	0.66645
C	1.73157	-0.77685	1.85000	F	8.74624	-0.46192	-0.44088
H	1.92567	-1.85255	1.92904	F	8.79689	-0.43759	1.73083
H	2.12928	-0.32097	2.76495	F	8.53044	-2.32027	0.66315

Zero-point correction= 0.695637 (Hartree/Particle)
Thermal correction to Energy= 0.743126
Thermal correction to Enthalpy= 0.744070
Thermal correction to Gibbs Free Energy= 0.607761
Sum of electronic and zero-point Energies= -2359.863427
Sum of electronic and thermal Energies= -2359.815938
Sum of electronic and thermal Enthalpies= -2359.814994
Sum of electronic and thermal Free Energies= -2359.951303

(1g) TS*(E)re*

Fe	-0.71599	-1.24259	-1.08378	C	-5.13818	-0.08854	2.47110
C	-0.89448	-1.01599	1.17119	H	-3.43911	-1.36737	2.80603
C	-2.15842	-1.29123	0.48352	C	-5.28653	0.91027	0.28242
C	-2.06461	-2.62192	-0.08335	H	-3.70416	0.41718	-1.08786
C	-0.71671	-3.09339	0.08562	C	-5.80896	0.73481	1.56442
C	0.04698	-2.05655	0.74866	H	-5.53332	-0.23124	3.47313
C	-1.74059	-0.71068	-2.40568	H	-5.80059	1.54624	-0.43351
C	0.62450	-1.62425	-2.15340	H	-6.72951	1.23356	1.85408
O	-0.63113	-0.03015	1.92753	N	-3.09962	-3.45466	-0.51370
O	-2.37213	-0.28088	-3.28290	N	-0.35191	-4.38993	-0.25767
O	1.51695	-1.80276	-2.87730	C	-2.71549	-4.86434	-0.63075
H	4.36533	1.84097	1.73715	H	-2.78165	-5.34499	0.35379
C	3.84305	1.66480	0.80393	H	-3.42487	-5.36602	-1.29362
C	4.55303	1.26333	-0.32663	C	-1.29441	-5.03858	-1.16376
C	2.46565	1.85868	0.72859	H	-1.04417	-6.10312	-1.21763
C	3.87566	1.03970	-1.53117	H	-1.21757	-4.61909	-2.18329
C	1.77073	1.64339	-0.47301	C	1.04420	-4.71774	-0.51895
H	1.92965	2.20439	1.60413	H	1.12949	-5.80363	-0.61714
C	2.50201	1.22698	-1.60129	H	1.41638	-4.25303	-1.44551
H	4.42396	0.72177	-2.41176	H	1.67479	-4.39743	0.30728
C	0.31629	1.96833	-0.56389	C	-4.04695	-2.97514	-1.51347
H	1.99629	1.02211	-2.53656	H	-3.60792	-2.93874	-2.52459
H	-0.20605	0.23192	-1.01467	H	-4.91586	-3.63947	-1.53034
N	-0.32815	2.17525	0.58440	H	-4.39696	-1.97761	-1.25430
H	-0.20189	1.40510	1.29940	C	-1.61874	4.29081	0.25791
C	-0.18716	2.58484	-1.84471	C	-0.55583	5.14291	0.58678
H	0.25043	2.09295	-2.71165	C	-2.71459	4.81954	-0.43465
H	-1.27138	2.51794	-1.92541	C	-0.58531	6.48938	0.22157
H	0.09553	3.64352	-1.87299	H	0.30098	4.74658	1.12441
C	-1.64422	2.83593	0.71084	C	-2.75023	6.16787	-0.79397
C	1.38310	-2.18978	1.39679	H	-3.54724	4.16917	-0.69244
C	2.59248	-1.85945	0.77148	C	-1.68322	7.00695	-0.46945
C	1.42638	-2.66518	2.71936	H	0.24925	7.13552	0.47916
C	3.81067	-2.01971	1.43633	H	-3.60828	6.56002	-1.33258
H	2.58016	-1.48182	-0.24443	H	-1.70572	8.05508	-0.75322
C	2.64022	-2.82431	3.38643	H	-2.37406	2.28677	0.10283
H	0.49580	-2.91242	3.22215	C	-2.08821	2.74811	2.18093
C	3.83860	-2.50459	2.74440	H	-2.10314	1.70788	2.50920
H	4.73422	-1.75304	0.93270	H	-1.40472	3.31781	2.81910
H	2.64946	-3.19624	4.40742	H	-3.08763	3.17748	2.28292
H	4.78633	-2.62858	3.26109	C	6.03759	1.03075	-0.26696
C	-3.41886	-0.56729	0.80789	F	6.33635	-0.29442	-0.28098
C	-3.95903	-0.73175	2.09565	F	6.66928	1.57355	-1.33155
C	-4.10096	0.27027	-0.08911	F	6.59381	1.54968	0.84656

Zero-point correction= 0.694680 (Hartree/Particle)
Thermal correction to Energy= 0.740924
Thermal correction to Enthalpy= 0.741868
Thermal correction to Gibbs Free Energy= 0.612127
Sum of electronic and zero-point Energies= -2359.838288
Sum of electronic and thermal Energies= -2359.792044
Sum of electronic and thermal Enthalpies= -2359.791099

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 Sum of electronic and thermal Free Energies=     -2359.920841
Imaginary frequency                                -186.15
```

(1g) $TS_{(E)si}$

Fe	0.52288	-1.48281	-0.96957	C	-2.02118	-1.22146	4.24544
C	1.05340	-0.33481	0.90608	H	0.06498	-1.49051	3.78734
C	0.10366	-1.42756	1.12901	C	-3.49007	-0.96325	2.34891
C	0.79292	-2.66819	0.86527	H	-2.54630	-1.02833	0.41552
C	2.07034	-2.36634	0.27802	C	-3.30563	-1.03342	3.72998
C	2.20463	-0.92440	0.20351	H	-1.86624	-1.27356	5.31975
C	-0.96785	-2.23014	-1.52278	H	-4.48221	-0.81427	1.93477
C	1.28729	-1.62439	-2.54116	H	-4.15585	-0.94173	4.40026
O	0.88233	0.88646	1.19652	N	0.43306	-3.95305	1.24546
O	-1.96175	-2.67903	-1.92490	N	2.99454	-3.37409	0.00553
O	1.74375	-1.65437	-3.61127	C	1.49212	-4.95559	1.11232
H	-4.42948	2.43565	0.81813	H	2.11529	-4.96023	2.01642
C	-3.96754	1.90021	-0.00393	H	1.03059	-5.94240	1.02195
C	-4.73527	1.05168	-0.80294	C	2.38379	-4.69659	-0.10030
C	-2.61369	2.07494	-0.27371	H	3.18332	-5.44350	-0.13670
C	-4.13726	0.37380	-1.87047	H	1.79151	-4.78574	-1.02907
C	-1.99532	1.39934	-1.34049	C	4.05706	-3.14657	-0.96607
H	-2.03390	2.75834	0.33433	H	4.73713	-4.00263	-0.93764
C	-2.78471	0.54915	-2.13597	H	3.67150	-3.04179	-1.99283
H	-4.72995	-0.28745	-2.49285	H	4.62410	-2.25281	-0.71504
C	-0.56776	1.68668	-1.67520	C	-0.93293	-4.42959	1.06398
H	-2.34067	-0.00344	-2.95461	H	-1.12608	-4.74791	0.02657
H	-0.00472	-0.08878	-1.43913	H	-1.10975	-5.27876	1.73066
N	0.13374	2.35799	-0.76075	H	-1.64352	-3.64668	1.32220
H	0.14373	1.90623	0.19951	C	1.79862	3.74759	0.35922
C	-0.18732	1.70995	-3.13653	C	0.89477	4.49789	1.12309
H	-0.61344	2.59461	-3.62442	C	3.12120	3.63498	0.79641
H	0.89462	1.71495	-3.26742	C	1.30295	5.11369	2.30590
H	-0.58043	0.83254	-3.64745	H	-0.13610	4.59971	0.79421
C	1.37376	3.13998	-0.97437	C	3.53352	4.25795	1.97532
C	3.46208	-0.16467	-0.04840	H	3.83034	3.04937	0.22043
C	3.83701	0.32807	-1.30790	C	2.62647	4.99739	2.73496
C	4.33387	0.05501	1.03265	H	0.58806	5.68545	2.89102
C	5.05201	0.99521	-1.48704	H	4.56395	4.15488	2.30370
H	3.18587	0.16022	-2.15837	H	2.94615	5.47706	3.65573
C	5.54765	0.71953	0.85703	H	2.17044	2.46929	-1.31888
H	4.05305	-0.30804	2.01685	C	1.18628	4.28445	-1.99071
C	5.91456	1.18961	-0.40665	H	1.02684	3.93845	-3.01220
H	5.32639	1.35587	-2.47478	H	0.34373	4.91961	-1.70128
H	6.20737	0.86920	1.70728	H	2.08732	4.90340	-1.98625
H	6.86220	1.70176	-0.54746	C	-6.18716	0.82224	-0.48625
C	-1.10295	-1.27929	1.98920	F	-6.35573	-0.23309	0.35252
C	-0.93254	-1.34350	3.38321	F	-6.74843	1.89165	0.11756
C	-2.39620	-1.08146	1.48763	F	-6.90874	0.55207	-1.59493

```
Zero-point correction=                 0.694245 (Hartree/Particle)
 Thermal correction to Energy=             0.740567
 Thermal correction to Enthalpy=           0.741511
 Thermal correction to Gibbs Free Energy=      0.612273
 Sum of electronic and zero-point Energies=       -2359.829511
 Sum of electronic and thermal Energies=          -2359.783188
 Sum of electronic and thermal Enthalpies=        -2359.782244
 Sum of electronic and thermal Free Energies=     -2359.911482
Imaginary frequency                                -200.00
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(1g) $TS_{(Z)re}$

Fe	0.76570	-1.39841	-0.48424	C	4.37929	-0.28770	3.88029
C	1.96438	0.42214	0.21871	H	4.23854	0.65041	1.94949
C	2.49461	-0.87130	0.65982	C	2.98434	-2.22333	4.21319
C	2.93053	-1.58996	-0.52151	H	1.74365	-2.79040	2.55778
C	2.50109	-0.85468	-1.68330	C	3.92977	-1.32206	4.70322
C	1.77877	0.32061	-1.23544	H	5.10795	0.42751	4.25211
C	0.33152	-2.89456	0.33037	H	2.61619	-3.02650	4.84586
C	-0.35704	-1.69846	-1.80008	H	4.30718	-1.42038	5.71719
O	1.64290	1.39587	0.95932	N	3.82036	-2.66503	-0.60802
O	-0.02165	-3.84567	0.89812	N	2.88545	-1.23424	-2.96418
O	-1.14855	-1.88884	-2.63089	C	4.38064	-2.86272	-1.94760
H	-4.61146	-0.43254	-1.71160	H	5.22451	-2.17711	-2.09721
C	-4.30796	-0.56273	-0.67849	H	4.76457	-3.88332	-2.01864
C	-5.16039	-1.20922	0.22419	C	3.35125	-2.61456	-3.04810
C	-3.07139	-0.09605	-0.25301	H	3.80919	-2.76530	-4.03090
C	-4.76097	-1.39071	1.54754	H	2.51123	-3.32557	-2.94893
C	-2.65698	-0.26281	1.08011	C	2.14373	-0.77748	-4.13186
H	-2.40388	0.37562	-0.96353	H	2.68759	-1.09322	-5.02643
C	-3.51514	-0.92763	1.96930	H	1.12651	-1.19688	-4.17696
H	-5.42111	-1.88976	2.24813	H	2.07225	0.30806	-4.14273
C	-1.32791	0.22460	1.55850	C	3.55948	-3.88761	0.14341
H	-3.22110	-1.07634	3.00199	H	2.72583	-4.47247	-0.28071
H	-0.39113	-0.69024	0.31002	H	4.46135	-4.50654	0.13961
N	-0.93121	1.49081	1.43061	H	3.32654	-3.65160	1.17912
H	0.11282	1.59201	1.52063	C	-0.69060	3.86333	0.93763
C	-0.67057	-0.50547	2.70942	C	-0.30413	4.24905	2.22855
H	-0.74664	-1.58629	2.59986	C	-0.33279	4.67144	-0.14479
H	0.37916	-0.22052	2.78200	C	0.42960	5.41711	2.43021
H	-1.16397	-0.20173	3.64290	H	-0.56886	3.62753	3.07972
C	-1.55885	2.62842	0.72031	C	0.39487	5.84578	0.05644
C	1.36105	1.49571	-2.05225	H	-0.60882	4.37510	-1.15227
C	0.13806	1.57523	-2.73727	C	0.77807	6.22232	1.34363
C	2.24770	2.58142	-2.15891	H	0.72868	5.69880	3.43586
C	-0.17095	2.68063	-3.53406	H	0.67012	6.45908	-0.79683
H	-0.55931	0.74735	-2.67670	H	1.34857	7.13340	1.50034
C	1.94106	3.68757	-2.95113	H	-1.58871	2.42125	-0.35558
H	3.18804	2.54792	-1.61739	C	-2.98322	2.92103	1.23151
C	0.73260	3.73891	-3.64983	H	-3.68177	2.10756	1.03671
H	-1.11575	2.70918	-4.07048	H	-2.96480	3.11869	2.30719
H	2.64841	4.50901	-3.02432	H	-3.35639	3.81899	0.73165
H	0.49670	4.59487	-4.27599	C	-6.47498	-1.76146	-0.25846
C	2.95427	-1.07316	2.06243	F	-6.32208	-2.97253	-0.83919
C	3.89529	-0.16421	2.57860	F	-7.35911	-1.91426	0.75157
C	2.49670	-2.09465	2.91085	F	-7.04467	-0.95383	-1.18070

Zero-point correction= 0.694754 (Hartree/Particle)
 Thermal correction to Energy= 0.741042
 Thermal correction to Enthalpy= 0.741986
 Thermal correction to Gibbs Free Energy= 0.611769
 Sum of electronic and zero-point Energies= -2359.827860
 Sum of electronic and thermal Energies= -2359.781572
 Sum of electronic and thermal Enthalpies= -2359.780628
 Sum of electronic and thermal Free Energies= -2359.910845
Imaginary frequency -265.84

(1g) $TS_{(Z)si}$

Fe	2.07958	-0.05167	0.98247	C	0.58893	3.28333	-0.11674
C	2.02766	0.13950	-1.30349	C	1.14482	4.37505	-2.61807
C	2.24230	1.38989	-0.57519	H	2.50102	2.72061	-2.86046
C	3.52975	1.29118	0.08405	C	-0.05296	4.45436	-0.52781
C	4.00597	-0.06103	-0.04460	H	0.37022	2.86754	0.86075
C	3.01769	-0.81862	-0.79266	C	0.22153	5.00434	-1.78052
C	1.52509	0.98675	2.28570	H	1.36504	4.79191	-3.59699
C	2.35916	-1.40625	2.06799	H	-0.76810	4.93584	0.13395
O	1.11008	-0.10819	-2.14188	H	-0.27860	5.91378	-2.10124
O	1.10193	1.64293	3.14759	N	4.33351	2.32600	0.56066
O	2.48348	-2.31007	2.78823	N	5.28338	-0.41254	0.38212
H	-3.70766	-3.11127	3.35621	C	5.72741	1.94731	0.80508
C	-3.18533	-2.21917	3.02381	H	6.29927	2.02111	-0.12899
C	-3.27864	-1.03677	3.75690	H	6.16204	2.65288	1.51783
C	-2.41476	-2.26608	1.86208	C	5.85386	0.52427	1.34422
C	-2.59444	0.10040	3.32074	H	6.91016	0.27356	1.48443
H	-3.87038	-1.00299	4.66685	H	5.35177	0.44439	2.32533
C	-1.74088	-1.12263	1.40127	C	5.63583	-1.80380	0.62570
H	-2.35157	-3.19551	1.30728	H	6.71331	-1.85747	0.80518
C	-1.83659	0.05903	2.15397	H	5.11721	-2.22485	1.50207
H	-2.63955	1.01965	3.89696	H	5.40479	-2.41615	-0.24285
C	-0.94370	-1.20791	0.13936	C	3.78237	3.32301	1.47034
H	-1.27797	0.93472	1.84895	H	3.68028	2.93955	2.49895
H	0.58843	-0.54274	0.79434	H	4.44020	4.19699	1.48482
N	-1.20495	-0.43390	-0.91768	H	2.80314	3.64982	1.12583
H	-0.42298	-0.43542	-1.61800	C	-3.53288	0.44261	-0.77432
C	-0.31418	-2.53549	-0.21944	C	-4.11758	-0.68928	-1.36072
H	-1.10183	-3.21017	-0.58098	C	-4.34997	1.32856	-0.06609
H	0.40630	-2.40364	-1.02642	C	-5.48172	-0.92942	-1.23660
H	0.17720	-2.99079	0.63939	H	-3.49533	-1.38637	-1.91365
C	-2.05887	0.76625	-0.98409	C	-5.71999	1.09779	0.05903
C	3.13231	-2.17147	-1.41042	H	-3.91247	2.20893	0.39699
C	3.07063	-3.37731	-0.69201	C	-6.28802	-0.03358	-0.52561
C	3.27548	-2.24597	-2.80778	H	-5.92394	-1.81033	-1.69169
C	3.18014	-4.60846	-1.34020	H	-6.34369	1.78927	0.61411
H	2.93731	-3.35307	0.38331	H	-1.74199	1.49002	-0.22644
C	3.37878	-3.47565	-3.45777	C	-1.84818	1.41248	-2.36514
H	3.29335	-1.32709	-3.38387	H	-0.79082	1.63173	-2.52593
C	3.33637	-4.66357	-2.72622	H	-2.19335	0.74067	-3.15757
H	3.13578	-5.52564	-0.75909	H	-2.42264	2.33948	-2.42783
H	3.49097	-3.50400	-4.53817	C	-7.76103	-0.31279	-0.41496
H	3.41791	-5.62215	-3.23095	F	-8.35874	-0.31655	-1.62989
C	1.52617	2.64283	-0.94297	F	-7.99691	-1.52946	0.13070
C	1.78855	3.20939	-2.20293	F	-8.40279	0.60023	0.34507

Zero-point correction= 0.694839 (Hartree/Particle)
 Thermal correction to Energy= 0.740256
 Thermal correction to Enthalpy= 0.741200
 Thermal correction to Gibbs Free Energy= 0.613396
 Sum of electronic and zero-point Energies= -2359.834979
 Sum of electronic and thermal Energies= -2359.789562
 Sum of electronic and thermal Enthalpies= -2359.788618
 Sum of electronic and thermal Free Energies= -2359.916422
Imaginary frequency -306.10

(1g) adduct $E_{E(S,1'S)}$

Fe	-2.31565	0.23123	-0.64192	C	1.20163	4.73107	-1.08027
C	-0.73240	0.76941	0.78873	H	-0.36291	4.44581	0.36960
C	-1.10788	1.88676	-0.10658	C	1.68978	2.83537	-2.49025
C	-2.46129	2.24679	0.19635	H	0.49763	1.07407	-2.14829
C	-3.00373	1.27583	1.14364	C	1.94782	4.15378	-2.10944
C	-1.98293	0.31262	1.43996	H	1.40326	5.75147	-0.76642
C	-2.56296	0.69061	-2.33636	H	2.26939	2.37619	-3.28607
C	-3.60253	-0.98865	-0.67029	H	2.72669	4.72460	-2.60662
O	0.36362	0.18796	0.82544	N	-3.20406	3.32025	-0.21044
O	-2.75190	1.04835	-3.42156	N	-4.27078	1.43034	1.66585
O	-4.49972	-1.71953	-0.67668	C	-4.40573	3.62287	0.55854
H	0.59239	-4.12454	0.28333	H	-4.15804	4.18776	1.46930
C	0.86592	-3.44661	-0.51878	H	-5.06058	4.25060	-0.05198
C	0.12216	-3.43371	-1.70344	C	-5.14511	2.34326	0.93129
C	1.94361	-2.58171	-0.36445	H	-5.99801	2.58807	1.57218
C	0.47975	-2.57013	-2.74131	H	-5.53434	1.85973	0.01980
C	2.30006	-1.69033	-1.38648	C	-4.98169	0.30158	2.26536
H	2.50122	-2.56382	0.56512	H	-5.81748	0.69391	2.85133
C	1.56601	-1.71002	-2.57830	H	-5.37797	-0.38269	1.50200
H	-0.08794	-2.57030	-3.66563	H	-4.32555	-0.25609	2.92858
C	3.46336	-0.72665	-1.20332	C	-2.90429	4.12351	-1.38675
H	1.83966	-1.03648	-3.38685	H	-2.23122	3.58471	-2.05130
H	3.33954	0.08143	-1.95104	H	-3.83463	4.32262	-1.93042
N	3.42295	-0.18616	0.16101	H	-2.43673	5.08305	-1.13225
H	2.45282	0.03448	0.38222	C	5.67068	0.66759	0.84460
C	4.79709	-1.42984	-1.51664	C	5.92552	-0.40286	1.71153
H	4.77594	-1.84413	-2.53004	C	6.74366	1.47170	0.44121
H	5.63778	-0.73526	-1.44765	C	7.21989	-0.66095	2.16299
H	4.97330	-2.24550	-0.80938	H	5.09616	-1.03665	2.00947
C	4.24618	1.00369	0.40787	C	8.04114	1.21702	0.89107
C	-1.94948	-0.74586	2.48443	H	6.56129	2.30428	-0.23564
C	-1.86153	-2.10733	2.15998	C	8.28351	0.14842	1.75547
C	-1.92424	-0.37646	3.84054	H	7.40069	-1.49786	2.83267
C	-1.77642	-3.07253	3.16477	H	8.86155	1.84951	0.56219
H	-1.86194	-2.41477	1.11987	H	9.29207	-0.05532	2.10450
C	-1.84141	-1.34169	4.84387	H	4.31750	1.62586	-0.50424
H	-1.96987	0.67673	4.10570	C	3.56341	1.85813	1.49204
C	-1.76955	-2.69524	4.50822	H	2.57062	2.17844	1.16169
H	-1.71722	-4.12308	2.89431	H	3.44947	1.27670	2.41263
H	-1.82681	-1.03566	5.88623	H	4.16335	2.74388	1.71910
H	-1.70449	-3.44873	5.28790	C	-1.10358	-4.29022	-1.80868
C	-0.08305	2.67544	-0.83183	F	-1.50899	-4.46750	-3.08336
C	0.20103	3.99660	-0.44359	F	-0.92319	-5.51362	-1.26303
C	0.68746	2.10111	-1.85467	F	-2.15689	-3.73161	-1.14082

Zero-point correction= 0.699213 (Hartree/Particle)
Thermal correction to Energy= 0.747430
Thermal correction to Enthalpy= 0.748374
Thermal correction to Gibbs Free Energy= 0.609997
Sum of electronic and zero-point Energies= -2359.859003
Sum of electronic and thermal Energies= -2359.810786
Sum of electronic and thermal Enthalpies= -2359.809842
Sum of electronic and thermal Free Energies= -2359.948219

(1g) adduct $E_{E(R,1'S)}$

Fe	0.56693	-1.41944	-0.92581	C	-1.88288	-1.01231	4.29987
C	1.21392	-0.38702	1.00253	H	0.20160	-1.32036	3.85910
C	0.22194	-1.47523	1.19233	C	-3.35865	-0.89319	2.39345
C	0.86950	-2.70738	0.85629	H	-2.42710	-1.10604	0.46898
C	2.12080	-2.39394	0.17362	C	-3.16797	-0.85685	3.77496
C	2.30247	-0.96339	0.18102	H	-1.72369	-0.97397	5.37398
C	-0.85787	-2.34825	-1.41691	H	-4.34923	-0.75722	1.97064
C	1.27557	-1.51644	-2.53862	H	-4.01350	-0.70034	4.43881
O	1.06497	0.80271	1.31531	N	0.49551	-3.99890	1.08680
O	-1.72787	-3.05715	-1.70900	N	2.99846	-3.40820	-0.17257
O	1.72899	-1.61175	-3.60283	C	1.49958	-5.03816	0.88277
H	-4.73998	2.63165	0.44470	H	2.13167	-5.16113	1.77577
C	-4.20304	1.97530	-0.23210	H	0.98220	-5.98686	0.70910
C	-4.87524	0.92680	-0.86116	C	2.36979	-4.71729	-0.32573
C	-2.84517	2.18150	-0.47360	H	3.15861	-5.47047	-0.41020
C	-4.18355	0.09484	-1.74745	H	1.76023	-4.75682	-1.24456
C	-2.13146	1.34207	-1.33605	C	4.09031	-3.15754	-1.10835
H	-2.32195	2.99942	0.00551	H	4.75323	-4.02685	-1.10198
C	-2.82825	0.30771	-1.98044	H	3.73115	-2.99873	-2.13631
H	-4.70387	-0.71291	-2.25119	H	4.66365	-2.28619	-0.80068
C	-0.63058	1.54581	-1.59436	C	-0.73271	-4.37471	1.77457
H	-2.30847	-0.34970	-2.66953	H	-1.01575	-5.38136	1.45344
H	-0.13934	0.53693	-1.36170	H	-0.61797	-4.37576	2.86663
N	-0.10760	2.57473	-0.71807	H	-1.54024	-3.69166	1.51732
H	-0.03810	2.17772	0.22032	C	1.67969	3.87828	0.31117
C	-0.37657	1.77085	-3.09259	C	0.83888	4.65557	1.12023
H	-0.88503	2.67348	-3.44125	C	3.01724	3.72307	0.68944
H	0.69082	1.85493	-3.30945	C	1.32404	5.25850	2.28090
H	-0.76241	0.92505	-3.66564	H	-0.20235	4.78371	0.83953
C	1.16528	3.27404	-0.99255	C	3.50692	4.33174	1.84623
C	3.55055	-0.19347	-0.09028	H	3.67888	3.11497	0.08002
C	3.88421	0.33547	-1.34593	C	2.66220	5.10121	2.64710
C	4.43474	0.03056	0.97943	H	0.65672	5.85374	2.89856
C	5.07602	1.03931	-1.53421	H	4.54836	4.19517	2.12498
H	3.21557	0.18442	-2.18536	H	3.04126	5.57193	3.55011
C	5.62390	0.73525	0.79471	H	1.93556	2.57787	-1.36083
H	4.18164	-0.35303	1.96350	C	1.00269	4.41892	-2.01582
C	5.95212	1.23895	-0.46617	H	0.75602	4.06671	-3.01811
H	5.31686	1.43281	-2.51781	H	0.21229	5.10111	-1.68901
H	6.29275	0.89209	1.63627	H	1.93693	4.98550	-2.08068
H	6.87899	1.78584	-0.61338	C	-6.31140	0.64294	-0.53037
C	-0.97714	-1.26775	2.05436	F	-6.42242	-0.22562	0.51319
C	-0.79787	-1.21108	3.44711	F	-6.98503	1.75790	-0.17353
C	-2.26956	-1.09236	1.54119	F	-6.97303	0.08014	-1.56553

Zero-point correction= 0.698778 (Hartree/Particle)
Thermal correction to Energy= 0.746504
Thermal correction to Enthalpy= 0.747448
Thermal correction to Gibbs Free Energy= 0.611757
Sum of electronic and zero-point Energies= -2359.847811
Sum of electronic and thermal Energies= -2359.800086
Sum of electronic and thermal Enthalpies= -2359.799141
Sum of electronic and thermal Free Energies= -2359.934832

(1g) adduct $E_{Z(S,1'S)}$

Fe	1.09747	-1.09927	-0.68342	C	2.57962	-1.16072	4.78654
C	2.13941	0.41206	0.68142	H	3.07869	0.28178	3.26980
C	2.46297	-1.00574	1.00822	C	1.67019	-3.24870	3.99720
C	3.23860	-1.51966	-0.08136	H	1.44869	-3.44317	1.87470
C	3.08749	-0.61013	-1.21374	C	2.06868	-2.43097	5.05652
C	2.37944	0.56688	-0.77101	H	2.88525	-0.51134	5.60205
C	0.63257	-2.80121	-0.55015	H	1.25842	-4.23468	4.19375
C	0.35174	-0.94690	-2.27420	H	1.97397	-2.77768	6.08150
O	1.59250	1.23048	1.43468	N	4.05026	-2.60547	-0.16264
O	0.41431	-3.94052	-0.51569	N	3.80689	-0.85462	-2.37621
O	-0.11325	-0.88292	-3.33529	C	4.71959	-2.91915	-1.42512
H	-4.24351	-2.65694	-1.88624	H	5.76685	-2.58636	-1.38004
C	-4.21345	-1.93219	-1.08039	H	4.72229	-4.00812	-1.55703
C	-5.40141	-1.47944	-0.50846	C	4.02133	-2.27899	-2.61618
C	-2.99027	-1.44804	-0.61328	H	4.65785	-2.39411	-3.49741
C	-5.35946	-0.54116	0.53019	H	3.06574	-2.79128	-2.81864
C	-2.93294	-0.50846	0.41972	C	3.55448	-0.07162	-3.58215
H	-2.07020	-1.80459	-1.06532	H	4.31606	-0.33095	-4.32217
C	-4.13688	-0.06292	0.98750	H	2.56328	-0.27150	-4.01587
H	-6.28439	-0.19004	0.97778	H	3.63288	0.99175	-3.36738
C	-1.59963	-0.04123	0.99925	C	4.43163	-3.44133	0.96873
H	-4.09617	0.67204	1.78442	H	3.80489	-4.33908	1.04663
H	-0.79547	-0.29115	0.23912	H	5.47031	-3.75622	0.82780
N	-1.58621	1.36760	1.34743	H	4.36591	-2.88773	1.90211
H	-0.84323	1.51091	2.02750	C	-1.23253	3.73868	0.94622
C	-1.29490	-0.85074	2.27251	C	-2.19182	4.19017	1.86418
H	-1.29131	-1.92298	2.06265	C	-0.16024	4.57949	0.62744
H	-0.31826	-0.57180	2.67551	C	-2.08653	5.45589	2.44066
H	-2.06061	-0.64907	3.02793	H	-3.01511	3.53537	2.13296
C	-1.37071	2.37183	0.28604	C	-0.05509	5.84872	1.20080
C	2.33278	1.91359	-1.41168	H	0.60123	4.23526	-0.06530
C	1.41246	2.28613	-2.40317	C	-1.01810	6.29217	2.10776
C	3.26318	2.87431	-0.97722	H	-2.83802	5.78977	3.15136
C	1.44090	3.56445	-2.96424	H	0.78591	6.48697	0.94300
H	0.67263	1.57283	-2.74581	H	-0.93517	7.27828	2.55667
C	3.28978	4.15345	-1.53262	H	-0.42767	2.15795	-0.24009
H	3.96794	2.61142	-0.19396	C	-2.49105	2.39856	-0.76653
C	2.38049	4.50217	-2.53363	H	-2.55896	1.45811	-1.31976
H	0.72050	3.82763	-3.73342	H	-3.46397	2.59250	-0.30608
H	4.01960	4.87745	-1.18138	H	-2.28615	3.19883	-1.48422
H	2.39905	5.49750	-2.96796	C	-6.73583	-1.96381	-1.00011
C	2.31252	-1.53030	2.39207	F	-7.45109	-0.96608	-1.57344
C	2.69973	-0.71339	3.47057	F	-7.49679	-2.44414	0.01247
C	1.78336	-2.80092	2.68162	F	-6.62120	-2.94870	-1.91785

Zero-point correction= 0.698816 (Hartree/Particle)
Thermal correction to Energy= 0.746745
Thermal correction to Enthalpy= 0.747689
Thermal correction to Gibbs Free Energy= 0.610124
Sum of electronic and zero-point Energies= -2359.850506
Sum of electronic and thermal Energies= -2359.802577
Sum of electronic and thermal Enthalpies= -2359.801632
Sum of electronic and thermal Free Energies= -2359.939198

(1g) adduct $E_{Z(R,1'S)}$

Fe	-1.49717	-0.48379	-0.81778	C	-2.03577	5.01243	0.77961
C	-2.36848	0.56202	1.04166	H	-3.18469	3.31831	1.44472
C	-2.38559	1.37611	-0.19851	C	-0.50306	4.59691	-1.03510
C	-3.32623	0.75945	-1.09211	H	-0.45613	2.58810	-1.79174
C	-3.61592	-0.57990	-0.59232	C	-1.06713	5.47842	-0.11179
C	-2.97463	-0.74231	0.69160	H	-2.47435	5.68643	1.51002
C	-0.81668	0.06776	-2.35111	H	0.25908	4.94547	-1.72638
C	-1.22461	-2.18215	-1.22497	H	-0.74985	6.51676	-0.08199
O	-1.79692	0.85321	2.10559	N	-3.95657	1.25327	-2.19044
O	-0.46233	0.41972	-3.39950	N	-4.57476	-1.34418	-1.24208
O	-1.07298	-3.29046	-1.53008	C	-4.88582	0.40306	-2.93542
H	5.56661	-2.02440	1.05569	H	-5.92073	0.66500	-2.67261
C	4.68955	-1.75837	0.47548	H	-4.75542	0.59727	-4.00655
C	4.73532	-1.82132	-0.92135	C	-4.64161	-1.07735	-2.67572
C	3.52116	-1.36143	1.11586	H	-5.47204	-1.64838	-3.09922
C	3.60771	-1.47849	-1.66672	H	-3.71559	-1.40371	-3.17808
C	2.37754	-1.01517	0.38028	C	-4.81307	-2.73492	-0.87439
H	3.49538	-1.30038	2.19827	H	-5.72295	-3.06890	-1.38020
C	2.44075	-1.07879	-1.01447	H	-3.98739	-3.39995	-1.16981
H	3.63810	-1.52859	-2.74999	H	-4.96543	-2.82329	0.19868
C	1.09022	-0.64294	1.10963	C	-3.73417	2.58674	-2.73645
H	1.57007	-0.80961	-1.60246	H	-2.88018	2.60986	-3.42681
H	0.31694	-0.41556	0.29292	H	-4.63179	2.88595	-3.28420
N	1.23811	0.48104	2.00774	H	-3.56217	3.31077	-1.94333
H	0.35112	0.59784	2.49599	C	3.15912	1.96334	1.40391
C	0.55630	-1.83771	1.91563	C	3.93932	1.71922	2.54285
H	1.27489	-2.11269	2.69265	C	3.78886	2.45324	0.25573
H	-0.39024	-1.57825	2.39568	C	5.31289	1.95566	2.53057
H	0.39616	-2.70457	1.26976	H	3.45884	1.32578	3.43420
C	1.64479	1.78127	1.44592	C	5.16560	2.69045	0.23751
C	-3.21233	-1.76172	1.75416	H	3.19661	2.64581	-0.63610
C	-2.79786	-3.10122	1.67660	C	5.93250	2.44254	1.37585
C	-3.87184	-1.34237	2.92361	H	5.90325	1.75892	3.42181
C	-3.06061	-3.99585	2.71453	H	5.63807	3.06242	-0.66757
H	-2.26425	-3.45079	0.80101	H	7.00376	2.62291	1.36391
C	-4.12978	-2.23427	3.96392	H	1.26244	1.88818	0.41674
H	-4.17228	-0.30421	3.01716	C	1.01093	2.89634	2.29554
C	-3.72919	-3.56731	3.86217	H	-0.07722	2.79667	2.30199
H	-2.73138	-5.02752	2.62763	H	1.37702	2.84151	3.32633
H	-4.64178	-1.88451	4.85592	H	1.27524	3.87743	1.89300
H	-3.92813	-4.26319	4.67213	C	6.01393	-2.19561	-1.61632
C	-1.89391	2.78289	-0.19519	F	6.79300	-1.11388	-1.85823
C	-2.44156	3.67872	0.74061	F	6.75821	-3.05225	-0.87968
C	-0.90710	3.26115	-1.07156	F	5.78655	-2.78454	-2.81317

```
Zero-point correction=                 0.698856 (Hartree/Particle)
 Thermal correction to Energy=             0.746526
 Thermal correction to Enthalpy=           0.747471
 Thermal correction to Gibbs Free Energy=      0.612062
 Sum of electronic and zero-point Energies=       -2359.852314
 Sum of electronic and thermal Energies=          -2359.804644
 Sum of electronic and thermal Enthalpies=        -2359.803699
 Sum of electronic and thermal Free Energies=     -2359.939108
```

(S,1'S)-N-(1-(4-trifluoromethylphenyl)ethyl)-(S)-α-methylbenzylamine

```
Zero-point correction=                 0.316898 (Hartree/Particle)
 Thermal correction to Energy=             0.336071
 Thermal correction to Enthalpy=           0.337015
 Thermal correction to Gibbs Free Energy=      0.266140
 Sum of electronic and zero-point Energies=       -1012.644036
 Sum of electronic and thermal Energies=          -1012.624864
 Sum of electronic and thermal Enthalpies=        -1012.623920
 Sum of electronic and thermal Free Energies=     -1012.694795
```

(R,1'S)-N-(1-(4-trifluoromethylphenyl)ethyl)-(S)-α-methylbenzylamine

```
Zero-point correction=                 0.316906 (Hartree/Particle)
 Thermal correction to Energy=             0.336118
 Thermal correction to Enthalpy=           0.337062
 Thermal correction to Gibbs Free Energy=      0.266125
 Sum of electronic and zero-point Energies=       -1012.643705
 Sum of electronic and thermal Energies=          -1012.624493
 Sum of electronic and thermal Enthalpies=        -1012.623549
 Sum of electronic and thermal Free Energies=     -1012.694486
```

Internal Reaction Coordinate (IRC) calculation

IRC calculations were performed for all the transition states related to the energy pathway of compound (**1a**). The data revealed that the transfer of the hydride from the iron atom to the carbon atom happens when the proton transfer from the hydroxy group of hydrogenated catalyst B to the imine nitrogen has already almost completely occurred in a mechanism that we can define concerted but asynchronous.

A picture related to **(1a)-TS(E)re** is reported as example in figure S6.

FIGURE S6

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