

Supplementary Information for:

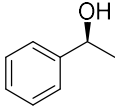
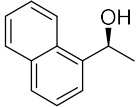
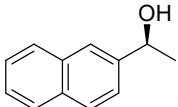
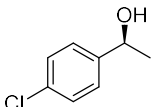
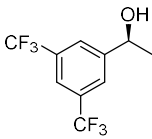
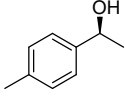
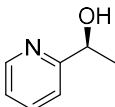
Enantioselective direct, base-free hydrogenation of ketones by a manganese amido complex of a homochiral, unsymmetrical P-N-P' ligand

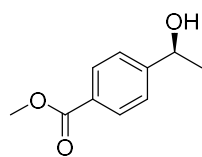
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Department of Chemistry, University of Toronto, 80 Saint George St., Toronto, Ontario, M5S3H6, Canada.

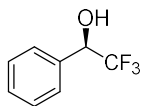
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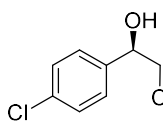
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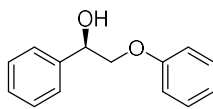
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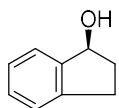
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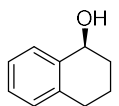
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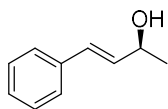
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General comments

All manipulations that involved air- or moisture-sensitive materials were performed using Schlenk techniques or a glovebox under an argon or nitrogen atmosphere. All solvents and substrates were degassed and dried using standard procedures prior to all manipulations and reactions unless stated otherwise.^{1,2} Deuterated solvents were purchased from Cambridge Isotope Laboratories, INC, and dried over activated molecular sieves in argon or nitrogen glovebox. (1*S*,2*S*)-2-(diphenylphosphino)-1,2-diphenylethylamine was purchased from ACROS Organics and ligand **P-NH-P'** was prepared according to the previous literature.³

NMR spectra of the samples that were prepared under argon in degassed solvents were recorded at ambient temperature and pressure unless specified, using a Bruker Advance III 400 MHz, Agilent DD2 500 MHz or Agilent DD2 600 MHz [¹H (400 MHz, 500 MHz and 600 MHz), ¹³C{¹H} (100 MHz, 125 MHz and 150 MHz) and ³¹P{¹H} (162 MHz, 202 MHz and 243 MHz)]. All NMR spectra shown in **Figure S8-16** were recorded on an Agilent DD2 500 MHz, spectrometer at 25°C and in deuterated toluene. Data for ¹H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant (Hz), integration. The IR spectra were obtained using a Bruker Alpha IR spectrometer with an ATR platinum-diamond attachment. Elemental analyses were performed using a PerkinElmer 2400 CHN elemental analyzer at the Department of Chemistry at the University of Toronto. The conversions and *ee* for each reaction were obtained either on Shimadzu GC-2014 gas chromatograph equipped with a chiral column (CP Chirasil-Dex CB 25 m x 2.5 mm), using hydrogen gas as the carrier gas and 1,4-di-*tert*-butylbenzene as an external standard, or HPLC analysis performed on an Agilent HP 1100 Series modular system operated by ChemStation LC 3D software, v.10.02. on chiral column DAICEL CHIRALPAK AD-H or OD-H. Enantiomeric purity (reported as % *ee*) was determined by comparison with the racemic assay and calculated as follows:

$$\% ee = [(Area A - Area B)/(Area A + Area B)] \times 100.$$

Synthesis of manganese complex **4**

P-NH-P' (150 mg, 2.9x10⁻¹ mmol) and Mn(CO)₅Br (78.4 mg, 2.9x10⁻¹ mmol, 1 equiv.) was dissolved in 5 mL toluene, and the reaction mixture was refluxed for 16 h. All volatiles were evaporated off. The residue was taken up in pentane, filtered, and washed with 2x5 mL pentane to afford **4** as yellow solid (155 mg, 76% yield).

¹H NMR (500 MHz, toluene-d₈): δ 7.95 (m, 2H), 7.68 (m, 2H), 7.02 (m, 4H), 6.87 (m, 4H), 6.78 (m, 2H), 6.63 (m, 6H), 4.60 (m, 1H), 4.29 (m, 1H), 4.00 (m, 1H), 3.31 (m, 1H), 2.64-2.59 (m, 1H), 2.33 (m, 1H), 2.17 (m, 1H), 1.55 (m, 1H), 1.46-1.24 (m, 12H). ³¹P{¹H} NMR (202 MHz, toluene-d₈): δ 84.5 (d, *J*_{PP} = 92.7 Hz), 81.0 (d, *J*_{PP} = 92.7 Hz). ¹³C{¹H} NMR (125 MHz, C₆D₆): δ 140.06 (m), 136.67-136.16 (m), 134.45 (m), 133.56 (m), 130.24 (s), 129.55 (s), 128.86 (s), 126.20 (s), 74.06 (m), 55.70 (s), 50.68 (m), 26.30-26.01 (m), 24.12 (m), 19.98-19.90 (m), 18.75 (m), 18.34 (m). FTIR 1944, 1908 cm⁻¹ ν_(CO). HRMS (ESI-TOF, CH₂Cl₂) m/z calculated for [C₃₆H₄₁MnNO₂P₂]⁺: 636.1988, found: 636.1992.

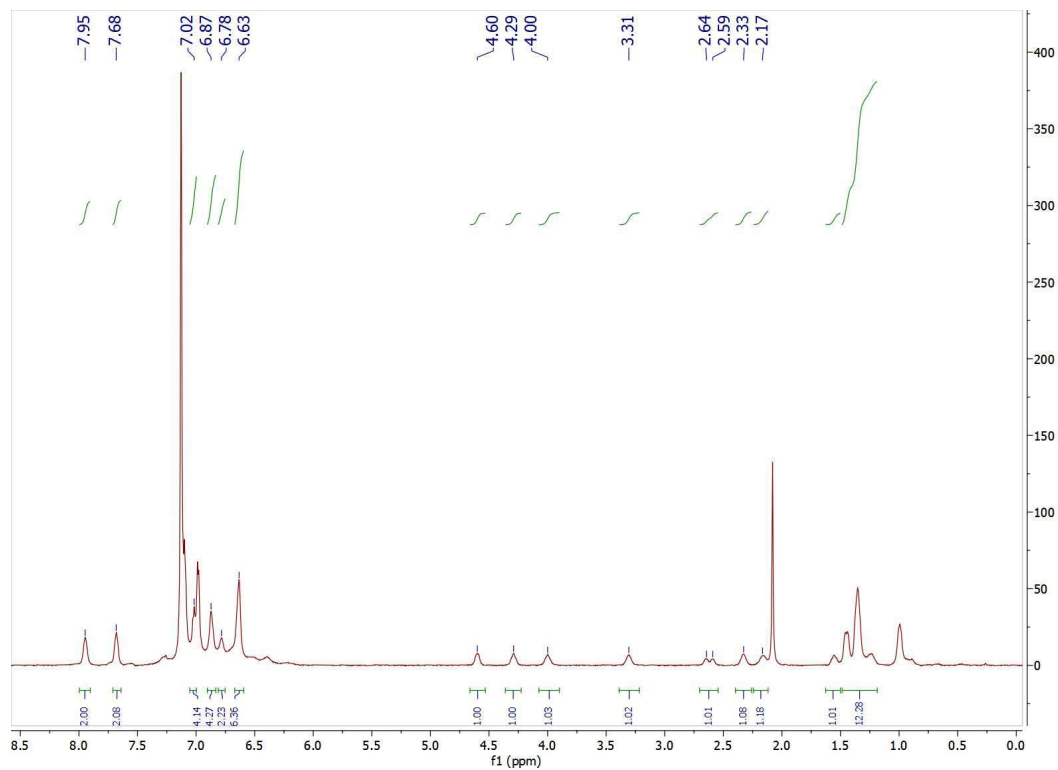


Figure S1. ^1H NMR spectrum of manganese complex **4** (25°C, 500 MHz, toluene- d_8).

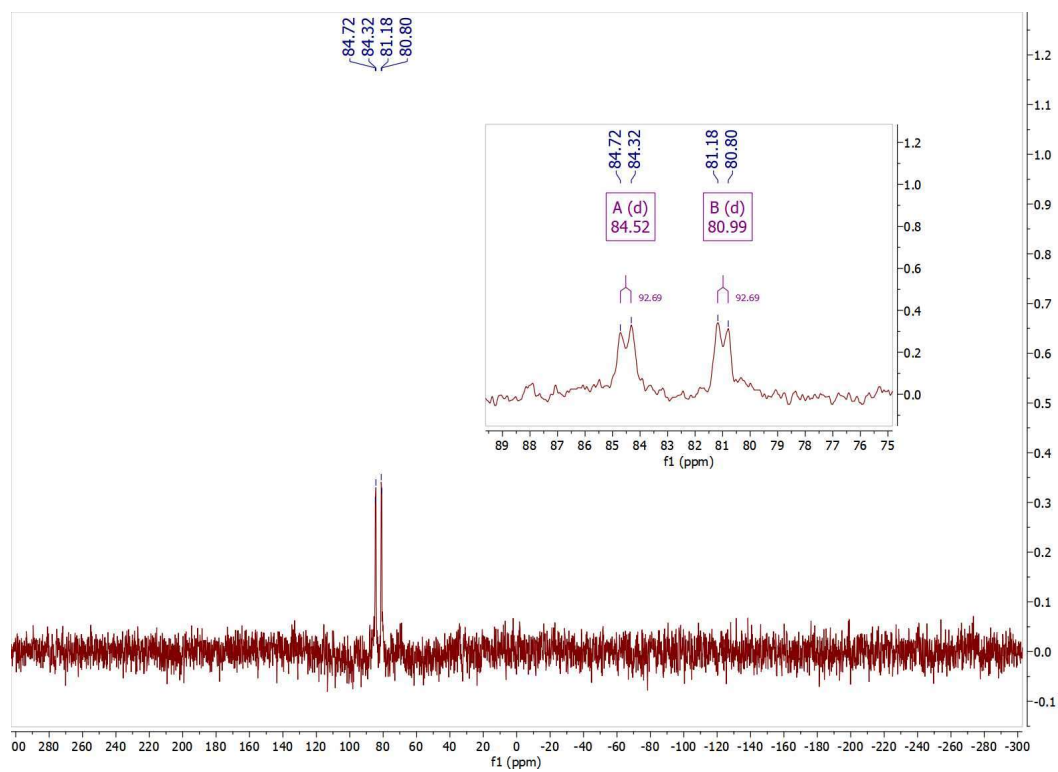


Figure S2. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of manganese complex **4** (25°C, 202 MHz, toluene- d_8).

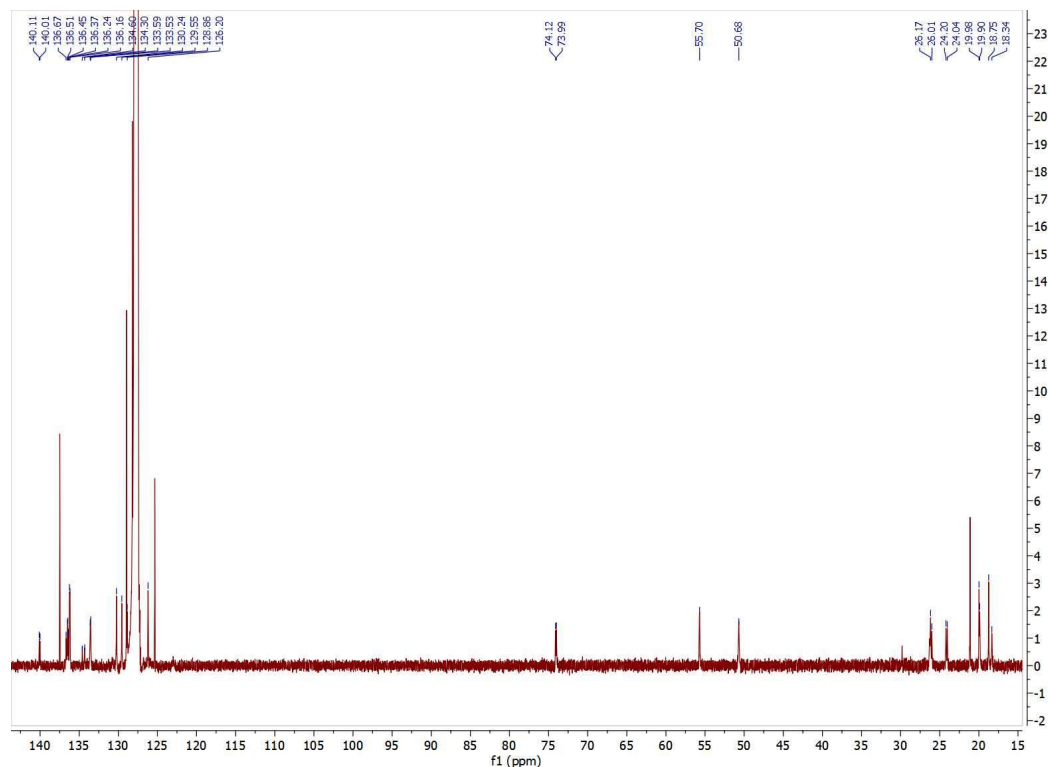


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of manganese complex **4** (25°C, 125 MHz, C_6D_6).

Synthesis of manganese amido complex **1Mn**

4 (50 mg, 7.0×10^{-2} mmol) was dissolved in 10 mL THF in a scintillation vial in argon glovebox. KO^tBu (13.7 mg, 1.4×10^{-1} mmol, 2 equiv.) was added at room temperature while stirring vigorously. The reaction mixture was stirred for 15 minutes and all volatiles were evaporated off. The residue was taken up in *n*-heptane and filtered. The filtrate was concentrated *in vacuo* to afford **1Mn** as a dark red solid (40 mg, 90% yield). The catalyst is air and water sensitive as a solid and in solution. It is stable in room temperature under argon atmosphere for at least 3 weeks.

^1H NMR (500 MHz, C_6D_6): δ 7.93 (t, $J_{\text{HH}} = 8.6$ Hz, 2H), 7.39-7.29 (m, 2H), 7.11-6.76 (m, 14H), 6.59-6.50 (m, 2H), 4.75 (d, $J_{\text{HH}} = 8.2$ Hz, 1H), 4.23 (dd, $J_{\text{HH}} = 8.0, 7.2$ Hz, 1H), 3.24-2.84 (m, 2H), 2.44-2.04 (m, 2H), 1.62-1.42 (m, 2H), 1.22 (dddd, $J_{\text{HH}} = 64.5, 51.6, 14.1, 7.0$, 12H) $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz, C_6D_6): δ 110.04 (d, $J_{\text{PP}} = 96$ Hz), 96.68 (d, $J_{\text{PP}} = 96$ Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, C_6D_6): δ 145.64 (d, $J^1_{\text{CH}} = 11.4$ Hz), 138.37 (d, $J^1_{\text{CH}} = 7.8$ Hz), 135.59 (s), 135.53 (s), 135.14 (d, $J^1_{\text{CH}} = 10.6$ Hz), 134.88 (s), 134.58 (s), 133.12 (d, $J^1_{\text{CH}} = 9.9$ Hz), 129.95 (s), 129.76-129.69 (m), 127.52 (m), 127.04 (s), 126.65 (s), 85.63-85.42 (m), 62.37-62.30 (m), 62.11-61.93 (m), 26.78 (d, $J^1_{\text{CH}} = 19.6$ Hz), 26.31 (d, $J^1_{\text{CH}} = 20.2$ Hz), 23.86-23.77 (m), 18.74-18.63 (m), 18.01-17.93 (m).

FTIR 1895, 1782 cm^{-1} $\nu_{(\text{CO})}$.

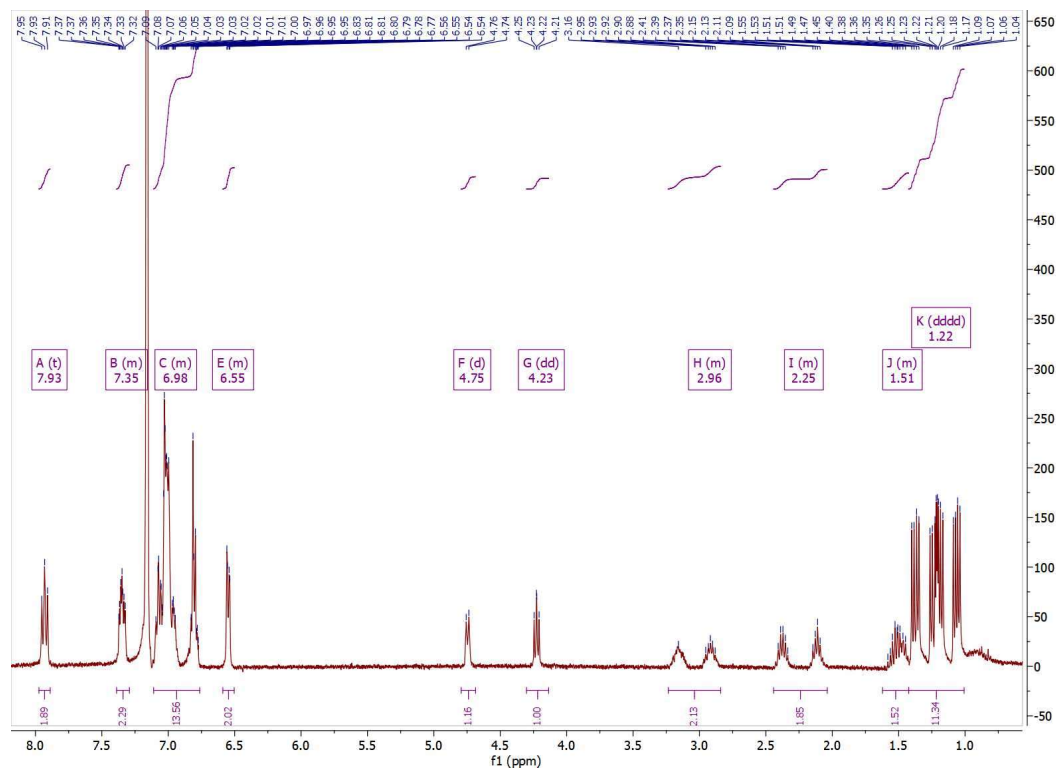


Figure S4. ^1H NMR spectrum of manganese complex **1Mn** (25°C, 500 MHz, C_6D_6).

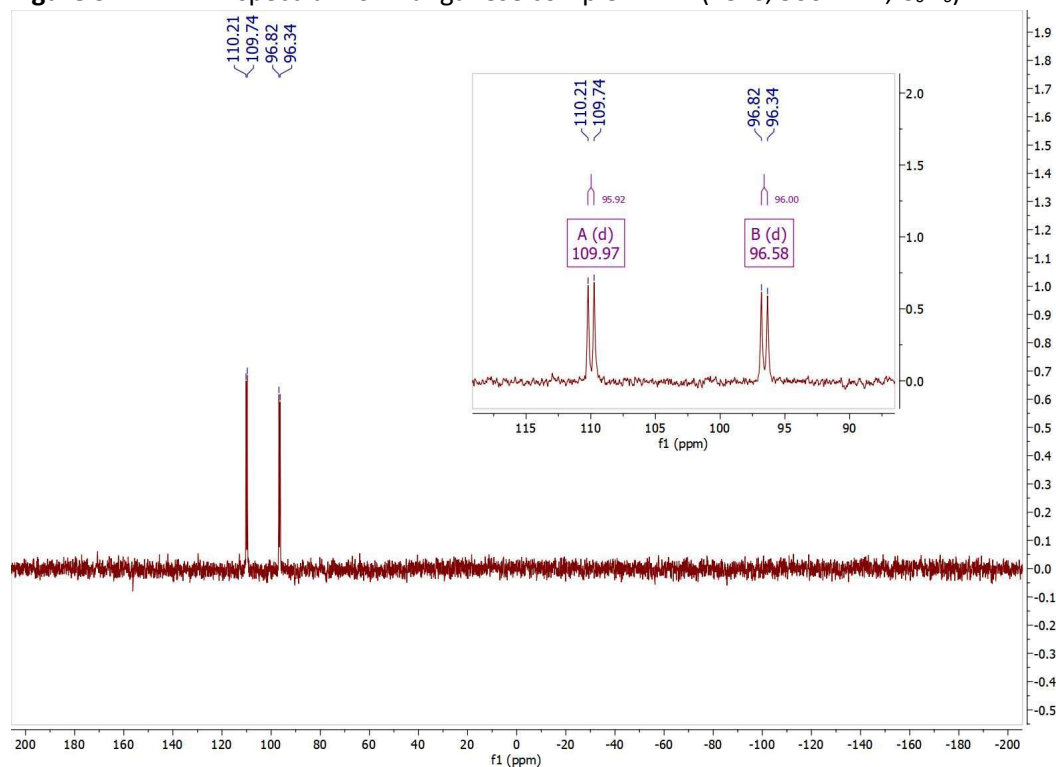


Figure S5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of manganese complex **1Mn** (25°C, 202 MHz, C_6D_6).

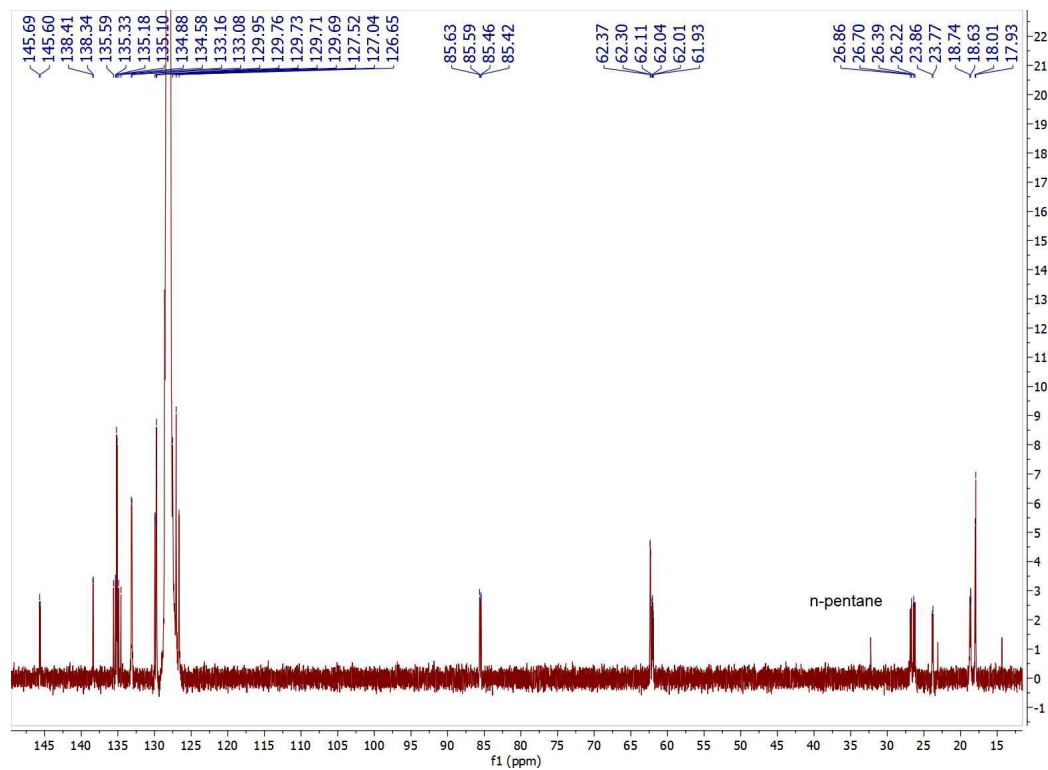


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of manganese complex **1Mn** (25°C, 125 MHz, C_6D_6).

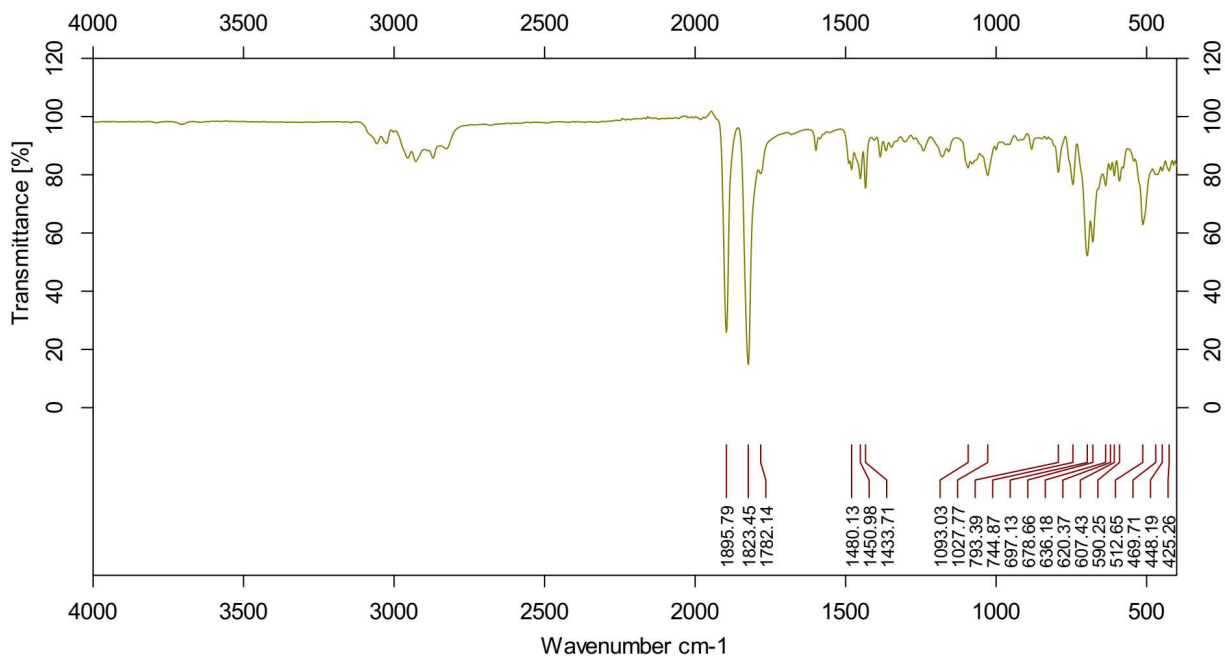


Figure S7. FT-IR spectrum of manganese complex **1Mn**.

NMR study of manganese complex **1Mn** under a hydrogen atmosphere

A dry NMR tube with J. Young valve was charged with **1Mn** (25 mg, 0.05 mmol) and toluene- d_8 in a glovebox. It was taken outside, degassed, and connected to stainless steel line flushed with hydrogen. The line was set to hold 100 psi of hydrogen and the NMR tube was opened to the line. The J. Young valve was closed and the NMR tube was taken back into the box to be agitated to mix the solution. All of the NMR spectra were acquired using an Agilent DD2 500 MHz spectrometer (**Figure S8-11**). The sample was allowed to stay at room temperature for 2 days to observe further changes in the equilibrium (**Figure S12-14**). Hydrogen pressure was relieved and ^1H and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra were found to be identical from **Figure S12** and **S13**. Excess acetophenone was added to the sample and further change was observed (**Figure S15-16**).

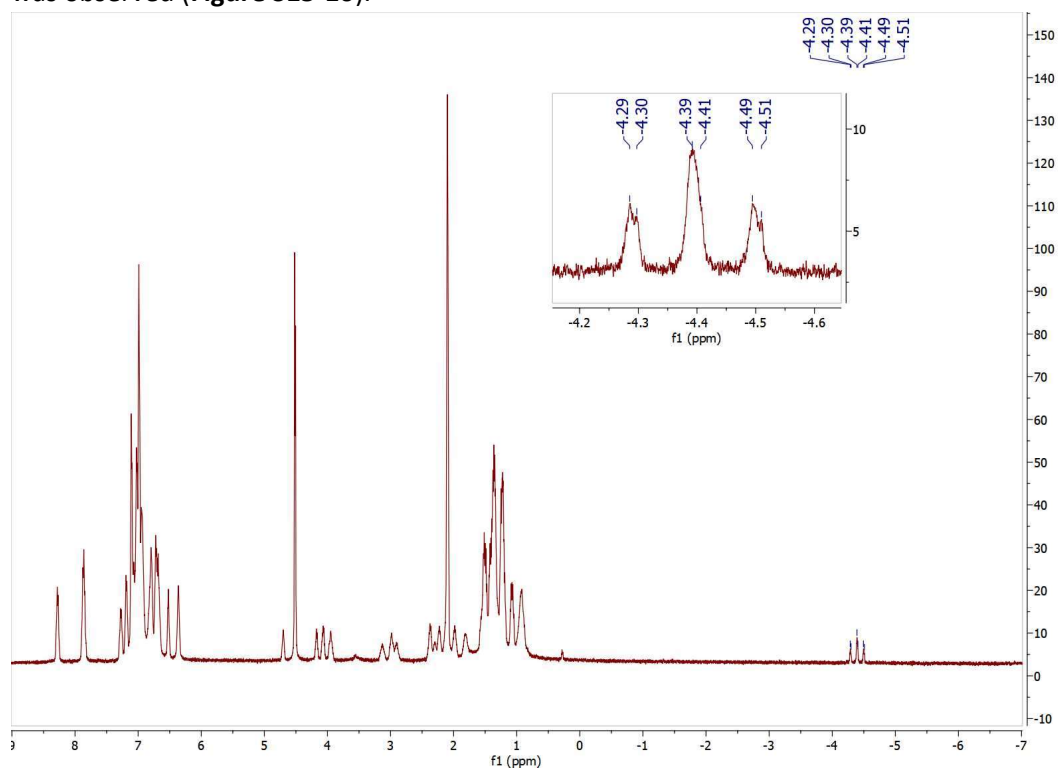


Figure S8. complex **1Mn** in toluene- d_8 under a hydrogen atmosphere; the insert is an expansion of the hydride signals.

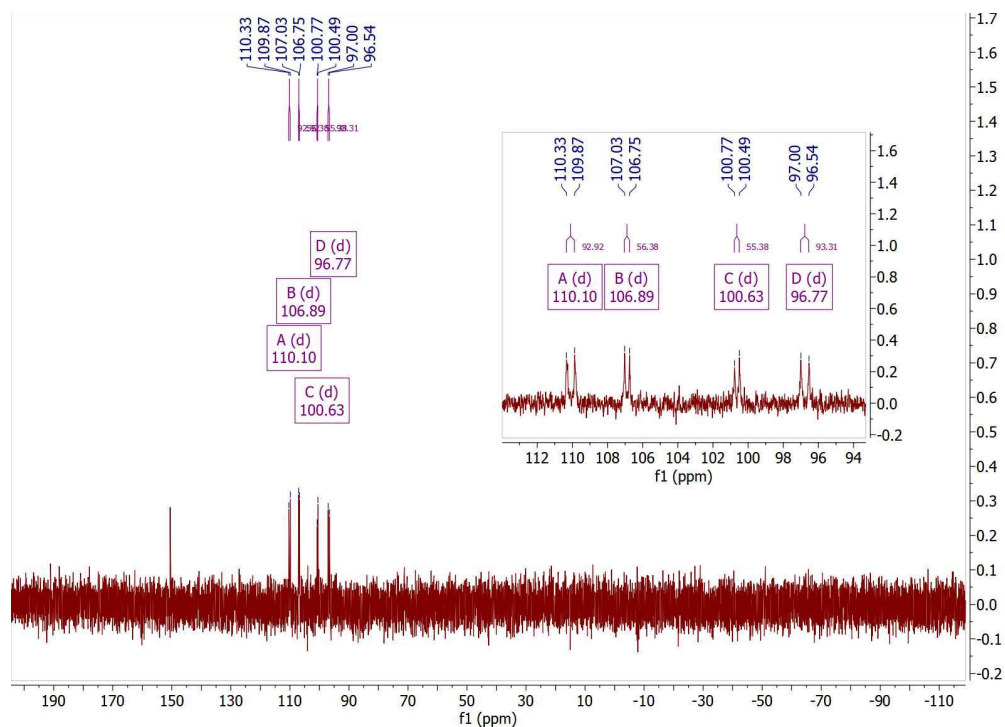


Figure S9. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (202 MHz) of manganese complex **1Mn** in toluene- d_8 under a hydrogen atmosphere with a spectrometer artifact near 150 ppm. New peaks at 106.9 ppm and 100.6 ppm were observed.

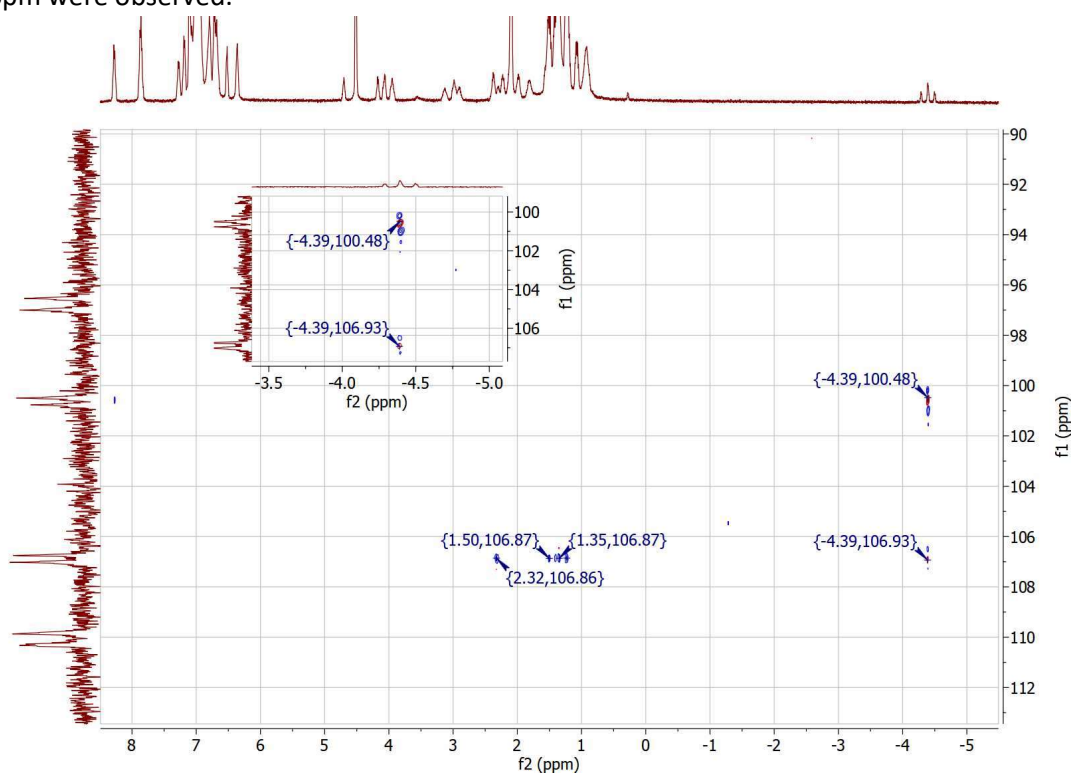


Figure S10. ^1H - ^{31}P HSQC spectrum of manganese complex **1Mn** under a H_2 atmosphere. The hydride peak correlated to the new peaks at 106.9 ppm and 100.6 ppm in the ^{31}P NMR spectrum.

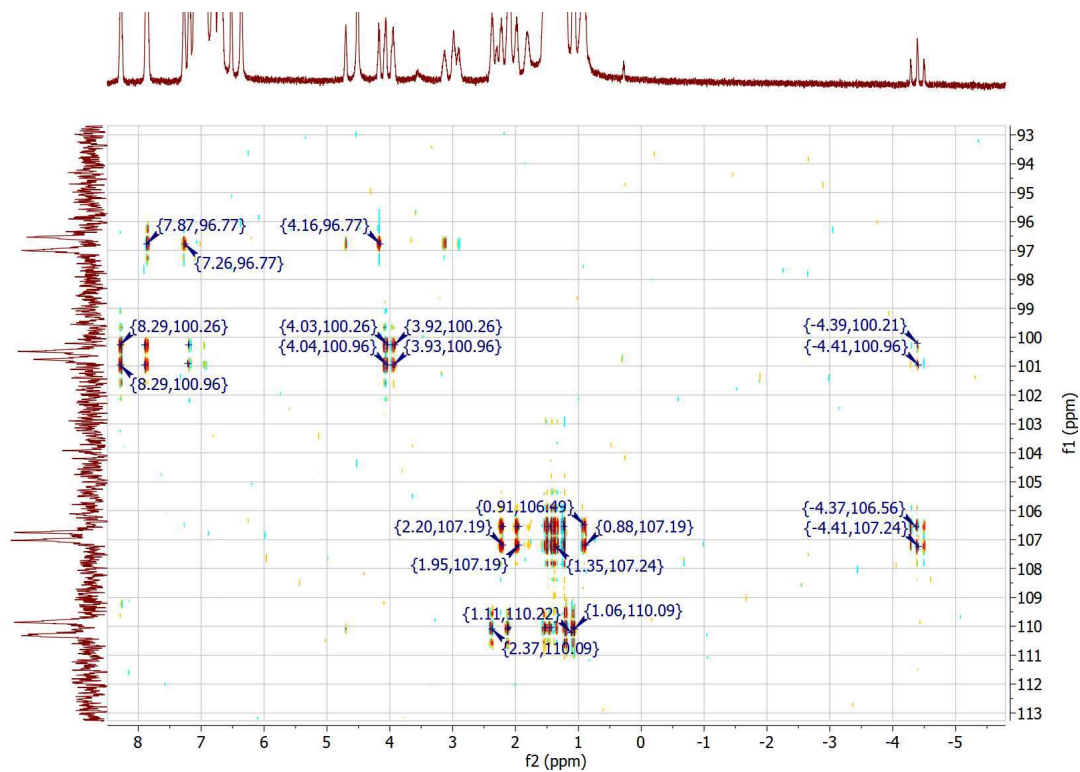


Figure S11. ^1H - ^{31}P HMBC spectrum of manganese complex **1Mn** under a H_2 atmosphere.

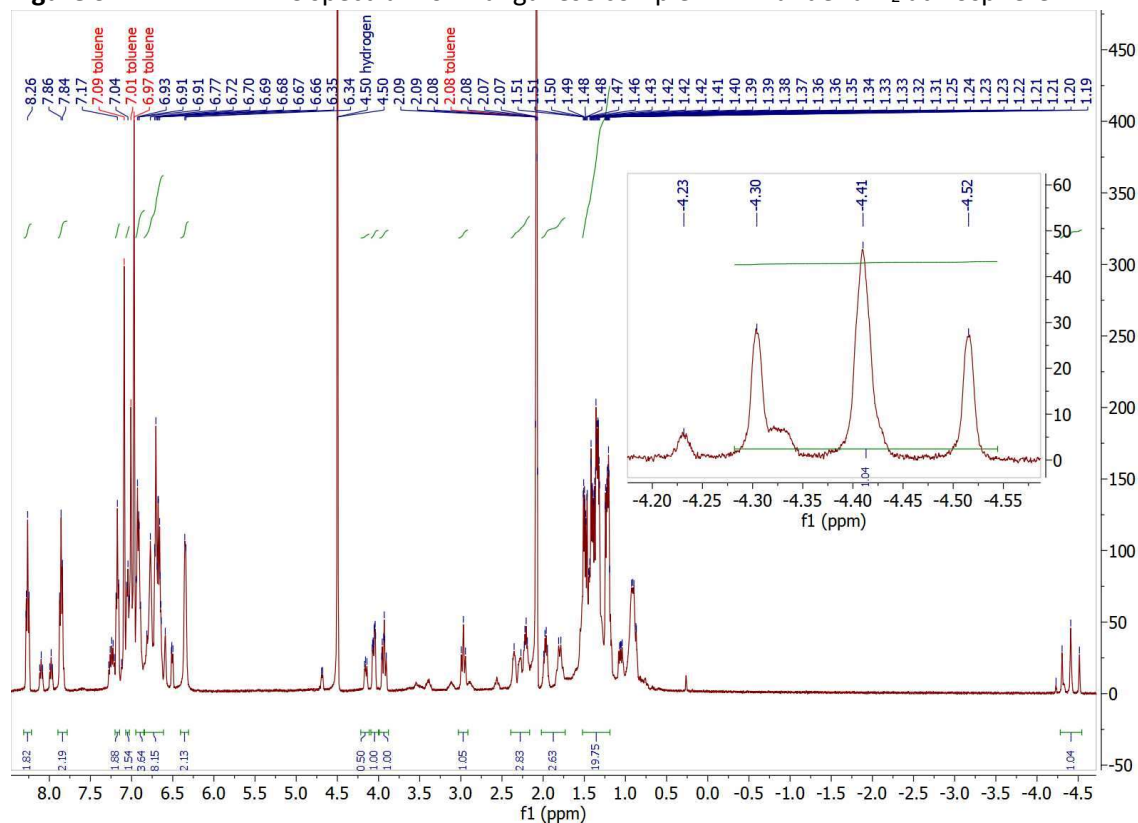


Figure S12. ^1H NMR spectrum of **1Mn** under H_2 atmosphere for 2 days; the insert is an expansion of the hydride signals.

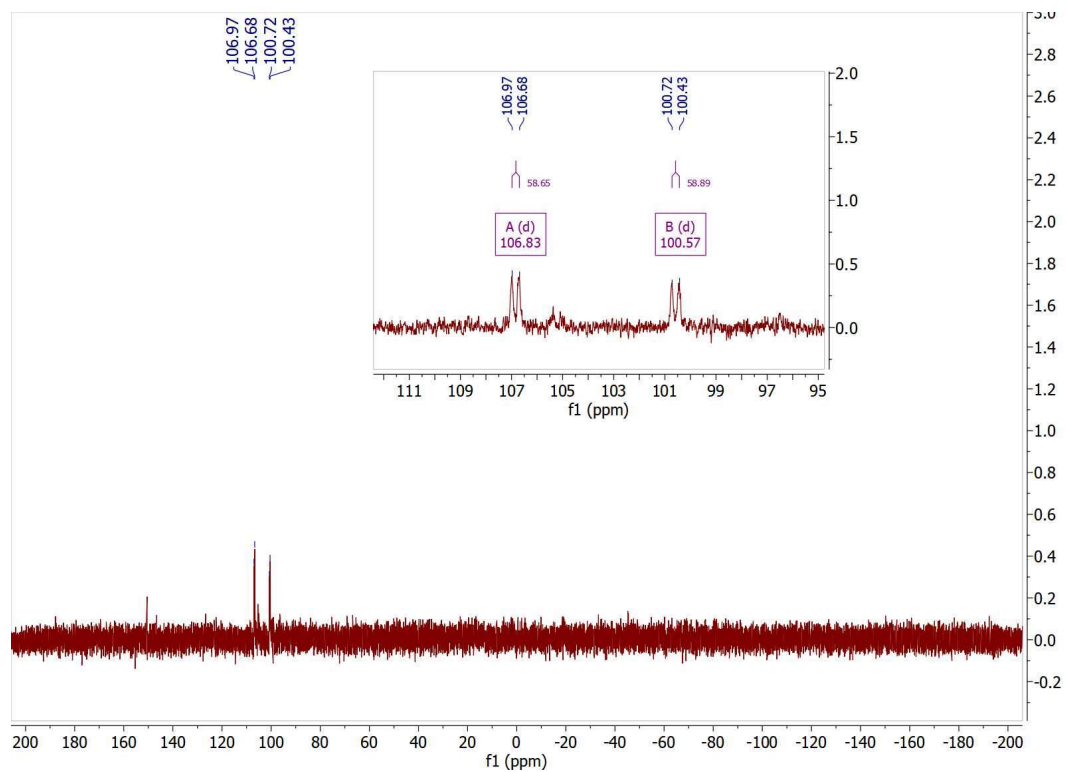


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of manganese complex **1Mn** in toluene- d_8 under a H_2 atmosphere for 2 days.

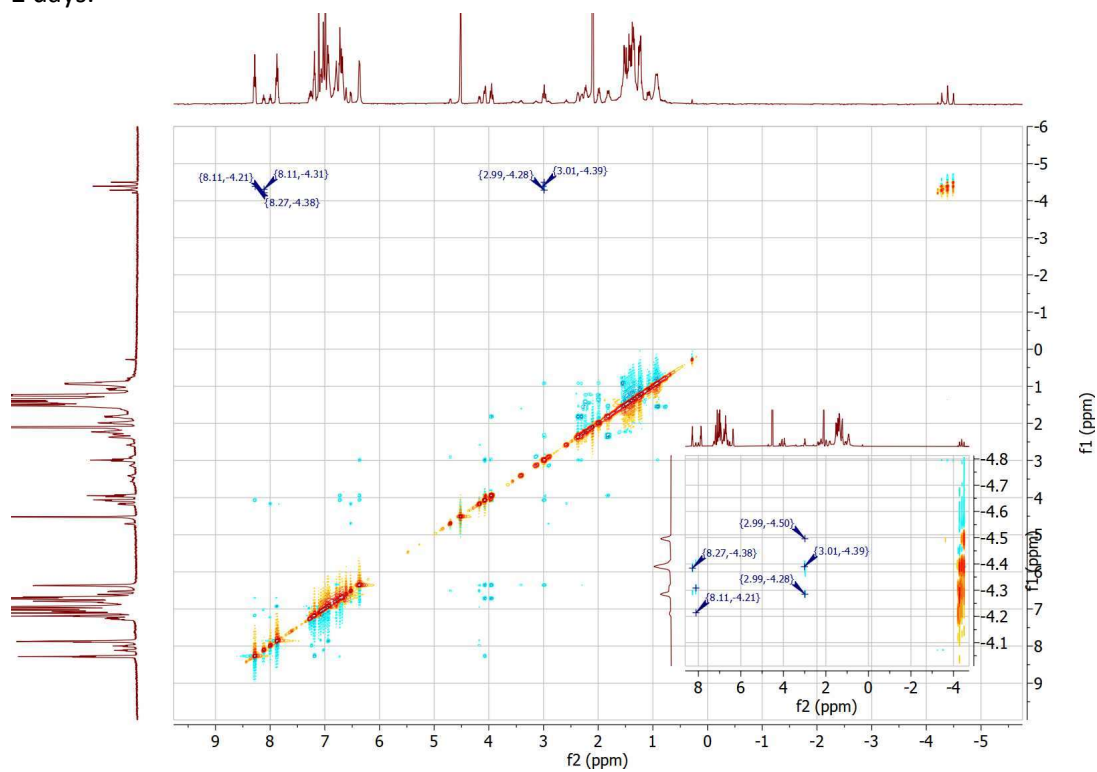


Figure S14. $^1\text{H}\text{-}^1\text{H}$ NOESY spectrum of manganese complex **1Mn** in toluene- d_8 under a H_2 atmosphere for 2.5 days.

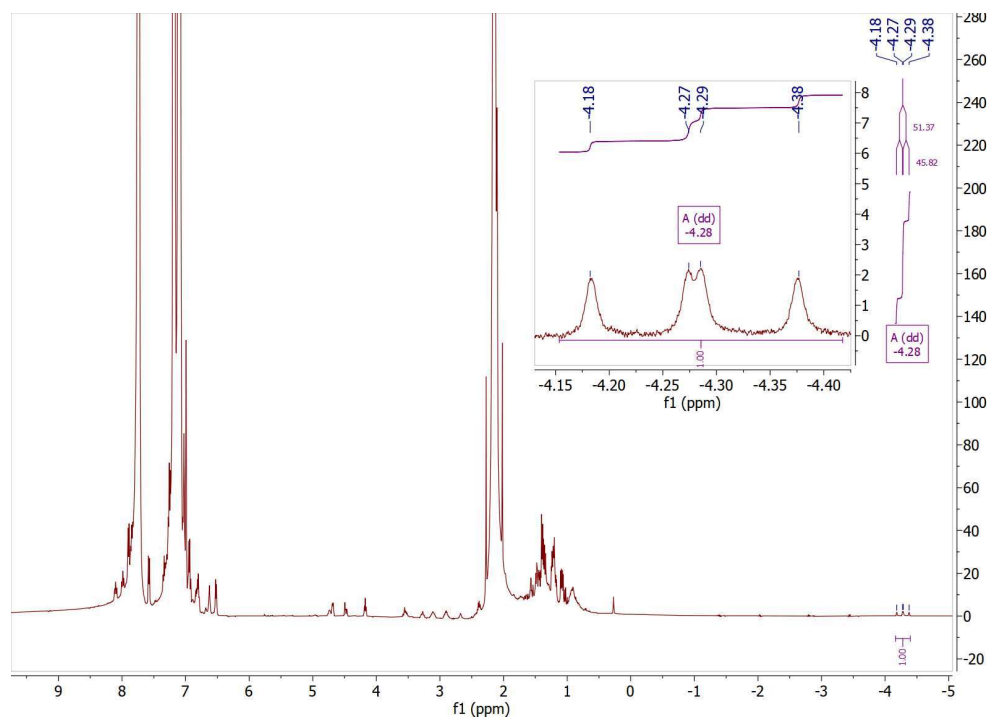


Figure S15. ^1H NMR spectrum of the reaction mixture upon depressurization and addition of excess acetophenone. There were artifacts from the spectrometer observed from -1 to -4 ppm. Aside from those, one hydride species remains while mainly the **1Mn** was reformed with no obvious evidence of 1-phenylethanol formation.

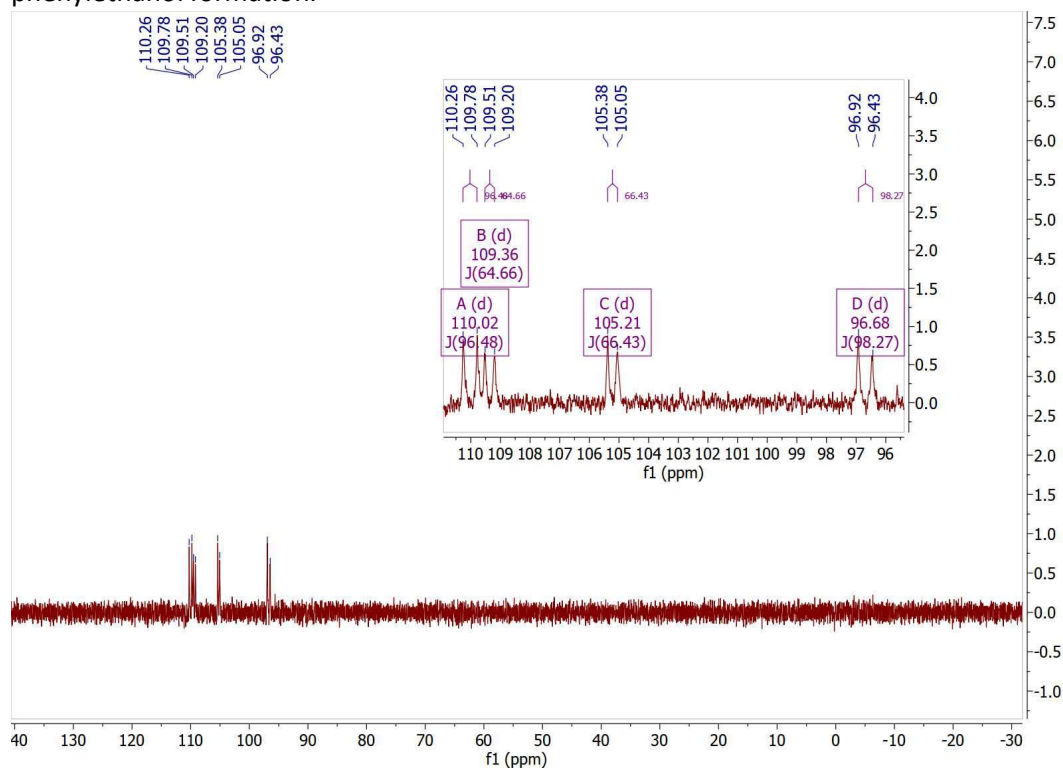
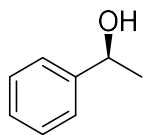


Figure S16. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the reaction mixture upon addition of excess acetophenone. The manganese amido complex **1Mn** has reappeared along with a hydride isomer that does not lose H_2 .

General procedure for the direct hydrogenation of ketones

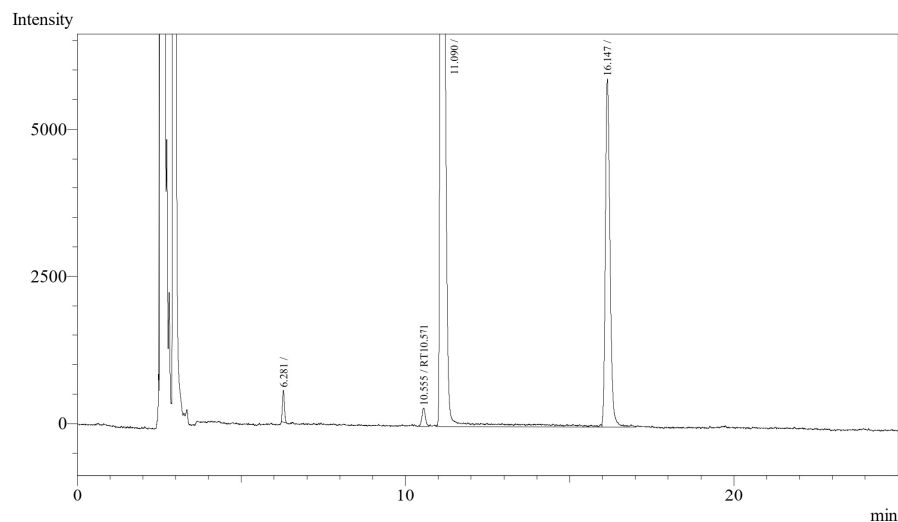
All of the hydrogenation reactions were performed at constant pressures using a stainless steel 50 mL Parr hydrogenation reactor. The reactor was maintained at the appropriate temperature in oil bath. The reactor was flushed several times with hydrogen gas at 10 bar prior to addition of the catalytic mixture. In an argon glovebox, the catalyst (5×10^{-3} mmol), substrate (0.5 mmol) and di-tert-butylbenzene were weighed out, dissolved in 3 mL toluene and taken up in 6 mL syringe with 12 in. needles; the needles were then stoppered well. The syringe was taken out of the glovebox and injected into the prepared Parr reactor against a flow of hydrogen gas. The reaction was stopped after a given reaction time by exposing it to air, and the reactor was allowed to cool down. The catalytic mixture was filtered through a silica plug, then it was analyzed by gas chromatography.



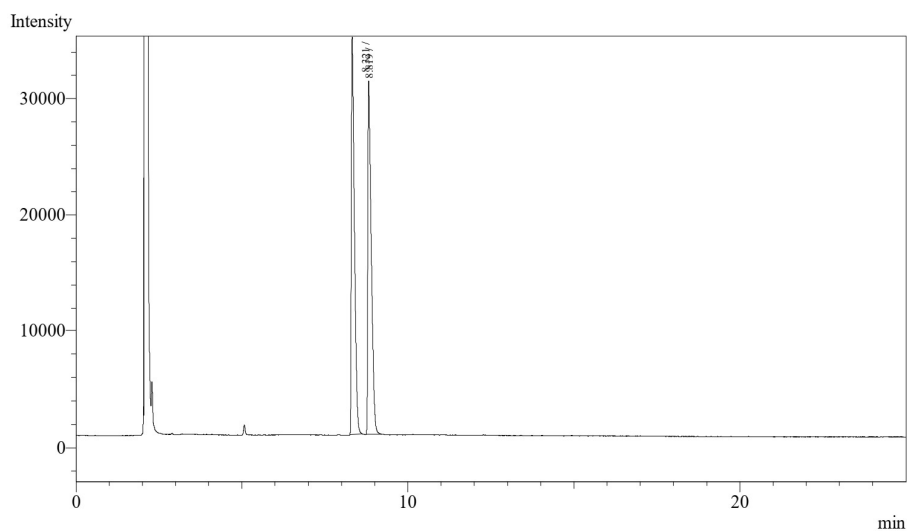
(S)-1-phenylethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 0.58 mL/min, progression: 130/25, detector temperature: 275°C, t_{maj} : 11.1 min, t_{min} : 10.6 min, t_{SM} : 6.3 min, $[\alpha_D^{20}]$: -30.0 (c = 0.01 g/mL, CHCl₃)

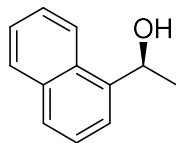


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	6.281	2177	530	0.000				
2	10.555	2388	317	0.000 %		V	4	RT10.571
3	11.090	181548	20467	0.000		SV		
4	16.147	57611	5903	0.000		SV		
Total		243724	27217					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.321	219179	34006	0.000				
2	8.819	219821	30352	0.000				
Total		439000	64358					

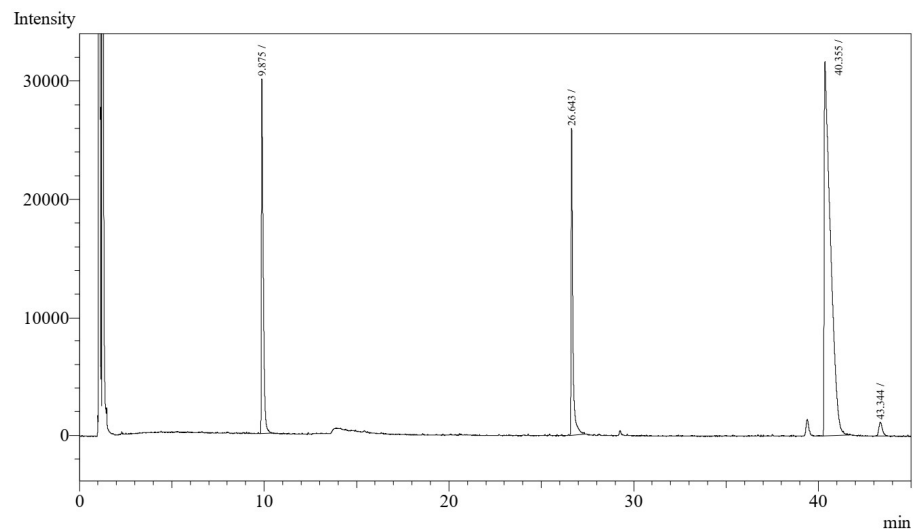
Figure S17. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-phenylethanol.



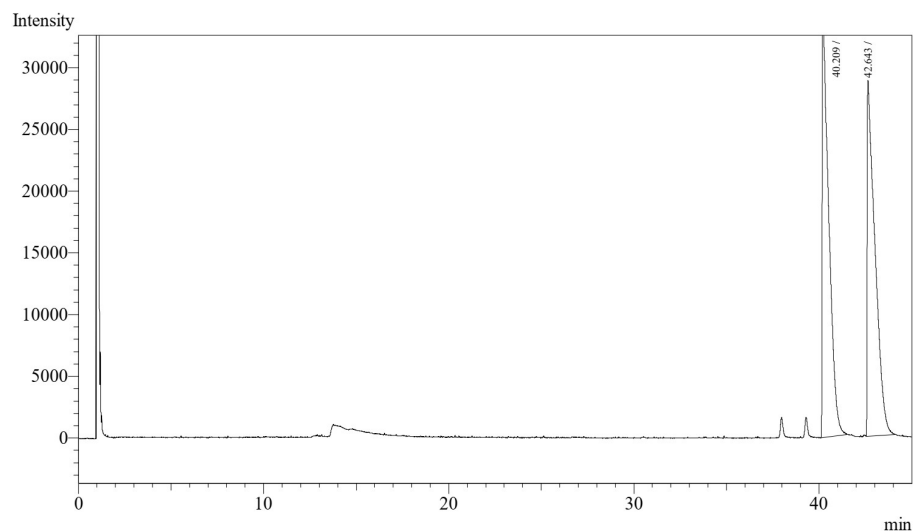
(S)-1-(1-naphthyl)ethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.45 mL/min, progression: 120/20-5-150/20, detector temperature: 275°C, t_{maj} : 40.4 min, t_{min} : 43.3 min, t_{SM} : 26.6 min, $[\alpha_D^{20}]$: -45.2 (c = 0.01 g/mL, CHCl₃)

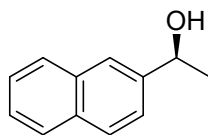


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	9.875	205548	29977	18.217	S			
2	26.643	164831	25940	14.608	S			
3	40.355	742776	31657	65.830	SV			
4	43.344	15176	1173	1.345	V			
Total		1128331	88747					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	40.209	844603	34323	50.092	S			
2	42.643	841507	28834	49.908	SV			
Total		1686110	63157					

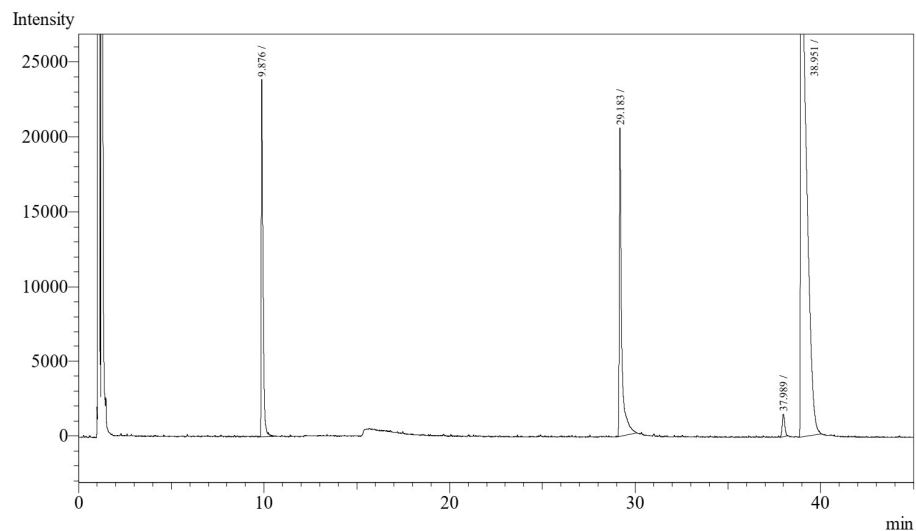
Figure S18. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-(1-naphthyl)ethanol.



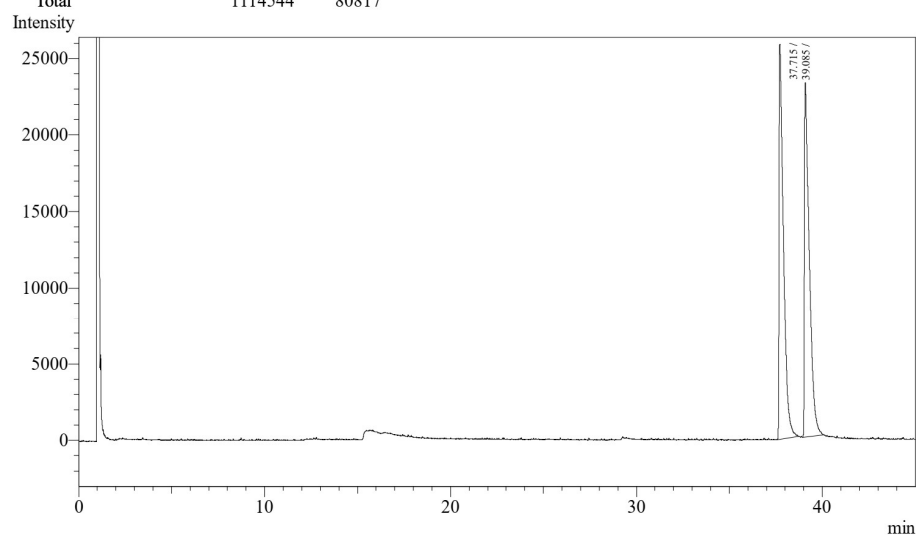
(S)-1-(2-naphthyl)ethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.45 mL/min, progression: 120/20-5-150/20, detector temperature: 275°C, t_{maj} : 39.0 min, t_{min} : 38.0 min, t_{SM} : 29.2 min, $[\alpha_D^{20}]$: -31.4 (c = 0.01 g/mL, CHCl₃)

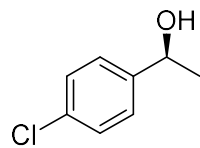


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	9.876	154322	23804	13.846		S		
2	29.183	180357	20619	16.182		S		
3	37.989	14187	1504	1.273				
4	38.951	765678	34890	68.699		S		
Total		1114544	80817					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	37.715	424771	25845	50.206		S		
2	39.085	421293	23197	49.794		S		
Total		846064	49042					

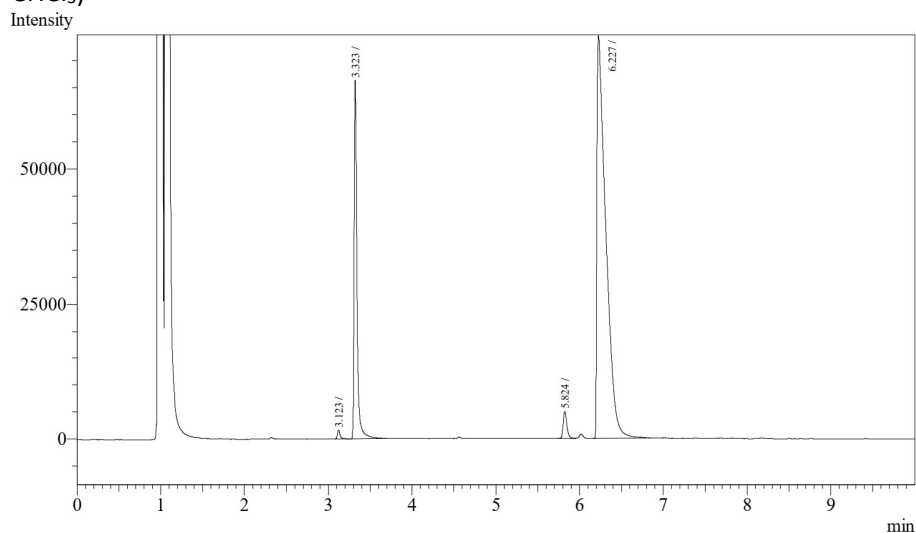
Figure S19. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-(2-naphthyl)ethanol.



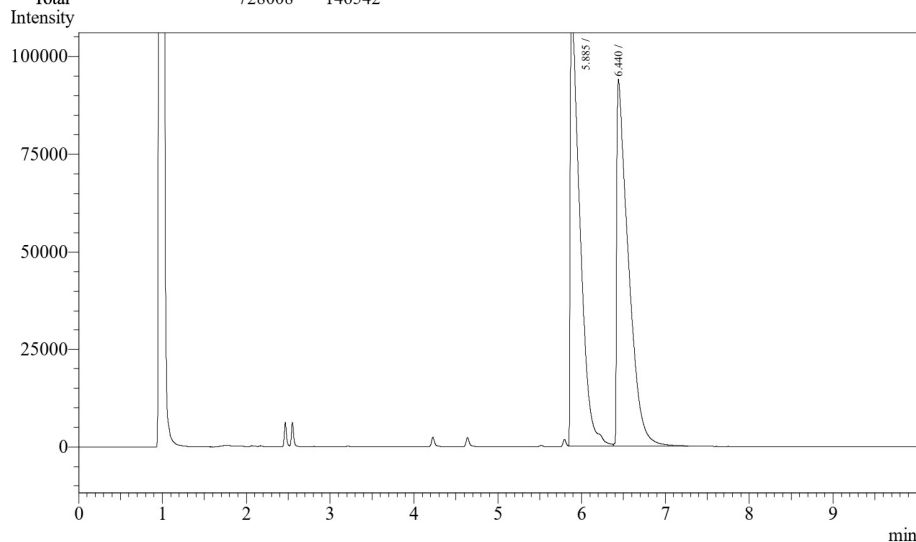
(S)-1-(4'-chlorophenyl)ethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.47 mL/min, progression: 145/10, detector temperature: 275°C, t_{maj}: 6.2 min, t_{min}: 5.8 min, t_{SM}: 3.1 min, [α_D^{20}]: -31.4 (c = 0.01 g/mL, CHCl₃)

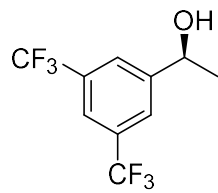


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Compd Name
1	3.123	3674	1610	0.505				
2	3.323	156554	65674	21.504		V		
3	5.824	15194	4976	2.087				
4	6.227	552586	74282	75.904		S		
Total		728008	146542					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Compd Name
1	5.885	907641	112297	49.963				
2	6.440	908985	93824	50.037		SV		
Total		1816626	206121					

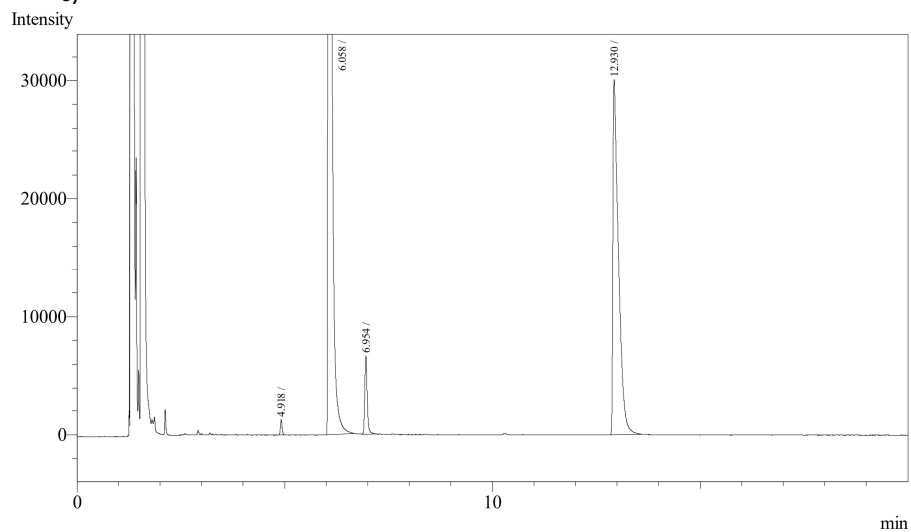
Figure S20. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-(4'-chlorophenyl)ethanol.



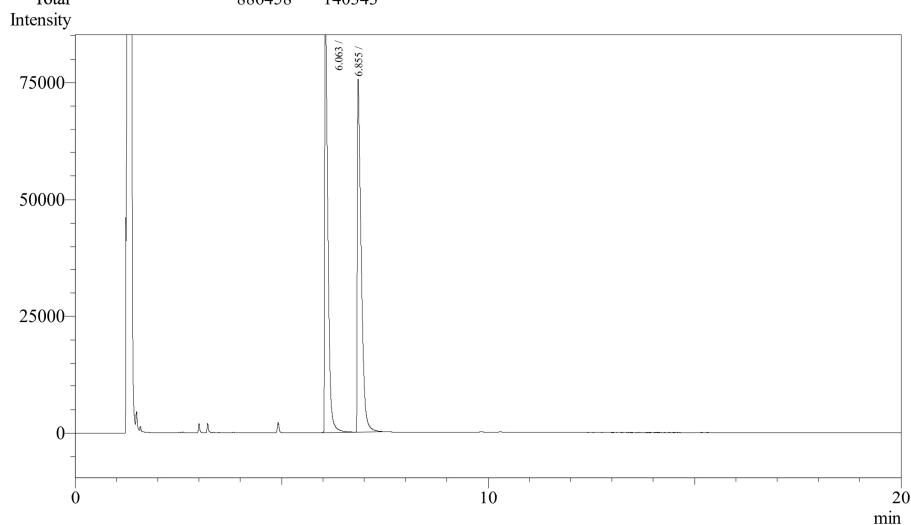
(S)-1-(3',5'-bis(trifluoromethyl)phenyl)ethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.02 mL/min, progression: 120/20, detector temperature: 275°C, t_{maj} : 6.1 min, t_{min} : 7.0 min, t_{SM} : 4.9 min, $[\alpha_D^{20}]$: -45.2 (c = 0.01 g/mL, CHCl₃)

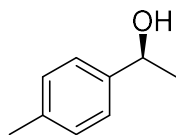


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	4.918	3496	1291	0.394				
2	6.058	573679	102356	64.716				
3	6.954	27080	6638	3.055				
4	12.930	282203	30058	31.835		S		
Total		886458	140343					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	6.063	494318	93592	50.183		S		
2	6.855	490710	75388	49.817		S		
Total		985028	168980					

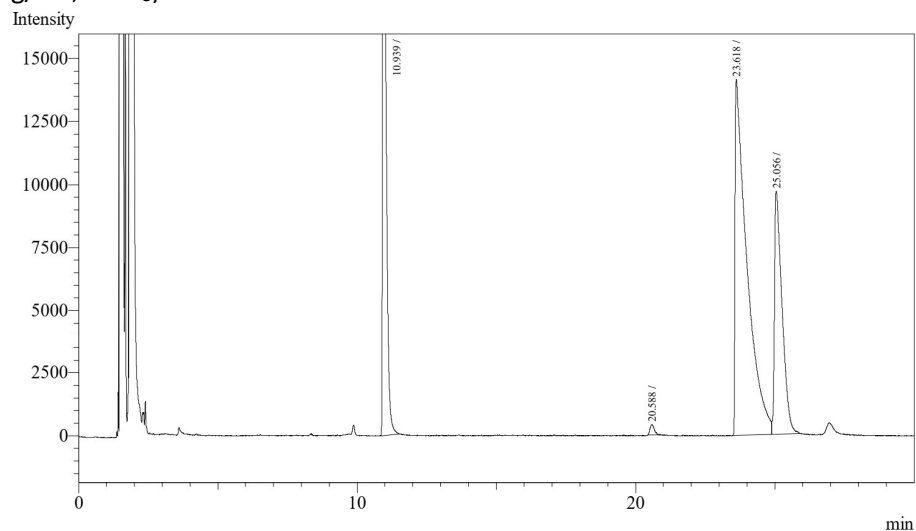
Figure S21. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-(3',5'-(bistrifluoromethyl)phenyl)ethanol.



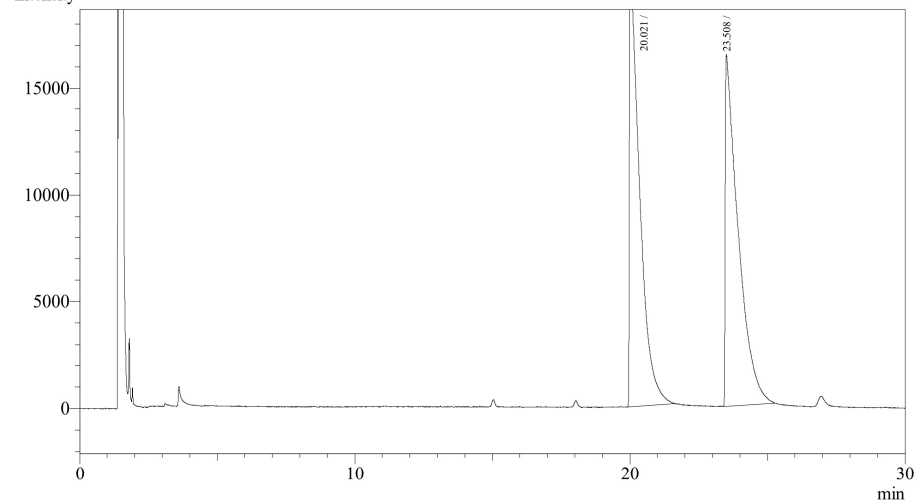
(S)-1-(4'-methylphenyl)ethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 0.97 mL/min, progression: 110/30, detector temperature: 275°C, t_{maj} : 23.6 min, t_{min} : 20.6 min, t_{SM} : 25.1 min, $[\alpha_D^{20}]$: -15.0 (c = 0.01 g/mL, CHCl₃)

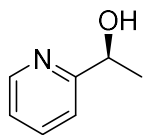


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	10.939	252870	31602	29.406				
2	20.588	4656	425	0.541				
3	23.618	418955	14163	48.721				
4	25.056	183433	9684	21.332		SV		
Total		859914	55874					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	20.021	530301	21057	49.720				
2	23.508	536279	16485	50.280		S		
Total		1066580	37542					

Figure S22. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-(4'-methylphenyl)ethanol.



(S)-1-(2-pyridyl)ethanol

$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 8.52 (ddd, $J = 5.1, 1.8, 1.1$ Hz, 1H), 7.67 (td, $J = 7.7, 1.8$ Hz, 1H), 7.28 (dq, $J = 8.1, 0.9$ Hz, 1H), 7.18 (ddd, $J = 7.4, 4.9, 1.1$ Hz, 1H), 4.88 (q, $J = 6.6$ Hz, 1H), 1.49 (d, $J = 6.6$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ 163.18, 148.21, 136.94, 122.33, 119.93, 68.97, 24.36.

Product ratio was determined by HPLC, Chiralpak OD-H column, 2% iPrOH in hexanes (30 min), 1.0 mL/min. t_{maj} : 17.9 min, t_{min} : 16.0 min, $[\alpha]_D^{20}$: -13.4 ($c = 0.01$ g/mL, CHCl_3)

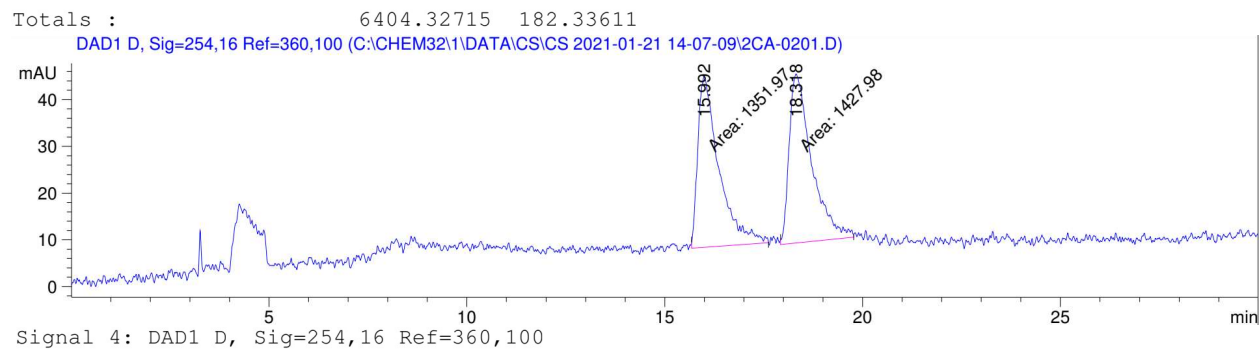
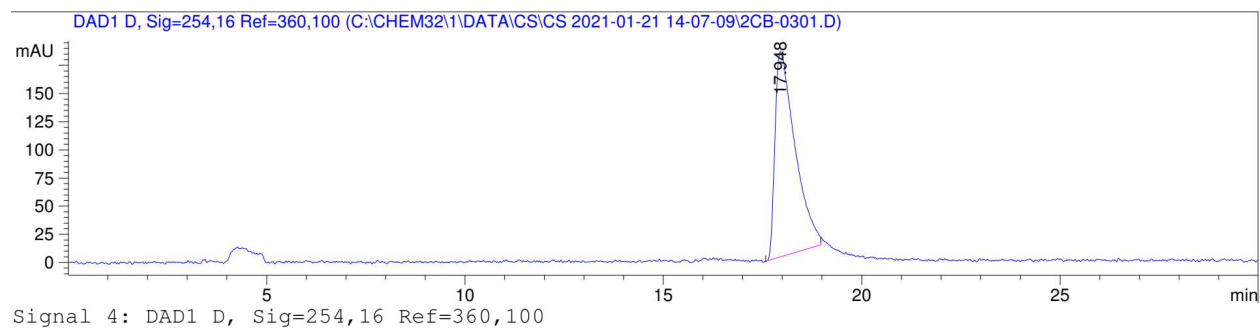
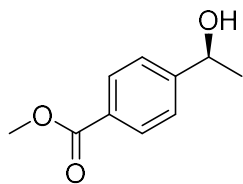


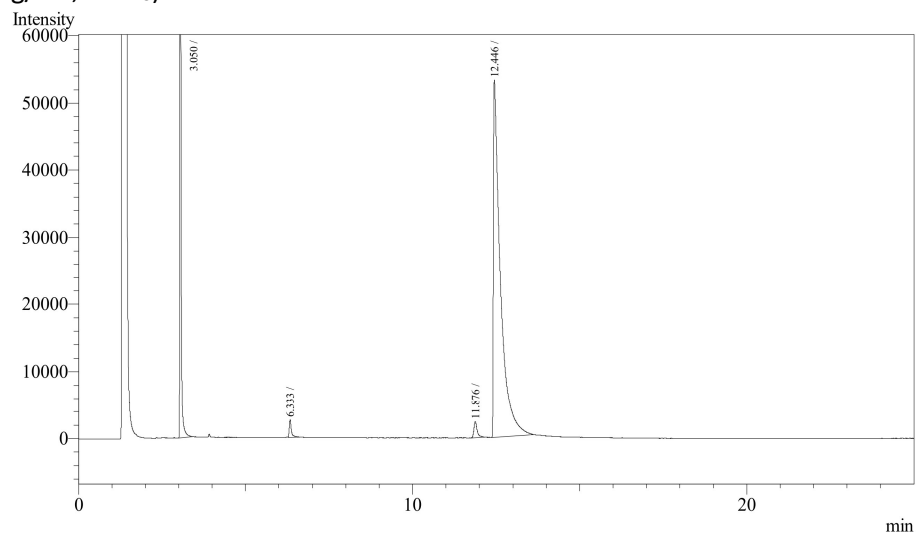
Figure S23. HPLC chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 2-pyridylethanol.



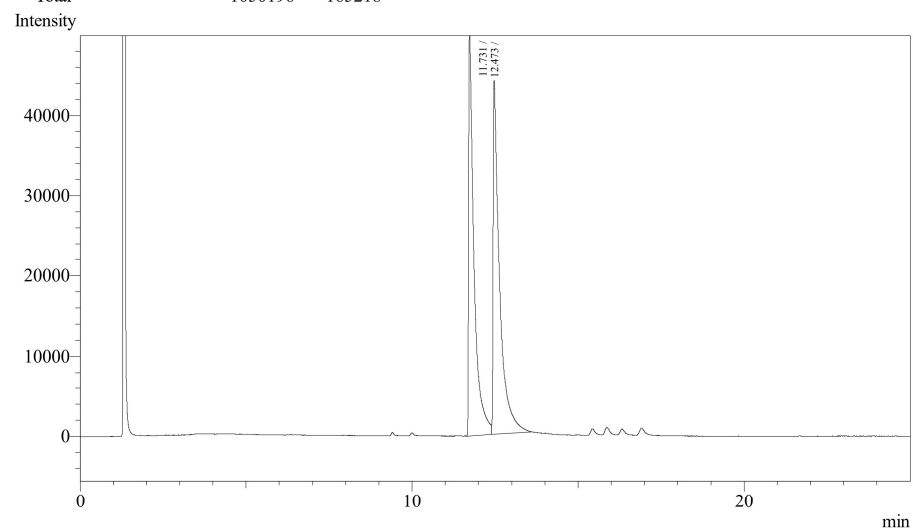
Methyl 4-((1S)-1-hydroxyethyl)benzoate

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 0.96 mL/min, progression: 160/25, detector temperature: 275°C, t_{maj} : 12.4 min, t_{min} : 11.9 min, t_{SM} : 6.3 min, $[\alpha_D^{20}]$: -23.8 (c = 0.01 g/mL, CHCl₃)

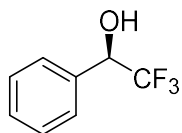


Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.050	249930	107014	23.798				
2	6.333	11777	2635	1.121		SV		
3	11.876	16025	2378	1.526				
4	12.446	772464	53191	73.554				
Total		1050196	165218					



Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	11.731	565134	50561	48.791				
2	12.473	593133	44106	51.209		V		
Total		1158267	94667					

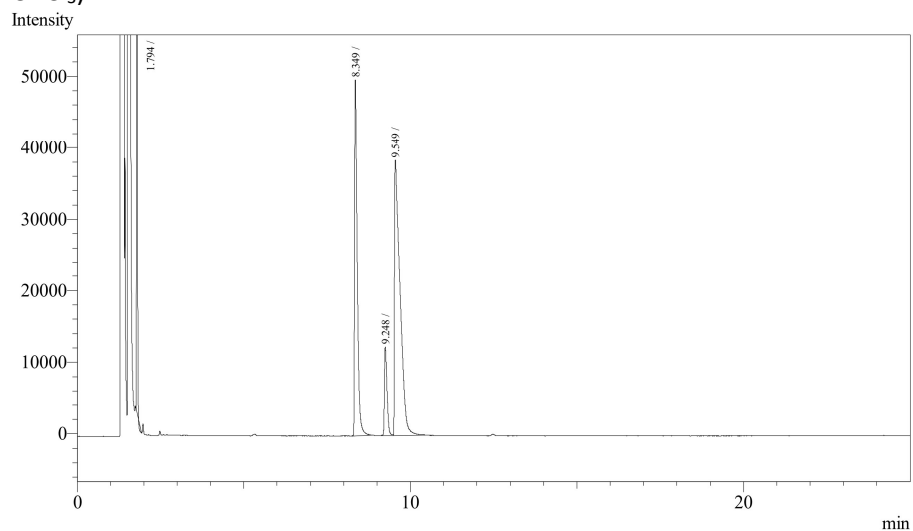
Figure S24. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of methyl 4-(1-hydroxyethyl)benzoate.



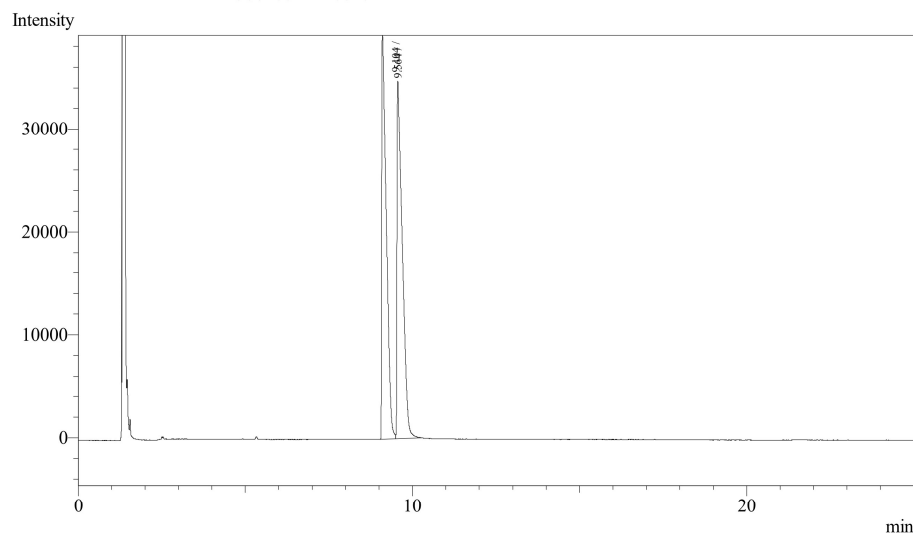
(*R*)-1-phenyl-2,2,2-trifluoroethanol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.01 mL/min, progression: 130/25, detector temperature: 275°C, t_{maj} : 9.5 min, t_{min} : 9.2 min, t_{SM} : 1.8 min, $[\alpha_D^{20}]$: -7.6 (c = 0.01 g/mL, CHCl₃)

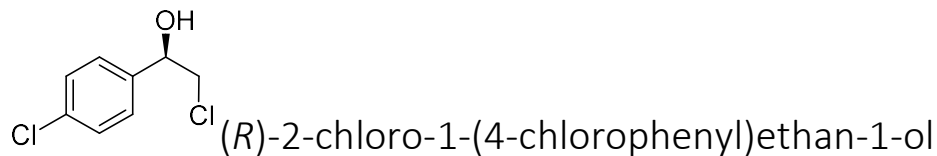


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	1.794	170350	99725	17.796				
2	8.349	275346	49664	28.764		S		
3	9.248	66607	12421	6.958				
4	9.549	444963	38454	46.483		SV		
Total		957266	200264					



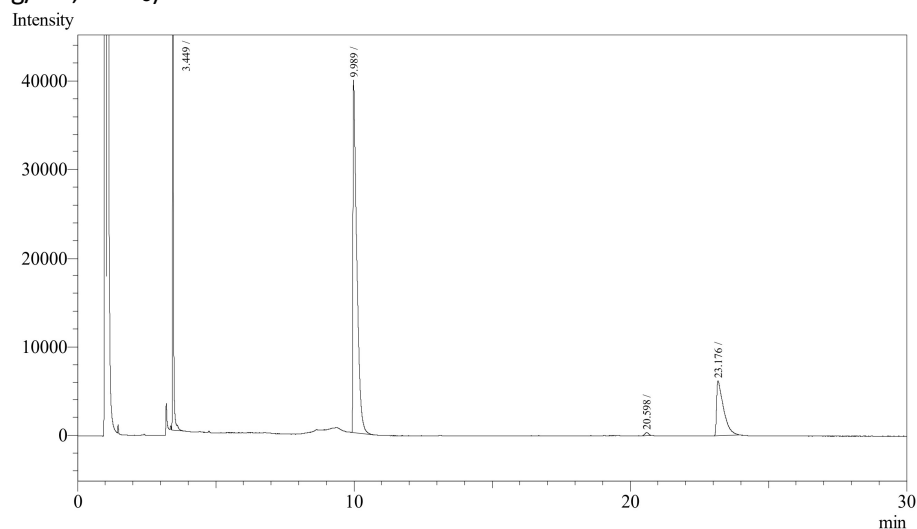
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	9.104	378237	39519	49.685				
2	9.564	383041	34689	50.315		SV		
Total		761278	74208					

Figure S25. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-phenyl-2,2,2-trifluoroethanol.

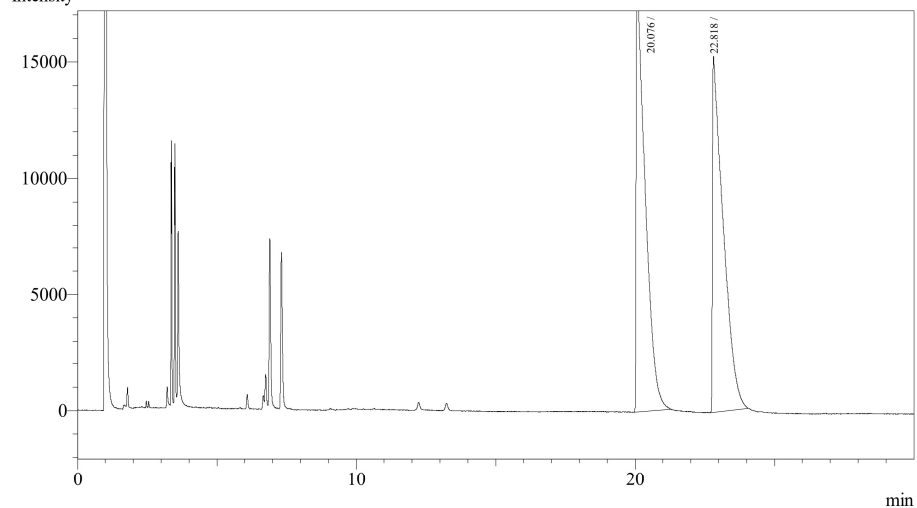


Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.47 mL/min, progression: 145/30, detector temperature: 275°C, t_{maj}: 23.2 min, t_{min}: 20.6 min, t_{SM}: 10.0 min, [α_D^{20}]: -26.6 (c = 0.01 g/mL, CHCl₃)

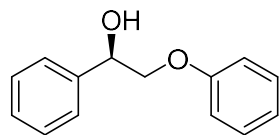


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	3.449	131699	53407	21.126		S		
2	9.989	381640	39764	61.220				
3	20.598	3219	345	0.516		V		
4	23.176	106837	6229	17.138				
Total		623395	99745					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	20.076	416443	18388	50.351				
2	22.818	410635	15299	49.649				
Total		827078	33687					

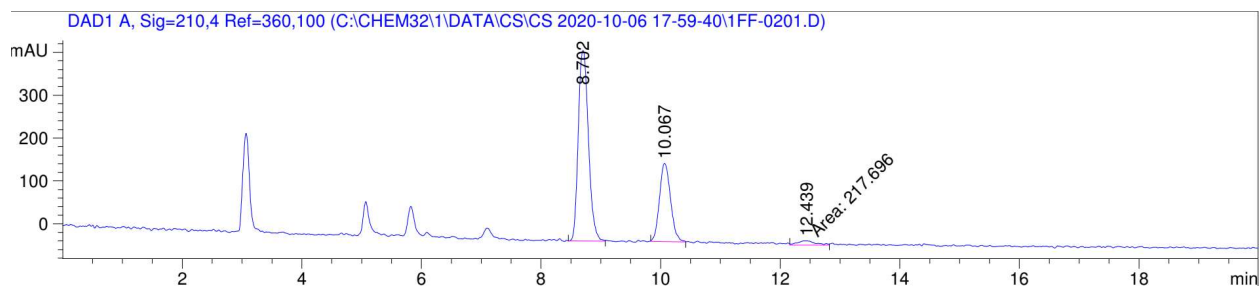
Figure S26. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 2-chloro-1-(4-chlorophenyl)ethan-1-ol.



2-phenoxy-1-phenylethanol

$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.52-7.46 (m, 2H), 7.43 (ddd, $J = 7.6, 6.4, 1.4$ Hz, 2H), 7.40-7.30 (m, 3H), 7.02 (tq, $J = 7.3, 1.0$ Hz, 1H), 6.98-6.94 (m, 2H), 5.14 (dd, $J = 8.8, 3.2$ Hz, 1H), 4.13 (dd, $J = 9.7, 3.3$ Hz, 1H), 4.05 (dd, $J = 9.6, 8.7$ Hz, 1H), 3.04 (br s, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3): δ 158.45, 139.81, 129.61, 128.60, 128.20, 126.36, 121.33, 114.71, 73.35, 72.60.

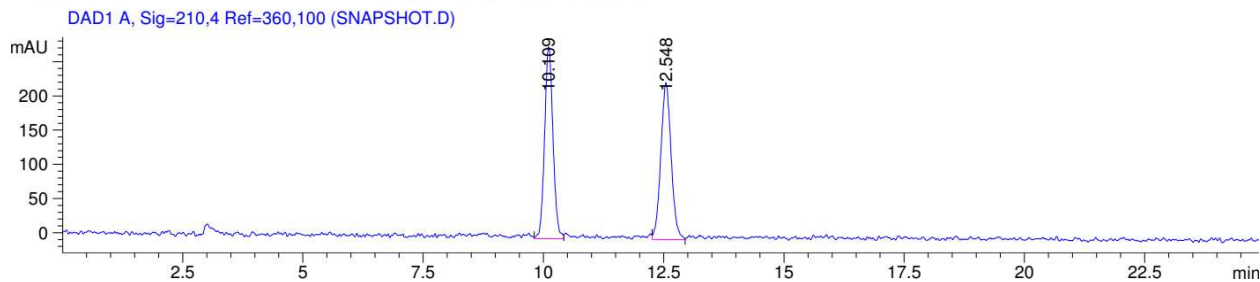
Product ratio was determined by HPLC, Chiralpak AD-H column, IPA/Hex = 10:90 – 25 – 30:70, 1.0 mL/min. t_{maj} : 10.1 min, t_{min} : 12.4 min, t_{SM} : 8.7 min, $[\alpha_D^{20}]$: -34.8 ($c = 0.01$ g/mL, CHCl_3)



Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.702	BB	0.1879	5257.26123	444.77356	67.2013
2	10.067	BB	0.1982	2348.19189	182.43895	30.0159
3	12.439	MM	0.3544	217.69557	10.23825	2.7827

Totals : 7823.14870 637.45076

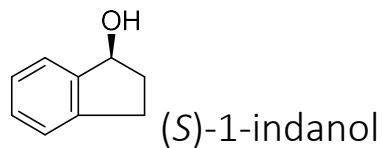


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.109	VV	0.1839	3408.36499	280.24716	49.8309
2	12.548	VV	0.2047	3431.49976	229.13759	50.1691

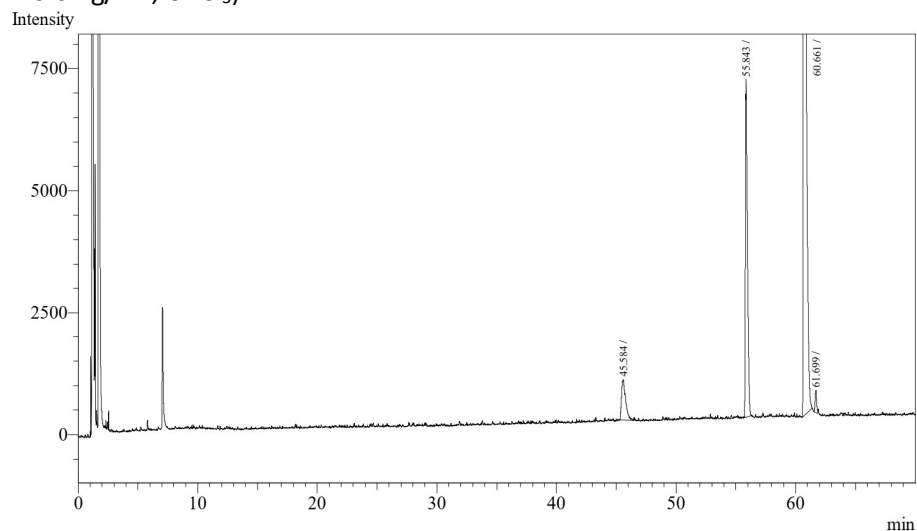
Totals : 6839.86475 509.38475

Figure S27. HPLC chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 2-phenoxy-1-phenylethanol.

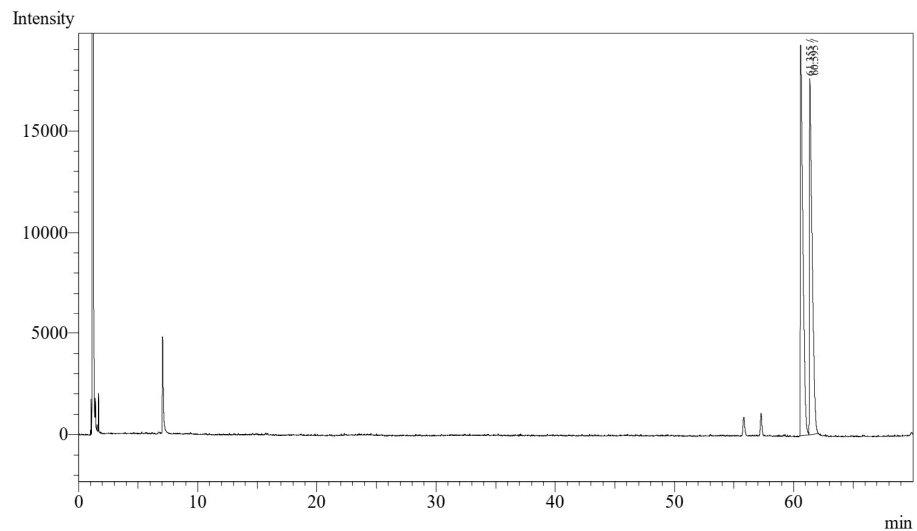


Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.48 mL/min, progression: 90/50-13-120/10, detector temperature: 275°C, t_{maj} : 60.7 min, t_{min} : 61.7 min, t_{SM} : 45.6 min, $[\alpha_D^{20}]$: 6.8 (c = 0.01 g/mL, CHCl₃)

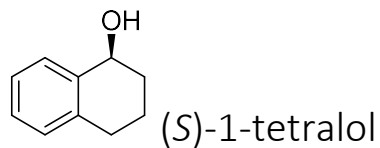


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	45.584	19507	825	5.194				
2	55.843	82612	6926	21.996		V		
3	60.661	269488	17801	71.754				
4	61.699	3963	450	1.055				
Total		375570	26002					



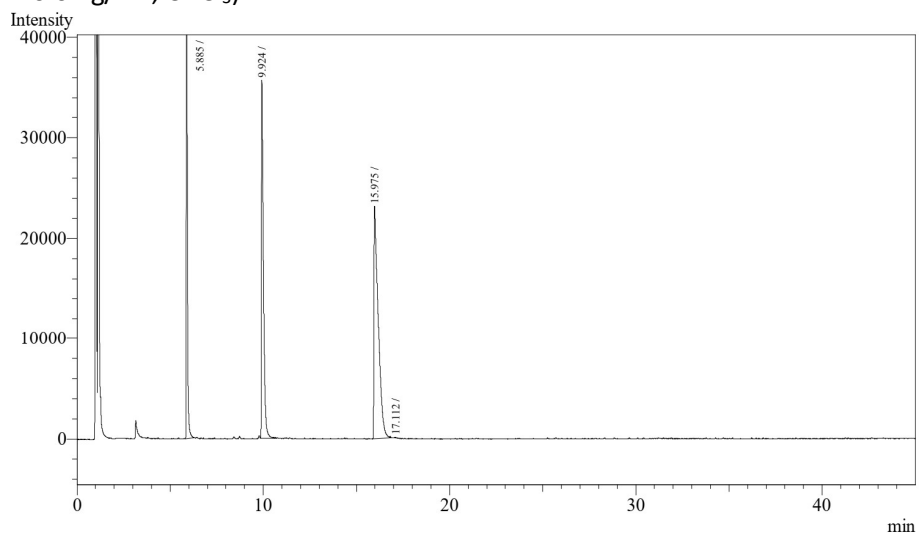
Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	60.595	281515	19303	50.124		S		
2	61.355	280118	17577	49.876		V		
Total		561633	36880					

Figure S28. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-indanol.

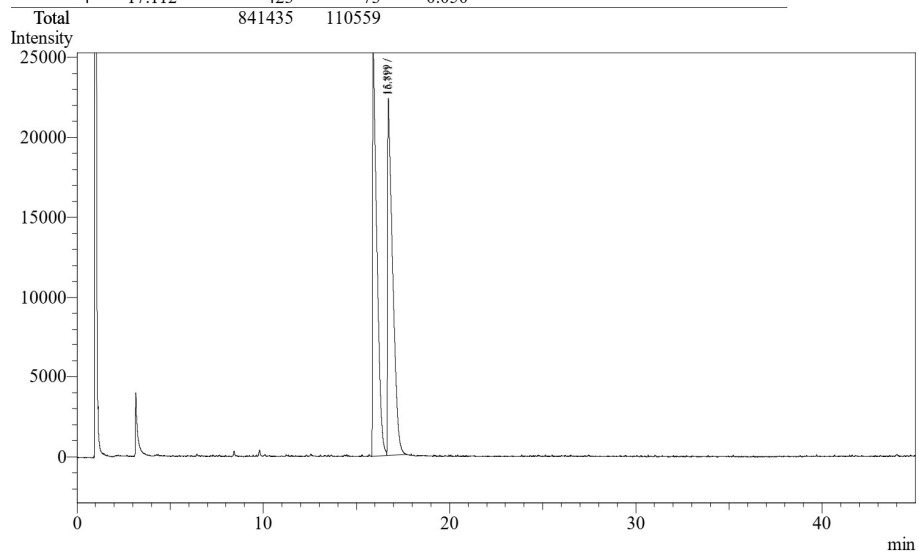


Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 1.51 mL/min, progression: 110/40-4-130/10, detector temperature: 275°C, t_{maj}: 16.0 min, t_{min}: 17.1 min, t_{SM}: 5.9 min, [α_D²⁰]: 28.0 (c = 0.01 g/mL, CHCl₃)

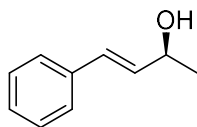


Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	5.885	205393	51678	24.410				
2	9.924	267491	35628	31.790		S		
3	15.975	368128	23180	43.750		S		
4	17.112	423	73	0.050				
Total		841435	110559					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	15.899	413427	25927	49.935				
2	16.711	414501	22359	50.065		SV		
Total		827928	48286					

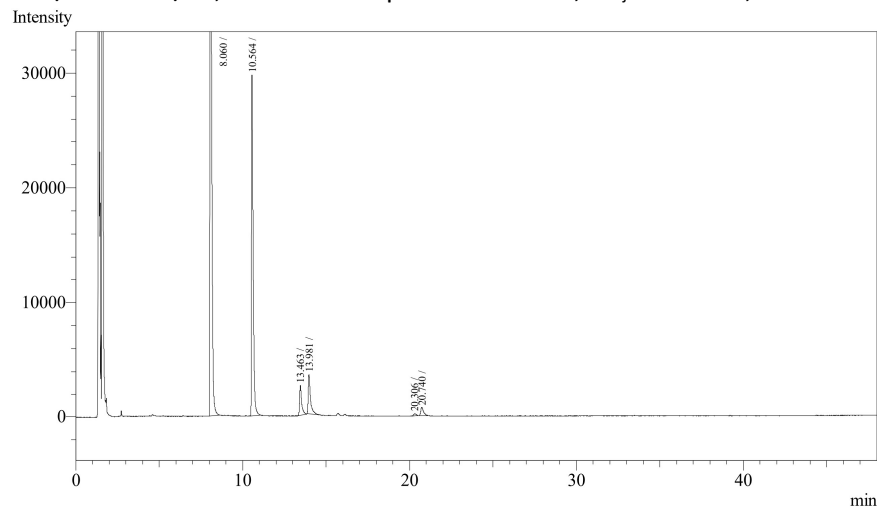
Figure S29. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of 1-tetralol.



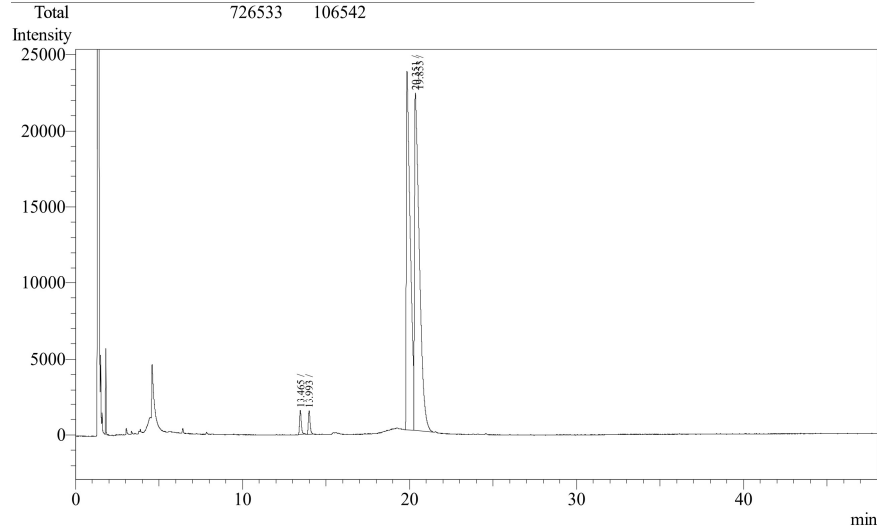
trans-4-phenyl-3-buten-2-ol

Gas chromatograph was developed using following condition:

Carrier gas H₂, Injector temperature: 250°C, Split ratio: 50, column flow: 0.98 mL/min, progression: 125/20-5-140/25, detector temperature: 275°C, t_{maj}: 20.7 min, t_{min}: 20.3 min, t_{SM}: 8.1 min



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	8.060	459866	69724	63.296				
2	10.564	200418	29732	27.586				
3	13.463	22950	2655	3.159				
4	13.981	33181	3519	4.567				
5	20.306	1918	186	0.264				
6	20.740	8200	726	1.129				
Total		726533	106542					



Peak#	Ret.Time	Area	Height	Conc.	Unit	Mark	ID#	Cmpd Name
1	13.465	10911	1572	1.266				
2	13.993	11139	1531	1.293				
3	19.853	385350	23580	44.718				
4	20.351	454342	22217	52.724		V		
Total		861742	48900					

Figure S30. Gas chromatogram of catalytic mixture (top) and racemic mixture (bottom) of *trans*-4-phenyl-3-buten-2-ol.

Calculations

In order for comparison with past work with iron catalysts,³ the calculations were standardized using Gaussian09⁴ with the functional M11L and basis set 6-31G** for all non-metal elements and SDD for the manganese. An ultrafine integration grid, a temperature of 353 K and the smd toluene solvation model were employed during optimization. An entropy value of 17.2 eu was used for dihydrogen⁵ in toluene at 353 K instead of the gas phase (1 atm, 353 K) value of 32.3 eu (provided by the Gaussian09 calculation) in order to obtain exoergic hydrogenation reactions as observed experimentally (Table S1). This may still have an error of up to 3 eu but there is no experimental value for comparison. Transition states were located using the qst3 method and verified using IRC calculations. The Python program Goodvibes was used to correct for frequency modes of less than 50 cm⁻¹ using the Truhlar method.⁵

Table S1. Free energies of hydrogenation of the ketones using an entropy of 17.2 eu for H₂ at 353 K, corrected from the gas phase value of 32.3 eu.

Ketone	ΔG^{hydrog} kcal/mol with $S = 32.3$	ΔG^{hydrog} kcal/mol with $S = 17.2$
MeCOPh	1.6	-3.7
MeCOC ₆ H ₂ (3,5-CF ₃) ₂	0.5	-4.8
CF ₃ COPh	-6.2	-11.6
MeCO(2-C ₅ H ₄ N)	2.0	-3.3
1-indanone	5.6	0.2

Energies, transition state wavenumbers, Cartesian coordinates.

1Mn

ΔH^{353} -2387.243149 Hartrees, ΔS^{353} 274.6 eu, ΔG^{353} -2387.397628 Hartrees

```

15  3.387031000  0.553181000  0.350720000
 1  3.548443000  2.967066000  0.631155000
 6 -1.555304000  0.649300000  -0.166249000
 6  1.269741000 -0.726207000  2.085736000
 1 -1.567220000  0.973401000  -1.225021000
25  1.403388000 -0.488305000  0.354883000
 8  1.151156000 -0.772732000  3.232719000
 1 -0.870196000  1.582873000  1.659337000
 6 -0.626486000  1.632154000  0.562604000
 1  3.356520000  2.131878000  2.164557000
 6  2.999728000  2.144140000  1.122106000
15 -0.707407000 -0.996720000  -0.239172000
 6  4.922506000 -0.027068000  1.183148000
 1  5.621485000  0.835498000  1.203382000
 6  3.839824000  1.068945000  -1.366261000
 1  3.040812000  1.812789000  -1.573922000
 6  1.494334000  2.362419000  1.072530000
 1  1.299368000  3.363970000  0.636075000
 1  1.102592000  2.443168000  2.119492000
 7  0.765608000  1.333870000  0.369749000
 6  5.171272000  1.772047000  -1.491646000
 1  5.272890000  2.226582000  -2.490913000
 1  5.296447000  2.585071000  -0.758511000

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1	6.024159000	1.085263000	-1.369256000
6	3.679172000	-0.046025000	-2.375500000
1	2.655197000	-0.458372000	-2.372185000
1	3.875732000	0.323679000	-3.395538000
1	4.367673000	-0.888262000	-2.197810000
6	4.610857000	-0.438588000	2.605728000
1	5.540895000	-0.676038000	3.147351000
1	4.085181000	0.333626000	3.188178000
1	3.983759000	-1.345942000	2.623403000
6	5.583732000	-1.179929000	0.460068000
1	4.902018000	-2.040919000	0.362379000
1	5.942080000	-0.923665000	-0.546932000
1	6.459353000	-1.530407000	1.030963000
6	-0.959485000	-1.498453000	-1.980757000
6	-2.061600000	-1.094410000	-2.731788000
6	-0.029875000	-2.344872000	-2.580706000
6	-2.222650000	-1.514776000	-4.039893000
6	-0.191732000	-2.766639000	-3.888805000
6	-1.286061000	-2.349113000	-4.624355000
1	-2.823033000	-0.442656000	-2.290713000
1	0.838433000	-2.693532000	-2.014406000
1	-3.096408000	-1.184603000	-4.609324000
1	0.553191000	-3.429800000	-4.337870000
1	-1.412142000	-2.677643000	-5.659883000
6	-1.700135000	-2.257285000	0.620206000
6	-3.029631000	-2.513612000	0.287854000
6	-1.096879000	-3.030024000	1.606378000
6	-3.739050000	-3.500043000	0.944302000
6	-1.807336000	-4.023065000	2.259952000
6	-3.130179000	-4.255353000	1.933807000
1	-3.527400000	-1.927223000	-0.492035000
1	-0.045730000	-2.861636000	1.859323000
1	-4.783764000	-3.683447000	0.677777000
1	-1.315132000	-4.623026000	3.030481000
1	-3.693420000	-5.038521000	2.449689000
6	-2.953641000	0.719097000	0.360151000
6	-3.247978000	0.349259000	1.670510000
6	-3.986076000	1.207092000	-0.433070000
6	-4.536798000	0.442803000	2.160768000
6	-5.278451000	1.299581000	0.054333000
6	-5.558666000	0.912823000	1.352473000
1	-2.450602000	-0.035385000	2.317729000
1	-3.761323000	1.545369000	-1.452081000
1	-4.746796000	0.140435000	3.190791000
1	-6.073863000	1.690419000	-0.587127000
1	-6.578528000	0.985435000	1.740971000
6	-1.041212000	3.020537000	0.107407000
6	-1.877358000	3.810966000	0.880729000

6	-0.637814000	3.495219000	-1.135933000
6	-2.303830000	5.048339000	0.426852000
6	-1.053466000	4.732809000	-1.588949000
6	-1.891868000	5.513841000	-0.808653000
1	-2.205141000	3.441344000	1.860087000
1	0.034718000	2.876373000	-1.743870000
1	-2.966008000	5.657927000	1.049416000
1	-0.718568000	5.096861000	-2.565618000
1	-2.222664000	6.493443000	-1.166468000
6	2.078101000	-2.116312000	0.051304000
8	2.516895000	-3.177935000	-0.083329000

3TS

ΔH^{353} -2387.232044 Hartrees, ΔS^{353} 270.4 eu, ΔG^{353} -2387.384168 Hartrees, $93i$ cm⁻¹

15	3.387031000	0.553181000	0.350720000
1	3.548443000	2.967066000	0.631155000
6	-1.555304000	0.649300000	-0.166249000
6	1.269741000	-0.726207000	2.085736000
1	-1.567220000	0.973401000	-1.225021000
25	1.403388000	-0.488305000	0.354883000
8	1.151156000	-0.772732000	3.232719000
1	-0.870196000	1.582873000	1.659337000
6	-0.626486000	1.632154000	0.562604000
1	3.356520000	2.131878000	2.164557000
6	2.999728000	2.144140000	1.122106000
15	-0.707407000	-0.996720000	-0.239172000
6	4.922506000	-0.027068000	1.183148000
1	5.621485000	0.835498000	1.203382000
6	3.839824000	1.068945000	-1.366261000
1	3.040812000	1.812789000	-1.573922000
6	1.494334000	2.362419000	1.072530000
1	1.299368000	3.363970000	0.636075000
1	1.102592000	2.443168000	2.119492000
7	0.765608000	1.333870000	0.369749000
6	5.171272000	1.772047000	-1.491646000
1	5.272890000	2.226582000	-2.490913000
1	5.296447000	2.585071000	-0.758511000
1	6.024159000	1.085263000	-1.369256000
6	3.679172000	-0.046025000	-2.375500000
1	2.655197000	-0.458372000	-2.372185000
1	3.875732000	0.323679000	-3.395538000
1	4.367673000	-0.888262000	-2.197810000
6	4.610857000	-0.438588000	2.605728000
1	5.540895000	-0.676038000	3.147351000
1	4.085181000	0.333626000	3.188178000
1	3.983759000	-1.345942000	2.623403000
6	5.583732000	-1.179929000	0.460068000
1	4.902018000	-2.040919000	0.362379000

1	5.942080000	-0.923665000	-0.546932000
1	6.459353000	-1.530407000	1.030963000
6	-0.959485000	-1.498453000	-1.980757000
6	-2.061600000	-1.094410000	-2.731788000
6	-0.029875000	-2.344872000	-2.580706000
6	-2.222650000	-1.514776000	-4.039893000
6	-0.191732000	-2.766639000	-3.888805000
6	-1.286061000	-2.349113000	-4.624355000
1	-2.823033000	-0.442656000	-2.290713000
1	0.838433000	-2.693532000	-2.014406000
1	-3.096408000	-1.184603000	-4.609324000
1	0.553191000	-3.429800000	-4.337870000
1	-1.412142000	-2.677643000	-5.659883000
6	-1.700135000	-2.257285000	0.620206000
6	-3.029631000	-2.513612000	0.287854000
6	-1.096879000	-3.030024000	1.606378000
6	-3.739050000	-3.500043000	0.944302000
6	-1.807336000	-4.023065000	2.259952000
6	-3.130179000	-4.255353000	1.933807000
1	-3.527400000	-1.927223000	-0.492035000
1	-0.045730000	-2.861636000	1.859323000
1	-4.783764000	-3.683447000	0.677777000
1	-1.315132000	-4.623026000	3.030481000
1	-3.693420000	-5.038521000	2.449689000
6	-2.953641000	0.719097000	0.360151000
6	-3.247978000	0.349259000	1.670510000
6	-3.986076000	1.207092000	-0.433070000
6	-4.536798000	0.442803000	2.160768000
6	-5.278451000	1.299581000	0.054333000
6	-5.558666000	0.912823000	1.352473000
1	-2.450602000	-0.035385000	2.317729000
1	-3.761323000	1.545369000	-1.452081000
1	-4.746796000	0.140435000	3.190791000
1	-6.073863000	1.690419000	-0.587127000
1	-6.578528000	0.985435000	1.740971000
6	-1.041212000	3.020537000	0.107407000
6	-1.877358000	3.810966000	0.880729000
6	-0.637814000	3.495219000	-1.135933000
6	-2.303830000	5.048339000	0.426852000
6	-1.053466000	4.732809000	-1.588949000
6	-1.891868000	5.513841000	-0.808653000
1	-2.205141000	3.441344000	1.860087000
1	0.034718000	2.876373000	-1.743870000
1	-2.966008000	5.657927000	1.049416000
1	-0.718568000	5.096861000	-2.565618000
1	-2.222664000	6.493443000	-1.166468000
6	2.078101000	-2.116312000	0.051304000
8	2.516895000	-3.177935000	-0.083329000

6Mn

ΔH^{353} -2387.234535 Hartrees ΔS^{353} 272.9 eu ΔG^{353} -2387.388064 Hartrees

1	6.186344000	1.486464000	0.100439000
1	4.311226000	0.222424000	-3.549659000
1	-3.683945000	-1.271295000	-2.618699000
6	-4.637101000	-0.995162000	-2.139057000
6	0.605133000	1.673890000	-0.327121000
15	0.745931000	-0.991375000	0.310282000
6	-2.993883000	2.218014000	0.163026000
1	-0.800471000	-2.604710000	2.140355000
1	3.365205000	-1.398932000	4.529359000
6	3.031595000	0.403596000	-1.837444000
7	-0.742433000	1.348931000	0.048460000
1	3.571938000	-1.931311000	0.372124000
6	1.704993000	-3.917654000	-2.362915000
1	-0.033054000	-2.782309000	-1.820340000
6	5.388328000	0.850264000	-1.794285000
6	-2.010437000	-2.140612000	-0.059130000
1	3.005760000	-0.593752000	2.240494000
6	-4.580117000	0.411373000	-1.578344000
6	1.683609000	-2.226883000	-0.642188000
6	2.234901000	-1.211474000	2.714790000
6	3.044505000	-4.157392000	-2.122026000
6	-1.604500000	2.415650000	-0.380465000
1	1.172141000	-4.484012000	-3.131913000
1	3.580823000	-4.913081000	-2.703427000
6	4.249611000	0.472260000	-2.486510000
25	-1.385593000	-0.464953000	-0.163193000
1	-4.875783000	1.289034000	-3.522028000
15	-3.451448000	0.483261000	-0.116948000
1	-1.635867000	2.486327000	-1.500084000
1	6.352440000	0.902616000	-2.308213000
1	-5.419586000	-1.067361000	-2.912340000
6	4.074388000	1.102464000	0.195444000
1	-4.217627000	2.436062000	-2.345379000
1	1.768352000	0.918804000	1.281752000
6	-4.186062000	1.384655000	-2.666987000
6	1.029448000	-2.957961000	-1.627796000
1	-5.591885000	0.688912000	-1.217339000
6	3.030840000	-2.489763000	-0.398855000
6	2.926579000	0.707148000	-0.481955000
1	3.999551000	1.383668000	1.252978000
8	-2.400551000	-3.228768000	-0.054378000
6	1.609778000	0.645426000	0.221210000
6	1.069640000	-1.536090000	2.023335000
6	5.296411000	1.169712000	-0.451507000
1	0.703764000	1.684997000	-1.447032000

6	0.330291000	-2.785806000	3.953106000
1	1.653830000	-2.806983000	5.649953000
1	-1.241385000	3.409885000	-0.049337000
1	-3.173806000	1.180945000	-3.053281000
1	-2.956966000	2.355396000	1.260165000
1	-0.428512000	-3.407812000	4.436477000
6	1.490122000	-2.452149000	4.628468000
6	0.121741000	-2.330654000	2.662879000
1	-4.851922000	-1.765805000	-1.384059000
1	2.139622000	0.087378000	-2.392676000
6	2.442884000	-1.665140000	4.004756000
1	4.764763000	-3.629525000	-0.938248000
1	-3.714515000	2.954893000	-0.228817000
6	3.705635000	-3.442263000	-1.136421000
6	-4.542748000	0.134727000	1.337288000
1	-6.338020000	1.235006000	0.769176000
6	-5.179867000	-1.235109000	1.309360000
6	-5.593003000	1.195938000	1.581361000
1	-4.461347000	-2.047344000	1.123254000
1	-3.823680000	0.160712000	2.183470000
1	-5.667365000	-1.447119000	2.274906000
1	-5.968611000	-1.299917000	0.540831000
1	-5.176041000	2.206990000	1.698339000
1	-6.150795000	0.970227000	2.505487000
6	1.094096000	3.029722000	0.147584000
6	1.814861000	3.865758000	-0.691089000
6	0.881834000	3.427095000	1.463596000
6	2.313726000	5.073627000	-0.231163000
6	1.369805000	4.635095000	1.923969000
6	2.090456000	5.463154000	1.076979000
1	1.992232000	3.555874000	-1.728111000
1	0.300193000	2.772020000	2.124646000
1	2.882322000	5.720326000	-0.906467000
1	1.185296000	4.939316000	2.959245000
1	2.478045000	6.419311000	1.441113000
6	-1.201100000	-0.517125000	-1.905877000
8	-1.027126000	-0.461642000	-3.045948000

H₂

ΔH^{353} -1.164092 Hartrees ΔS^{353} 17.2 eu ΔG^{353} -1.174287 Hartrees

1	0.000000000	0.000000000	0.374939000
1	0.000000000	0.000000000	-0.374939000

1TS^{H2}

ΔH^{353} -2388.388076 Hartrees, ΔS^{353} 272.9 eu, ΔG^{353} -2388.541617 Hartrees, 914.6075i cm⁻¹

1	6.152360000	1.444885000	0.566432000
1	4.513710000	0.487745000	-3.285015000
1	-3.732424000	-1.016005000	-2.629181000
6	-4.681073000	-0.757247000	-2.131013000

6	0.639266000	1.665651000	-0.194405000
15	0.694885000	-1.057918000	0.248395000
6	-2.964195000	2.266878000	0.363288000
1	-0.785084000	-2.898085000	1.898595000
1	3.460202000	-2.009072000	4.286213000
6	3.133434000	0.503952000	-1.643408000
7	-0.698664000	1.457411000	0.251148000
1	3.501859000	-2.056766000	0.132450000
6	1.537650000	-3.663151000	-2.777662000
1	-0.160852000	-2.560447000	-2.071180000
6	5.477015000	0.969816000	-1.421018000
6	-2.087539000	-2.098707000	-0.190680000
1	3.022145000	-0.903709000	2.141240000
6	-4.601686000	0.608083000	-1.478950000
6	1.590428000	-2.179555000	-0.874809000
6	2.268851000	-1.584807000	2.551744000
6	2.874264000	-3.961807000	-2.593284000
6	-1.578576000	2.493921000	-0.183605000
1	0.976319000	-4.125642000	-3.594301000
1	3.379673000	-4.659008000	-3.267981000
6	4.386675000	0.642765000	-2.209688000
25	-1.434075000	-0.444687000	-0.120788000
1	-4.919671000	1.623896000	-3.349946000
15	-3.460741000	0.557331000	-0.024042000
1	-1.616627000	2.535496000	-1.304365000
1	6.468583000	1.076836000	-1.869992000
1	-5.465500000	-0.767611000	-2.905692000
6	4.044924000	1.033053000	0.500366000
1	-4.222010000	2.675660000	-2.109651000
1	1.676372000	0.761318000	1.428100000
6	-4.212488000	1.648742000	-2.504300000
6	0.900727000	-2.778354000	-1.923593000
1	-5.606387000	0.870061000	-1.088926000
6	2.933533000	-2.505212000	-0.688943000
6	2.944365000	0.687067000	-0.275604000
1	3.903673000	1.224160000	1.571135000
8	-2.501548000	-3.173592000	-0.269069000
6	1.584728000	0.576091000	0.338505000
6	1.081585000	-1.819588000	1.862553000
6	5.301618000	1.168563000	-0.063335000
1	0.678430000	1.626809000	-1.317612000
6	0.414840000	-3.332534000	3.621680000
1	1.796850000	-3.578189000	5.254121000
1	-1.226683000	3.498081000	0.135470000
1	-3.211493000	1.458901000	-2.924391000
1	-2.925511000	2.340138000	1.467306000
1	-0.325082000	-4.021268000	4.039494000
6	1.596164000	-3.085558000	4.298440000

6	0.158692000	-2.702188000	2.417143000
1	-4.906564000	-1.572013000	-1.426443000
1	2.282153000	0.230320000	-2.278123000
6	2.522286000	-2.209926000	3.760172000
1	4.626577000	-3.618800000	-1.388494000
1	-3.673250000	3.038737000	0.022572000
6	3.570196000	-3.382530000	-1.544425000
6	-4.562483000	0.165124000	1.409481000
1	-5.208781000	2.225179000	1.812607000
6	-5.190175000	-1.206767000	1.333326000
6	-5.618766000	1.212026000	1.685803000
1	-4.461445000	-2.006313000	1.131988000
1	-3.844927000	0.164977000	2.256082000
1	-5.686695000	-1.451921000	2.286386000
1	-5.969630000	-1.255850000	0.554037000
1	-6.157917000	0.966586000	2.616023000
1	-6.380327000	1.258205000	0.889745000
6	1.214655000	3.006239000	0.217559000
6	1.921285000	3.792381000	-0.679801000
6	1.082745000	3.444908000	1.530006000
6	2.489861000	4.989223000	-0.277591000
6	1.643300000	4.642151000	1.934126000
6	2.352003000	5.417876000	1.030435000
1	2.033285000	3.450636000	-1.715763000
1	0.507894000	2.834513000	2.237628000
1	3.046372000	5.596637000	-0.997736000
1	1.524035000	4.978943000	2.968771000
1	2.796302000	6.365516000	1.348917000
6	-1.240732000	-0.292802000	-1.885482000
8	-1.076724000	-0.130867000	-3.015760000
1	-1.087738000	0.607709000	1.218032000
1	-1.479905000	-0.224145000	1.558282000

5Mn

ΔH^{353} -2388.416589 Hartrees, ΔS^{353} 272.75 eu, ΔG^{353} -2388.570027 Hartrees

1	6.179733000	1.152964000	0.686352000
1	4.463764000	0.618552000	-3.212880000
1	-3.945263000	-0.875301000	-2.574426000
6	-4.867487000	-0.466694000	-2.126093000
6	0.664755000	1.690402000	-0.043620000
15	0.631395000	-1.067079000	0.225529000
6	-2.979756000	2.225207000	0.571227000
1	-0.815601000	-3.117468000	1.571522000
1	3.193385000	-2.277537000	4.353128000
6	3.097039000	0.580954000	-1.560991000
7	-0.701782000	1.451357000	0.406462000
1	3.398367000	-2.198436000	0.274761000
6	1.715639000	-3.300767000	-3.019321000

1	-0.016387000	-2.229380000	-2.341179000
6	5.465076000	0.886615000	-1.325917000
6	-2.074848000	-2.041818000	-0.553990000
1	2.848238000	-0.982423000	2.300708000
6	-4.589162000	0.833111000	-1.403572000
6	1.603433000	-2.098569000	-0.929329000
6	2.103488000	-1.734150000	2.583428000
6	3.016941000	-3.676827000	-2.745139000
6	-1.600066000	2.543029000	0.060380000
1	1.232139000	-3.621393000	-3.946641000
1	3.573243000	-4.293238000	-3.457541000
6	4.352342000	0.692457000	-2.127393000
25	-1.442719000	-0.426851000	-0.218302000
1	-4.782525000	1.990360000	-3.207902000
15	-3.433061000	0.540014000	0.014267000
1	-1.592761000	2.629385000	-1.043469000
1	6.458742000	0.970136000	-1.775020000
1	-5.586986000	-0.310242000	-2.947082000
6	4.050618000	0.875971000	0.609453000
1	-3.918607000	2.855913000	-1.933173000
1	1.671359000	0.673453000	1.530586000
6	-4.064285000	1.860648000	-2.380985000
6	1.014614000	-2.517354000	-2.117345000
1	-5.538843000	1.222818000	-0.985585000
6	2.909373000	-2.503227000	-0.656595000
6	2.928151000	0.659051000	-0.180441000
1	3.929360000	0.981154000	1.694360000
8	-2.484133000	-3.104755000	-0.754082000
6	1.567217000	0.548157000	0.433094000
6	0.983031000	-1.952402000	1.787171000
6	5.309975000	0.982460000	0.045094000
1	0.624505000	1.680620000	-1.151849000
6	0.290605000	-3.683514000	3.321503000
1	1.565404000	-4.028545000	5.023033000
1	-1.245679000	3.513093000	0.460353000
1	-3.111479000	1.550171000	-2.837624000
1	-2.965194000	2.222821000	1.677946000
1	-0.431775000	-4.454096000	3.606189000
6	1.403226000	-3.446928000	4.110969000
6	0.079748000	-2.938721000	2.176460000
1	-5.284305000	-1.249041000	-1.473682000
1	2.228521000	0.400882000	-2.206610000
6	2.308238000	-2.469833000	3.739265000
1	4.639132000	-3.576545000	-1.331473000
1	-3.699286000	3.007544000	0.277527000
6	3.611641000	-3.277954000	-1.558829000
6	-4.525195000	-0.000560000	1.410788000
1	-6.555228000	0.511218000	0.805926000

6	-4.797523000	-1.485547000	1.444151000
6	-5.803886000	0.790573000	1.563432000
1	-3.871345000	-2.077197000	1.412785000
1	-3.871977000	0.223232000	2.279499000
1	-5.326583000	-1.751768000	2.374625000
1	-5.441017000	-1.816263000	0.612677000
1	-5.653742000	1.881034000	1.496517000
1	-6.263544000	0.589511000	2.545540000
1	-0.694466000	1.370599000	1.426218000
6	1.241214000	3.016606000	0.388602000
6	1.794928000	3.880025000	-0.544945000
6	1.255744000	3.385520000	1.729533000
6	2.351319000	5.085308000	-0.152759000
6	1.801787000	4.592678000	2.124217000
6	2.353313000	5.445952000	1.182581000
1	1.795282000	3.592757000	-1.602756000
1	0.826797000	2.718260000	2.488607000
1	2.787125000	5.752326000	-0.902066000
1	1.799806000	4.871143000	3.182108000
1	2.788449000	6.399553000	1.494476000
6	-1.158007000	-0.029764000	-1.936148000
1	-1.688742000	-0.670263000	1.325442000
8	-0.962868000	0.213105000	-3.053692000

2TS^{H2}

ΔH^{353} -2388.381058 Hartrees, ΔS^{353} 273.2 eu, ΔG^{353} -2388.534774 Hartrees, 538i cm⁻¹

15	3.469503000	0.516857000	0.060386000
1	3.636534000	2.654908000	-1.153314000
6	-1.433127000	0.535500000	-0.588641000
6	2.009294000	-2.099444000	0.778672000
1	-1.054405000	0.524739000	-1.632631000
25	1.446666000	-0.503198000	0.217586000
8	2.341471000	-3.129549000	1.173973000
1	-0.900760000	1.465421000	1.256435000
6	-0.652677000	1.625065000	0.175812000
1	3.065076000	2.864836000	0.509563000
6	2.975189000	2.222028000	-0.383389000
15	-0.740504000	-1.021483000	0.157138000
6	4.586132000	0.755612000	1.514220000
1	5.315224000	1.538888000	1.218068000
6	4.569920000	0.048537000	-1.348864000
1	3.945458000	0.347505000	-2.218390000
6	1.531726000	2.212515000	-0.843811000
1	1.491896000	1.810508000	-1.893005000
1	1.182012000	3.262482000	-0.914750000
7	0.767301000	1.435052000	0.069255000
6	5.863822000	0.827133000	-1.423960000
1	6.367730000	0.639147000	-2.386307000

1	5.721762000	1.916610000	-1.345150000
1	6.573088000	0.529408000	-0.634316000
6	4.818865000	-1.439394000	-1.467057000
1	3.896361000	-2.035166000	-1.407338000
1	5.291395000	-1.669420000	-2.435893000
1	5.498231000	-1.813719000	-0.685683000
6	3.826184000	1.246609000	2.726691000
1	4.533831000	1.570385000	3.507366000
1	3.157890000	2.097785000	2.521518000
1	3.208082000	0.442981000	3.157565000
6	5.337197000	-0.507552000	1.873090000
1	4.648813000	-1.358336000	2.019481000
1	6.079991000	-0.806860000	1.120271000
1	5.881993000	-0.371009000	2.822086000
6	-1.212633000	-2.412856000	-0.909323000
6	-1.381362000	-2.286222000	-2.284393000
6	-1.264757000	-3.690277000	-0.351142000
6	-1.625872000	-3.396707000	-3.073403000
6	-1.503379000	-4.799092000	-1.140743000
6	-1.692722000	-4.655222000	-2.504667000
1	-1.304020000	-1.306484000	-2.763497000
1	-1.117010000	-3.820288000	0.726792000
1	-1.762159000	-3.272375000	-4.151536000
1	-1.541535000	-5.790869000	-0.681119000
1	-1.885699000	-5.531988000	-3.129290000
6	-1.756578000	-1.341514000	1.632345000
6	-3.073286000	-1.790835000	1.524321000
6	-1.223554000	-1.133814000	2.900448000
6	-3.835986000	-2.009391000	2.655418000
6	-1.989732000	-1.352291000	4.033638000
6	-3.296593000	-1.787435000	3.912272000
1	-3.511807000	-1.966075000	0.535519000
1	-0.184857000	-0.803396000	2.999618000
1	-4.868376000	-2.355941000	2.553308000
1	-1.553888000	-1.188072000	5.023425000
1	-3.901747000	-1.963747000	4.806542000
1	1.189855000	0.852476000	1.237414000
6	-2.919636000	0.680831000	-0.605845000
6	-3.628469000	1.096551000	0.520898000
6	-3.643228000	0.403243000	-1.762680000
6	-5.005418000	1.212441000	0.491714000
6	-5.021675000	0.512769000	-1.792367000
6	-5.710387000	0.915564000	-0.661976000
1	-3.096348000	1.325810000	1.450296000
1	-3.107461000	0.101991000	-2.670010000
1	-5.537024000	1.540514000	1.389859000
1	-5.563551000	0.286532000	-2.715545000
1	-6.800145000	1.006746000	-0.682262000

6	-1.097863000	3.029313000	-0.139641000
6	-1.024148000	3.994343000	0.856664000
6	-1.512188000	3.418547000	-1.407274000
6	-1.354809000	5.312606000	0.599823000
6	-1.845308000	4.735539000	-1.669275000
6	-1.768274000	5.687153000	-0.667051000
1	-0.696872000	3.695338000	1.859760000
1	-1.577768000	2.678239000	-2.212522000
1	-1.295208000	6.056122000	1.400432000
1	-2.173561000	5.022755000	-2.672673000
1	-2.036844000	6.727144000	-0.873866000
6	1.534032000	-0.906375000	-1.515836000
8	1.596290000	-1.131094000	-2.644775000
1	1.338806000	0.102739000	1.794767000

7Mn

ΔH^{353} -2388.407017 Hartrees, ΔS^{353} 273.4 eu, ΔG^{353} -2388.56083 Hartrees

15	3.445365000	0.446977000	0.029945000
1	3.567823000	2.189760000	-1.705861000
6	-1.389365000	0.509253000	-0.592417000
6	2.022097000	-2.152657000	0.754011000
1	-1.027722000	0.466242000	-1.640116000
25	1.470042000	-0.568103000	0.202141000
8	2.357834000	-3.166753000	1.191840000
1	-0.853716000	1.516493000	1.210077000
6	-0.650235000	1.635453000	0.124445000
1	3.268794000	2.894035000	-0.124905000
6	2.993663000	2.045059000	-0.775598000
15	-0.694971000	-1.039850000	0.198923000
6	4.439336000	1.004635000	1.489870000
1	5.252438000	1.652866000	1.102128000
6	4.688346000	-0.212875000	-1.174571000
1	4.168826000	-0.038262000	-2.140585000
6	1.508074000	2.091373000	-1.070354000
1	1.269255000	1.555760000	-2.006767000
1	1.187898000	3.141733000	-1.206916000
7	0.810292000	1.431345000	0.026123000
6	5.997179000	0.541153000	-1.212311000
1	6.598548000	0.224909000	-2.080785000
1	5.864490000	1.632893000	-1.294448000
1	6.612538000	0.350234000	-0.317201000
6	4.904871000	-1.704911000	-1.059630000
1	3.967253000	-2.269799000	-1.164674000
1	5.585445000	-2.051902000	-1.854903000
1	5.358177000	-1.998689000	-0.099468000
6	3.611620000	1.818064000	2.459490000
1	4.250848000	2.199738000	3.272898000
1	3.132408000	2.699374000	2.001462000

1	2.821009000	1.205544000	2.920648000
6	5.046860000	-0.177829000	2.210432000
1	4.271140000	-0.909821000	2.496409000
1	5.802288000	-0.708612000	1.612119000
1	5.544567000	0.146706000	3.139511000
6	-1.229879000	-2.435502000	-0.835796000
6	-1.320547000	-2.349226000	-2.222076000
6	-1.381804000	-3.689164000	-0.243547000
6	-1.594981000	-3.468619000	-2.987544000
6	-1.647650000	-4.809017000	-1.009357000
6	-1.764766000	-4.701539000	-2.384250000
1	-1.154389000	-1.394528000	-2.729918000
1	-1.289402000	-3.792622000	0.843017000
1	-1.668748000	-3.373475000	-4.074795000
1	-1.763016000	-5.781133000	-0.521259000
1	-1.978641000	-5.586422000	-2.990401000
6	-1.748445000	-1.261681000	1.673159000
6	-3.069985000	-1.699369000	1.573099000
6	-1.241814000	-0.955383000	2.932145000
6	-3.860327000	-1.817482000	2.700315000
6	-2.037141000	-1.069348000	4.061027000
6	-3.346416000	-1.499178000	3.947175000
1	-3.493338000	-1.944867000	0.592535000
1	-0.198242000	-0.635545000	3.018472000
1	-4.895161000	-2.158590000	2.602493000
1	-1.620862000	-0.828815000	5.043939000
1	-3.973335000	-1.594416000	4.838958000
1	1.188492000	1.833435000	0.885013000
6	-2.877495000	0.657245000	-0.601867000
6	-3.575968000	1.161625000	0.493524000
6	-3.611869000	0.256709000	-1.714482000
6	-4.955145000	1.248953000	0.478132000
6	-4.992531000	0.337179000	-1.729785000
6	-5.671359000	0.832770000	-0.630688000
1	-3.036520000	1.479580000	1.392498000
1	-3.084614000	-0.126709000	-2.594777000
1	-5.478938000	1.646628000	1.352211000
1	-5.544128000	0.013427000	-2.617290000
1	-6.762832000	0.901814000	-0.640654000
6	-1.080941000	3.029171000	-0.249594000
6	-0.990253000	4.034587000	0.704843000
6	-1.502417000	3.366008000	-1.530394000
6	-1.304341000	5.345010000	0.392612000
6	-1.818653000	4.674630000	-1.846517000
6	-1.719396000	5.668118000	-0.887394000
1	-0.672440000	3.776557000	1.722974000
1	-1.590026000	2.591057000	-2.300027000
1	-1.232459000	6.121255000	1.159964000

1	-2.152258000	4.922018000	-2.858369000
1	-1.974886000	6.701504000	-1.138265000
6	1.561152000	-0.945993000	-1.537580000
8	1.674492000	-1.230122000	-2.656410000
1	1.458966000	-0.261437000	1.751048000

4TS

ΔH^{353} -2388.353399 Hartrees, ΔS^{353} 273.2 eu, ΔG^{353} -2388.507382 Hartrees, 570i cm⁻¹

15	3.413881000	0.700488000	0.033178000
1	3.309615000	2.722106000	-1.342898000
6	-1.360149000	0.452154000	-0.479396000
6	2.363320000	-2.323021000	0.413207000
1	-0.937545000	0.498369000	-1.504863000
25	1.661844000	-0.738448000	0.146657000
8	2.815799000	-3.354011000	0.659685000
1	-1.203044000	1.558953000	1.351659000
6	-0.887400000	1.702546000	0.297409000
1	3.023360000	3.087553000	0.356502000
6	2.756112000	2.383492000	-0.450098000
15	-0.559820000	-1.114144000	0.252717000
6	4.396132000	1.134517000	1.536270000
1	5.061688000	1.974280000	1.245325000
6	4.648762000	0.431752000	-1.321756000
1	4.044354000	0.673622000	-2.222482000
6	1.266835000	2.505976000	-0.728770000
1	1.022964000	2.062959000	-1.723625000
1	0.996305000	3.573916000	-0.785907000
7	0.561221000	1.885354000	0.375864000
6	5.837683000	1.364592000	-1.293045000
1	6.419755000	1.271490000	-2.224731000
1	5.557450000	2.426116000	-1.195599000
1	6.527680000	1.129297000	-0.465972000
6	5.079471000	-1.012031000	-1.451917000
1	4.225359000	-1.692280000	-1.584391000
1	5.734856000	-1.135283000	-2.329888000
1	5.646217000	-1.366314000	-0.576432000
6	3.501815000	1.601820000	2.663525000
1	4.115740000	2.017404000	3.479716000
1	2.779302000	2.377868000	2.366201000
1	2.920314000	0.763735000	3.076492000
6	5.239223000	-0.031429000	2.000716000
1	4.619405000	-0.932706000	2.152559000
1	6.046835000	-0.293131000	1.301020000
1	5.715428000	0.200030000	2.967906000
6	-1.094907000	-2.494823000	-0.795014000
6	-1.235700000	-2.373858000	-2.173956000
6	-1.157524000	-3.770071000	-0.232981000
6	-1.480022000	-3.484634000	-2.961337000

6	-1.398146000	-4.879315000	-1.021843000
6	-1.570516000	-4.739984000	-2.388137000
1	-1.127317000	-1.399736000	-2.657555000
1	-1.010480000	-3.899469000	0.844692000
1	-1.593250000	-3.363796000	-4.042495000
1	-1.446209000	-5.868974000	-0.558714000
1	-1.762212000	-5.617655000	-3.011715000
6	-1.502053000	-1.353904000	1.790157000
6	-2.751994000	-1.972228000	1.816290000
6	-0.991718000	-0.825679000	2.973342000
6	-3.464333000	-2.066848000	2.997206000
6	-1.715314000	-0.906155000	4.151034000
6	-2.949692000	-1.531104000	4.166115000
1	-3.184572000	-2.374007000	0.894262000
1	-0.002919000	-0.354350000	2.965805000
1	-4.441484000	-2.558495000	3.001136000
1	-1.300127000	-0.485741000	5.071580000
1	-3.516407000	-1.605617000	5.099068000
1	0.950787000	0.955185000	0.294491000
6	-2.855739000	0.399564000	-0.586386000
6	-3.677835000	0.640651000	0.513990000
6	-3.468525000	0.143134000	-1.809799000
6	-5.054570000	0.602257000	0.394818000
6	-4.845207000	0.101475000	-1.930855000
6	-5.645702000	0.326144000	-0.825353000
1	-3.239568000	0.857097000	1.493849000
1	-2.847336000	-0.011302000	-2.698672000
1	-5.675010000	0.793777000	1.275154000
1	-5.297240000	-0.102203000	-2.905884000
1	-6.735098000	0.296101000	-0.916971000
6	-1.525248000	2.986724000	-0.166533000
6	-1.784517000	3.975350000	0.773623000
6	-1.796392000	3.251276000	-1.503647000
6	-2.303996000	5.199557000	0.392966000
6	-2.318149000	4.473400000	-1.887181000
6	-2.573132000	5.451063000	-0.940739000
1	-1.570878000	3.772909000	1.829293000
1	-1.602875000	2.488976000	-2.266330000
1	-2.505839000	5.964490000	1.148265000
1	-2.532519000	4.663639000	-2.942761000
1	-2.990093000	6.415031000	-1.245848000
6	1.632579000	-0.847996000	-1.640160000
8	1.667661000	-0.947242000	-2.791754000
1	1.770642000	-0.691449000	1.708797000

8Mn

ΔH^{353} -2388.417328 Hartrees, ΔS^{353} 273.7 eu, ΔG^{353} -2388.571299 Hartrees

1	6.141582000	1.136371000	1.089035000
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1	4.761809000	0.814186000	-2.963331000
1	-3.363038000	-0.836999000	-2.819342000
6	-4.356364000	-0.464173000	-2.520187000
6	0.716013000	1.645032000	-0.043122000
15	0.616081000	-1.087798000	0.090425000
6	-2.920512000	2.378732000	0.313574000
1	-0.572382000	-3.480978000	1.044781000
1	3.454509000	-2.805612000	3.844592000
6	3.268571000	0.632869000	-1.435552000
7	-0.655122000	1.495743000	0.450303000
1	3.204739000	-2.473350000	-0.290084000
6	1.324781000	-2.555124000	-3.660337000
1	-0.256297000	-1.500555000	-2.643632000
6	5.601664000	0.980513000	-0.988794000
6	-2.115363000	-1.961227000	-0.544469000
1	2.940689000	-1.210593000	2.055857000
6	-4.235879000	0.876798000	-1.828845000
6	1.403535000	-1.903605000	-1.340681000
6	2.262894000	-2.052403000	2.224177000
6	2.582487000	-3.120510000	-3.554440000
6	-1.478180000	2.593844000	-0.049225000
1	0.786003000	-2.588544000	-4.612040000
1	3.045923000	-3.598291000	-4.422970000
6	4.562540000	0.811339000	-1.887850000
25	-1.493299000	-0.421378000	0.054326000
1	-4.067544000	1.909076000	-3.710010000
15	-3.403147000	0.689204000	-0.184793000
1	-1.349681000	2.605948000	-1.146791000
1	6.625102000	1.118328000	-1.348993000
1	-4.963097000	-0.371411000	-3.436430000
6	4.036338000	0.810694000	0.817554000
1	-3.497580000	2.879328000	-2.346180000
1	1.605066000	0.526528000	1.540443000
6	-3.535676000	1.853632000	-2.745267000
6	0.737453000	-1.951041000	-2.561145000
1	-5.253192000	1.269876000	-1.628684000
6	2.663216000	-2.492190000	-1.242164000
6	2.985081000	0.614556000	-0.071757000
1	3.825541000	0.848663000	1.893411000
8	-2.500386000	-2.966488000	-0.967134000
6	1.578982000	0.474803000	0.430554000
6	1.135709000	-2.219927000	1.425952000
6	5.333153000	0.984593000	0.367925000
1	0.632551000	1.597189000	-1.147891000
6	0.629035000	-4.239730000	2.651121000
1	1.985171000	-4.767583000	4.239139000
1	-1.119960000	3.572078000	0.326030000
1	-2.504500000	1.530314000	-2.964429000

1	-3.039509000	2.438889000	1.413219000
1	-0.023853000	-5.102049000	2.814210000
6	1.748102000	-4.053651000	3.445150000
6	0.324127000	-3.329483000	1.657038000
1	-4.819695000	-1.244280000	-1.897747000
1	2.461549000	0.490696000	-2.163081000
6	2.563471000	-2.958538000	3.228120000
1	4.242936000	-3.539386000	-2.248013000
1	-3.550384000	3.182225000	-0.104994000
6	3.250071000	-3.089756000	-2.340965000
6	-4.787513000	0.370306000	1.002282000
1	-6.550542000	1.264961000	0.081519000
6	-5.317003000	-1.043302000	0.930793000
6	-5.919131000	1.371965000	0.978828000
1	-4.513729000	-1.797226000	0.923589000
1	-4.262510000	0.474582000	1.975448000
1	-5.960643000	-1.259177000	1.799314000
1	-5.937196000	-1.203764000	0.032965000
1	-5.576180000	2.418184000	1.021299000
1	-6.584200000	1.217852000	1.845136000
1	-0.621788000	1.589244000	1.469603000
6	1.345066000	2.963611000	0.335382000
6	1.803402000	3.836424000	-0.640296000
6	1.485717000	3.324727000	1.670807000
6	2.386618000	5.043200000	-0.294506000
6	2.061540000	4.531920000	2.020801000
6	2.514752000	5.395186000	1.037029000
1	1.703566000	3.556820000	-1.695579000
1	1.140238000	2.646757000	2.462131000
1	2.744965000	5.718206000	-1.077033000
1	2.162678000	4.801082000	3.076298000
1	2.973811000	6.348774000	1.312479000
6	-1.800006000	-0.785302000	1.774493000
1	-1.228357000	0.017590000	-1.443740000
8	-2.015913000	-1.008450000	2.890119000

Acetophenone

ΔH^{353} -384.668121 Hartrees, ΔS^{353} 93.4 eu, ΔG^{353} -384.720678 Hartrees

6	0.000000000	0.213092000	0.000000000
6	-1.045835000	-0.707674000	0.000000000
6	1.313700000	-0.252293000	0.000000000
6	-0.782139000	-2.066474000	0.000000000
6	1.577223000	-1.607961000	0.000000000
6	0.528621000	-2.517427000	0.000000000
1	-2.086225000	-0.364355000	0.000000000
1	2.123700000	0.484100000	0.000000000
1	-1.609075000	-2.783725000	0.000000000
1	2.611949000	-1.965584000	0.000000000

1	0.736227000	-3.592679000	0.000000000
6	-0.218399000	1.688078000	0.000000000
6	-1.628478000	2.197532000	0.000000000
1	-1.617502000	3.294621000	0.000000000
1	-2.184444000	1.844411000	0.883699000
1	-2.184444000	1.844411000	-0.883699000
8	0.717708000	2.444695000	0.000000000

TS^S

ΔH^{353} -2773.061633 Hartrees, ΔS^{353} 314.4 eu, ΔG^{353} -2773.238522 Hartrees, 995i cm⁻¹

1	-6.377771000	1.080086000	-2.065885000
1	-5.812846000	0.839959000	2.183923000
1	1.756121000	-0.424442000	4.190312000
6	2.820816000	-0.175053000	4.062313000
6	-1.312822000	1.705419000	0.114896000
15	-1.165569000	-1.071948000	0.043117000
6	2.274147000	2.488094000	0.767371000
1	0.264613000	-3.452849000	-0.540007000
1	-2.901793000	-2.848078000	-4.298225000
6	-4.047939000	0.658530000	0.979176000
7	0.138039000	1.537090000	0.110228000
1	-3.956652000	-2.048809000	-0.203953000
6	-2.568612000	-3.327543000	3.161767000
1	-0.759810000	-2.292186000	2.667818000
6	-6.250486000	0.966564000	0.079504000
6	1.480651000	-1.875435000	1.231420000
1	-2.871512000	-1.217873000	-2.466223000
6	3.003772000	1.110064000	3.278989000
6	-2.269774000	-2.023760000	1.151655000
6	-2.176673000	-2.063284000	-2.436142000
6	-3.854915000	-3.650833000	2.775105000
6	0.780084000	2.677562000	0.760400000
1	-2.162182000	-3.710215000	4.102239000
1	-4.478108000	-4.285495000	3.412071000
6	-5.406564000	0.825463000	1.168509000
25	0.791300000	-0.289286000	0.815570000
1	2.533604000	2.337609000	4.981320000
15	2.652610000	0.853349000	1.471927000
1	0.376081000	2.750066000	1.789321000
1	-7.325879000	1.096652000	0.230324000
1	3.247035000	-0.069012000	5.073951000
6	-4.361401000	0.788927000	-1.385774000
1	2.390944000	3.209120000	3.450468000
1	-1.819723000	0.536474000	-1.594824000
6	2.224661000	2.231465000	3.927727000
6	-1.782571000	-2.520523000	2.355679000
1	4.077657000	1.385004000	3.328794000
6	-3.557344000	-2.389959000	0.757450000

6	-3.505540000	0.626738000	-0.303191000
1	-3.943602000	0.811551000	-2.399311000
8	1.943399000	-2.902286000	1.486465000
6	-2.026681000	0.492870000	-0.505024000
6	-1.285043000	-2.207627000	-1.380006000
6	-5.723103000	0.951263000	-1.199160000
1	-1.614301000	1.778147000	1.180447000
6	-0.470232000	-4.239924000	-2.395285000
1	-1.361821000	-4.794321000	-4.275869000
1	0.518555000	3.625251000	0.251238000
1	1.140972000	2.037049000	3.939337000
1	2.625794000	2.463746000	-0.280970000
1	0.204851000	-5.100273000	-2.370186000
6	-1.343919000	-4.070451000	-3.456279000
6	-0.440168000	-3.314978000	-1.368037000
1	3.301716000	-1.048266000	3.596522000
1	-3.393925000	0.529111000	1.850273000
6	-2.199553000	-2.983710000	-3.470368000
1	-5.356352000	-3.449274000	1.243620000
1	2.780620000	3.333401000	1.262063000
6	-4.345816000	-3.183343000	1.566656000
6	4.341013000	0.492570000	0.821596000
1	5.499539000	2.045513000	1.850970000
6	4.979474000	-0.717389000	1.463875000
6	5.283270000	1.674547000	0.834045000
1	4.327254000	-1.605219000	1.445230000
1	4.149620000	0.234493000	-0.228902000
1	5.899586000	-0.984480000	0.917481000
1	5.275568000	-0.533391000	2.511362000
1	4.912669000	2.524553000	0.240647000
1	6.251676000	1.380517000	0.393823000
1	0.481368000	1.549832000	-0.865503000
6	-1.779101000	2.959601000	-0.586156000
6	-2.684154000	3.817087000	0.022244000
6	-1.340752000	3.246618000	-1.875317000
6	-3.148972000	4.939795000	-0.640524000
6	-1.798241000	4.373569000	-2.533849000
6	-2.705939000	5.221042000	-1.920527000
1	-3.038330000	3.591625000	1.035011000
1	-0.609294000	2.591504000	-2.367605000
1	-3.865355000	5.604381000	-0.148783000
1	-1.438335000	4.593736000	-3.543297000
1	-3.068088000	6.109899000	-2.445154000
6	-0.007179000	0.033560000	2.366489000
1	1.437045000	-0.391300000	-0.809488000
6	1.803702000	0.234403000	-2.275353000
6	3.226236000	-0.263543000	-2.321044000
6	3.577735000	-1.579518000	-2.043106000

6	4.218949000	0.642452000	-2.670607000
6	4.901607000	-1.973619000	-2.081063000
1	2.800558000	-2.293337000	-1.741160000
6	5.545391000	0.246951000	-2.717617000
1	3.926387000	1.675472000	-2.882974000
6	5.890788000	-1.058988000	-2.414423000
1	5.171048000	-3.005561000	-1.836051000
1	6.321752000	0.969382000	-2.989064000
1	6.939168000	-1.371121000	-2.439041000
6	0.861792000	-0.566793000	-3.137141000
8	1.614353000	1.463517000	-2.214622000
1	0.918829000	-1.655521000	-3.009068000
1	1.131655000	-0.337511000	-4.183556000
1	-0.174899000	-0.233706000	-2.991572000
8	-0.596461000	0.302060000	3.325200000

TS^R

ΔH^{353} -2773.053028 Hartrees, ΔS^{353} 313.3 eu, ΔG^{353} -2773.229255 Hartrees, 1061i cm⁻¹

1	-5.917990000	1.856801000	-1.207354000
1	-4.352533000	3.297918000	2.521860000
1	3.584141000	0.771476000	3.339302000
6	4.527302000	0.559651000	2.813779000
6	-0.427401000	1.918010000	-0.284285000
15	-0.793783000	-0.586090000	0.820775000
6	3.218565000	1.700944000	-1.080765000
1	-0.283062000	-3.281508000	1.474505000
1	-4.469464000	-3.326001000	-1.164946000
6	-3.011824000	2.141315000	1.312161000
7	0.869253000	1.331921000	-0.611202000
1	-3.589131000	-0.558061000	1.808721000
6	-1.281390000	-0.781265000	4.890663000
1	0.356634000	-0.732182000	3.514811000
6	-5.278897000	2.631374000	0.696424000
6	1.936338000	-1.688416000	1.494761000
1	-3.232307000	-1.226055000	-0.893755000
6	4.593749000	1.282582000	1.481975000
6	-1.538330000	-0.558454000	2.498613000
6	-2.841237000	-2.136308000	-0.431153000
6	-2.652932000	-0.759229000	5.053922000
6	1.897765000	2.356332000	-0.759918000
1	-0.623577000	-0.882264000	5.758547000
1	-3.089878000	-0.832874000	6.054118000
6	-4.226347000	2.739863000	1.589566000
25	1.425843000	-0.228133000	0.613279000
1	5.018174000	3.168309000	2.419958000
15	3.552687000	0.440579000	0.190876000
1	1.946009000	2.934033000	0.183567000
1	-6.239984000	3.104092000	0.917752000

1	5.342350000	0.901341000	3.473311000
6	-3.882596000	1.337871000	-0.760732000
1	4.422136000	3.352186000	0.767272000
1	-1.559150000	0.362225000	-1.212672000
6	4.308933000	2.754015000	1.683816000
6	-0.729971000	-0.683058000	3.623570000
1	5.633331000	1.203700000	1.100793000
6	-2.922605000	-0.588952000	2.676930000
6	-2.825258000	1.415540000	0.138102000
1	-3.735129000	0.814896000	-1.713614000
8	2.282102000	-2.636823000	2.055123000
6	-1.494019000	0.812716000	-0.197047000
6	-1.667495000	-2.103262000	0.309362000
6	-5.101156000	1.932013000	-0.483712000
1	-0.325389000	2.392708000	0.714238000
6	-1.906922000	-4.467856000	0.731685000
1	-3.652765000	-5.415340000	-0.102254000
1	1.632777000	3.077104000	-1.556870000
1	3.301039000	2.933629000	2.088432000
1	3.109316000	1.174071000	-2.046559000
1	-1.529524000	-5.384878000	1.193661000
6	-3.088125000	-4.484909000	0.008430000
6	-1.204119000	-3.288334000	0.879928000
1	4.611378000	-0.533635000	2.733152000
1	-2.194901000	2.226117000	2.037850000
6	-3.545708000	-3.320080000	-0.578165000
1	-4.560706000	-0.679891000	4.056007000
1	4.016927000	2.450552000	-1.211577000
6	-3.473015000	-0.670415000	3.940672000
6	4.800444000	-0.695965000	-0.570212000
1	6.504071000	-0.728161000	-1.892815000
6	5.501639000	-1.575045000	0.441538000
6	5.802321000	0.004139000	-1.459274000
1	4.801314000	-2.126464000	1.088140000
1	4.187568000	-1.367149000	-1.191721000
1	6.111107000	-2.327730000	-0.084971000
1	6.193050000	-1.011138000	1.089805000
1	6.415806000	0.736812000	-0.906698000
1	5.334682000	0.536440000	-2.301856000
1	0.790365000	0.885847000	-1.543195000
6	-0.873854000	2.987630000	-1.253267000
6	-1.237717000	4.245121000	-0.794678000
6	-0.951833000	2.720257000	-2.616520000
6	-1.678973000	5.219058000	-1.673617000
6	-1.384926000	3.695700000	-3.496082000
6	-1.753469000	4.946041000	-3.027566000
1	-1.180670000	4.460742000	0.278804000
1	-0.644326000	1.738311000	-2.998347000

1	-1.966329000	6.204402000	-1.295217000
1	-1.434014000	3.476341000	-4.566898000
1	-2.098848000	5.714508000	-3.725178000
6	1.349704000	0.864661000	2.004867000
1	1.429263000	-1.096745000	-0.964324000
6	0.065006000	-2.052682000	-2.745553000
6	0.106524000	-3.376601000	-2.323068000
6	-1.020093000	-1.624584000	-3.501456000
6	-0.898330000	-4.256689000	-2.673753000
6	-2.028712000	-2.505148000	-3.852692000
6	-1.963164000	-3.826764000	-3.450393000
1	0.935462000	-3.720146000	-1.693329000
1	-1.030040000	-0.586994000	-3.850927000
1	-0.858107000	-5.294553000	-2.328876000
1	-2.868354000	-2.158476000	-4.463756000
1	-2.754826000	-4.528709000	-3.730142000
6	1.233477000	-1.109440000	-2.616360000
6	2.541036000	-1.762186000	-3.006842000
1	3.349714000	-1.018715000	-3.006413000
1	2.428727000	-2.112285000	-4.048524000
1	2.827444000	-2.631637000	-2.398628000
8	1.064952000	0.071892000	-2.974721000
8	1.257884000	1.646740000	2.851668000

MnNH-S-alkoxide

ΔH^{353} -2773.07802 Hartrees, ΔS^{353} 317.4 eu, ΔG^{353} -2773.256584 Hartrees

1	5.979038000	1.635289000	2.450671000
1	6.041926000	0.733790000	-1.746535000
1	-1.873753000	-1.260175000	-4.171438000
6	-2.947568000	-1.040735000	-4.056904000
6	1.215070000	1.576762000	-0.472501000
15	1.221860000	-1.120419000	0.052143000
6	-2.392214000	2.103220000	-1.209221000
1	-0.570539000	-3.138475000	1.042617000
1	2.654743000	-2.236924000	4.689815000
6	4.129701000	0.626410000	-0.781016000
7	-0.225959000	1.337849000	-0.454823000
1	3.989661000	-1.945181000	0.739930000
6	3.063729000	-3.599076000	-2.623768000
1	1.171269000	-2.613315000	-2.446783000
6	6.166924000	1.193670000	0.352552000
6	-1.265669000	-2.257606000	-1.314799000
1	2.831952000	-0.992884000	2.579533000
6	-3.174548000	0.335685000	-3.465767000
6	2.471868000	-2.144628000	-0.790538000
6	2.040419000	-1.740999000	2.694114000
6	4.302236000	-3.826972000	-2.055248000
6	-0.906735000	2.349162000	-1.254477000

1	2.792539000	-4.079206000	-3.568002000
1	5.021934000	-4.484910000	-2.550790000
6	5.494351000	0.843778000	-0.806055000
25	-0.734120000	-0.575894000	-0.979890000
1	-2.831023000	1.318629000	-5.347268000
15	-2.710261000	0.375949000	-1.672871000
1	-0.517042000	2.319149000	-2.294128000
1	7.247056000	1.363905000	0.331403000
1	-3.393994000	-1.101323000	-5.063076000
6	4.094266000	1.126935000	1.554962000
1	-2.685164000	2.414290000	-3.967019000
1	1.562941000	0.760510000	1.464286000
6	-2.482565000	1.386823000	-4.303419000
6	2.154832000	-2.764954000	-1.994420000
1	-4.263367000	0.545287000	-3.494705000
6	3.716651000	-2.403228000	-0.216158000
6	3.409822000	0.752595000	0.404323000
1	3.532186000	1.274782000	2.485119000
8	-1.595611000	-3.331616000	-1.565614000
6	1.925284000	0.559969000	0.433878000
6	1.140122000	-1.975188000	1.658996000
6	5.461471000	1.339377000	1.533550000
1	1.568975000	1.420357000	-1.516522000
6	0.055957000	-3.639235000	3.030855000
1	0.874350000	-3.938191000	4.999109000
1	-0.692874000	3.366546000	-0.873884000
1	-1.390235000	1.247482000	-4.328129000
1	-2.714563000	2.204000000	-0.154796000
1	-0.731417000	-4.388002000	3.156265000
6	0.951327000	-3.389228000	4.056420000
6	0.148722000	-2.935675000	1.843551000
1	-3.382098000	-1.855269000	-3.458470000
1	3.614706000	0.334993000	-1.704277000
6	1.943481000	-2.440198000	3.884220000
1	5.598365000	-3.414927000	-0.384838000
1	-2.951188000	2.849918000	-1.796093000
6	4.624716000	-3.230116000	-0.847087000
6	-4.290618000	-0.007950000	-0.803901000
1	-5.695057000	1.161601000	-2.011767000
6	-4.835740000	-1.378341000	-1.130077000
6	-5.353206000	1.055256000	-0.967947000
1	-4.084784000	-2.177164000	-1.019599000
1	-3.990869000	-0.016066000	0.258396000
1	-5.665630000	-1.619914000	-0.445481000
1	-5.241797000	-1.434605000	-2.154949000
1	-5.025612000	2.046005000	-0.617718000
1	-6.240043000	0.786111000	-0.370038000
1	-0.619930000	1.514086000	0.580561000

6	1.634358000	2.975968000	-0.081196000
6	2.444309000	3.715900000	-0.930823000
6	1.259968000	3.523440000	1.142819000
6	2.880439000	4.979908000	-0.573541000
6	1.690611000	4.790629000	1.494083000
6	2.503318000	5.520729000	0.642377000
1	2.745295000	3.284369000	-1.893292000
1	0.593349000	2.960212000	1.808732000
1	3.521140000	5.548375000	-1.254240000
1	1.383244000	5.217694000	2.453783000
1	2.842722000	6.520696000	0.928641000
6	0.035720000	-0.402648000	-2.556806000
1	-1.274429000	-0.304768000	1.529573000
6	-1.547323000	0.534443000	2.287500000
6	-3.036600000	0.311870000	2.514816000
6	-3.567978000	-0.963157000	2.677144000
6	-3.898682000	1.398624000	2.526719000
6	-4.930963000	-1.152728000	2.818853000
1	-2.893007000	-1.831094000	2.663168000
6	-5.264254000	1.215000000	2.676818000
1	-3.464389000	2.394395000	2.389847000
6	-5.786573000	-0.060518000	2.813910000
1	-5.335609000	-2.164310000	2.928931000
1	-5.935620000	2.080799000	2.676118000
1	-6.865845000	-0.207158000	2.920485000
6	-0.791482000	0.200659000	3.569934000
8	-1.247321000	1.734243000	1.822288000
1	-0.940057000	-0.832704000	3.929354000
1	-1.123314000	0.889932000	4.365062000
1	0.289156000	0.364930000	3.428312000
8	0.577397000	-0.240616000	-3.560957000

Mn(S-alkoxide)

ΔH^{353} -2773.100996 Hartrees, ΔS^{353} 317.7 eu, ΔG^{353} -2773.279745 Hartrees

1	6.222769000	1.658241000	-1.226543000
1	5.580642000	-2.538974000	-0.588042000
1	-2.240242000	-4.324155000	0.545808000
6	-3.295566000	-4.157515000	0.276694000
6	1.109973000	-0.452582000	-1.686608000
15	0.983534000	-0.166348000	1.083575000
6	-2.528448000	-0.893517000	-2.358378000
1	-0.677176000	0.769736000	3.185526000
1	2.459977000	4.472505000	2.207451000
6	3.835642000	-1.293112000	-0.542767000
7	-0.331256000	-0.405637000	-1.479810000
1	3.687200000	0.432317000	2.144100000
6	2.651026000	-3.049275000	3.452579000
1	0.822628000	-2.772080000	2.369150000

6	6.056336000	-0.463919000	-0.910180000
6	-1.578503000	-1.559064000	2.008959000
1	2.618035000	2.384675000	0.933165000
6	-3.420056000	-3.357360000	-1.004616000
6	2.155522000	-1.094685000	2.127011000
6	1.845034000	2.478710000	1.703074000
6	3.876750000	-2.514056000	3.800302000
6	-1.048371000	-0.986587000	-2.604830000
1	2.347541000	-4.028207000	3.834107000
1	4.553537000	-3.070650000	4.455146000
6	5.192142000	-1.520444000	-0.675947000
25	-0.990988000	-1.063726000	0.395666000
1	-3.034142000	-5.078965000	-2.237320000
15	-2.919974000	-1.594702000	-0.722084000
1	-0.718168000	-2.039264000	-2.699969000
1	7.130272000	-0.644162000	-1.011286000
1	-3.755297000	-5.152110000	0.152838000
6	4.191673000	1.042940000	-0.895120000
1	-2.782971000	-3.554096000	-3.095877000
1	1.659938000	1.323043000	-0.661741000
6	-2.665065000	-4.046577000	-2.118573000
6	1.795981000	-2.343278000	2.622359000
1	-4.491276000	-3.331163000	-1.291810000
6	3.385537000	-0.557074000	2.504973000
6	3.315755000	-0.004750000	-0.638417000
1	3.792643000	2.056920000	-1.018070000
8	-1.931891000	-1.934263000	3.039358000
6	1.841463000	0.236628000	-0.529378000
6	0.966429000	1.428749000	1.958865000
6	5.551269000	0.818856000	-1.023894000
1	1.388170000	-1.527013000	-1.700218000
6	-0.057281000	2.758981000	3.689907000
1	0.735393000	4.739394000	3.973165000
1	-0.785017000	-0.489847000	-3.558030000
1	-1.587183000	-4.124294000	-1.902529000
1	-2.813559000	0.175055000	-2.311721000
1	-0.823329000	2.864445000	4.463336000
6	0.807279000	3.802396000	3.413506000
6	0.026910000	1.579942000	2.972722000
1	-3.778276000	-3.681895000	1.143341000
1	3.164717000	-2.136357000	-0.336764000
6	1.764293000	3.656476000	2.424223000
1	5.204404000	-0.828415000	3.606757000
1	-3.100208000	-1.331834000	-3.192865000
6	4.240567000	-1.263240000	3.327364000
6	-4.518884000	-0.762424000	-0.330425000
1	-5.812384000	-1.720853000	-1.817377000
6	-5.180627000	-1.337711000	0.900881000

6	-5.496371000	-0.717543000	-1.484078000
1	-4.488043000	-1.455373000	1.748866000
1	-4.211741000	0.273007000	-0.091490000
1	-5.992140000	-0.674117000	1.240707000
1	-5.636517000	-2.322915000	0.698823000
1	-5.108798000	-0.180899000	-2.362788000
1	-6.414205000	-0.190874000	-1.173139000
1	-0.642168000	0.567682000	-1.363071000
6	1.566515000	0.159763000	-2.989395000
6	2.420131000	-0.532161000	-3.835227000
6	1.175998000	1.447997000	-3.339521000
6	2.878364000	0.047014000	-5.006027000
6	1.624285000	2.025741000	-4.512734000
6	2.479842000	1.326489000	-5.348356000
1	2.739698000	-1.544019000	-3.559980000
1	0.496653000	2.014694000	-2.687286000
1	3.554924000	-0.510752000	-5.659796000
1	1.302220000	3.036608000	-4.779004000
1	2.837555000	1.784587000	-6.274736000
6	-0.240950000	-2.641724000	0.097415000
6	-2.374577000	1.652848000	0.948819000
6	-2.320693000	3.037078000	0.401843000
6	-3.401691000	3.913639000	0.467218000
6	-1.155137000	3.484847000	-0.216738000
6	-3.313793000	5.192744000	-0.050144000
1	-4.340886000	3.569786000	0.912822000
6	-1.060672000	4.767089000	-0.725467000
1	-0.295983000	2.806697000	-0.262877000
6	-2.141700000	5.628610000	-0.646140000
1	-4.180314000	5.859583000	0.002216000
1	-0.126504000	5.102209000	-1.188206000
1	-2.073832000	6.640759000	-1.055878000
6	-3.154234000	1.395995000	2.023863000
8	-1.625483000	0.823585000	0.304410000
1	-3.689523000	2.196049000	2.534390000
1	-3.200979000	0.400397000	2.467226000
8	0.286055000	-3.643863000	-0.139217000

$T_{\text{NH-O}}$

ΔH^{353} -2773.076955 Hartrees, ΔS^{353} 315.0 eu, ΔG^{353} -2773.254181 Hartrees, 1735i cm⁻¹

1	-6.018131000	1.479054000	-2.498203000
1	-6.038034000	0.827061000	1.745434000
1	1.848375000	-1.001562000	4.247889000
6	2.920762000	-0.778238000	4.129268000
6	-1.222919000	1.604524000	0.381678000
15	-1.225614000	-1.111806000	0.007487000
6	2.368282000	2.192530000	1.100109000
1	0.554463000	-3.194213000	-0.874825000

1	-2.662250000	-2.459248000	-4.567094000
6	-4.134812000	0.669677000	0.769513000
7	0.211093000	1.356420000	0.391571000
1	-3.990816000	-1.980535000	-0.633281000
6	-3.046796000	-3.477974000	2.797764000
1	-1.158381000	-2.493861000	2.569672000
6	-6.185275000	1.162434000	-0.375757000
6	1.276410000	-2.160381000	1.408908000
1	-2.827456000	-1.102454000	-2.526977000
6	3.138682000	0.564917000	3.463116000
6	-2.467298000	-2.103843000	0.899889000
6	-2.041045000	-1.860795000	-2.601926000
6	-4.287085000	-3.734435000	2.245378000
6	0.880077000	2.426869000	1.111793000
1	-2.770182000	-3.915240000	3.761043000
1	-5.002675000	-4.371660000	2.772887000
6	-5.500106000	0.883487000	0.794706000
25	0.720337000	-0.499437000	1.013688000
1	2.768184000	1.651548000	5.281761000
15	2.688661000	0.497729000	1.667474000
1	0.489983000	2.484090000	2.153754000
1	-7.265800000	1.330190000	-0.354217000
1	3.359935000	-0.777565000	5.140533000
6	-4.123485000	1.031021000	-1.591576000
1	2.621147000	2.663147000	3.838392000
1	-1.588575000	0.682331000	-1.503461000
6	2.427731000	1.654683000	4.233020000
6	-2.143229000	-2.669198000	2.128705000
1	4.224936000	0.788143000	3.489783000
6	-3.713232000	-2.392412000	0.342490000
6	-3.425839000	0.728485000	-0.427666000
1	-3.571648000	1.126709000	-2.534645000
8	1.622324000	-3.219986000	1.700049000
6	-1.941010000	0.539268000	-0.459882000
6	-1.143560000	-2.047464000	-1.554528000
6	-5.491307000	1.239511000	-1.569965000
1	-1.596174000	1.523077000	1.430915000
6	-0.075130000	-3.793013000	-2.834906000
1	-0.898052000	-4.191588000	-4.783839000
1	0.666907000	3.414578000	0.656948000
1	1.336977000	1.504202000	4.256622000
1	2.710953000	2.235112000	0.048299000
1	0.704533000	-4.555538000	-2.919524000
6	-0.968584000	-3.590908000	-3.872760000
6	-0.161301000	-3.025833000	-1.686866000
1	3.368100000	-1.620593000	3.580738000
1	-3.610630000	0.434130000	1.703217000
6	-1.951431000	-2.624514000	-3.752417000

1	-5.591082000	-3.401244000	0.563452000
1	2.915109000	2.974219000	1.652179000
6	-4.616340000	-3.192997000	1.013287000
6	4.281001000	0.073130000	0.837150000
1	5.659694000	1.341643000	1.973021000
6	4.840243000	-1.265114000	1.258859000
6	5.330976000	1.156949000	0.936011000
1	4.101136000	-2.079789000	1.195618000
1	3.990353000	-0.009541000	-0.224614000
1	5.680367000	-1.540464000	0.599807000
1	5.236570000	-1.246822000	2.288847000
1	4.998212000	2.116581000	0.512069000
1	6.227531000	0.854742000	0.369010000
1	0.698292000	1.492570000	-0.831897000
6	-1.635030000	2.977299000	-0.104929000
6	-2.420201000	3.790701000	0.699393000
6	-1.271281000	3.432590000	-1.369089000
6	-2.839054000	5.034655000	0.259877000
6	-1.684945000	4.678659000	-1.804980000
6	-2.471195000	5.482363000	-0.995991000
1	-2.713962000	3.434690000	1.694385000
1	-0.627102000	2.815080000	-2.007279000
1	-3.459689000	5.661257000	0.907580000
1	-1.384634000	5.029803000	-2.797174000
1	-2.797453000	6.466028000	-1.346765000
6	-0.056308000	-0.265780000	2.577666000
1	1.285776000	-0.408716000	-1.546486000
6	1.585074000	0.348628000	-2.355467000
6	3.074990000	0.118637000	-2.529964000
6	3.603550000	-1.167021000	-2.577514000
6	3.941049000	1.199363000	-2.610838000
6	4.968163000	-1.370838000	-2.675567000
1	2.924606000	-2.028861000	-2.508273000
6	5.308379000	0.999594000	-2.717865000
1	3.513802000	2.205893000	-2.562285000
6	5.827647000	-0.284038000	-2.741908000
1	5.370103000	-2.389103000	-2.694939000
1	5.982916000	1.860860000	-2.772171000
1	6.908053000	-0.441544000	-2.814987000
6	0.851059000	-0.052647000	-3.625311000
8	1.281741000	1.601049000	-1.988539000
1	1.004536000	-1.105950000	-3.915650000
1	1.198309000	0.584298000	-4.456151000
1	-0.230814000	0.120547000	-3.509606000
8	-0.606037000	-0.053380000	3.568169000

1-phenylethanol

ΔH^{353} -385.846516 Hartrees, ΔS^{353} 95.7 eu, ΔG^{353} -385.900375 Hartrees

1	-1.891030000	1.153959000	-1.530796000
1	-1.847004000	-1.106908000	-1.019854000
6	-0.154115000	-0.126027000	-0.169658000
6	0.690802000	-1.212954000	-0.360493000
6	0.398743000	1.102208000	0.175397000
6	2.060470000	-1.080475000	-0.205903000
6	1.769406000	1.238684000	0.325699000
6	2.603868000	0.148232000	0.137259000
1	0.262146000	-2.183759000	-0.642352000
1	-0.265740000	1.961018000	0.324286000
1	2.714451000	-1.944773000	-0.364201000
1	2.194026000	2.211973000	0.594960000
1	3.687211000	0.257083000	0.253341000
6	-1.650926000	-0.282158000	-0.291620000
6	-2.274336000	-0.659725000	1.027668000
1	-1.854501000	-1.601688000	1.411353000
1	-2.087482000	0.128333000	1.775830000
8	-2.276470000	0.892312000	-0.694109000
1	-3.363783000	-0.780440000	0.920210000
1	-1.891030000	1.153959000	-1.530796000
1	-1.847004000	-1.106908000	-1.019854000
6	-0.154115000	-0.126027000	-0.169658000
6	0.690802000	-1.212954000	-0.360493000
6	0.398743000	1.102208000	0.175397000
6	2.060470000	-1.080475000	-0.205903000
6	1.769406000	1.238684000	0.325699000
6	2.603868000	0.148232000	0.137259000
1	0.262146000	-2.183759000	-0.642352000
1	-0.265740000	1.961018000	0.324286000
1	2.714451000	-1.944773000	-0.364201000
1	2.194026000	2.211973000	0.594960000
1	3.687211000	0.257083000	0.253341000
6	-1.650926000	-0.282158000	-0.291620000
6	-2.274336000	-0.659725000	1.027668000
1	-1.854501000	-1.601688000	1.411353000
1	-2.087482000	0.128333000	1.775830000
8	-2.276470000	0.892312000	-0.694109000
1	-3.363783000	-0.780440000	0.920210000

3,5-bis(trifluoromethyl)acetophenone

ΔH^{353} -1058.486733 Hartrees, ΔS^{353} 136.3 eu, ΔG^{353} -1058.563417 Hartrees

6	-0.189468000	1.626696000	0.001861000
6	-1.290749000	0.779057000	-0.017972000
6	1.090214000	1.081949000	0.021068000
6	-1.109750000	-0.594016000	-0.020614000
6	1.262534000	-0.288298000	0.021049000
6	0.164488000	-1.134824000	-0.001105000
1	-2.308041000	1.182793000	-0.035201000

1	1.946559000	1.763210000	0.038622000
1	0.303598000	-2.220815000	-0.002730000
6	-0.308475000	3.118963000	0.003206000
6	-1.678351000	3.718596000	-0.021769000
1	-1.596761000	4.812310000	-0.020603000
1	-2.270061000	3.401689000	0.852429000
1	-2.239412000	3.400917000	-0.915640000
8	0.683356000	3.796709000	0.024002000
6	-2.293498000	-1.513526000	-0.000178000
9	-3.388556000	-0.909071000	-0.414750000
9	-2.102596000	-2.567083000	-0.769260000
9	-2.538037000	-1.968585000	1.215023000
6	2.639149000	-0.882656000	0.000004000
9	3.547658000	-0.030200000	0.422764000
9	2.712377000	-1.957575000	0.761391000
9	2.989233000	-1.254756000	-1.217634000

TS^S 3,5-CF3

ΔH^{353} -3446.865899 Hartrees, ΔS^{353} 351.9 eu, ΔG^{353} -3447.063794 Hartrees, 909i cm⁻¹

1	-6.789825000	0.875981000	-3.112523000
1	-7.085082000	0.511907000	1.155436000
1	0.100609000	-0.344791000	4.622669000
6	1.155230000	-0.034453000	4.676804000
6	-2.315620000	1.692690000	0.071694000
15	-1.981900000	-1.063779000	-0.047023000
6	1.052995000	2.653288000	1.359825000
1	-0.318622000	-3.333599000	-0.388006000
1	-2.753242000	-2.816609000	-4.668327000
6	-5.104734000	0.470833000	0.333181000
7	-0.877545000	1.610846000	0.318180000
1	-4.611451000	-2.176862000	-0.838273000
6	-3.812176000	-3.490106000	2.700545000
1	-2.003246000	-2.350219000	2.581730000
6	-7.093773000	0.690260000	-0.990107000
6	0.458333000	-1.754558000	1.589846000
1	-3.176634000	-1.240369000	-2.834677000
6	1.390298000	1.272410000	3.945089000
6	-3.215256000	-2.107910000	0.813476000
6	-2.444625000	-2.041456000	-2.689755000
6	-4.982752000	-3.865846000	2.070251000
6	-0.425345000	2.765164000	1.091904000
1	-3.568775000	-3.882095000	3.692044000
1	-5.677791000	-4.551681000	2.563504000
6	-6.481185000	0.556347000	0.244648000
25	-0.245831000	-0.198987000	1.087811000
1	0.543446000	2.438016000	5.540992000
15	1.390070000	1.026286000	2.103384000
1	-1.008862000	2.788291000	2.032893000

1	-8.183197000	0.755748000	-1.059625000
1	1.399184000	0.078409000	5.746216000
6	-4.939339000	0.671028000	-2.041627000
1	0.617677000	3.324835000	4.014237000
1	-2.401685000	0.566420000	-1.737412000
6	0.434932000	2.330283000	4.448738000
6	-2.935005000	-2.618391000	2.076252000
1	2.417645000	1.616385000	4.185994000
6	-4.382393000	-2.527440000	0.173901000
6	-4.312468000	0.514456000	-0.811274000
1	-4.327145000	0.754805000	-2.947623000
8	0.934037000	-2.756881000	1.907935000
6	-2.817585000	0.468914000	-0.712173000
6	-1.758659000	-2.160159000	-1.487044000
6	-6.317864000	0.751433000	-2.133701000
1	-2.802873000	1.694406000	1.068806000
6	-0.636451000	-4.109957000	-2.362092000
1	-1.120607000	-4.664115000	-4.386060000
1	-0.645206000	3.711578000	0.561572000
1	-0.617959000	2.065299000	4.265371000
1	1.582890000	2.673916000	0.389229000
1	0.075756000	-4.928236000	-2.222350000
6	-1.304152000	-3.963649000	-3.566547000
6	-0.860590000	-3.213949000	-1.333088000
1	1.756920000	-0.871540000	4.293077000
1	-4.635264000	0.346031000	1.316251000
6	-2.211714000	-2.931551000	-3.724673000
1	-6.177933000	-3.692261000	0.285866000
1	1.418497000	3.513568000	1.944863000
6	-5.263149000	-3.385756000	0.801102000
6	3.188798000	0.761550000	1.776900000
1	4.045371000	2.396160000	2.957948000
6	3.773522000	-0.400095000	2.547773000
6	4.043105000	1.999699000	1.927871000
1	3.194223000	-1.329687000	2.428400000
1	3.199167000	0.475285000	0.717281000
1	4.793363000	-0.610229000	2.184066000
1	3.862072000	-0.189830000	3.627392000
1	3.739548000	2.817742000	1.256600000
1	5.093281000	1.762582000	1.681888000
1	-0.379270000	1.674744000	-0.584162000
6	-2.736637000	2.950449000	-0.650955000
6	-3.775715000	3.730922000	-0.165804000
6	-2.114244000	3.320760000	-1.839010000
6	-4.193192000	4.857878000	-0.852322000
6	-2.524805000	4.452348000	-2.520003000
6	-3.567525000	5.221597000	-2.031156000
1	-4.274199000	3.440196000	0.766338000

1	-1.276754000	2.728411000	-2.231191000
1	-5.016912000	5.460624000	-0.458930000
1	-2.020544000	4.738349000	-3.447841000
1	-3.892574000	6.114006000	-2.573646000
6	-1.317699000	0.012567000	2.485712000
1	0.669967000	-0.215988000	-0.411664000
6	1.248699000	0.492085000	-1.807163000
6	2.685830000	0.102958000	-1.564292000
6	3.077480000	-1.198241000	-1.276087000
6	3.642569000	1.102698000	-1.618522000
6	4.402551000	-1.480437000	-1.012302000
1	2.324560000	-1.991276000	-1.203744000
6	4.970943000	0.812324000	-1.349744000
1	3.317003000	2.124972000	-1.832845000
6	5.359512000	-0.475846000	-1.037423000
1	6.404535000	-0.701414000	-0.808168000
6	0.554020000	-0.356082000	-2.837321000
8	0.964067000	1.699095000	-1.759783000
1	0.654137000	-1.440562000	-2.702316000
1	1.007075000	-0.094457000	-3.810172000
1	-0.510027000	-0.092555000	-2.896010000
8	-2.070527000	0.198756000	3.343309000
6	4.825143000	-2.858470000	-0.617021000
9	5.930148000	-3.224981000	-1.239268000
9	5.080814000	-2.935070000	0.677620000
9	3.902350000	-3.757135000	-0.885525000
6	5.993374000	1.901452000	-1.396569000
9	5.479144000	3.068974000	-1.063608000
9	6.996789000	1.662062000	-0.573085000
9	6.513876000	2.042911000	-2.601818000

TS^R 3,5-CF3

ΔH^{353} -3446.865925 Hartrees, ΔS^{353} 350.8 eu, ΔG^{353} -3447.057644 Hartrees, 953i cm⁻¹

1	-2.726978000	5.527743000	-0.334449000
1	0.785791000	5.935974000	2.100548000
1	5.070232000	-1.243307000	1.986563000
6	5.366803000	-2.112177000	1.380181000
6	1.439048000	1.872618000	-0.769277000
15	0.184043000	0.485489000	1.263895000
6	3.462002000	-0.905280000	-2.240721000
1	-0.818089000	-1.745831000	2.691250000
1	-4.781513000	0.947212000	1.442036000
6	0.494028000	4.027521000	1.166509000
7	1.834520000	0.515639000	-1.139051000
1	-1.264206000	2.581625000	2.787479000
6	1.483721000	1.167471000	5.094740000
1	2.028400000	-0.105244000	3.463704000
6	-1.017863000	5.875360000	0.927171000

6	1.697244000	-2.103517000	1.660913000
1	-2.574421000	1.577934000	0.590726000
6	5.263871000	-1.815008000	-0.103861000
6	0.415379000	1.223989000	2.928293000
6	-2.659653000	0.701261000	1.237980000
6	0.641863000	2.163138000	5.551010000
6	3.077032000	0.513942000	-1.905038000
1	2.240240000	0.737205000	5.757036000
1	0.733217000	2.535059000	6.575716000
6	0.142743000	5.333177000	1.452764000
25	1.826339000	-0.824593000	0.428062000
1	7.059222000	-0.636018000	-0.084276000
15	3.501095000	-1.868369000	-0.694860000
1	3.853782000	1.014138000	-1.294922000
1	-1.295342000	6.908308000	1.155493000
1	6.410521000	-2.345254000	1.648910000
6	-1.460359000	3.800328000	-0.187706000
1	6.053507000	-0.316043000	-1.500796000
1	-0.652470000	1.441669000	-0.738018000
6	6.014384000	-0.542056000	-0.424677000
6	1.370071000	0.702006000	3.795046000
1	5.770615000	-2.636305000	-0.652052000
6	-0.460134000	2.193196000	3.420847000
6	-0.311170000	3.234828000	0.352512000
1	-2.081572000	3.203921000	-0.868058000
8	1.616111000	-2.947652000	2.443751000
6	0.097244000	1.840211000	-0.018372000
6	-1.534870000	-0.036867000	1.582555000
6	-1.817334000	5.105305000	0.101741000
1	2.220920000	2.259030000	-0.082253000
6	-2.939136000	-1.498940000	2.892464000
1	-5.035715000	-1.011208000	2.951653000
1	2.976181000	1.106511000	-2.834019000
1	5.596070000	0.333459000	0.095337000
1	2.665591000	-1.333321000	-2.877023000
1	-3.043278000	-2.375454000	3.538069000
6	-4.050424000	-0.740070000	2.562366000
6	-1.693771000	-1.151127000	2.405810000
1	4.750051000	-2.960244000	1.711063000
1	1.408725000	3.609681000	1.602478000
6	-3.908268000	0.351263000	1.726072000
1	-1.026069000	3.439154000	5.070108000
1	4.393055000	-0.937541000	-2.831136000
6	-0.336607000	2.669742000	4.711010000
6	3.365344000	-3.635237000	-1.227886000
1	3.951798000	-5.005557000	-2.786244000
6	3.756149000	-4.615133000	-0.143927000
6	4.089615000	-3.944595000	-2.518017000

1	3.224637000	-4.439568000	0.804211000
1	2.284559000	-3.767559000	-1.391652000
1	3.506829000	-5.639570000	-0.465471000
1	4.838944000	-4.608194000	0.065106000
1	5.178336000	-3.780933000	-2.439905000
1	3.728860000	-3.349584000	-3.371131000
1	1.114987000	0.141171000	-1.779884000
6	1.355593000	2.822621000	-1.940387000
6	2.057275000	4.018970000	-1.924649000
6	0.557634000	2.526707000	-3.040787000
6	1.962569000	4.909700000	-2.979717000
6	0.468532000	3.412285000	-4.099328000
6	1.167466000	4.607683000	-4.070476000
1	2.684770000	4.259937000	-1.058465000
1	0.012942000	1.574978000	-3.081764000
1	2.519258000	5.850776000	-2.948893000
1	-0.157180000	3.164564000	-4.961888000
1	1.092674000	5.308422000	-4.906941000
6	3.010419000	0.187631000	1.273529000
1	0.659446000	-1.665883000	-0.639291000
6	-1.609156000	-1.659859000	-1.531635000
6	-2.167734000	-2.629837000	-0.710454000
6	-2.418556000	-0.639534000	-2.005113000
6	-3.513176000	-2.592330000	-0.400337000
6	-3.762989000	-0.599634000	-1.679414000
6	-4.324447000	-1.580587000	-0.886402000
1	-1.540424000	-3.424400000	-0.293694000
1	-1.977096000	0.110402000	-2.669560000
1	-5.386618000	-1.551723000	-0.632023000
6	-0.213160000	-1.757436000	-2.094242000
6	0.155143000	-3.161742000	-2.508331000
1	1.143435000	-3.165496000	-2.986567000
1	-0.573635000	-3.474552000	-3.277293000
1	0.125770000	-3.908814000	-1.703480000
8	0.174925000	-0.824931000	-2.815693000
8	3.766606000	0.917138000	1.755273000
6	-4.585408000	0.557998000	-2.136976000
9	-5.877035000	0.306028000	-2.083613000
9	-4.376384000	1.631403000	-1.383590000
9	-4.298047000	0.912358000	-3.373290000
6	-4.114442000	-3.692281000	0.413721000
9	-4.526414000	-4.690126000	-0.351548000
9	-3.252354000	-4.203865000	1.268972000
9	-5.165563000	-3.287287000	1.099320000

1-(3,5-bis(trifluoromethyl)phenyl)ethanol

ΔH^{353} -1059.667354 Hartrees, ΔS^{353} 137.8 eu, ΔG^{353} -1059.744881 Hartrees

1	2.094089000	2.763172000	-1.741026000
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1	0.171134000	3.547602000	-0.777900000
6	0.447743000	1.522561000	-0.168597000
6	-0.906537000	1.234337000	-0.133126000
6	1.359621000	0.474264000	-0.111344000
6	-1.346741000	-0.078224000	-0.039185000
6	0.914862000	-0.832390000	-0.022382000
6	-0.441702000	-1.120794000	0.015536000
1	-1.638228000	2.050679000	-0.186386000
1	2.431100000	0.695754000	-0.144943000
1	-0.789993000	-2.155554000	0.079156000
6	0.936829000	2.951301000	-0.226889000
6	1.088318000	3.527836000	1.157189000
1	0.137432000	3.498737000	1.709752000
1	1.835111000	2.952966000	1.729111000
8	2.181015000	3.053790000	-0.832649000
1	1.429005000	4.572864000	1.100352000
6	-2.821184000	-0.340691000	-0.023505000
9	-3.098470000	-1.615700000	0.152432000
9	-3.423014000	0.332036000	0.940746000
9	-3.393847000	0.033905000	-1.154005000
6	1.888253000	-1.968451000	0.059551000
9	3.122108000	-1.584340000	-0.193999000
9	1.890301000	-2.524552000	1.258075000
9	1.587973000	-2.927464000	-0.797740000

1,1,1-trifluoroacetophenone

ΔH^{353} -1058.486733 Hartrees, ΔS^{353} 136.3 eu, ΔG^{353} -1058.563417 Hartrees

6	-0.040365000	0.723345000	0.000000000
6	-1.395044000	0.387027000	0.000000000
6	0.337277000	2.067466000	0.000000000
6	-2.351402000	1.385827000	0.000000000
6	-0.621317000	3.059026000	0.000000000
6	-1.967444000	2.717892000	0.000000000
1	-1.717474000	-0.657840000	0.000000000
1	1.404605000	2.309777000	0.000000000
1	-3.412898000	1.121272000	0.000000000
1	-0.321557000	4.111293000	0.000000000
1	-2.729449000	3.504195000	0.000000000
6	1.045564000	-0.270957000	0.000000000
6	0.672336000	-1.773506000	0.000000000
8	2.210000000	0.005574000	0.000000000
9	1.749523000	-2.508938000	0.000000000
9	-0.040365000	-2.090532000	1.065056000
9	-0.040365000	-2.090532000	-1.065056000

TS^S 1,1,1-F3

ΔH^{353} -682.283409 Hartrees, ΔS^{353} 326.4 eu, ΔG^{353} -682.342952 Hartrees, 351i cm⁻¹

1	6.408132000	0.416803000	2.293014000
1	5.931972000	1.487669000	-1.837799000

1	-2.828672000	1.587807000	-5.203351000
6	-2.473276000	1.174974000	-4.244427000
6	1.384193000	1.718340000	0.312943000
15	1.242806000	-0.951961000	-0.453986000
6	-2.167452000	2.717314000	-0.269871000
1	-0.057636000	-3.425998000	-0.806272000
1	2.734434000	-3.984008000	3.242807000
6	4.140748000	0.969292000	-0.778179000
7	-0.069165000	1.569887000	0.217746000
1	4.009326000	-1.994841000	-0.397731000
6	2.788296000	-2.172650000	-4.052795000
1	0.954080000	-1.319426000	-3.352480000
6	6.325543000	0.964217000	0.213022000
6	-1.336190000	-1.329462000	-1.961755000
1	2.724581000	-1.832393000	2.066967000
6	-2.710771000	2.170248000	-3.125673000
6	2.390436000	-1.537249000	-1.757541000
6	2.104457000	-2.648737000	1.684034000
6	4.056599000	-2.611334000	-3.725031000
6	-0.680186000	2.863981000	-0.086567000
1	2.427343000	-2.247418000	-5.082522000
1	4.711244000	-3.028562000	-4.495829000
6	5.503998000	1.170705000	-0.882483000
25	-0.681397000	0.049973000	-1.050187000
1	-2.116124000	3.836909000	-4.348447000
15	-2.489813000	1.376356000	-1.459398000
1	-0.199971000	3.244100000	-1.009372000
1	7.404577000	1.121702000	0.128998000
1	-2.986132000	0.212985000	-4.095421000
6	4.404995000	0.371216000	1.519616000
1	-2.099942000	4.215659000	-2.622849000
1	1.872005000	0.089867000	1.600039000
6	-1.889983000	3.419291000	-3.352913000
6	1.962024000	-1.640454000	-3.076241000
1	-3.778598000	2.468904000	-3.162705000
6	3.659302000	-2.020634000	-1.435543000
6	3.571080000	0.555337000	0.423351000
1	3.966219000	0.088944000	2.484104000
8	-1.780517000	-2.229456000	-2.532104000
6	2.088878000	0.373558000	0.552892000
6	1.318649000	-2.470108000	0.553125000
6	5.771198000	0.566649000	1.416446000
1	1.711692000	2.110503000	-0.671467000
6	0.579208000	-4.758476000	0.748234000
1	1.359818000	-5.876436000	2.415228000
1	-0.463416000	3.602993000	0.708448000
1	-0.807606000	3.219213000	-3.338167000
1	-2.614216000	2.399441000	0.689787000

1	-0.025324000	-5.588381000	0.370886000
6	1.351467000	-4.919162000	1.886381000
6	0.563716000	-3.544742000	0.089222000
1	-1.402931000	0.952091000	-4.370944000
1	3.506046000	1.115178000	-1.660874000
6	2.115388000	-3.863543000	2.348827000
1	5.483297000	-2.901014000	-2.136387000
1	-2.626708000	3.685439000	-0.530312000
6	4.488236000	-2.538957000	-2.410245000
6	-4.225221000	0.884326000	-1.067889000
1	-5.308990000	2.685408000	-1.695068000
6	-4.810578000	-0.077571000	-2.076155000
6	-5.166407000	2.039416000	-0.811722000
1	-4.159854000	-0.946147000	-2.266072000
1	-4.115846000	0.332713000	-0.124266000
1	-5.770094000	-0.470859000	-1.700237000
1	-5.025772000	0.405496000	-3.045092000
1	-4.842897000	2.681124000	0.022294000
1	-6.164059000	1.651126000	-0.543073000
1	-0.437849000	1.293307000	1.137025000
6	1.819947000	2.704461000	1.370136000
6	2.712720000	3.720679000	1.062555000
6	1.360655000	2.585681000	2.678109000
6	3.143711000	4.602489000	2.038374000
6	1.783462000	3.472234000	3.651757000
6	2.678038000	4.481177000	3.335360000
1	3.084850000	3.813068000	0.035473000
1	0.648599000	1.793557000	2.944363000
1	3.850822000	5.396175000	1.780395000
1	1.407931000	3.372724000	4.674350000
1	3.013470000	5.179218000	4.107706000
6	0.209888000	0.811689000	-2.383168000
1	-1.440351000	-0.541551000	0.380925000
6	-2.090298000	-0.267102000	2.060425000
6	-3.477514000	-0.768199000	1.831762000
6	-3.775149000	-1.933497000	1.132336000
6	-4.511082000	0.011922000	2.337993000
6	-5.091904000	-2.300160000	0.932073000
1	-2.967142000	-2.528193000	0.695087000
6	-5.828075000	-0.360489000	2.138878000
1	-4.257678000	0.927531000	2.880643000
6	-6.120190000	-1.513991000	1.430528000
1	-5.322180000	-3.205475000	0.363220000
1	-6.636899000	0.258529000	2.538296000
1	-7.161202000	-1.805480000	1.262627000
6	-1.153629000	-1.259568000	2.763579000
8	-1.876563000	0.905068000	2.352136000
8	0.850136000	1.344180000	-3.186463000

9	-1.118206000	-2.474773000	2.278084000
9	0.074588000	-0.786805000	2.810194000
9	-1.570402000	-1.359691000	4.017742000

TS^R 1,1,1-F3

ΔH^{353} -3070.674752 Hartrees, ΔS^{353} 327.2 eu, ΔG^{353} -3070.858813 Hartrees, 506i cm⁻¹

1	6.335094000	0.118370000	-1.991844000
1	5.691682000	-1.932908000	1.724930000
1	-1.887013000	-1.963572000	3.922504000
6	-2.940537000	-2.173950000	3.680559000
6	1.270427000	-1.765743000	-0.642405000
15	0.995098000	0.667637000	0.667686000
6	-2.254358000	-3.005880000	-0.453526000
1	-0.121406000	3.059095000	1.655975000
1	2.803932000	4.428728000	-2.095223000
6	3.937678000	-1.229627000	0.710848000
7	-0.191916000	-1.674139000	-0.603702000
1	3.731361000	1.726984000	1.026013000
6	2.317330000	1.019163000	4.543361000
1	0.542074000	0.341428000	3.559926000
6	6.168861000	-0.917262000	-0.112614000
6	-1.635362000	0.642754000	2.116798000
1	2.469389000	2.047674000	-1.630990000
6	-3.073914000	-2.964991000	2.394274000
6	2.054134000	0.940636000	2.143251000
6	1.964539000	2.783560000	-1.000435000
6	3.592244000	1.531474000	4.401311000
6	-0.757925000	-3.023927000	-0.611787000
1	1.899612000	0.846230000	5.539398000
1	4.196301000	1.758940000	5.284671000
6	5.300987000	-1.408303000	0.848316000
25	-0.927514000	-0.490650000	0.946283000
1	-2.519131000	-4.794731000	3.380308000
15	-2.704163000	-1.892363000	0.921774000
1	-0.289947000	-3.566602000	0.233008000
1	7.248178000	-1.055691000	-0.002171000
1	-3.355054000	-2.748221000	4.525811000
6	4.294097000	-0.086452000	-1.355453000
1	-2.428479000	-4.912874000	1.620887000
1	1.736693000	0.114023000	-1.520737000
6	-2.254201000	-4.233432000	2.468587000
6	1.555758000	0.726395000	3.423402000
1	-4.136560000	-3.263945000	2.292867000
6	3.327578000	1.498879000	2.018547000
6	3.412604000	-0.554354000	-0.388464000
1	3.895912000	0.407926000	-2.249075000
8	-2.103013000	1.399546000	2.852796000
6	1.932235000	-0.386243000	-0.553275000

6	1.157896000	2.380023000	0.054757000
6	5.660359000	-0.258994000	-1.217913000
1	1.555713000	-2.353558000	0.253568000
6	0.711745000	4.699214000	0.554210000
1	1.693664000	6.153008000	-0.696144000
1	-0.473790000	-3.573501000	-1.529381000
1	-1.173358000	-4.033581000	2.529063000
1	-2.723909000	-2.602392000	-1.365073000
1	0.199928000	5.448825000	1.164867000
6	1.537647000	5.090523000	-0.486796000
6	0.525690000	3.357451000	0.821553000
1	-3.463977000	-1.205872000	3.656441000
1	3.265326000	-1.599855000	1.494464000
6	2.155011000	4.130148000	-1.266168000
1	5.093920000	2.200506000	3.008416000
1	-2.635907000	-4.034403000	-0.349089000
6	4.093538000	1.776130000	3.132942000
6	-4.390634000	-1.333633000	0.418163000
1	-4.925408000	-3.099682000	-0.771873000
6	-5.037475000	-0.432772000	1.444740000
6	-5.335134000	-2.442910000	0.010749000
1	-4.377244000	0.384451000	1.776409000
1	-4.180146000	-0.724608000	-0.476733000
1	-5.946824000	0.030351000	1.028141000
1	-5.353817000	-0.992214000	2.341989000
1	-6.266282000	-2.011988000	-0.393629000
1	-5.633258000	-3.081435000	0.858684000
1	-0.491019000	-1.189263000	-1.456134000
6	1.786071000	-2.497478000	-1.858313000
6	2.627889000	-3.591446000	-1.723346000
6	1.437132000	-2.069740000	-3.135617000
6	3.115144000	-4.250185000	-2.838970000
6	1.916041000	-2.733297000	-4.250571000
6	2.757471000	-3.824034000	-4.105532000
1	2.913347000	-3.926020000	-0.719066000
1	0.776667000	-1.201855000	-3.264068000
1	3.781476000	-5.108864000	-2.715852000
1	1.629909000	-2.391046000	-5.249507000
1	3.137652000	-4.345359000	-4.988675000
6	-0.080583000	-1.523248000	2.120960000
1	-1.672731000	0.367041000	-0.291851000
6	-1.793107000	2.605543000	-1.505321000
6	-2.754717000	2.907062000	-0.547458000
6	-1.187887000	3.635782000	-2.214422000
6	-3.095665000	4.221903000	-0.298492000
6	-1.545650000	4.949682000	-1.976236000
6	-2.497544000	5.245434000	-1.016994000
1	-3.218137000	2.098083000	0.027527000

1	-0.430355000	3.385595000	-2.963300000
1	-3.839215000	4.453245000	0.469485000
1	-1.063409000	5.754138000	-2.539671000
1	-2.774569000	6.285654000	-0.821392000
6	-1.437599000	1.218434000	-1.930628000
6	-2.593758000	0.485600000	-2.634391000
8	-0.335559000	0.901892000	-2.345778000
8	0.507287000	-2.217278000	2.836673000
9	-2.644015000	0.943115000	-3.873730000
9	-3.790123000	0.665525000	-2.119445000
9	-2.372941000	-0.813169000	-2.719010000

2,2,2-trifluoro-1-phenylethanol

ΔH^{353} -683.474095 Hartrees, ΔS^{353} 108.6 eu, ΔG^{353} -683.535185 Hartrees

1	0.668991000	-1.861649000	-1.757183000
1	1.024467000	0.477539000	-1.699960000
6	-0.613715000	-0.090310000	-0.432474000
6	-1.352633000	1.044396000	-0.741798000
6	-1.213045000	-1.125003000	0.276624000
6	-2.676251000	1.145566000	-0.349141000
6	-2.538417000	-1.025433000	0.664361000
6	-3.271578000	0.109112000	0.353095000
1	-0.880372000	1.861036000	-1.301256000
1	-0.624301000	-2.014675000	0.524484000
1	-3.253093000	2.041465000	-0.600403000
1	-3.005728000	-1.844168000	1.221173000
1	-4.320145000	0.185520000	0.658821000
6	0.829746000	-0.202698000	-0.839466000
6	1.747826000	0.291182000	0.265031000
8	1.242287000	-1.496950000	-1.082748000
9	3.011518000	0.226428000	-0.098096000
9	1.617112000	-0.414277000	1.367885000
9	1.480292000	1.548921000	0.556757000

2-acetylpyridine

ΔH^{353} -400.705156 Hartrees, ΔS^{353} 93.3 eu, ΔG^{353} -400.757629 Hartrees

6	0.000000000	0.188618000	0.000000000
7	-0.919031000	-0.770471000	0.000000000
6	1.369269000	-0.049369000	0.000000000
6	-0.485131000	-2.016746000	0.000000000
6	1.805549000	-1.360606000	0.000000000
6	0.857081000	-2.369724000	0.000000000
1	2.058397000	0.799581000	0.000000000
1	-1.259222000	-2.796162000	0.000000000
1	2.874585000	-1.597113000	0.000000000
1	1.148692000	-3.423785000	0.000000000
6	-0.497640000	1.602709000	0.000000000
6	-1.978114000	1.799459000	0.000000000
1	-2.207037000	2.872768000	0.000000000

1	-2.437764000	1.316688000	0.876194000
1	-2.437764000	1.316688000	-0.876194000
8	0.283406000	2.517323000	0.000000000

TS^S Acpy

ΔH^{353} -2789.098644 Hartrees, ΔS^{353} 314.3 eu, ΔG^{353} -2789.275459 Hartrees, 848i cm⁻¹

1	-6.362728000	1.297598000	-1.986319000
1	-5.756350000	0.929416000	2.248504000
1	3.231857000	-1.179090000	3.613927000
6	2.784082000	-0.286186000	4.074911000
6	-1.262852000	1.701682000	0.145934000
15	-1.186381000	-1.074974000	-0.000957000
6	2.357603000	2.366480000	0.751805000
1	0.185771000	-3.456318000	-0.692442000
1	-3.119595000	-2.733261000	-4.307065000
6	-4.013243000	0.717583000	1.017395000
7	0.182680000	1.496353000	0.104626000
1	-4.016636000	-1.951081000	-0.197881000
6	-2.584243000	-3.377172000	3.088115000
1	-0.755663000	-2.386614000	2.576727000
6	-6.214202000	1.124167000	0.153675000
6	1.458759000	-1.968726000	1.132501000
1	-2.981438000	-1.130982000	-2.453597000
6	3.007089000	0.987661000	3.282817000
6	-2.294516000	-2.021591000	1.110629000
6	-2.306055000	-1.992642000	-2.462948000
6	-3.890695000	-3.645685000	2.728047000
6	0.871417000	2.612632000	0.747105000
1	-2.165827000	-3.801614000	4.005149000
1	-4.517937000	-4.278748000	3.362669000
6	-5.362882000	0.926655000	1.227947000
25	0.797722000	-0.354577000	0.778045000
1	2.544006000	2.237865000	4.970332000
15	2.673756000	0.724953000	1.472907000
1	0.474931000	2.704226000	1.777254000
1	-7.282478000	1.287926000	0.321409000
1	1.712486000	-0.497546000	4.209234000
6	-4.349748000	0.919514000	-1.339400000
1	2.438815000	3.101421000	3.431761000
1	-1.819834000	0.588591000	-1.587763000
6	2.245437000	2.130980000	3.913825000
6	-1.793216000	-2.571672000	2.285492000
1	4.086097000	1.239113000	3.345252000
6	-3.603525000	-2.333587000	0.741595000
6	-3.487438000	0.699479000	-0.272215000
1	-3.942961000	0.955095000	-2.357092000
8	1.904004000	-3.012690000	1.340010000
6	-2.015688000	0.525401000	-0.495858000

6	-1.378270000	-2.175089000	-1.443700000
6	-5.702685000	1.123610000	-1.131541000
1	-1.540330000	1.748808000	1.219345000
6	-0.650235000	-4.207940000	-2.518593000
1	-1.627816000	-4.715874000	-4.368733000
1	0.645606000	3.568548000	0.236349000
1	1.157741000	1.959323000	3.913715000
1	2.704359000	2.320782000	-0.298125000
1	0.010167000	-5.079639000	-2.534133000
6	-1.561412000	-4.004165000	-3.540911000
6	-0.557938000	-3.299077000	-1.481335000
1	3.218340000	-0.188139000	5.083905000
1	-3.353865000	0.542812000	1.876490000
6	-2.390366000	-2.897182000	-3.508037000
1	-5.424372000	-3.346170000	1.245017000
1	2.896513000	3.198667000	1.235101000
6	-4.397066000	-3.124734000	1.548196000
6	4.364415000	0.303135000	0.859848000
1	5.529147000	1.860353000	1.870311000
6	4.964470000	-0.904720000	1.542035000
6	5.333955000	1.462943000	0.859269000
1	4.293454000	-1.777944000	1.530526000
1	4.181004000	0.016524000	-0.184376000
1	5.888351000	-1.203044000	1.018059000
1	5.247804000	-0.703354000	2.589487000
1	4.998529000	2.302896000	0.231275000
1	6.308970000	1.135228000	0.458667000
1	0.495786000	1.507985000	-0.880777000
6	-1.712456000	2.990300000	-0.501135000
6	-2.546222000	3.867678000	0.176678000
6	-1.326721000	3.296543000	-1.802448000
6	-2.993136000	5.028977000	-0.429421000
6	-1.766103000	4.461387000	-2.404991000
6	-2.602632000	5.328916000	-1.722140000
1	-2.858642000	3.626164000	1.199489000
1	-0.653276000	2.623183000	-2.349111000
1	-3.653202000	5.708960000	0.116987000
1	-1.449113000	4.696039000	-3.425531000
1	-2.950892000	6.247922000	-2.202423000
6	0.001867000	-0.057249000	2.334532000
1	1.479139000	-0.433709000	-0.821660000
6	1.801802000	0.206554000	-2.326177000
6	3.261537000	-0.178776000	-2.329199000
7	3.577514000	-1.453923000	-2.141393000
6	4.201991000	0.813077000	-2.580564000
6	4.858104000	-1.766807000	-2.153955000
6	5.539746000	0.465589000	-2.596798000
1	3.858803000	1.836368000	-2.751386000

6	5.881995000	-0.853333000	-2.362605000
1	5.094306000	-2.825186000	-1.983309000
1	6.311454000	1.218803000	-2.785661000
1	6.924312000	-1.181228000	-2.353544000
6	0.946460000	-0.709710000	-3.154115000
8	1.528585000	1.418909000	-2.294889000
1	1.095787000	-1.774085000	-2.939585000
1	1.223367000	-0.530997000	-4.209045000
1	-0.113660000	-0.444926000	-3.049965000
8	-0.578644000	0.202190000	3.301628000

TS^R Acpy

ΔH^{353} -2789.096041 Hartrees, ΔS^{353} 312.5 eu, ΔG^{353} -2789.271855 Hartrees, 558i cm⁻¹

1	6.376552000	-0.126208000	-1.391662000
1	5.233707000	-1.954172000	2.321496000
1	-2.941096000	-1.599485000	3.396703000
6	-3.860620000	-2.058631000	2.995603000
6	1.135448000	-1.788470000	-0.575796000
15	0.762935000	0.688851000	0.600457000
6	-2.421417000	-2.896142000	-0.914955000
1	-0.543129000	3.107789000	1.237135000
1	3.070203000	4.339959000	-1.916714000
6	3.635242000	-1.252111000	1.075730000
7	-0.310629000	-1.643754000	-0.759792000
1	3.477561000	1.682830000	1.255308000
6	1.587428000	1.232565000	4.586568000
1	-0.064732000	0.541653000	3.414655000
6	5.956668000	-1.052767000	0.504735000
6	-2.045432000	0.770183000	1.691229000
1	2.646924000	1.976329000	-1.424118000
6	-3.580574000	-2.868255000	1.748955000
6	1.639673000	1.014762000	2.181352000
6	2.025186000	2.736186000	-0.943204000
6	2.886680000	1.701786000	4.586639000
6	-0.918446000	-2.970074000	-0.853085000
1	1.037142000	1.130677000	5.526420000
1	3.376703000	1.966839000	5.528275000
6	4.966230000	-1.464910000	1.380448000
25	-1.205086000	-0.409209000	0.657183000
1	-3.100168000	-4.650888000	2.842674000
15	-3.010986000	-1.751629000	0.381717000
1	-0.599947000	-3.527057000	0.050059000
1	7.010196000	-1.218278000	0.747573000
1	-4.277658000	-2.698470000	3.791060000
6	4.269371000	-0.232657000	-0.988644000
1	-2.494327000	-4.687130000	1.186699000
1	1.750432000	0.044903000	-1.460020000
6	-2.654164000	-4.024870000	2.051575000

6	0.970036000	0.892387000	3.393708000
1	-4.532847000	-3.313973000	1.405462000
6	2.937310000	1.528988000	2.195734000
6	3.265343000	-0.619890000	-0.109105000
1	3.994680000	0.223413000	-1.947096000
8	-2.591218000	1.539886000	2.354473000
6	1.821438000	-0.422723000	-0.458448000
6	1.023432000	2.372136000	-0.052997000
6	5.603515000	-0.439532000	-0.683846000
1	1.266080000	-2.337102000	0.379755000
6	0.506255000	4.707563000	0.266052000
1	1.723820000	6.114515000	-0.820239000
1	-0.525486000	-3.534990000	-1.719866000
1	-1.670286000	-3.707141000	2.421525000
1	-2.741484000	-2.500624000	-1.893870000
1	-0.106296000	5.479992000	0.740510000
6	1.520478000	5.060291000	-0.609353000
6	0.258131000	3.376585000	0.537576000
1	-4.581561000	-1.243107000	2.824216000
1	2.863772000	-1.561504000	1.791516000
6	2.269933000	4.071805000	-1.219989000
1	4.580947000	2.243725000	3.370986000
1	-2.855393000	-3.908710000	-0.849552000
6	3.558730000	1.854601000	3.384697000
6	-4.602728000	-1.116430000	-0.337400000
1	-6.195956000	-2.144275000	0.748077000
6	-4.971138000	0.257359000	0.173152000
6	-5.779723000	-2.062177000	-0.270100000
1	-4.176048000	0.996716000	-0.006127000
1	-4.340591000	-1.010401000	-1.405839000
1	-5.878929000	0.618720000	-0.339645000
1	-5.197998000	0.256398000	1.252617000
1	-5.541182000	-3.080445000	-0.619983000
1	-6.595254000	-1.686756000	-0.910532000
1	-0.446281000	-1.136378000	-1.645881000
6	1.801304000	-2.596512000	-1.664209000
6	2.579344000	-3.700507000	-1.349144000
6	1.660197000	-2.229935000	-2.999165000
6	3.208898000	-4.428866000	-2.343776000
6	2.281774000	-2.963034000	-3.993814000
6	3.059057000	-4.062837000	-3.669319000
1	2.700478000	-3.986669000	-0.297618000
1	1.048402000	-1.357799000	-3.264472000
1	3.822716000	-5.294810000	-2.079089000
1	2.159623000	-2.669078000	-5.040726000
1	3.552501000	-4.638474000	-4.457754000
6	-0.559209000	-1.394479000	1.986762000
1	-1.707084000	0.483525000	-0.682619000

6	-1.640653000	2.457294000	-2.048065000
7	-2.701275000	2.838148000	-1.350107000
6	-0.810809000	3.342840000	-2.720798000
6	-2.946995000	4.131894000	-1.281980000
6	-1.100038000	4.691596000	-2.662483000
6	-2.192070000	5.101822000	-1.921468000
1	0.043374000	2.950994000	-3.278070000
1	-3.819390000	4.422402000	-0.682220000
1	-0.470520000	5.419727000	-3.184181000
1	-2.461253000	6.157530000	-1.835533000
6	-1.423121000	0.979508000	-2.284716000
6	-2.643620000	0.350258000	-2.908547000
1	-2.556721000	-0.744010000	-2.946850000
1	-2.675775000	0.702471000	-3.955726000
1	-3.581530000	0.656190000	-2.428453000
8	-0.304358000	0.569876000	-2.610595000
8	-0.077388000	-2.023239000	2.831394000

1-(2-pyridyl)-ethanol

ΔH^{353} -401.883311 Hartrees, ΔS^{353} 94.8 eu, ΔG^{353} -401.936634 Hartrees

6	-0.122156000	-0.024000000	-0.185332000
7	0.526281000	-1.171471000	-0.344995000
6	0.507315000	1.173142000	0.129876000
6	1.837272000	-1.154460000	-0.191792000
6	1.882755000	1.168500000	0.284984000
6	2.570246000	-0.020519000	0.121437000
1	-0.080832000	2.085835000	0.246085000
1	2.347450000	-2.118004000	-0.331391000
1	2.416010000	2.093063000	0.532650000
1	3.656838000	-0.074697000	0.231850000
6	-1.614037000	-0.117532000	-0.356716000
6	-2.224132000	-1.015337000	0.695115000
1	-3.309085000	-1.134296000	0.531061000
1	-2.074653000	-0.585163000	1.699478000
1	-1.769429000	-2.016793000	0.671596000
8	-2.128036000	1.171071000	-0.304319000
1	-3.080026000	1.103762000	-0.359784000
1	-1.789534000	-0.580742000	-1.357462000

1-indanone

ΔH^{353} -422.770816 Hartrees, ΔS^{353} 93.8 eu, ΔG^{353} -422.823591 Hartrees

8	-2.168575000	-1.657384000	0.000043000
6	-1.554765000	-0.626534000	-0.000004000
6	-2.151527000	0.769167000	-0.000024000
1	-2.809520000	0.875085000	-0.877987000
1	-2.809546000	0.875094000	0.877917000
6	-0.091220000	-0.463688000	-0.000030000
6	0.235755000	0.886589000	-0.000001000
6	0.883135000	-1.453577000	-0.000037000

6	1.567849000	1.271235000	0.000002000
6	2.208803000	-1.067387000	0.000009000
6	2.542713000	0.286638000	0.000013000
1	0.591237000	-2.509470000	-0.000051000
1	1.849729000	2.330359000	0.000011000
1	3.004523000	-1.819073000	0.000027000
1	3.599476000	0.575767000	0.000033000
6	-0.987744000	1.747592000	0.000003000
1	-0.997652000	2.415605000	-0.879222000
1	-0.997637000	2.415489000	0.879338000

TS^S indanone

ΔH^{353} -2811.165657 Hartrees, ΔS^{353} 314.6 eu, ΔG^{353} -2811.34266 Hartrees, 868i cm⁻¹

1	6.118501000	1.545366000	2.236634000
1	5.821488000	1.370017000	-2.042922000
1	-1.689506000	-1.245057000	-4.163091000
6	-2.777707000	-1.092250000	-4.087168000
6	1.079193000	1.767043000	-0.378813000
15	1.289661000	-0.955072000	0.067775000
6	-2.570685000	1.999636000	-1.146551000
1	1.360010000	-3.742137000	0.510419000
1	2.123534000	-1.711804000	4.954940000
6	3.995042000	1.097148000	-0.951603000
7	-0.341489000	1.407358000	-0.335352000
1	4.150501000	-1.528176000	0.488963000
6	3.142340000	-3.189273000	-2.842916000
1	1.178161000	-2.417087000	-2.490926000
6	6.124472000	1.479188000	0.085424000
6	-1.126637000	-2.272973000	-1.135788000
1	1.810590000	-0.264972000	3.011435000
6	-3.110824000	0.252922000	-3.473741000
6	2.552383000	-1.825203000	-0.937840000
6	1.800664000	-1.346218000	2.866270000
6	4.441309000	-3.292442000	-2.384418000
6	-1.120702000	2.391630000	-1.079711000
1	2.843328000	-3.686007000	-3.770397000
1	5.182278000	-3.862814000	-2.952529000
6	5.354363000	1.323985000	-1.054895000
25	-0.739044000	-0.554982000	-0.885568000
1	-2.753567000	1.296713000	-5.321896000
15	-2.707212000	0.256245000	-1.663050000
1	-0.684350000	2.447273000	-2.096905000
1	7.200819000	1.655335000	0.003241000
1	-3.184184000	-1.159175000	-5.110064000
6	4.158987000	1.195700000	1.429589000
1	-2.759527000	2.371128000	-3.919432000
1	1.615987000	0.915276000	1.475526000
6	-2.461001000	1.368334000	-4.260870000

6	2.206585000	-2.462084000	-2.124553000
1	-4.208594000	0.394512000	-3.540600000
6	3.858883000	-1.974895000	-0.467682000
6	3.376110000	1.024611000	0.293773000
1	3.684136000	1.157648000	2.416656000
8	-1.366842000	-3.394529000	-1.265351000
6	1.909344000	0.763239000	0.421702000
6	1.587216000	-1.894202000	1.607600000
6	5.521582000	1.415034000	1.329175000
1	1.374590000	1.726798000	-1.447471000
6	1.659891000	-4.098752000	2.600577000
1	1.988061000	-4.179725000	4.728743000
1	-1.018168000	3.403786000	-0.643325000
1	-1.361785000	1.313287000	-4.235674000
1	-3.015411000	2.061693000	-0.136982000
1	1.597394000	-5.184622000	2.484501000
6	1.876591000	-3.539517000	3.848899000
6	1.526006000	-3.284197000	1.493088000
1	-3.182578000	-1.943783000	-3.518891000
1	3.407689000	0.938407000	-1.863764000
6	1.952461000	-2.164779000	3.973704000
1	5.815963000	-2.780065000	-0.806232000
1	-3.137289000	2.709730000	-1.771186000
6	4.795570000	-2.687564000	-1.189088000
6	-4.308379000	-0.229664000	-0.887547000
1	-5.797684000	0.728755000	-2.178156000
6	-4.717734000	-1.650906000	-1.195221000
6	-5.458239000	0.722604000	-1.128534000
1	-3.895999000	-2.373945000	-1.071116000
1	-4.060089000	-0.179281000	0.184954000
1	-5.532031000	-1.963939000	-0.519482000
1	-5.104441000	-1.756581000	-2.223848000
1	-5.230013000	1.761073000	-0.842274000
1	-6.326784000	0.413715000	-0.521972000
1	-0.617175000	1.416597000	0.659231000
6	1.351901000	3.164029000	0.124817000
6	2.027772000	4.082800000	-0.663640000
6	0.935275000	3.544969000	1.397122000
6	2.287788000	5.359745000	-0.196522000
6	1.187050000	4.823173000	1.860875000
6	1.865150000	5.733489000	1.066382000
1	2.362079000	3.784679000	-1.664394000
1	0.398805000	2.828502000	2.033995000
1	2.825474000	6.072050000	-0.829055000
1	0.851422000	5.113736000	2.860939000
1	2.065395000	6.743000000	1.436794000
6	0.053998000	-0.280028000	-2.450463000
1	-1.548473000	-0.620441000	0.623932000

6	-1.489497000	-0.241906000	2.172394000
6	-2.901533000	0.232010000	2.328511000
6	-3.758683000	-0.846341000	2.504018000
6	-3.367389000	1.532969000	2.364133000
6	-5.113868000	-0.632013000	2.682069000
6	-4.724491000	1.749241000	2.537880000
1	-2.663794000	2.369434000	2.264991000
6	-5.589239000	0.671623000	2.689828000
1	-5.802753000	-1.472706000	2.821330000
1	-5.120255000	2.768896000	2.574061000
1	-6.657916000	0.857664000	2.835771000
6	-1.558037000	-1.699042000	2.640805000
8	0.575116000	-0.042652000	-3.455976000
6	-2.994432000	-2.123485000	2.417490000
1	-3.111270000	-2.561303000	1.403858000
1	-3.349096000	-2.889266000	3.125660000
1	-1.329723000	-1.676488000	3.724654000
1	-0.825791000	-2.359269000	2.165443000
8	-0.527179000	0.524019000	2.331368000

TS^R indanone

ΔH^{353} -2811.152104 Hartrees, ΔS^{353} 312.0 eu, ΔG^{353} -2811.327614 Hartrees, 1171i cm⁻¹

1	-6.302444000	-0.464244000	1.677636000
1	-5.140839000	-2.845897000	-1.700829000
1	3.848521000	-1.550103000	-3.194677000
6	3.508504000	-2.564909000	-2.944157000
6	-0.963644000	-1.709664000	0.827495000
15	-0.897950000	0.536952000	-0.801749000
6	2.712819000	-2.238403000	1.236150000
1	0.480482000	2.942756000	-1.444772000
1	-3.794876000	4.326799000	0.640054000
6	-3.575058000	-1.750033000	-0.728078000
7	0.457654000	-1.381471000	0.905347000
1	-3.746333000	0.980559000	-1.571673000
6	-1.769221000	0.235767000	-4.797265000
1	-0.047196000	0.011387000	-3.547510000
6	-5.872448000	-1.690644000	-0.037861000
6	1.901175000	0.713961000	-1.956205000
1	-3.195372000	1.947022000	0.563884000
6	3.616267000	-2.912311000	-1.470508000
6	-1.815315000	0.443219000	-2.389591000
6	-2.506971000	2.684004000	0.137930000
6	-3.123331000	0.501594000	-4.860612000
6	1.238924000	-2.561577000	1.261363000
1	-1.198979000	0.050492000	-5.711942000
1	-3.636785000	0.521189000	-5.826363000
6	-4.885815000	-2.157009000	-0.890446000
25	1.176701000	-0.346709000	-0.721232000

1	3.319163000	-5.002471000	-1.864713000
15	3.105568000	-1.493879000	-0.380568000
1	0.988321000	-3.364975000	0.542225000
1	-6.909608000	-2.012116000	-0.168591000
1	2.471817000	-2.652571000	-3.300706000
6	-4.220888000	-0.422142000	1.149895000
1	3.019988000	-4.583034000	-0.174348000
1	-1.745870000	0.199780000	1.390375000
6	2.904819000	-4.220093000	-1.206864000
6	-1.122507000	0.206926000	-3.572710000
1	4.688332000	-3.074268000	-1.232233000
6	-3.174413000	0.747876000	-2.475280000
6	-3.224279000	-0.864003000	0.287608000
1	-3.952583000	0.239568000	1.982296000
8	2.392616000	1.404458000	-2.739714000
6	-1.795952000	-0.460802000	0.497719000
6	-1.317545000	2.276218000	-0.457147000
6	-5.534947000	-0.824181000	0.986345000
1	-1.076190000	-2.435858000	-0.004123000
6	-0.817824000	4.580964000	-0.957069000
1	-2.292333000	6.031682000	-0.360688000
1	0.956193000	-2.939508000	2.262447000
1	1.828735000	-4.161674000	-1.433634000
1	2.910169000	-1.478202000	2.013635000
1	-0.137401000	5.327407000	-1.377033000
6	-2.014943000	4.973680000	-0.383604000
6	-0.470055000	3.243807000	-0.989674000
1	4.110790000	-3.266557000	-3.544717000
1	-2.808646000	-2.111374000	-1.424281000
6	-2.851924000	4.023998000	0.174509000
1	-4.892274000	0.991598000	-3.733243000
1	3.317292000	-3.123612000	1.498213000
6	-3.823452000	0.762525000	-3.694213000
6	4.739733000	-0.643665000	-0.158823000
1	5.944357000	-2.365462000	0.435543000
6	5.438786000	-0.336460000	-1.464890000
6	5.671510000	-1.357556000	0.793313000
1	4.802802000	0.223608000	-2.167926000
1	4.472182000	0.333686000	0.274362000
1	6.323326000	0.290578000	-1.266002000
1	5.805000000	-1.240445000	-1.979104000
1	5.253725000	-1.470323000	1.805608000
1	6.615196000	-0.795915000	0.896035000
1	0.591595000	-0.711370000	1.687652000
6	-1.511499000	-2.364904000	2.073704000
6	-2.161707000	-3.587787000	1.995218000
6	-1.398189000	-1.740027000	3.311932000
6	-2.693107000	-4.181202000	3.127138000

6	-1.922142000	-2.337116000	4.444189000
6	-2.572698000	-3.556913000	4.355597000
1	-2.260797000	-4.079530000	1.020069000
1	-0.875497000	-0.778792000	3.394451000
1	-3.206836000	-5.143754000	3.047389000
1	-1.819583000	-1.840795000	5.413903000
1	-2.988391000	-4.024183000	5.253092000
6	0.589242000	-1.612797000	-1.811292000
1	1.647254000	0.807890000	0.599710000
6	1.188604000	2.658795000	2.021243000
6	2.221371000	3.494764000	1.612719000
6	-0.028959000	3.168841000	2.426506000
6	2.026947000	4.862075000	1.561140000
6	-0.213684000	4.539651000	2.402415000
6	0.802664000	5.376531000	1.961076000
1	-0.813441000	2.493179000	2.787217000
1	2.835100000	5.533384000	1.250040000
1	-1.163691000	4.971451000	2.732295000
1	0.640432000	6.459132000	1.949036000
6	1.691310000	1.258534000	2.155957000
6	3.199608000	1.472859000	2.237098000
8	1.097920000	0.387634000	2.816781000
8	0.144618000	-2.466471000	-2.452185000
6	3.463717000	2.694802000	1.384451000
1	4.382943000	3.242233000	1.646955000
1	3.550718000	2.410155000	0.314257000
1	3.388555000	1.726674000	3.298844000
1	3.795487000	0.578617000	2.022442000

1-indanol

ΔH^{353} -423.944064 Hartrees, ΔS^{353} 94.1 eu, ΔG^{353} -423.996992 Hartrees

6	1.506836000	-0.733866000	0.319895000
6	2.045023000	0.658651000	0.598020000
1	2.029644000	0.837490000	1.687202000
1	3.087749000	0.757894000	0.257634000
6	0.024354000	-0.489584000	0.227163000
6	-0.216049000	0.853508000	-0.052862000
6	-1.018369000	-1.394976000	0.315607000
6	-1.511338000	1.300544000	-0.250671000
6	-2.317246000	-0.944635000	0.122590000
6	-2.558244000	0.393059000	-0.159727000
1	-0.827541000	-2.450181000	0.549215000
1	-1.713928000	2.356333000	-0.465914000
1	-3.156888000	-1.643158000	0.201288000
1	-3.588237000	0.737528000	-0.302584000
6	1.073388000	1.608848000	-0.092365000
1	1.011815000	2.596277000	0.395518000
1	1.375578000	1.798592000	-1.139704000

1	1.769775000	-1.457784000	1.124438000
8	2.038115000	-1.142482000	-0.908604000
1	1.536989000	-1.902434000	-1.204153000

syn-FeHNNH

ΔH^{298} -2066.958492 Hartrees, ΔS^{298} 192.581 eu, ΔG^{298} -2067.049994 Hartrees

17	-0.052201000	-2.085625000	1.108705000
26	-0.011047000	0.069983000	0.009577000
1	-0.001709000	1.391555000	-0.742511000
6	-0.022122000	0.922662000	1.549042000
8	-0.027287000	1.476780000	2.553447000
7	0.010287000	-0.892857000	-1.796714000
1	0.020726000	-0.124001000	-2.472292000
6	-1.199046000	-1.653529000	-2.059847000
1	-1.241095000	-2.475943000	-1.323871000
1	-1.169895000	-2.108486000	-3.069979000
6	-2.376298000	-0.726701000	-1.920066000
1	-3.327852000	-1.260641000	-2.069990000
1	-2.316566000	0.041455000	-2.709550000
15	-2.244339000	0.078719000	-0.284785000
6	-3.153992000	1.686600000	-0.411734000
1	-4.226420000	1.456813000	-0.263187000
6	-3.010392000	2.357842000	-1.758634000
1	-3.525625000	1.816359000	-2.565521000
1	-1.953047000	2.481193000	-2.051286000
1	-3.450991000	3.368091000	-1.717439000
6	-2.716421000	2.631869000	0.687752000
1	-3.358996000	3.527850000	0.695485000
6	-3.313150000	-0.993479000	0.772417000
1	-2.870472000	-1.994351000	0.594176000
6	-4.774530000	-1.036129000	0.387317000
1	-5.274960000	-1.869605000	0.907946000
1	-4.946109000	-1.182600000	-0.690437000
1	-5.305062000	-0.116987000	0.686131000
6	-3.163016000	-0.681801000	2.243939000
1	-3.627568000	0.284871000	2.502839000
1	-2.108552000	-0.657064000	2.558253000
1	-3.671613000	-1.449305000	2.851283000
6	1.215579000	-1.668667000	-2.038750000
1	1.200231000	-2.116057000	-3.052490000
1	1.230393000	-2.496147000	-1.307456000
6	2.400801000	-0.759610000	-1.863571000
1	2.382280000	0.015836000	-2.653013000
1	3.352992000	-1.298672000	-1.981626000
15	2.226276000	0.104779000	-0.261954000
6	2.985001000	1.742250000	-0.656221000
1	2.319476000	2.107350000	-1.465267000
6	2.904874000	2.725440000	0.487376000

1	3.576786000	2.443143000	1.315309000
1	1.885502000	2.820619000	0.895270000
1	3.218325000	3.727989000	0.152640000
6	4.391928000	1.670142000	-1.204837000
1	4.695661000	2.656914000	-1.592243000
1	4.498207000	0.951410000	-2.032329000
1	5.126805000	1.398423000	-0.429635000
6	3.414780000	-0.688205000	0.916608000
1	4.399002000	-0.213779000	0.731451000
6	3.002901000	-0.393886000	2.343932000
1	2.046726000	-0.888194000	2.582142000
1	2.880791000	0.681627000	2.547322000
1	3.763751000	-0.773650000	3.046517000
6	3.571469000	-2.178421000	0.712931000
1	4.265876000	-2.582622000	1.469071000
1	3.988364000	-2.438614000	-0.271459000
1	2.610911000	-2.703611000	0.832286000
1	-1.679744000	2.974244000	0.527914000
1	-2.764843000	2.185664000	1.693162000

TSFe

ΔH^{298} -2066.904560 Hartrees, ΔS^{298} 193.18 eu, ΔG^{298} -2066.996348 Hartrees, 400i cm⁻¹

1	17	0	-0.038941	-1.780584	-1.782843
2	26	0	-0.023510	-0.365862	0.050392
3	1	0	-0.029978	0.761109	1.059455
4	6	0	-0.022540	-1.546760	1.329105
5	8	0	-0.014441	-2.346109	2.148431
6	7	0	0.003786	1.922501	-1.579195
7	1	0	0.012575	1.225581	-0.839774
8	6	0	-1.172661	2.660347	-1.197904
9	1	0	-1.365325	3.451072	-1.944276
10	1	0	-1.055088	3.170047	-0.214403
11	6	0	-2.339612	1.691428	-1.183319
12	1	0	-2.443356	1.270962	-2.201359
13	1	0	-3.282252	2.225315	-0.974852
14	15	0	-2.215881	0.214361	-0.070406
15	6	0	-3.050450	0.723545	1.499862
16	1	0	-4.137732	0.632630	1.304826
17	6	0	-2.768999	2.155150	1.895668
18	1	0	-3.116828	2.890426	1.155158
19	1	0	-1.692870	2.327151	2.067965
20	1	0	-3.285440	2.382964	2.843017
21	6	0	-2.686975	-0.199525	2.642895
22	1	0	-3.326472	0.009865	3.516140
23	6	0	-3.390373	-0.932767	-0.906463
24	1	0	-2.864359	-1.137198	-1.860694
25	6	0	-4.753262	-0.362224	-1.222815
26	1	0	-5.341907	-1.101816	-1.791115

27	1	0	-4.711102	0.551433	-1.834222
28	1	0	-5.332178	-0.132779	-0.312916
29	6	0	-3.512133	-2.240015	-0.157524
30	1	0	-4.107305	-2.126357	0.764455
31	1	0	-2.530129	-2.658687	0.120334
32	1	0	-4.027611	-2.990449	-0.778778
33	6	0	1.294709	2.528774	-1.368085
34	1	0	1.355075	3.089234	-0.404968
35	1	0	1.491387	3.258420	-2.172761
36	6	0	2.328363	1.419885	-1.421743
37	1	0	3.350583	1.831853	-1.449747
38	1	0	2.187211	0.872771	-2.370785
39	15	0	2.188699	0.173571	-0.065994
40	6	0	2.820216	1.095125	1.405911
41	1	0	2.011950	1.824920	1.609943
42	6	0	2.936919	0.187414	2.609130
43	1	0	3.759091	-0.539424	2.494197
44	1	0	2.011923	-0.378824	2.807686
45	1	0	3.157536	0.779211	3.512055
46	6	0	4.102008	1.863963	1.183698
47	1	0	4.418306	2.336349	2.128568
48	1	0	3.994100	2.671658	0.444739
49	1	0	4.935039	1.218640	0.857982
50	6	0	3.496868	-1.082616	-0.429849
51	1	0	4.420217	-0.720632	0.065470
52	6	0	3.111892	-2.410364	0.189177
53	1	0	2.212172	-2.822911	-0.297250
54	1	0	2.901321	-2.338394	1.267981
55	1	0	3.928552	-3.140552	0.063768
56	6	0	3.788469	-1.248898	-1.903507
57	1	0	4.529287	-2.053692	-2.043701
58	1	0	4.206294	-0.340578	-2.362661
59	1	0	2.884991	-1.534144	-2.467438
60	1	0	-1.642996	-0.037507	2.960920
61	1	0	-2.799297	-1.267713	2.402687

anti-FeHNNH

ΔH^{298} -2066.963511 Hartrees, ΔS^{298} 191.677 eu, ΔG^{298} -2067.054583 Hartrees

17	-0.003037000	1.997940000	-1.378635000
26	0.020906000	0.030080000	0.036237000
1	0.021794000	-1.275438000	0.805528000
6	0.056569000	0.905649000	1.560324000
8	0.091026000	1.442696000	2.574023000
7	0.000411000	-1.038408000	-1.701560000
1	0.059966000	-0.278871000	-2.389841000
6	1.154003000	-1.898707000	-1.905715000
1	1.137200000	-2.346543000	-2.919269000
1	1.077044000	-2.732004000	-1.183899000

6	2.411794000	-1.104028000	-1.687366000
1	2.515169000	-0.351992000	-2.492229000
1	3.308354000	-1.742184000	-1.738971000
15	2.248837000	-0.184998000	-0.120038000
6	3.156872000	-1.189800000	1.138776000
1	4.234988000	-1.010321000	0.956918000
6	2.911190000	-2.676081000	1.007930000
1	3.224422000	-3.086441000	0.036073000
1	1.848601000	-2.929978000	1.159520000
1	3.483258000	-3.213616000	1.782670000
6	2.820305000	-0.740132000	2.544086000
1	3.460908000	-1.261719000	3.274338000
6	3.308429000	1.288972000	-0.446144000
1	2.823216000	1.700585000	-1.353431000
6	4.747855000	0.971102000	-0.778490000
1	5.253117000	1.871658000	-1.166017000
1	4.852329000	0.187103000	-1.545498000
1	5.316839000	0.649142000	0.109238000
6	3.216590000	2.344801000	0.630007000
1	3.730230000	2.037236000	1.556083000
1	2.173447000	2.594015000	0.882024000
1	3.703361000	3.275057000	0.292754000
6	-1.233941000	-1.756604000	-1.973489000
1	-1.279192000	-2.619666000	-1.282098000
1	-1.232720000	-2.169948000	-3.001305000
6	-2.396538000	-0.826154000	-1.762136000
1	-3.358883000	-1.321418000	-1.964742000
1	-2.313358000	0.016162000	-2.471474000
15	-2.223480000	-0.159394000	-0.077854000
6	-2.947782000	-1.473760000	0.999464000
1	-2.236140000	-2.316147000	0.889216000
6	-2.925004000	-1.036064000	2.447042000
1	-3.637363000	-0.213915000	2.634632000
1	-1.927208000	-0.695706000	2.770702000
1	-3.217601000	-1.868913000	3.106905000
6	-4.320993000	-1.962877000	0.603314000
1	-4.655242000	-2.745669000	1.304784000
1	-4.344919000	-2.406325000	-0.403199000
1	-5.081446000	-1.164906000	0.637332000
6	-3.420102000	1.246615000	0.079645000
1	-4.334714000	0.816790000	0.534411000
6	-2.882571000	2.300502000	1.023280000
1	-1.965780000	2.761301000	0.619055000
1	-2.642286000	1.896724000	2.019545000
1	-3.628518000	3.100499000	1.165747000
6	-3.811977000	1.860887000	-1.244247000
1	-4.510091000	2.697523000	-1.072682000
1	-4.319752000	1.146564000	-1.910516000

1	-2.938139000	2.266920000	-1.779931000
1	1.774513000	-0.985718000	2.796255000
1	2.953041000	0.340333000	2.705447000

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