Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

for

Highly Efficient Hydroboration of Carbonyl Compounds Catalyzed by Tris(methylcyclopentadienyl)lanthanide Complexes

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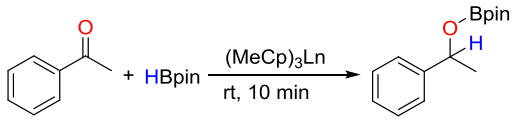
1. Optimization of the reaction conditions

Table S1. Optimization of the reaction conditions[a]



$(MeCp)_3Ln$ (Ln = Y (**a**), Yb (**b**), Nd (**c**), and La (**d**))

entry	cat (mol%)	solvent	time (min)	substrate ratio	conv[b] (%)
1	**a** (0.01)	THF	10	1:1	96
2	**a** (0.01)	Tol	10	1:1	94
3	**a** (0.01)	Tol	10	1:1.1	96
4	**a** (0.01)	Tol	10	1:1.2	97
5	**b** (0.01)	THF	10	1:1.2	93
6	**c** (0.01)	THF	10	1:1.2	95
7	**d** (0.01)	THF	10	1:1.2	99

[a] Reaction condition: all reaction were conduceted with acetophenone (1 mmol), pinacolborane (1-1.2 mmol) and $(MeCp)_3Ln$ (0.01 mmol%) under N_2 at 25 ^oC, 10 min.

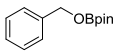
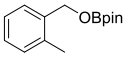
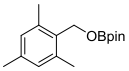
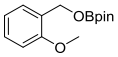
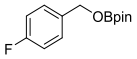
[b] NMR yield.

2. $(MeCp)_3La$ NMR data and elemental analysis

^1H NMR (400 MHz, $CDCl_3$) δ 5.97-5.85 (t, 6H), 5.86-5.85 (st, 6H), 3.95-3.92 (t, *J* = 6.3 Hz, 4H), 2.00 (m, 4H), 2.24 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 121.6, 114.3, 110.8, 70.4, 127.06, 25.3, 14.5. Elemental analysis: calculated C 58.93%, H 6.52%; found C 58.71%, H 6.24%.

3. TOF table for aldehyde hydroboration and ketone hydroboration

Table S2.

Product					
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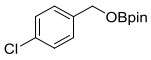
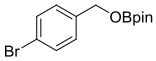
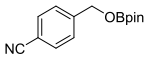
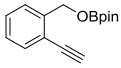
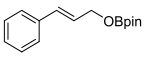
TOF (h^{-1})	97000	11800	19600	59400	59400
product					
	2f	**2g**	**2h**	**2i**	**2j**
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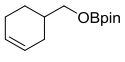
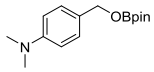
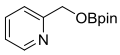
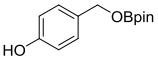
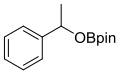
Product					
	2k	**2l**	**2m**	**2n**	**4a**
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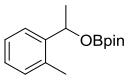
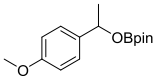
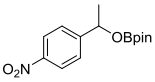
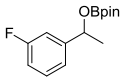
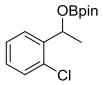
Product					
	4b	**4c**	**4d**	**4e**	**4f**
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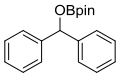
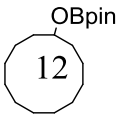
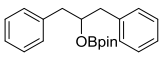
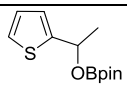
Product					
	4g	**4h**	**4i**	**4j**	
TOF (h^{-1})	5940	594	594	58200	

4. Spectroscopic data for aldehyde hydroboration products.

N,N-dimethyl-4-(((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methyl)aniline [1] ***(2l)*** NMR yield : 99%. colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.22 (m, 2H, Ar-H), 6.73-6.79 (t, J = 8.5 Hz, 2H, Ar-H), 4.81 (s, 2H, OCH_2), 1.25 (s, 12H, $C(CH_3)_2$). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.7 (Ar-C), 128.0 (Ar-C), 126.8 (Ar-C), 112.0 (Ar-C), 82.3 ($OC(CH_3)_2$), 66.3 (OCH_2), 40.2 (NCH_3), 24.2 (CH_3).

Spectral Data for 1° Alcohols. ***Phenylmethanol (3a)***.[2] colorless oil, 97.3 mg, 90% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.30 (m, 5H, Ar-H), 4.59 (s, 2H, OCH_2), 3.57 (s, 1H, CH_2OH). ^{13}C NMR (101 MHz, CDCl3) δ 140.5 (Ar-C), 128.0 (Ar-C), 127.1 (Ar-C), 126.6 (Ar-C), 64.4 (OCH_2).

o-tolylmethanol (3b).[2] white solid, 115.9 mg, 95% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.15 (m, 4H, Ar-H), 4.65 (s, 2H, OCH_2), 2.33 (s, 3H, CH_3),1.92 (s, 1H, CH_2OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.2 (Ar-H), 135.6 (Ar-H), 129.9 (Ar-H), 127.3 (Ar-H), 127.1 (Ar-H), 125.6 (Ar-H), 63.1 (OCH_2), 18.2 (CH_3).

2,4,6-trimethylbenzyl alcohol (3c).[3] white solid, 133.5 mg, 89% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (s, 2H, Ar-H), 4.67 (s, 2H, OCH_2), 2.41 (s, 6H, CH_3), 2.31 (s, 3H, CH_3), 1.81 (s, 1H, CH_2OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.6 (Ar-C), 137.3 (Ar-C), 133.8 (Ar-C), 129.1 (Ar-C), 59.0 (OCH_2), 21.0 (CH_3), 19.3 (CH_3).

(2-methoxyphenyl)methanol (3d).[4] colorless oil, 127.1 mg, 92% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.26 (m, 2H, Ar-H), 6.96-6.88 (m, 2H, Ar-H), 4.69 (s, 2H, OCH_2), 3.87 (s, 3H, OCH_3), 1.23 (s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0 (Ar-C), 128.5 (Ar-C), 128.3 (Ar-C), 120.2 (Ar-C), 109.7 (Ar-C), 61.7 (Ar-C), 54.8 (OCH_2), 24.4 (CH_3).

(4-fluorophenyl)methanol (3e).[5] colorless oil, 113.5 mg, 90% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H, Ar-H), 7.02-6.98 (t, J = 8.7 Hz, 2H, Ar-H), 4.56 (s, 2H, OCH_2) 2.77 (s, 1H, CH_2OH). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.78 (d, J_{C-F} = 244 Hz, Ar-C), 136.06 (Ar-C), 128.30 (Ar-C), 114.8 (d, J_{C-F} = 21 Hz, Ar-C), 63.88 (OCH_2).

(4-chlorophenyl)methanol (3f).[2] white solid, 124.4 mg, 87% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.24 (m, 4H, Ar-H), 4.58 (s, 2H, OCH_2), 2.63 (s, 1H, CH_2OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7 (Ar-C), 132.8 (Ar-C), 128.2 (Ar-C), 127.8 (Ar-C), 63.9 (OCH_2).

(4-bromophenyl)methanol (3g).[3] white solid, 151.5 mg, 81% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.45 (m, 2H, Ar-H), 7.21-7.19 (m, 2H, Ar-H), 4.60 (s, 2H, OCH_2), 2.26 (s, 1H, CH_2OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3 (Ar-C), 131.1 (Ar-C), 128.1 (Ar-C), 120.9 (Ar-C), 64.0 (OCH_2).

4-(hydroxymethyl)benzonitrile (3h). white solid, 113.2 mg, 85% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.58 (d, J = 8.1 Hz, 2H, Ar-H), 7.45-7.43 (d, J = 8.1 Hz, 2H, Ar-H), 4.73 (s, 2H, OCH_2), 2.69 (s, 1H,OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0 (Ar-C), 131.8 (Ar-C), 126.5 (Ar-C), 118.4 (CN), 110.4 (Ar-C), 63.5 (OCH_2). Elemental analysis: calculated C 72.17%, H 5.30%, N 10.52%; found C 71.81%, H 5.05%, N 10.26%.

(2-ethynylphenyl)methanol (3i).[6] white solid, 118.9 mg, 90% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.54 (m, 1H, Ar-H), 7.50-7.49 (d, J = 7.6 Hz, 1H, Ar-H), 7.43-7.39 (td, J = 7.6, 1,1 Hz, 1H, Ar-H), 7.33-7.29 (m, 1H, Ar-H), 4.88 (s, 2H, OCH_2), 3.39 (s, 1H, CH), 2.48 (s, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.8 (Ar-C), 132.4 (Ar-C), 128.8 (Ar-C), 126.9 (Ar-C), 126.8 (Ar-C), 119.7 (Ar-C), 81.5 (C), 80.8 (CH), 63.2 (OCH_2).

cinnamyl alcohol (3j).[2] white solid, 107.3 mg, 80% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.33 (m, 2H, Ar-H), 7.28-7.26 (m, 2H, Ar-H), 7.23-7.19 (m, 1H, Ar-H), 6.58-6.54 (d, J = 15.9 Hz, 1H, CH), 6.34-6.28 (dt, J = 15.9, 5.7 Hz, 1H, CH), 4.27-4.25 (dd, J = 5.7, 1.5 Hz, 2H, OCH_2), 2.57 (s, 1H, OH).^{13}C NMR (101 MHz, $CDCl_3$) δ 136.3 (Ar-C), 130.5 (Ar-C), 128.2 (Ar-C), 128.1 (Ar-C), 127.2 (Ar-C), 126.0 (Ar-C), 63.0 (OCH_2).

cyclohex-3-en-1-ylmethanol (3k).[7] colorless oil, 94.2 mg, 84% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.65-5.60 (d, 2H, CH=CH), 3.44 (s, 2H, CH2), 2.89-2.68 (d, 1H, OH), 2.08-1.64 (m, 6H, CH_2), 1.26-1.19 (m, 1H, CH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 126.6 (CH=CH), 125.4 (CH=CH), 67.1 (OCH_2), 35.7 (CH), 27.6 (CH_2), 24.7 (CH_2), 24.1 (CH_2).

pyridin-2-ylmethanol (3m). yellow oil, 92.7 mg, 85% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.40 (dd, J = 5.8, 1.6 Hz, 1H,Ar-H), 7.66-7.61 (dt, J = 7.7, 1.8 Hz, 1H, Ar-H), 7.42-7.40 (d, J = 7.9 Hz, 1H, Ar-H), 7.14-7.10 (m, 1H, Ar-H), 5.79 (s, CH_2), 4.75 (s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3 (Ar-C), 148.0 (Ar-C), 136.4 (Ar-C), 121.8 (Ar-C), 120.3 (Ar-C), 63.9 (OCH_2). HRMS (ESI^+) m/z calcd for $C6H8NOH^+$ 110.0600 $[M + H]^+$, found 110.0610.

4-(hydroxymethyl)phenol (3n). beige solid, 90.6 mg, 73% isolated yield. ^{1}H NMR (400 MHz, DMSO) δ7.11-7.09 (d, J = 8 Hz, 2H, Ar-H), 6.71-6.69 (d, J = 8 Hz, 2H, Ar-H), 4.35 (s, 2H, OCH_2), 3.37 (s, 1H, OH). ^{13}C NMR (100 MHz, CDCl3) δ 156.0 (Ar-C), 132.7 (Ar-C), 128.0 (Ar-C), 114.7 (Ar-C), 62.7 (OCH_2). Elemental analysis: calculated C 67.73%, H 6.50%; found C 67.46%, H 6.58%.

Spectral Data for 2° Alcohols. ***1-phenylethan-1-ol (5a)***.[2] colorless oil, 114.8 mg, 94% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.24 (m, 5H, Ar-H), 4.86 (q, J = 6.5 Hz, 1H, OCH), 2.09 (s, 1H, OH), 1.47 (d, J = 6.5 Hz, 3H, CH3). ^{13}C NMR (101 MHz, CDCl3) δ 145.8 (Ar-C), 128.5 (Ar-C), 127.5 (Ar-C), 125.4 (Ar-C), 70.4 (OCH), 25.2 (CH_3).

1-(o-tolyl)ethan-1-ol (5b).[3] colorless oil, 115.8 mg, 85% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.45 (d, J = 7.7 Hz, 1H, Ar-H), 7.19-6.98 (m, 3H, Ar-H), 5.04 (q, J = 6.4 Hz, 1H, OCH), 2.30 (s, 3H, Ar-CH_3), 1.40 (d, J = 6.4 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.9 (Ar-C), 134.2 (Ar-C), 130.4 (Ar-C), 127.1 (Ar-C), 126.4 (Ar-C), 124.6 (Ar-C), 66.7 (OCH), 29.9 (Ar-CH_3), 18.9 (CH_3).

1-(4-metoxyphenyl)ethan-1-ol (5c).[3] colorless oil, 123.3 mg, 81% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.25 (m, 2H, Ar-H), 6.88-6.84 (m, 2H, Ar-H), 4.83-4.78 (q, J = 6.4 Hz, 1H, OCH), 3.78 (s, 3H, OCH_3), 2.22 (s, 1H, OH),1.45 (d, J = 6.4 Hz, 3H, CH_3). ^{13}C NMR (101MHz, $CDCl_3$) δ 158.9 (Ar-C), 138.1 (Ar-C), 126.7 (Ar-C), 113.8 (Ar-C), 69.9 (OCH), 55.3 (OCH_3), 25.0 (CH_3).

1-(4-nitrophenyl)ethan-1-ol (5d).[3] brown oil, 145.4 mg, 87% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.14 (d, J = 8.8 Hz, 2H, Ar-H), 7.52-7.50 (d, J = 8.5 Hz, 2H, Ar-H), 4.99 (q, J = 6.4 Hz, 1H, OCH), 2.45 (s, 1H, OH), 1.50-1.48 (d, J = 6.5 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ153.2 (Ar-C), 147.1 (Ar-C), 126.1 (Ar-C), 123.7 (Ar-C), 69.4 (OCH), 25.5 (CH_3) .

1-(3-fluorophenyl)ethan-1-ol (5e).[8] colorless oil, 124.7 mg, 89% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.26 (m, 1H, Ar-H), 7.12-7.06 (m, 2H, Ar-H), 6.97-6.92 (m, 1H, Ar-H), 4.89-4.84 (q, J = 6.4 Hz, 1H, OCH), 2.20 (s, 1H, OH), 1.47-1.45 (d, J = 6.5 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, CDCl3) δ 162.5 (Ar-C), 148.1 (Ar-C), 129.4 (Ar-C), 120.5 (Ar-C), 113.5 (Ar-C), 111.7 (Ar-C), 69.2 (OCH), 24.6 (CH_3).

1-(2-cholophenyl)ethan-1-ol (5f).[8] colorless oil, 144.1 mg, 92% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.53 (dd, J = 7.7, 1.4 Hz, 1H, Ar-H), 7.30-7.24 (m, 2H, Ar-H), 7.19-7.14 (tt, J = 10.7, 5.4 Hz, 1H, Ar-H), 5.27-5.21 (qd, J = 6.2 3.9 Hz, 1H, OCH), 2.64 (s, 1H, OH), 1.45-1.43 (d, J = 6.5 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6 (Ar-C), 131.1 (Ar-C), 128.9 (Ar-C), 127.9 (Ar-C), 126.7 (Ar-C), 126.0 (Ar-C), 66.4 (OCH), 23.0 (CH_3).

Diphenylmethanol (5g).[9] white solid, 152.9 mg, 83% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.39 (m, 8H, Ar-H), 7.36-7.31 (m, 2H, Ar-H), 5.89 (s, 1H, OCH), 2.49 (s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.3 (Ar-C), 128.0 (Ar-C), 127.1 (Ar-C), 126.1 (Ar-C), 75.8 (OCH).

Cyclododecanol (5h).[9] white solid, 164.1 mg, 89% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.86-3.81 (dt, J = 7.8, 3.5 Hz, 1H, OCH), 1.69-1.61 (m, 2H, CH_2), 1.46-1.29 (m, 20H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 68.7 (OCH), 32.0 (CH_2), 23.7 (CH_2), 23.4 (CH_2), 22,9 (CH_2), 22.8 (CH_2), 20.5 (CH_2).

1,3-diphenylpropan-2-ol (5i)[8,9] Colorless oil, 197.4 mg, 93% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.25 (m, 4H, Ar-H), 7.21-7.17 (dd, J = 9.7, 4.5 Hz, 6H, Ar-H), 4.03-3.96 (m, 1H, OCH), 2.83-2.78 (m, 2H, CH_2), 2.73-2.68 (m, 2H, CH_2), 1.73 (s, 1H, OH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.1 (Ar-C),129.1 (Ar-C),128.1 (Ar-C), 126.1 (Ar-C), 73.2 (OCH), 43.0 (CH_3)

1-(thiophen-2-yl)ethan-1-ol (5j).[3] white oil, 102.4 mg, 80% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.23 (dd, J = 4.8, 1.4 Hz, 1H), 6.98-6.95 (m, 2H), 5.16-5.11 (q, J = 6.3 Hz, 1H, OCH), 2.07 (s, 1H, OH), 1.61-1.60 (d, J = 6.4 Hz, 3H, CH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.4 (Ar-C),126.2 (Ar-C),124.0 (Ar-C), 122.7 (Ar-C), 65.8 (OCH), 24.8 (CH_3).

Isolation of Secondary Amines. ***N-benzylaniline (6a)***.[10] brown oil, 144.8 mg, 79% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.29 (m, 5H, Ar-H), 7.22-7.18 (dd, J = 8.2, 7.5, Hz, 2H, Ar-H), 6.77-6.74 (dd, J = 16.3, 8.9, Hz, 1H, Ar-H), 6.69-6.67 (d, J = 8.6 Hz, 2H, Ar-H), 4.35 (s, 2H, CH_2). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.2 (Ar-C), 138.6 (Ar-C), 128.8 (Ar-C), 128.2 (Ar-C), 127.2 (Ar-C), 126.8 (Ar-C), 117.5 (Ar-C), 112.8 (Ar-C), 48.1 (CH_2).

N-(4-fluorobenzyl)aniline (6b).[10] yellow oil, 132.8 mg, 66% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.29 (dd, J = 8.4, 5.5, Hz, 2H, Ar-H), 7.17-7.13 (t, J = 7.9 Hz, 2H, Ar-H), 7.02-6.98 (t, J = 8.7 Hz, 2H, Ar-H), 6.72-6.69 (t, J = 7.3 Hz, 1H, Ar-H), 6.61-6.59 (d, J = 7.8 Hz, 2H, Ar-H), 4.28 (s, 2H, CH_2), 3.99 (s, 1H, NH). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6 (Ar-C), 147.5 (Ar-C), 134.6 (Ar-C), 128.8 (Ar-C), 128.5 (Ar-C), 117.3 (Ar-C), 115.0 (Ar-C), 112.4 (Ar-C), 47.1 (CH_2).

N-(4-methoxybenzyl)aniline (6c). white solid, 179.2 mg, 84% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-6.66 (m, 9H, Ar-H), 4.27 (s, 2H, CH_2), 3.82 (s, 3H, OCH_3). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.4 (Ar-C), 147.5 (Ar-C), 130.8 (Ar-C), 128.8 (Ar-C), 128.4 (Ar-C), 117.3 (Ar-C), 113.6 (Ar-C), 112.6 (Ar-C), 54.8 (OCH_3), 47.5 (CH_2). Elemental analysis: calculated C 78.84%, H 7.09%, N 6.57%; found C 78.47%, H 6.98%, N 6.37%.

5. Typical NMR-scale reaction for kinetic monitoring by ^{1}H-NMR arrays

In a glovebox, a certain amount of ketone/aldehyde and HBpin were mixed in a vial, then a stock solution containing an appropriate loading of $(MeCp)_3La$ was added. React for a certain amount of time, 25 μL reaction liquid was added to a J. Young tap NMR tube and move out of the glove box to be exposed to the air, then monitored by ^{1}H-NMR.

Kinetic Analysis. As described above, all kinetic experiment process was carried out and a large amount of data is collected. Boric acid esters concentration was tested by ^{1}H NMR, which indicated the completion of the reaction by the appearance of a new CH peak or a new CH_2 peak. For substrate aldehydes, the kinetic curves were obtained by internal standard method. [11]It is proved by experiment that the reaction is a pseudo-zero-order with respect to the substrate concentrations.

Initial concentrations of ketone and HBpin were 0.5 mol/L. Catalyst concentration was measured at 0.00246 mmol/mL [0.005 mol% of $(CpMe)_3La$ and 2 mL THF]. We use mesitylene as internal standard in aldehyde. The reaction condition is that the initial concentration of aldehyde is 2.2915 mmol/mL, and the HBpin concentration is 4.58 mmol/mL. For substrate HBpin ,The reaction condition is that the initial concentration of aldehyde is 4.6145 mmol/mL, and the initial concentrationof HBpin is 2.3072 mmol/mL. Catalyst concentration was measured at 0.0017 mmol/mL [0.005 mol% of $(CpMe)_3La$ and 4 mL THF]. Orders for each reactant were determined from the average rates (≥3 trials) at different time. A sraight line is obtained by drawing the experimental data, and the horizontal and vertical coordinates represent the time and ln(rate) (Figure S1, A, B, C, D,). (Eq. S1-S3, a: initial concentration of ketone; x: concentration of product at time t; b1and b2 are constant).

$$dx/dt=k[a-x] \quad \text{(Eq. S1)}$$

$$\ln[a-x]=-kt+b1 \text{ or } \ln(\text{rate}) = \ln k+\ln[\text{ketone}] \quad \text{(Eq. S2)}$$

$$-\ln[\text{ketone}]=kt+b2 \quad \text{(Eq. S3)}$$

Catalyst concentration was measured at 0.012 mol%, 0.017 mol%, and 0.023 mol% (for 4-methylacetophenone or p-methyl benzaldehyde). Datas were then plotted as ln(rate) vs. $\ln[(MeCp)_3La]$.[12] The negative rate of disappearance of ketone/aldehyde is proportional to the concentration of ketone/aldehyde to the order (α). Therefore, the order is the slope of a plot of ln(rate) vs. $\ln[(MeCp)_3La]$ (Figure S1, E, F).

Through the study of dynamics, the rates in both reaction were proven to be first order for substrates and catalyst.

$$\text{rate} = k[(MeCp)_3La]^1\,[HBpin]^1\,[\text{ketone}]^1$$

$$\text{rate} = k[(MeCp)_3La]^1\,[HBpin]^1[\text{aldehyde}]^1$$

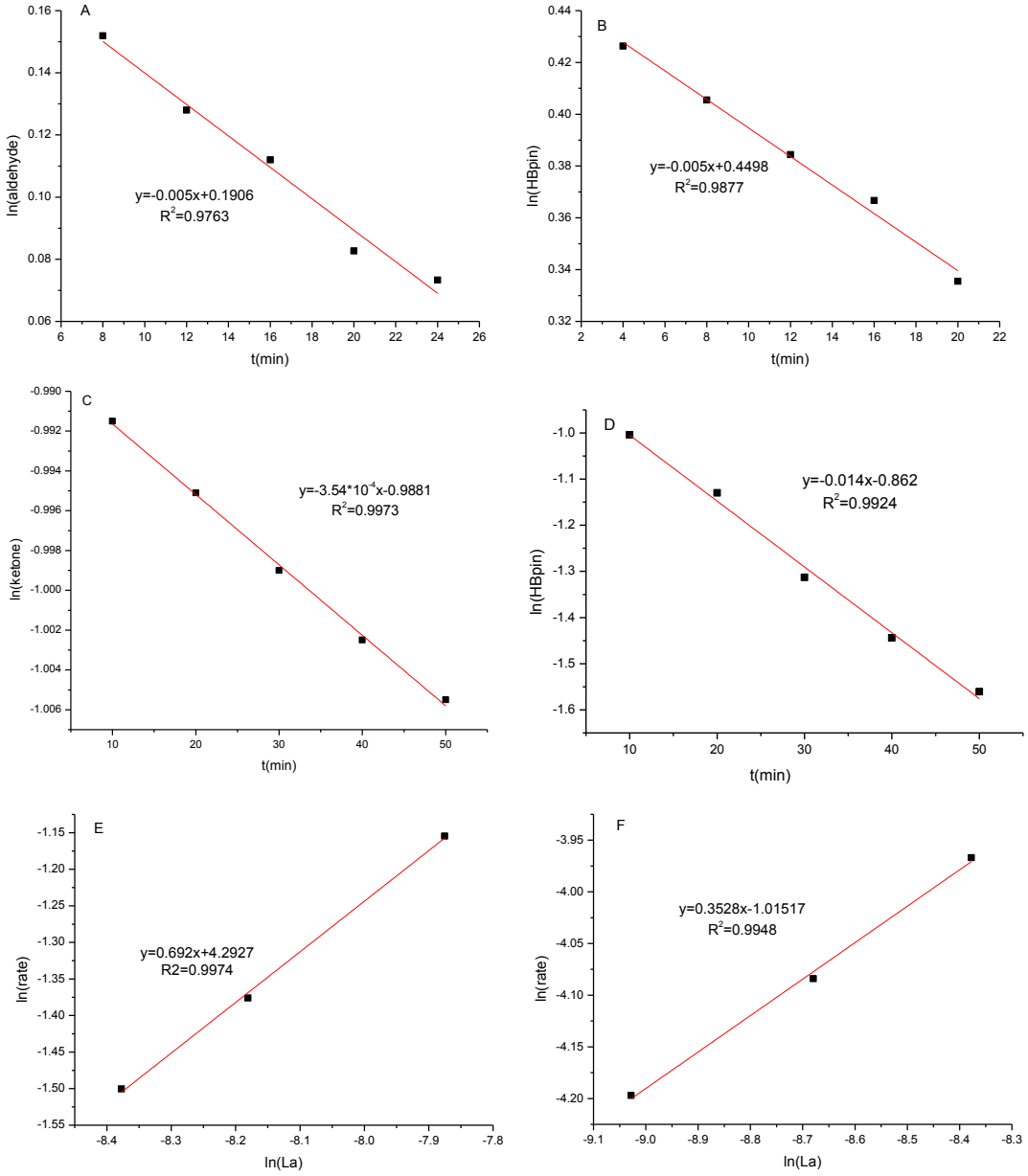


Figure S1. (A) Plot of ln[aldehyde] vs. t(min); (B) Plot of ln[HBpin] vs. t(min); (C) Plot of -ln[ketone] vs. t(min); (D) Plot of -ln[HBpin] vs. t(min); (E) Plot for reaction rate law order in $(MeCp)_3La$ for 2-methylbenzaldehyde; (F) Plot for reaction rate law order in $(MeCp)_3La$ for 2'-methylacetophenone.

6. NMR spectra

solvent THF (⋆), unreacted aldehyde/ketone (☆), aldehyde product (●) , ketone product (◆), unreacted HBpin (❇)

NMR spectra for aldehyde hydroboration product

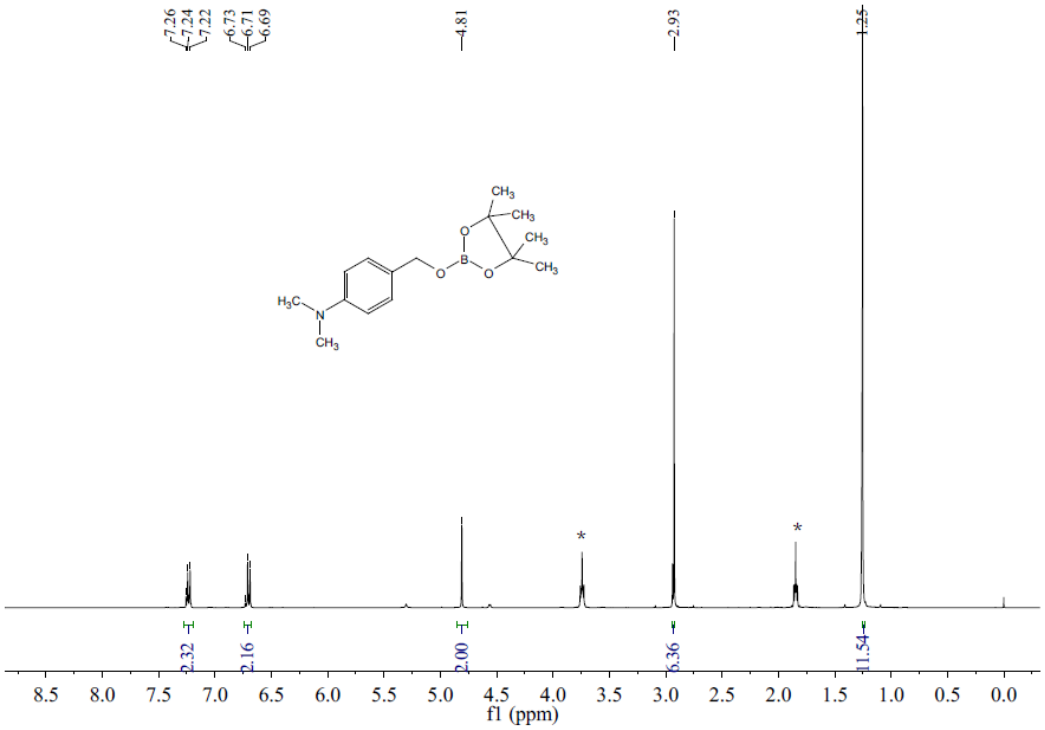


Figure S2. ^{1}H NMR spectrum of N,N-dimethyl-4-(((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methyl)anilinein **(2l)** acquired in $CDCl_3$

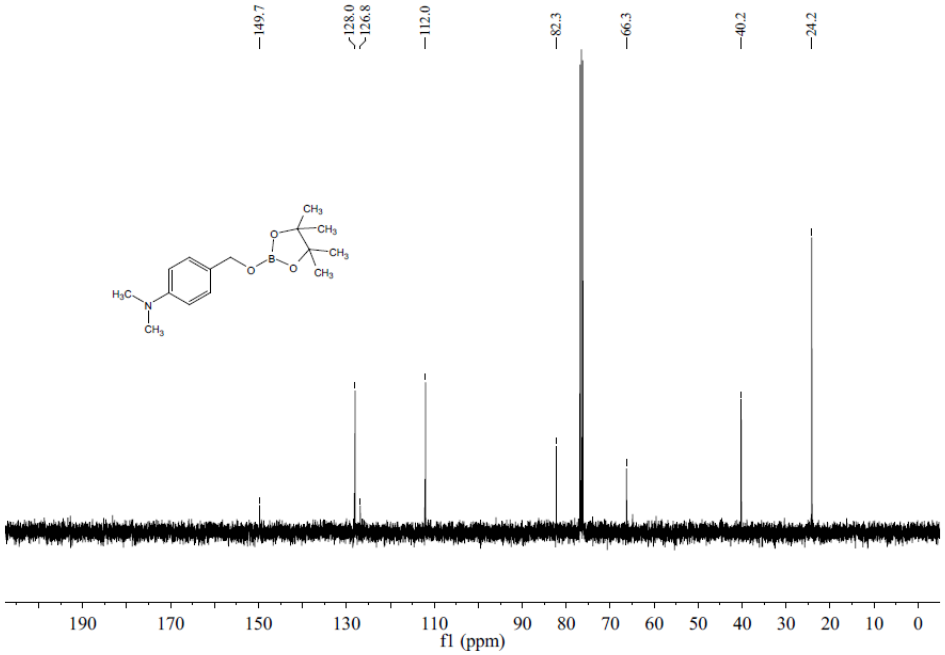


Figure S3. ^{13}C NMR spectrum of N,N-dimethyl-4-(((4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)oxy)methyl)anilinein **(2l)** acquired in $CDCl_3$

NMR spectra for 1^{o} alcohols

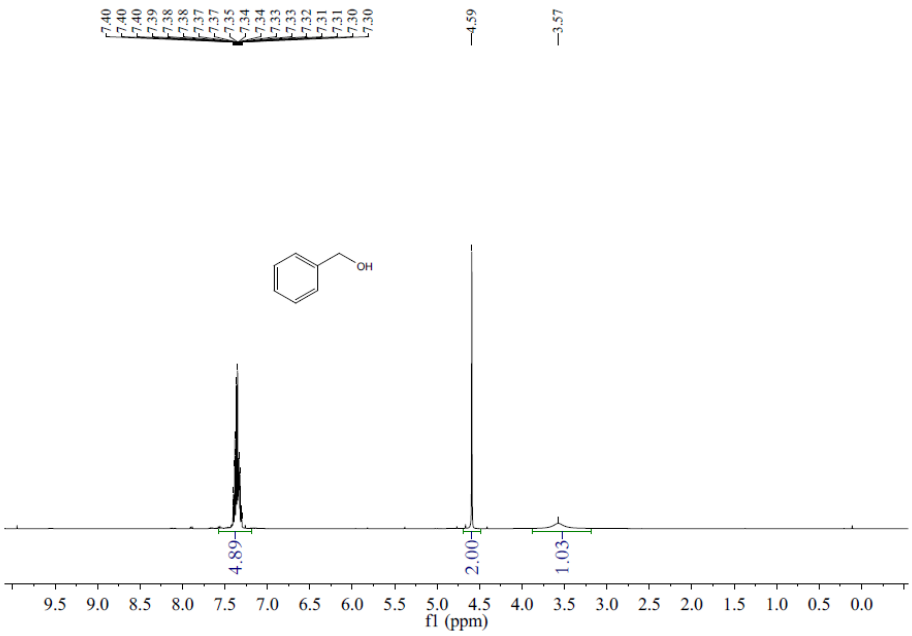


Figure S4. ^{1}H NMR spectrum of phenylmethanol **(3a)** acquired in $CDCl_3$

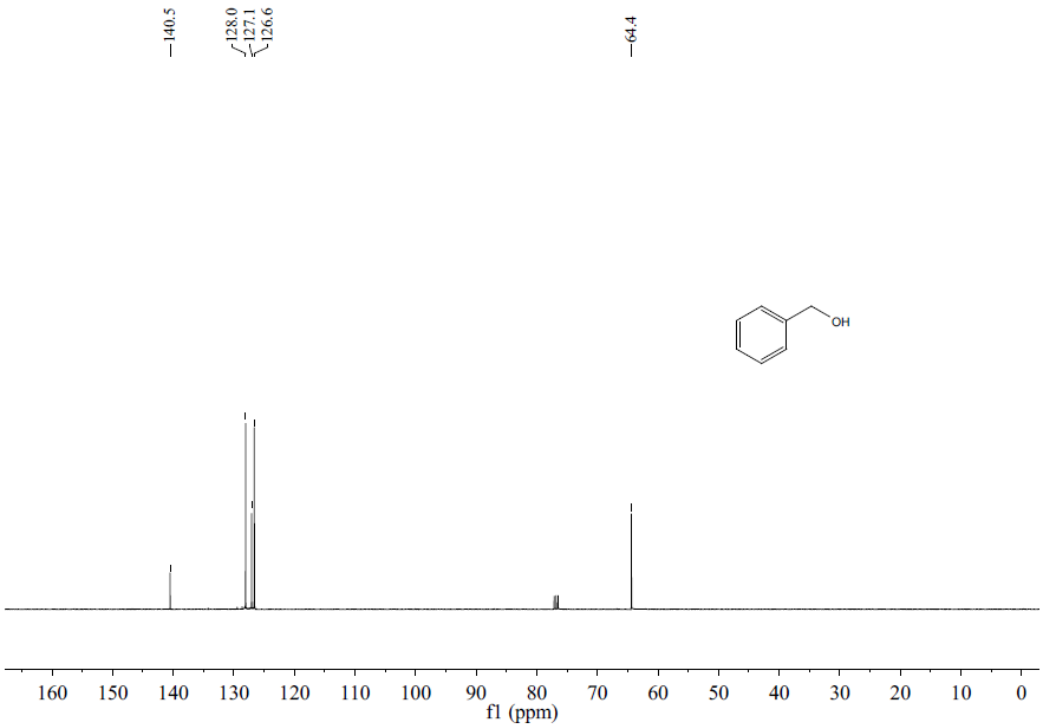


Figure S5. ^{13}C NMR spectrum of phenylmethanol **(3a)** acquired in $CDCl_3$

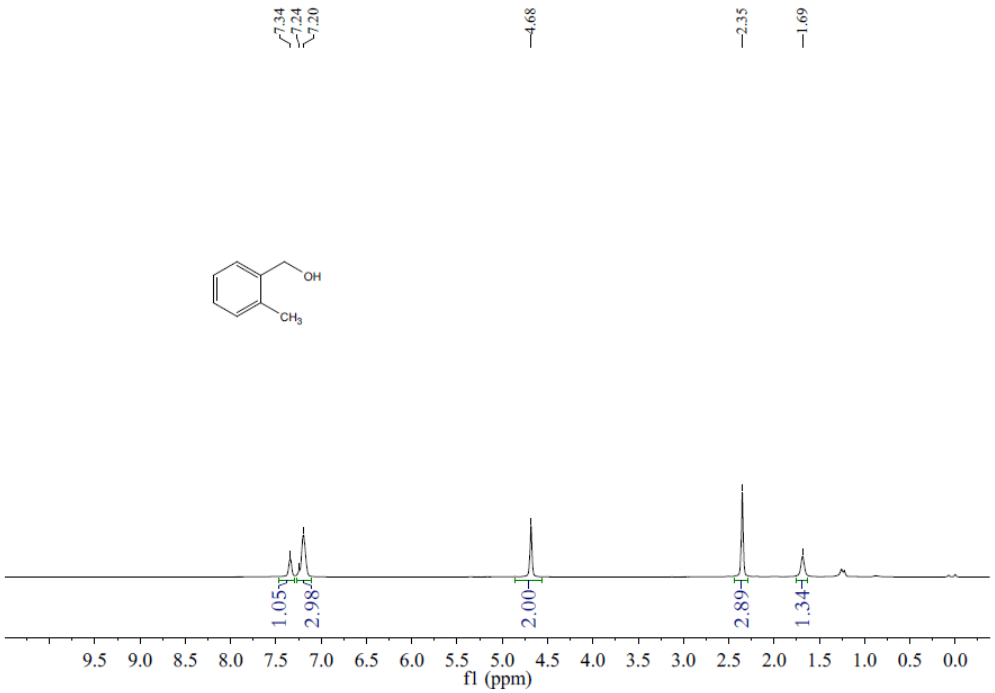


Figure S6. ^{1}H NMR spectrum of o-tolylmethanol **(3b)** acquired in $CDCl_3$

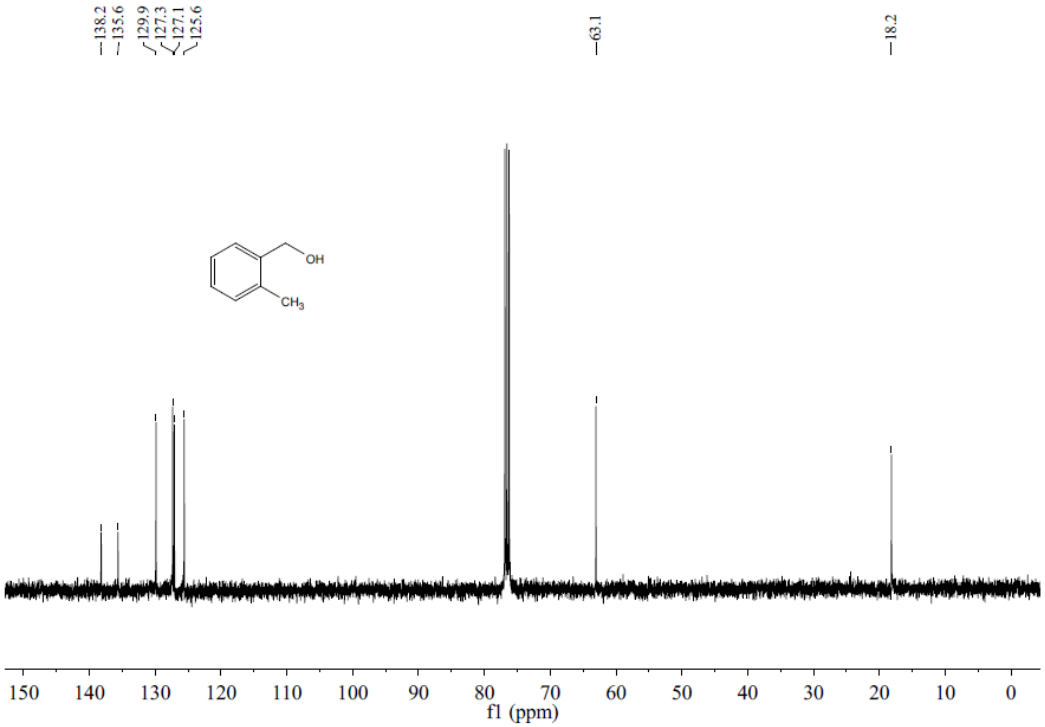


Figure S7. ^{13}C NMR spectrum of o-tolylmethanol **(3b)** acquired in $CDCl_3$

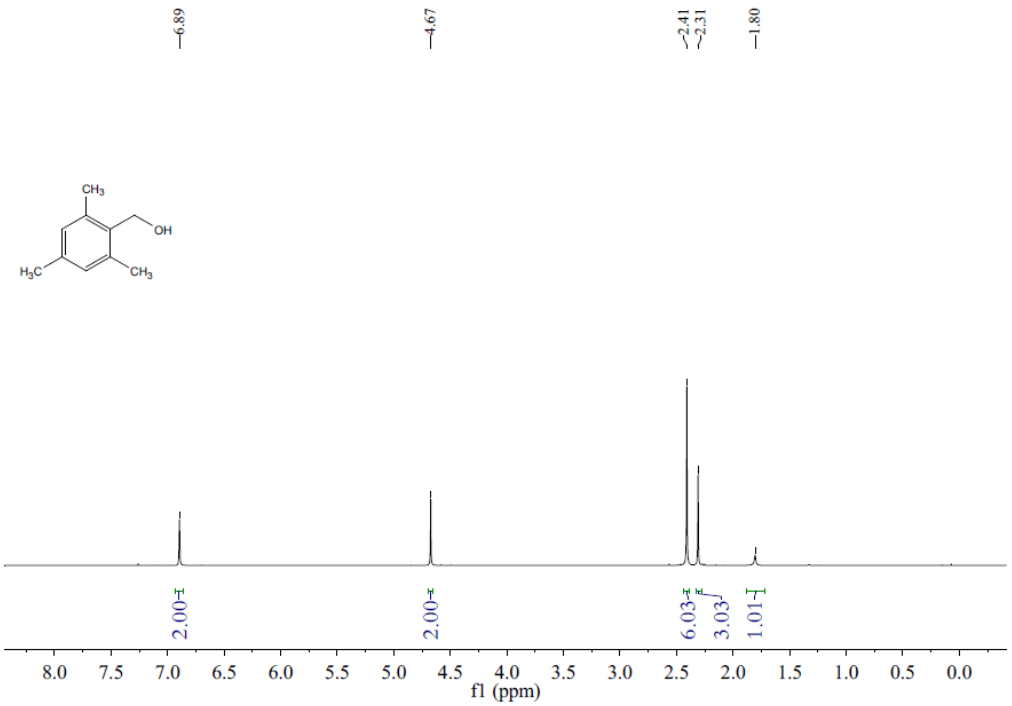


Figure S8. ^{1}H NMR spectrum of 2,4,6-trimethylbenzyl alcohol **(3c)** acquired in $CDCl_3$

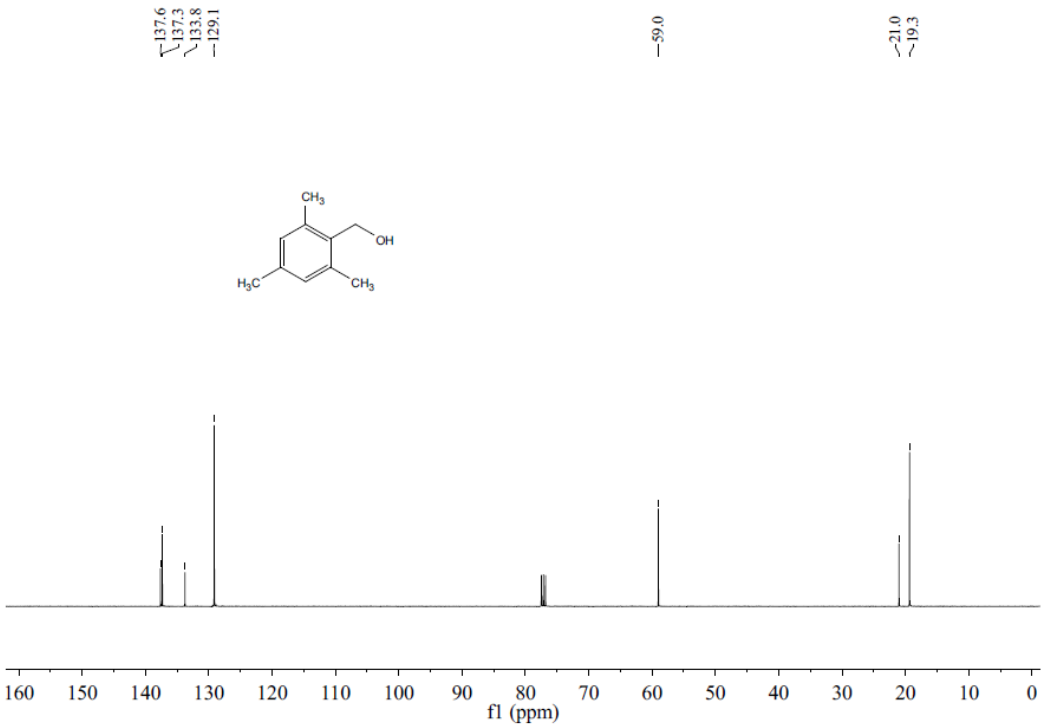


Figure S9.[13]C NMR spectrum of 2,4,6-trimethylbenzyl alcohol **(3c)** acquired in CDCl

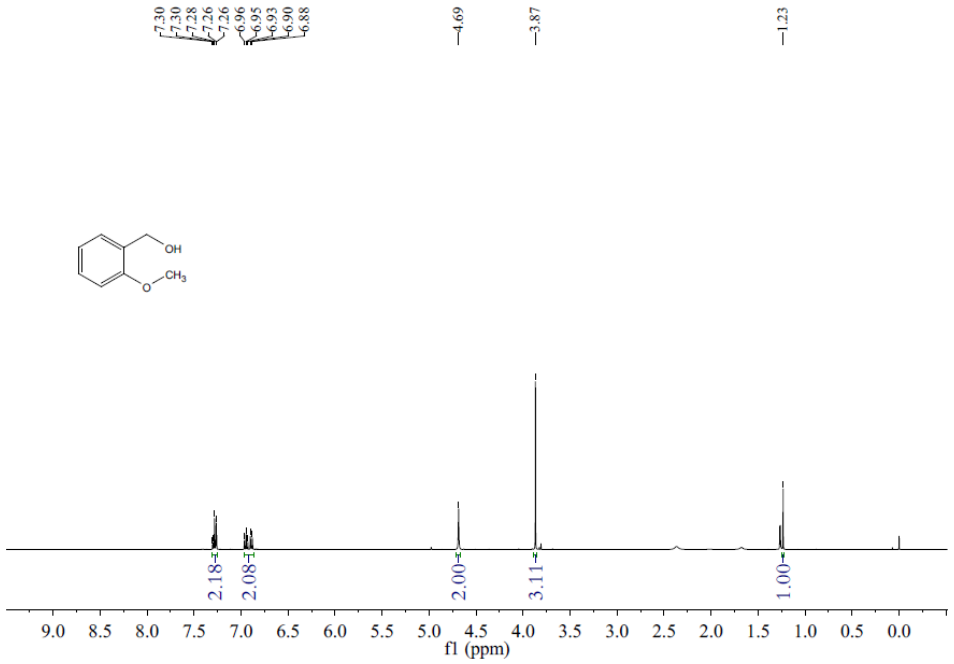


Figure S10.[1]H NMR spectrum of (2-methoxyphenyl)methanol **(3d)** acquired in $CDCl_3$

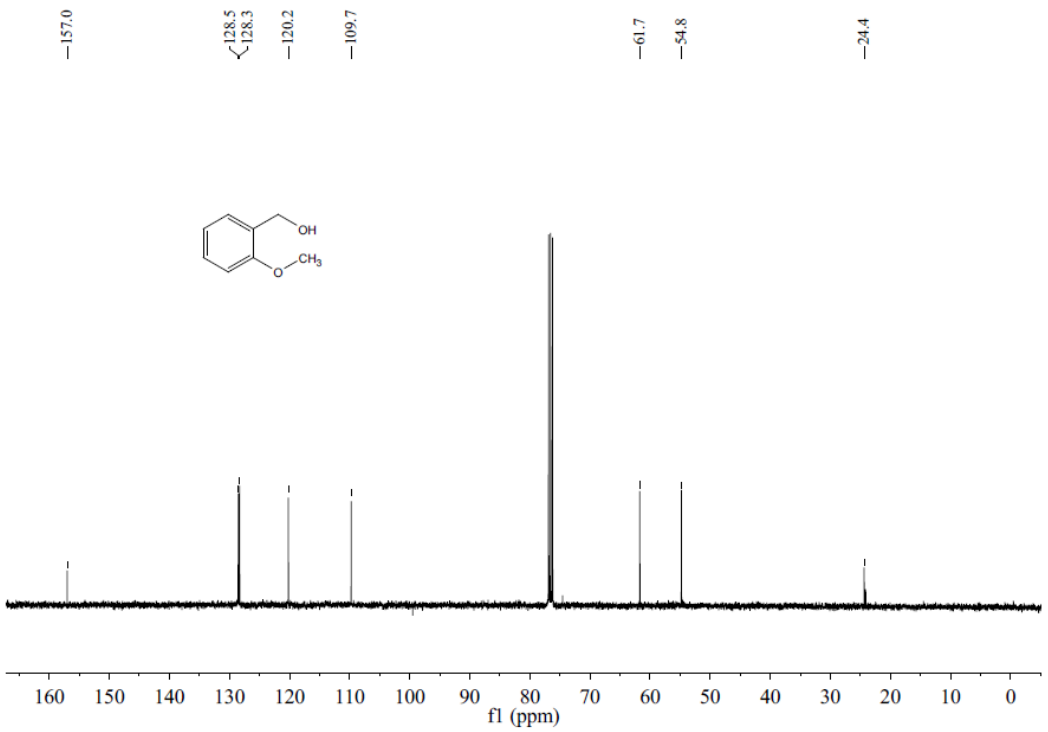


Figure S11.[13]C NMR spectrum of (2-methoxyphenyl)methanol **(3d)** acquired acquired in $CDCl_3$

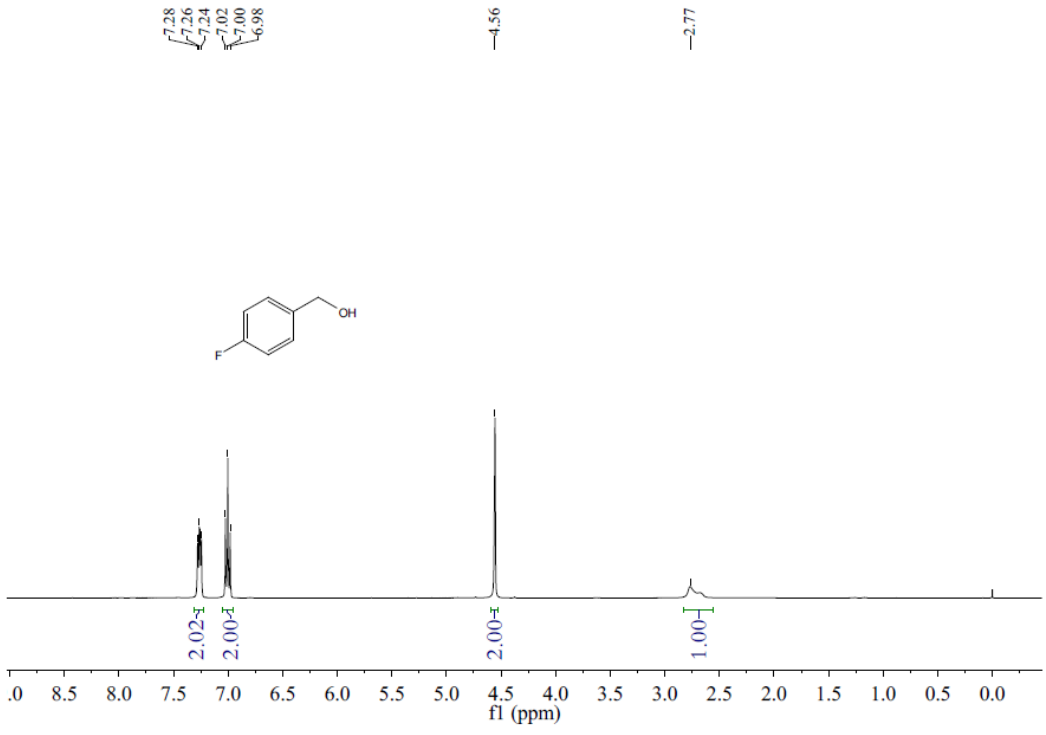


Figure S12.[1]H NMR spectrum of (4-fluorophenyl) methanol **(3e)** acquired in $CDCl_3$

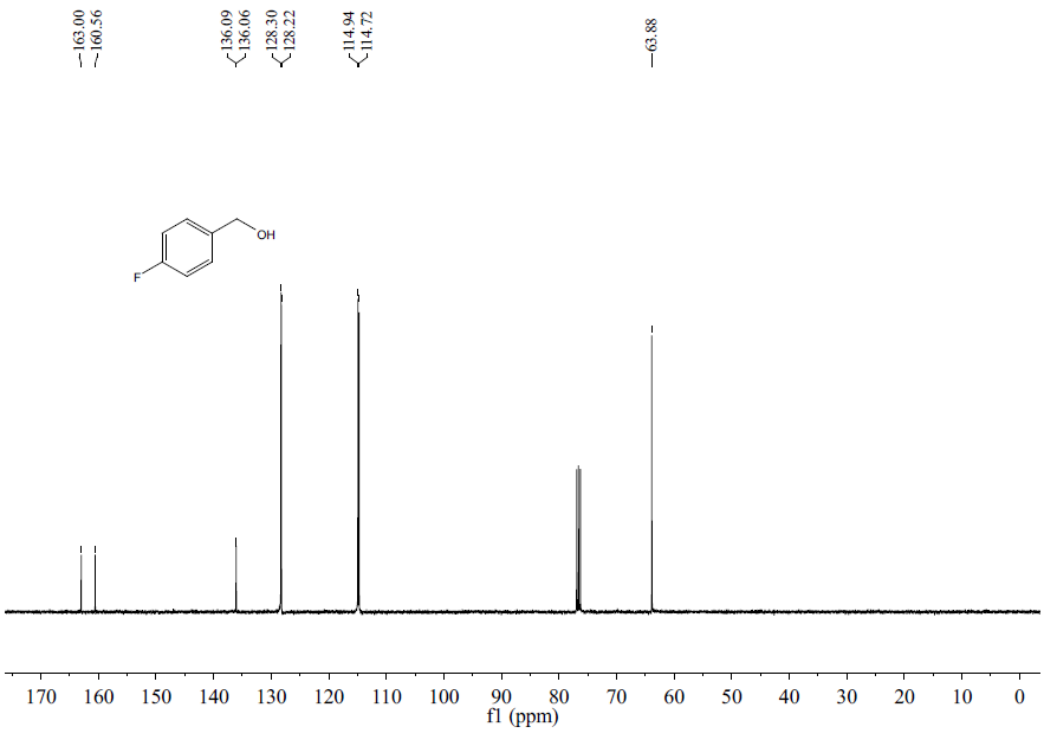


Figure S13. ^{13}C NMR spectrum of (4-fluorophenyl)methanol **(3e)** acquired in $CDCl_3$

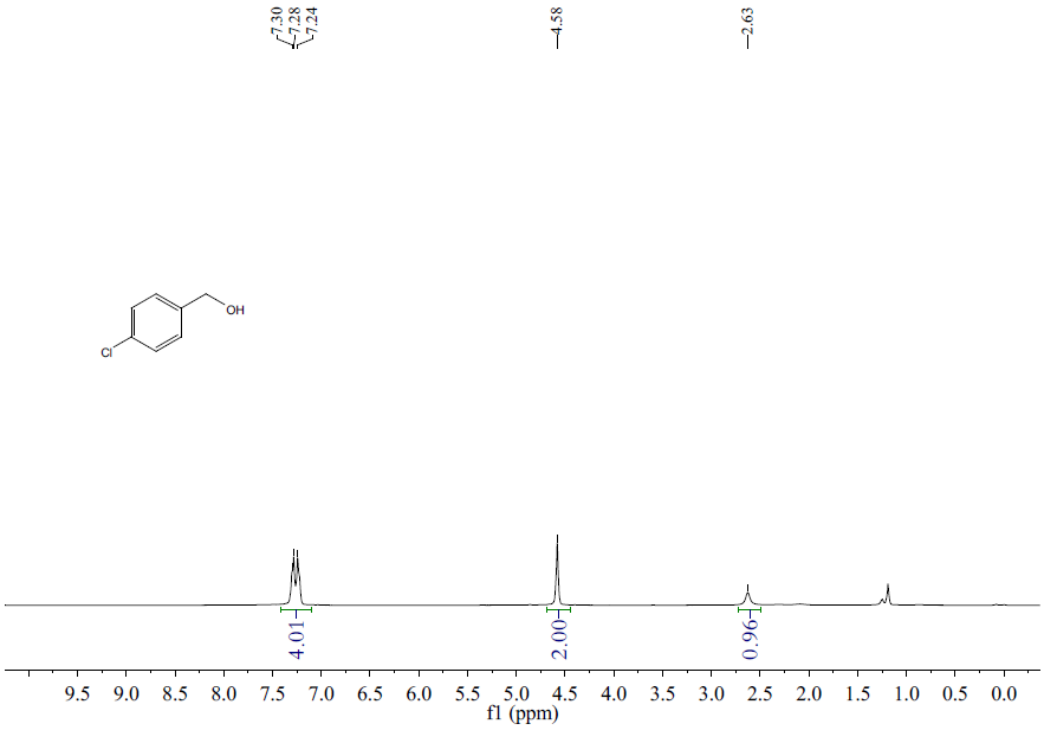


Figure S14. ^{1}H NMR spectrum of (4-chlorophenyl)methanol **(3f)** acquired in $CDCl_3$

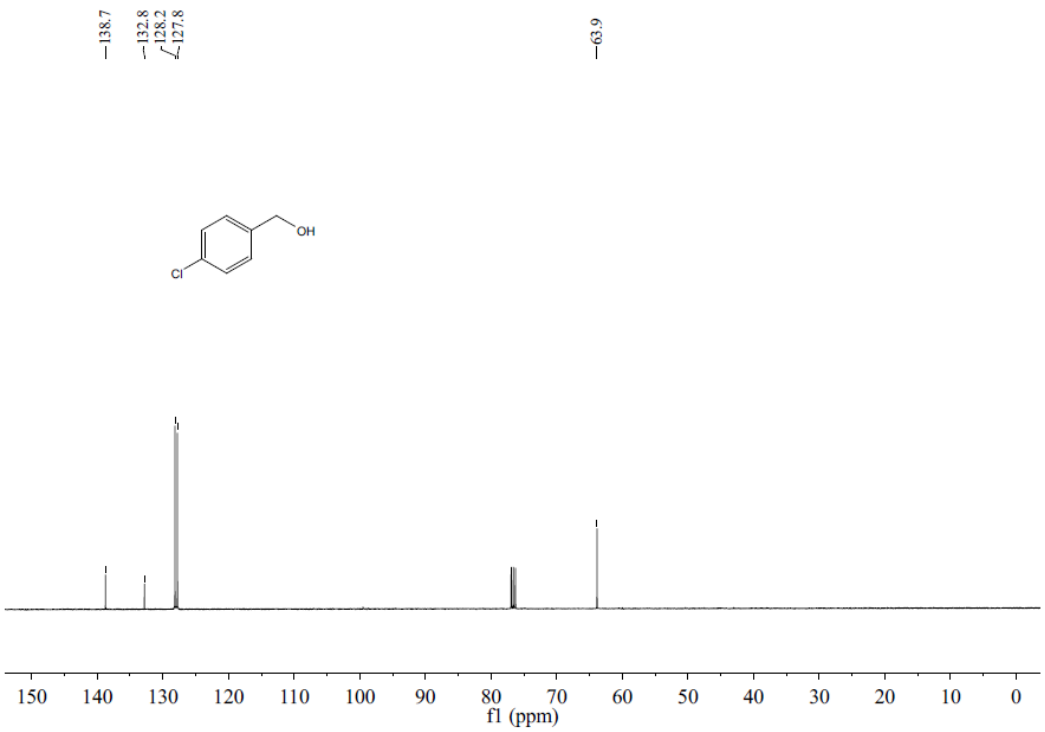


Figure S15. ^{13}C NMR spectrum of (4-chlorophenyl)methanol **(3f)** quired in $CDCl_3$

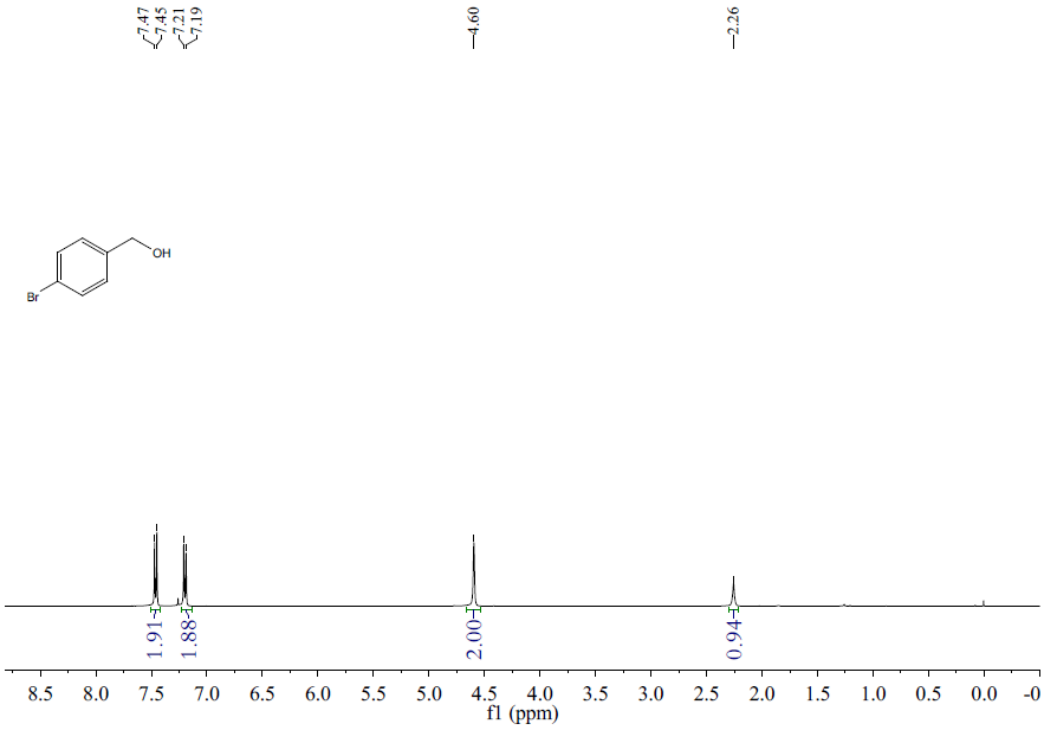


Figure S16. ^{1}H NMR spectrum of (4-bromophenyl)methanol **(3g)** cquired in $CDCl_3$

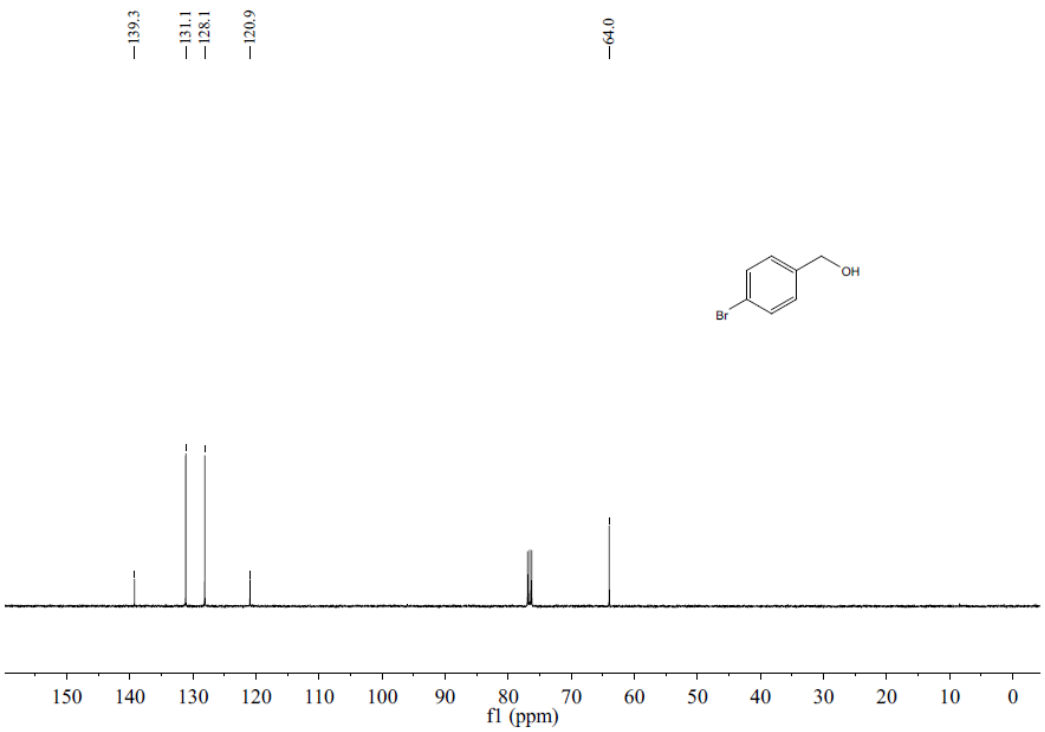


Figure S17. ^{13}C NMR spectrum of (4-bromophenyl)methanol **(3g)** acquired in $CDCl_3$

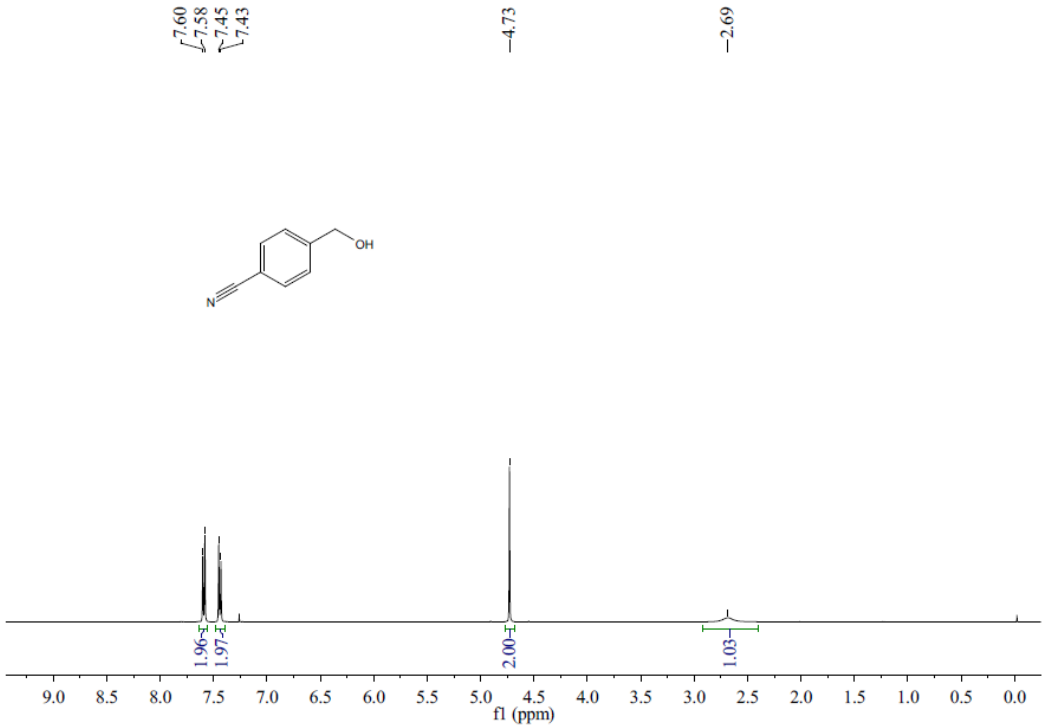


Figure S18. ^{1}H NMR spectrum of 4-(hydroxymethyl)benzonitrile **(3h)** acquired in $CDCl_3$

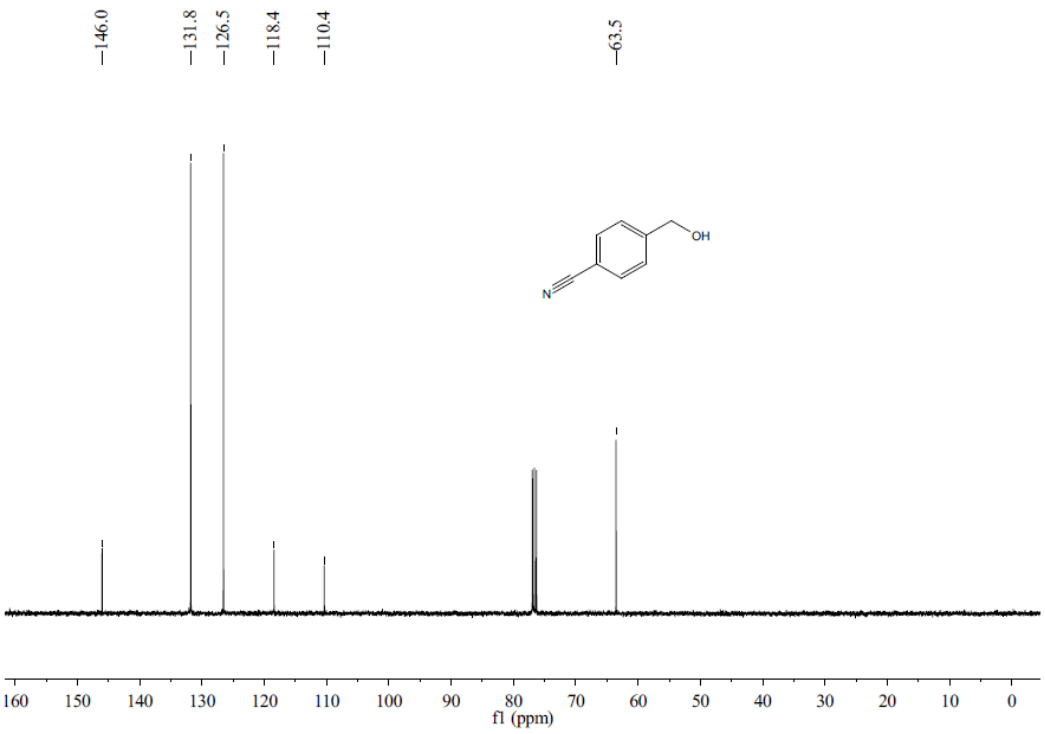


Figure S19. ^{13}C NMR spectrum of 4-(hydroxymethyl)benzonitrile **(3h)** acquired in $CDCl_3$

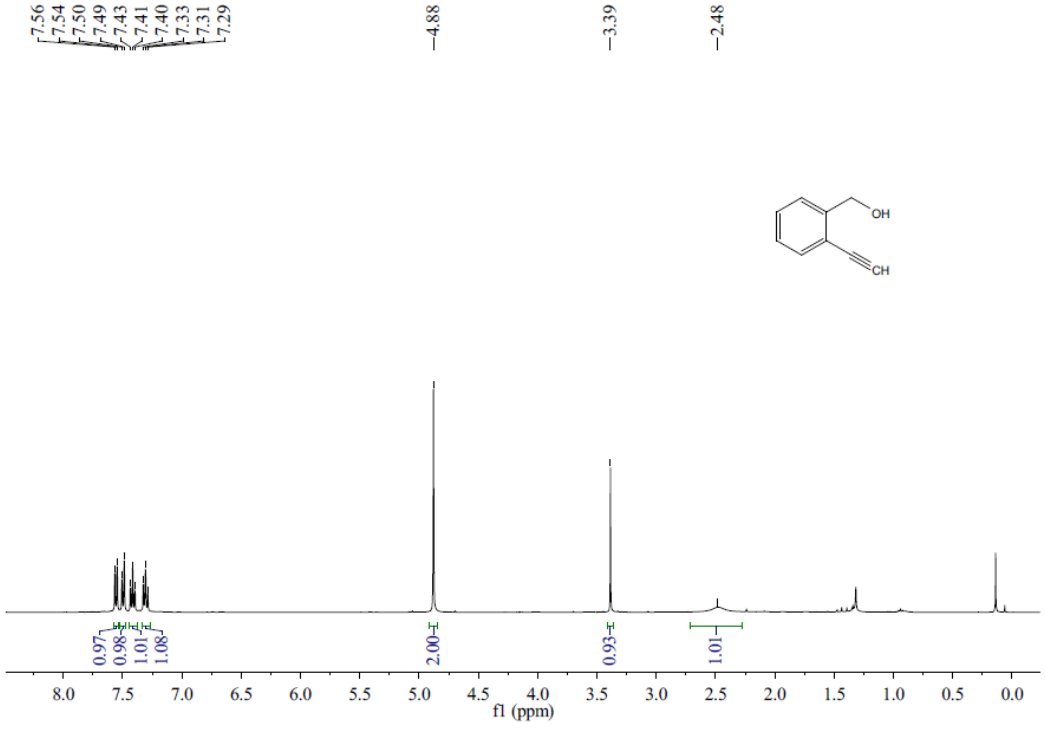


Figure S20. ^{1}H NMR spectrum of (2-ethynylphenyl)methanol **(3i)** acquired in $CDCl_3$

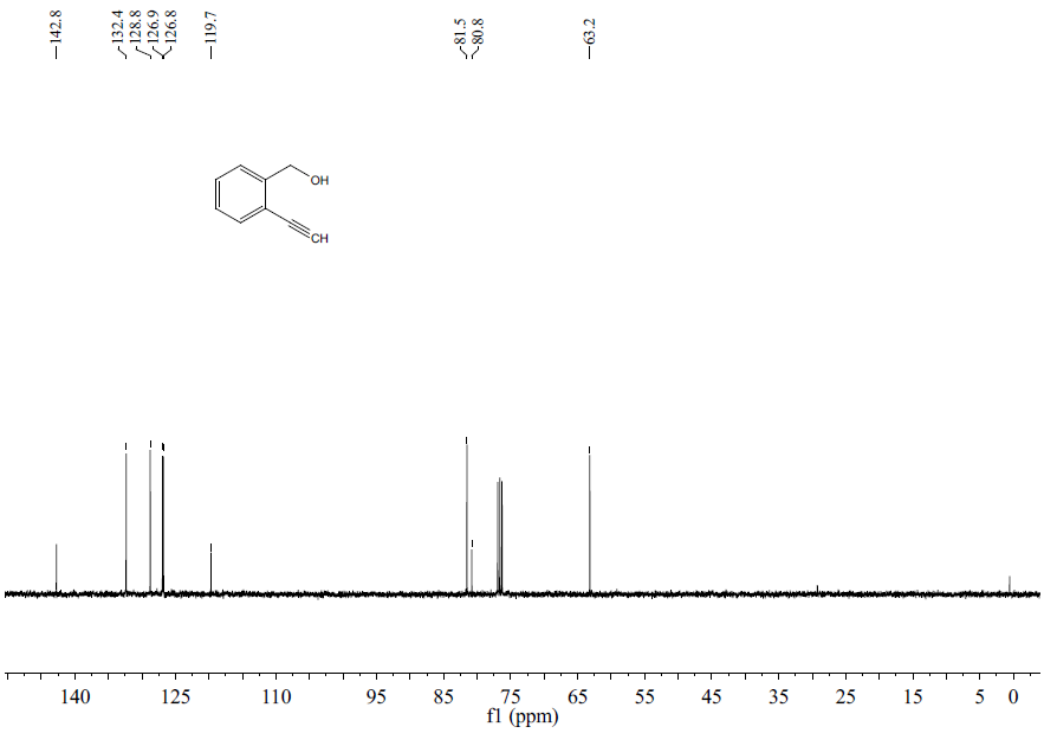


Figure S21.[1]H NMR spectrum of (2-ethynylphenyl)methanol **(3i)** acquired in $CDCl_3$

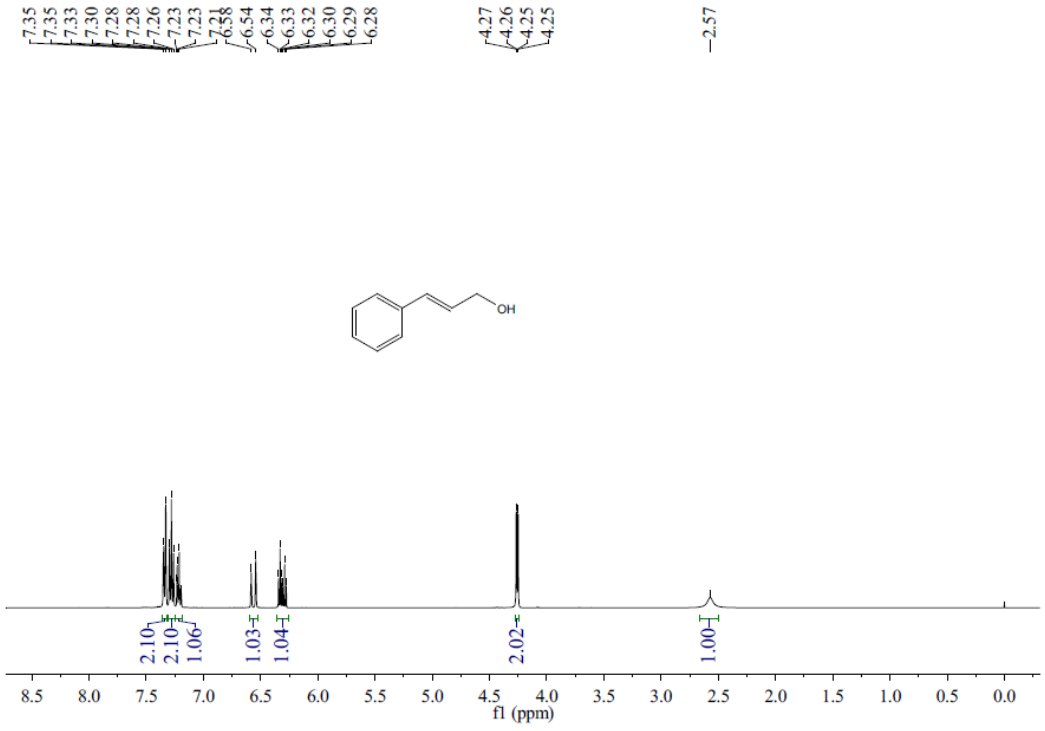


Figure S22.[1]H NMR spectrum of cinnamyl alcohol **(3j)** acquired in $CDCl_3$

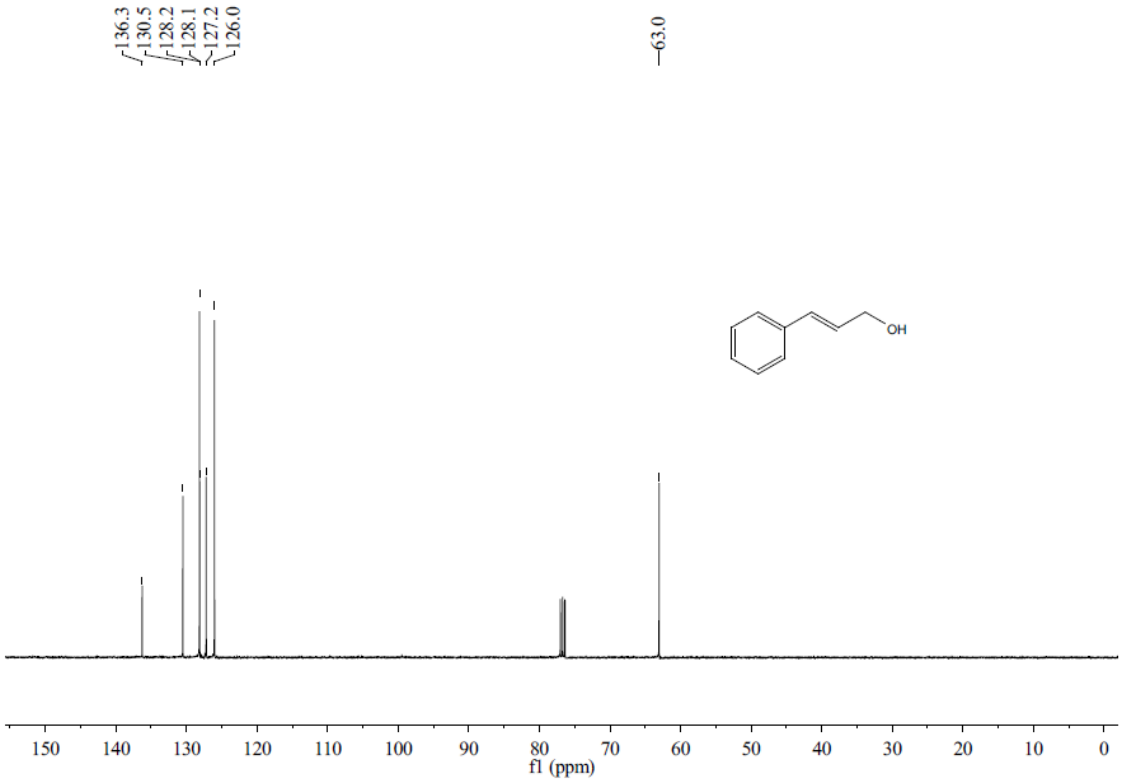


Figure S23. ^{13}C NMR spectrum of cinnamyl alcohol **(3j)** acquired in $CDCl_3$

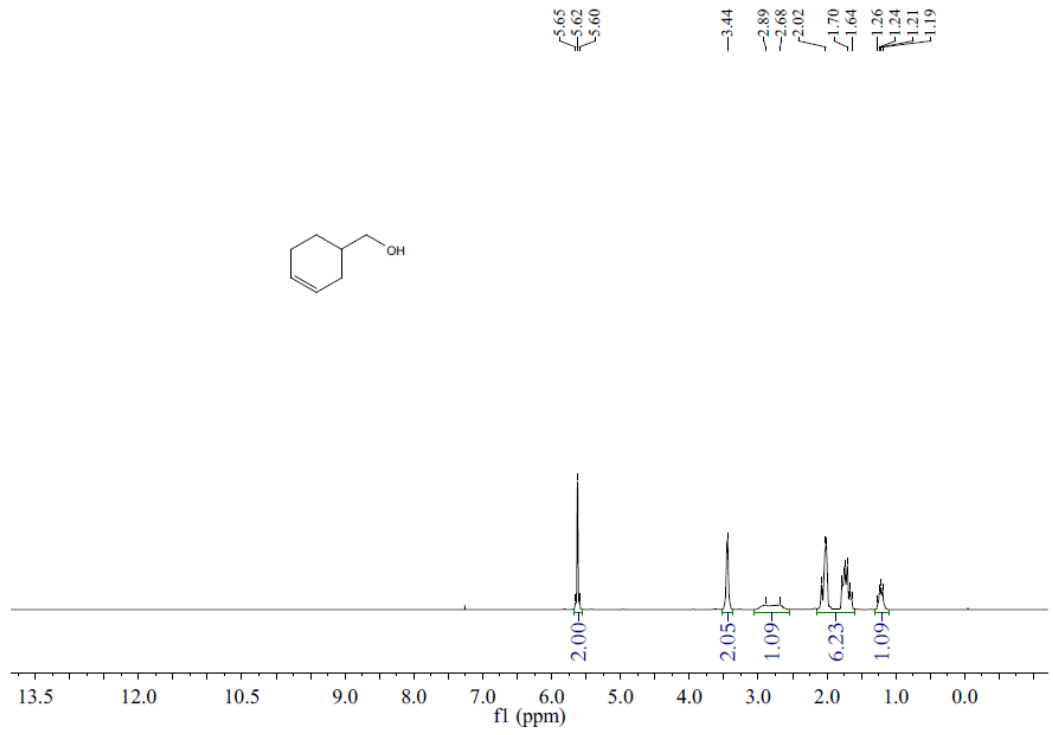


Figure S24. ^{1}H NMR spectrum of cyclohex-3-en-1-ylmethanol **(3k)** quired in $CDCl_3$

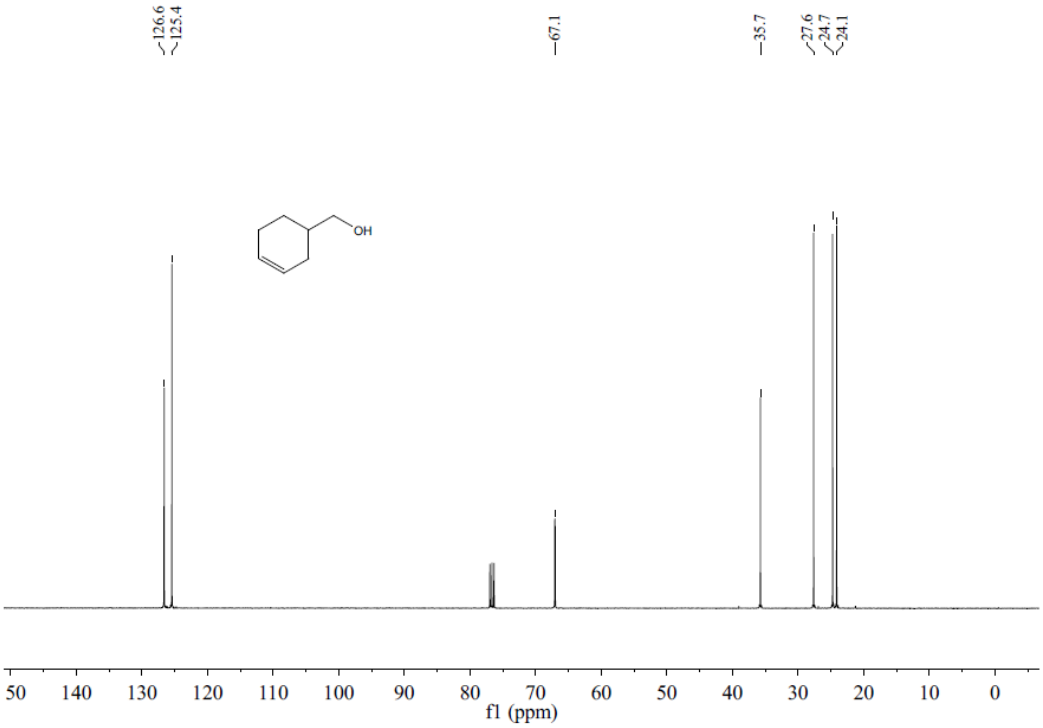


Figure S25. ^{13}C NMR spectrum of cyclohex-3-en-1-ylmethanol **(3k)** acquired in $CDCl_3$

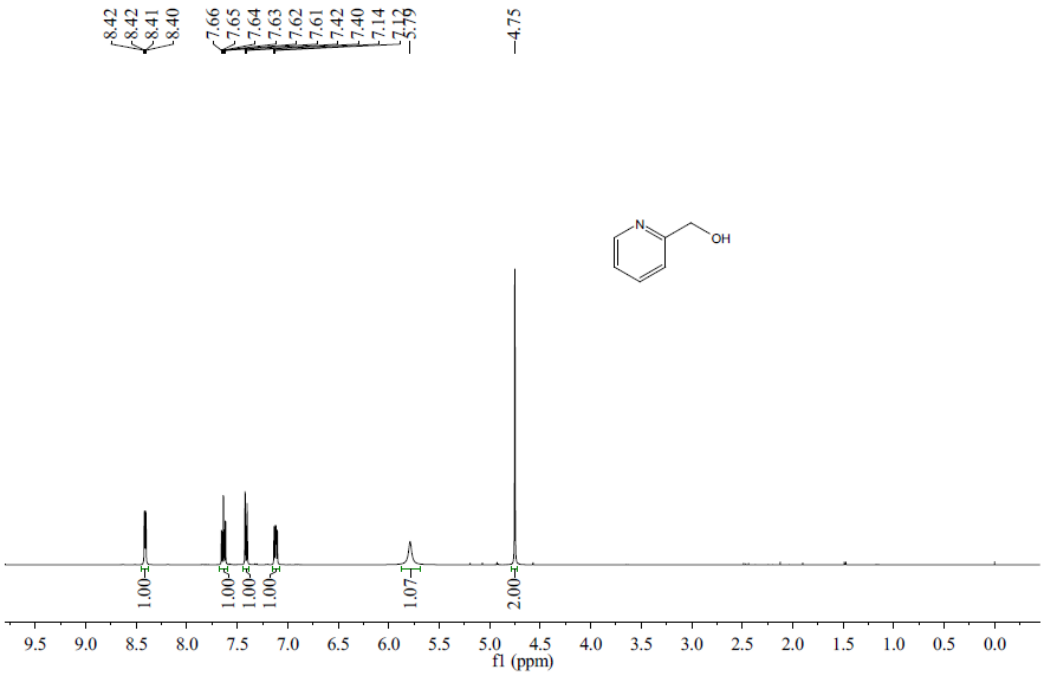


Figure S26. ^{1}H NMR spectrum of pyridin-2-ylmethanol **(3m)** acquired in $CDCl_3$

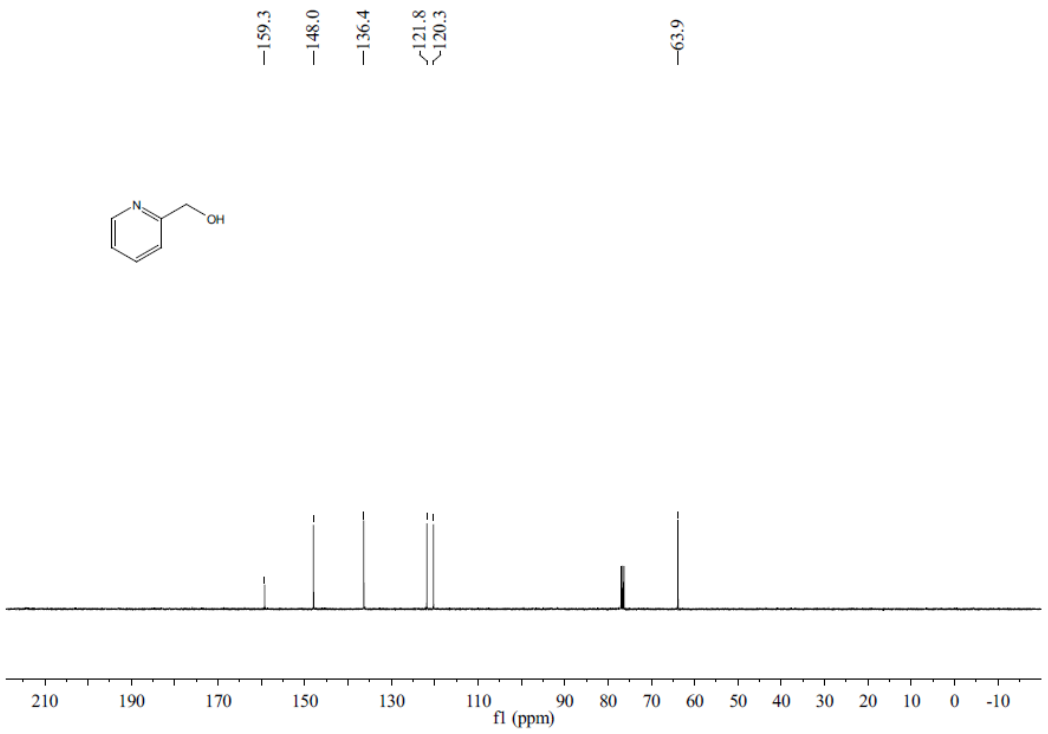


Figure S27. ^{13}**C NMR** spectrum of pyridin-2-ylmethanol **(3m)** acquired in $CDCl_3$

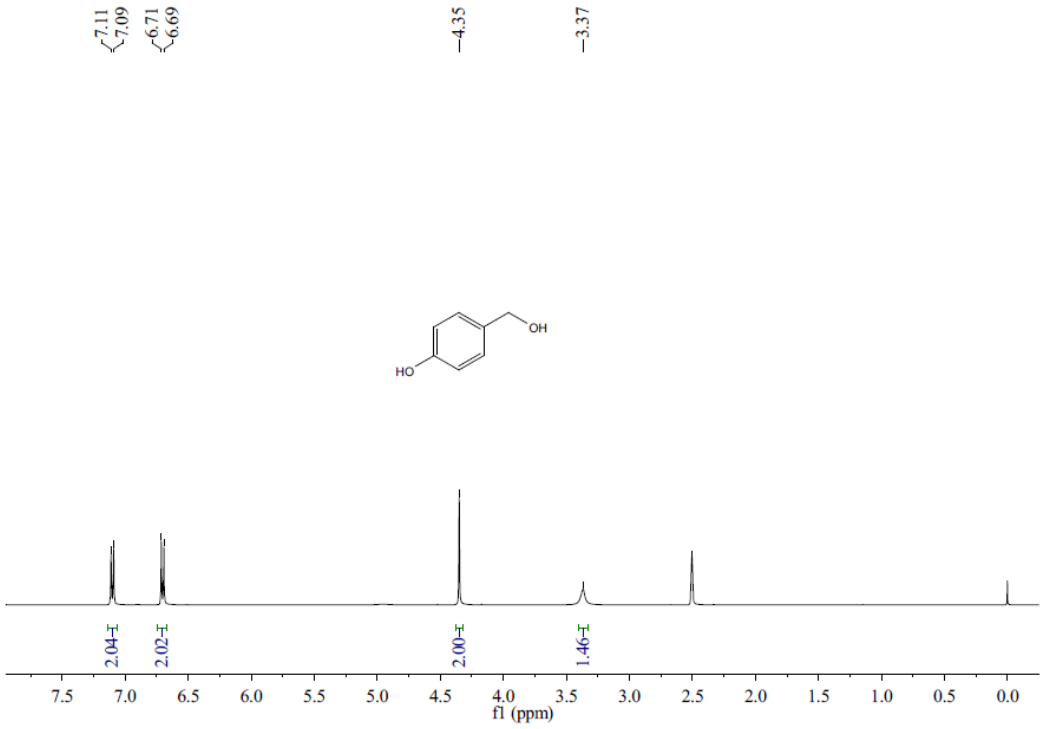


Figure S28. ^{1}H NMR spectrum of of 4-hydroxybenzyl alcohol **(3n)** acquired in DMSO

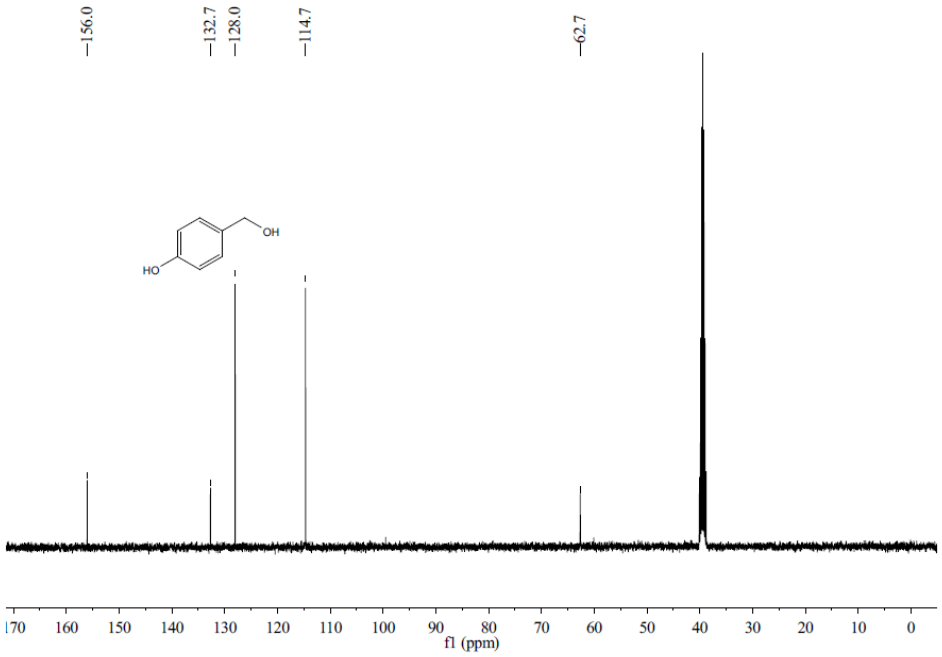


Figure S29. ^{13}C NMR spectrum of of 4-hydroxybenzyl alcohol **(3n)** acquired in DMSO

NMR spectra for 2^{o} alcohol

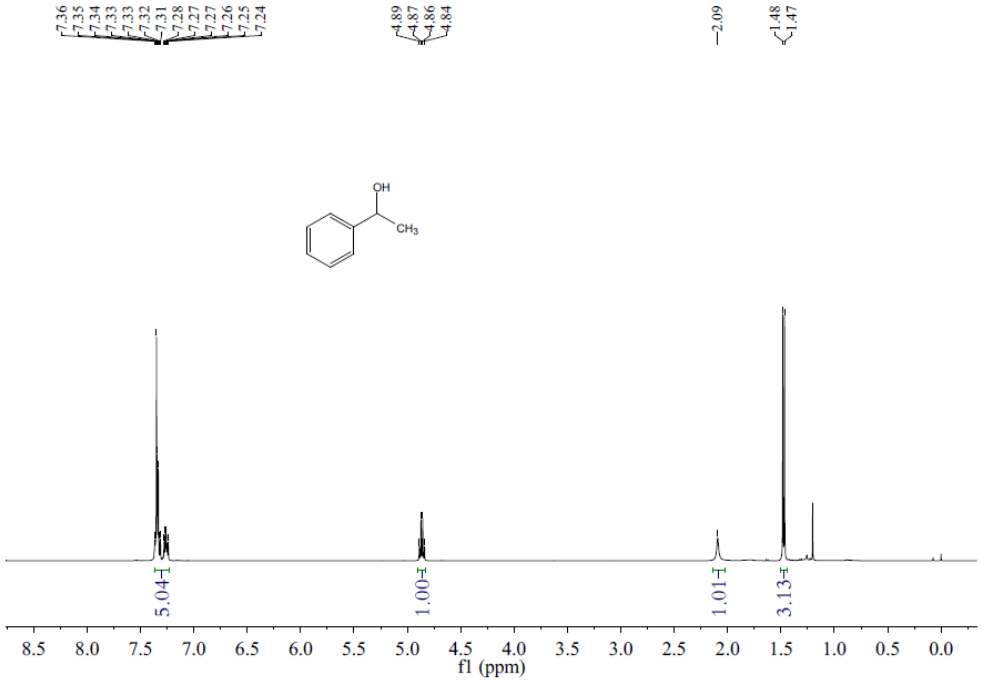


Figure S30.^{1}H NMR spectrum of 1-phenylethan-1-ol **(5a)** acquired in $CDCl_3$

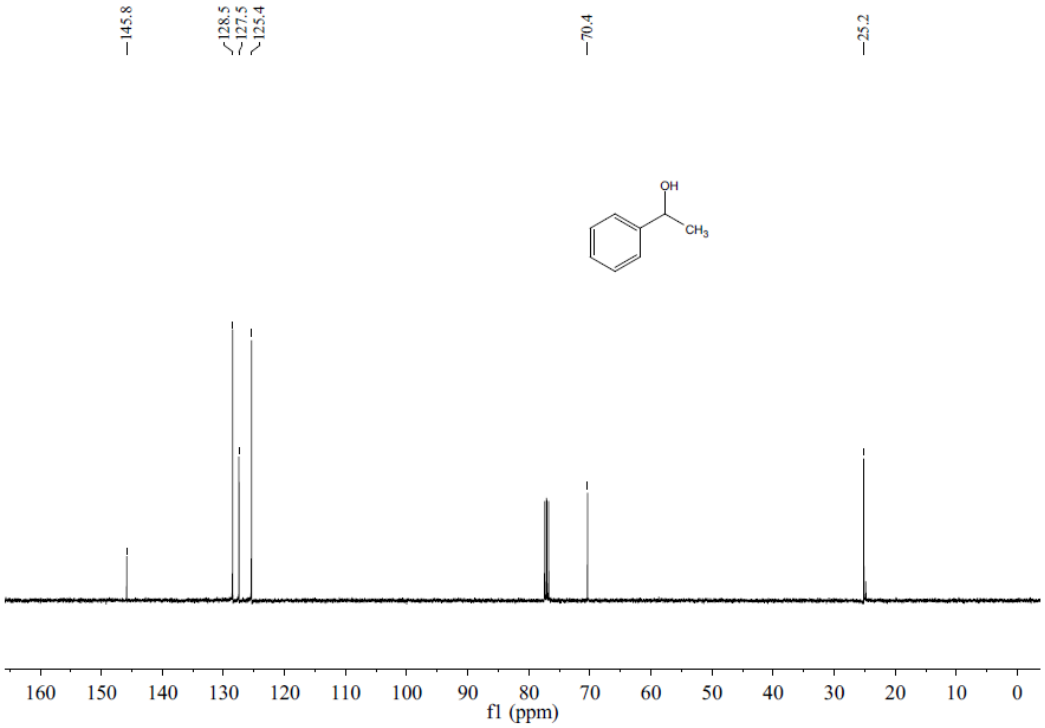


Figure S31. ^{13}C NMR spectrum of 1-phenylethan-1-ol **(5a)** acquired in $CDCl_3$

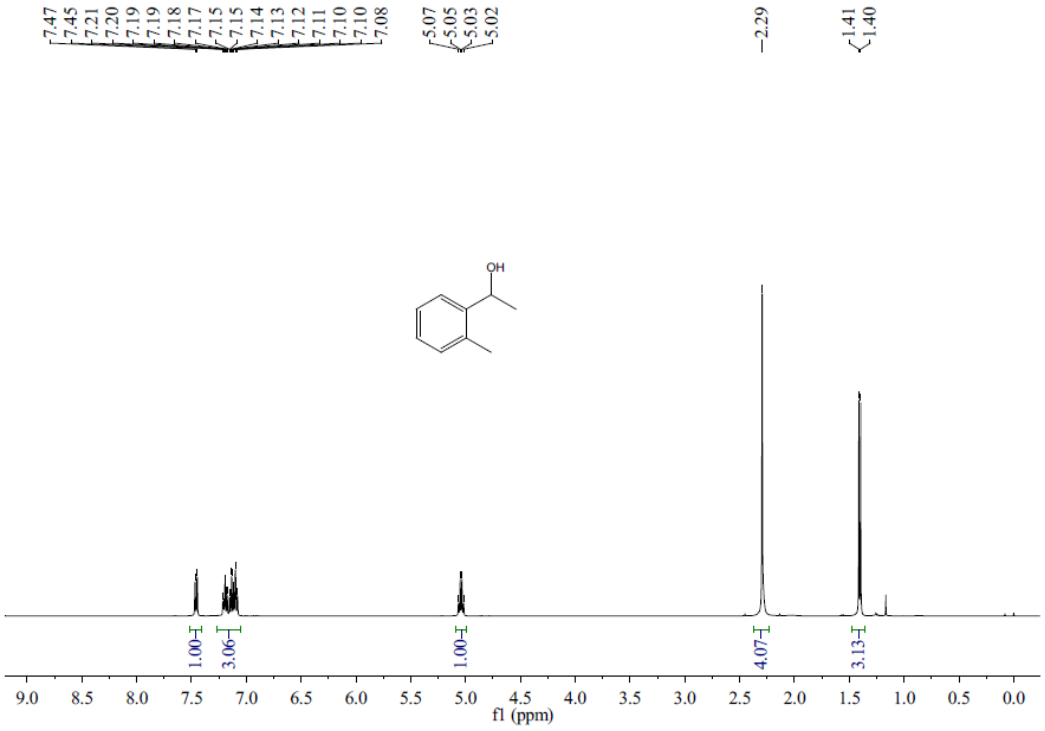


Figure S32. ^{1}H NMR spectrum of 1-(o-tolyl)ethan-1-ol **(5b)** acquired in $CDCl_3$

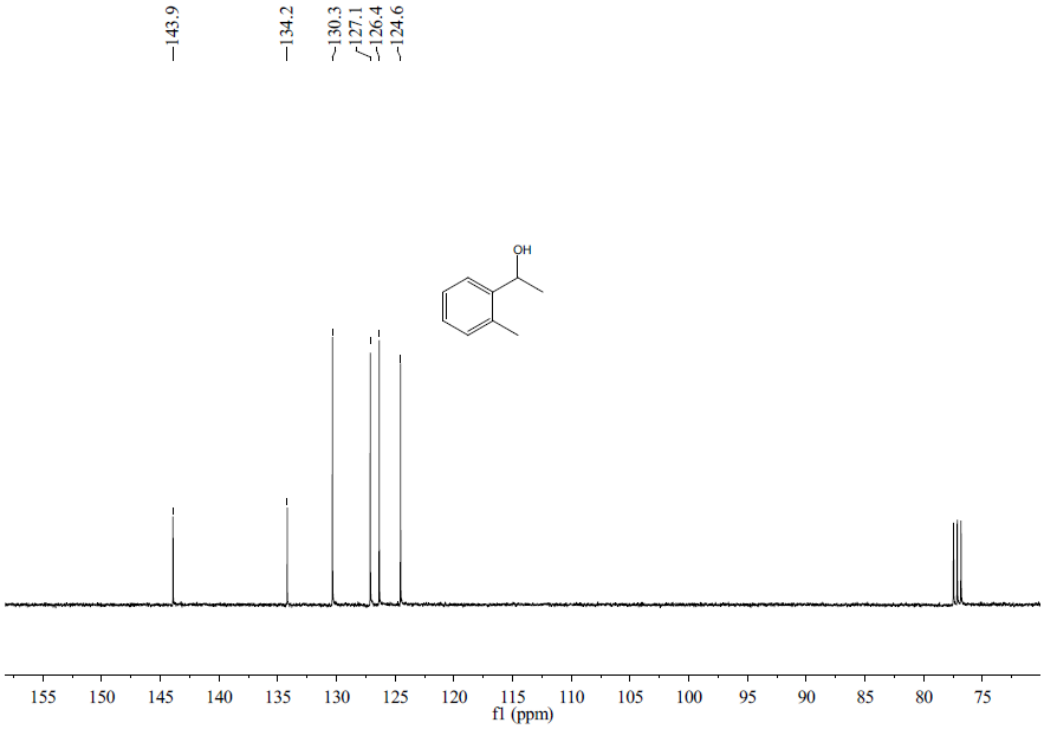


Figure S33. ^{13}C NMR spectrum of 1-(o-tolyl)ethan-1-ol **(5b)** acquired in $CDCl_3$

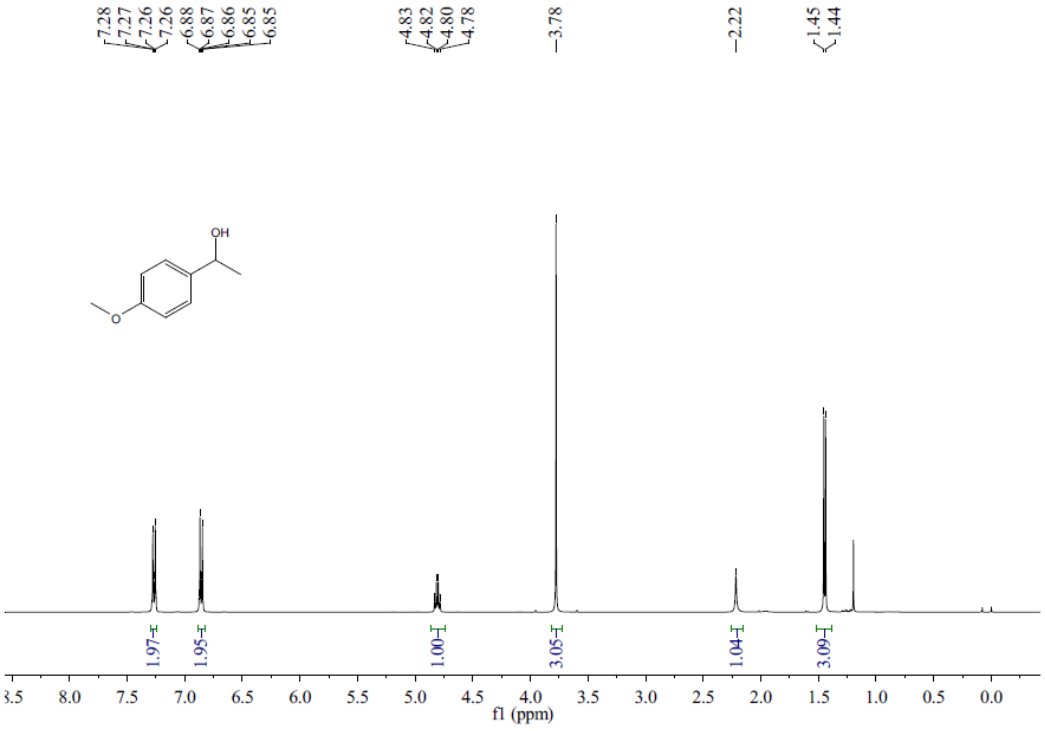


Figure S34. ^{1}H NMR spectrum of 1-(4-metoxyphenyl)ethan-1-ol **(5c)** acquired in $CDCl_3$

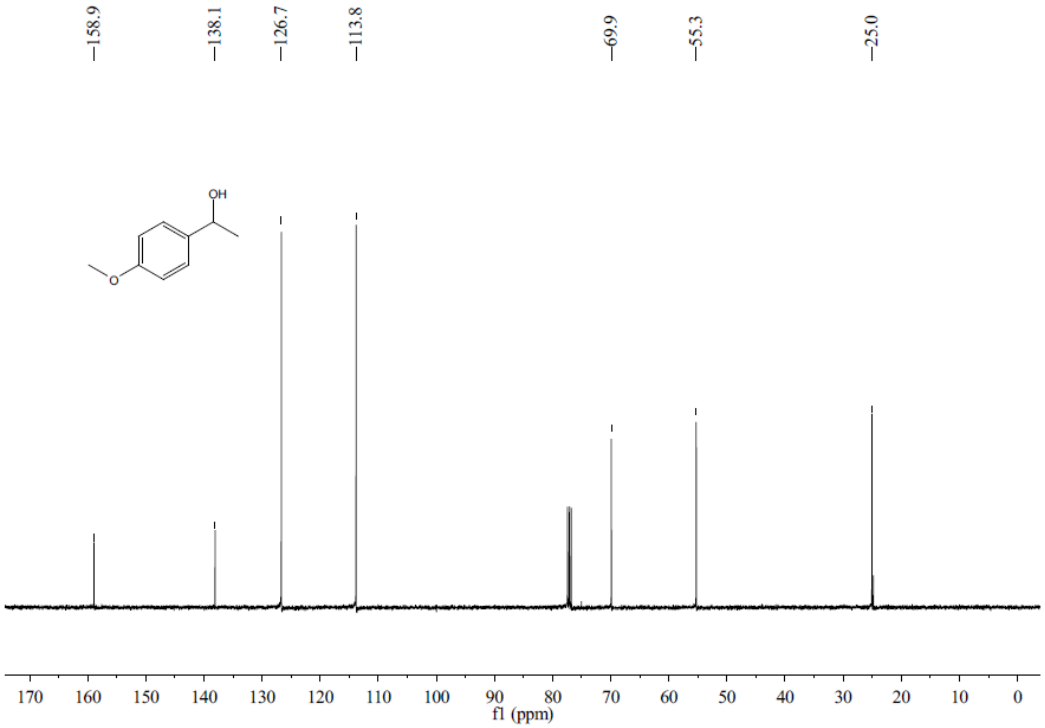


Figure S35. ^{13}C NMR spectrum of 1-(4-metoxyphenyl)ethan-1-ol **(5c)** acquired in $CDCl_3$

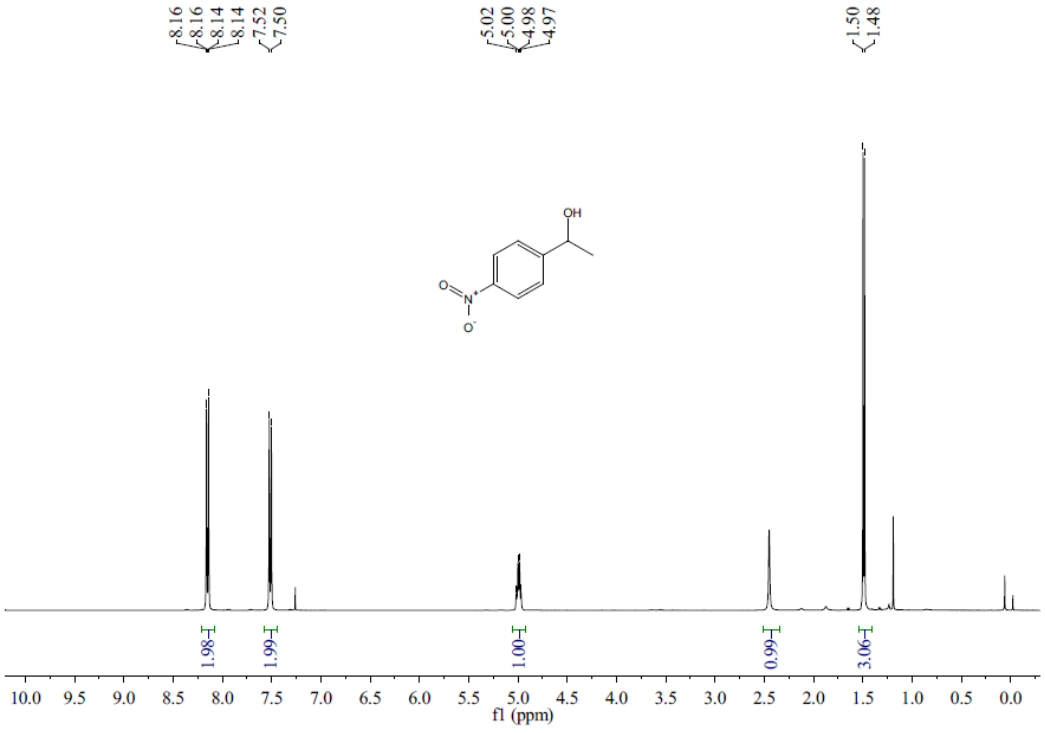


Figure S36. ^{1}H NMR spectrum of 1-(4-nitrophenyl)ethan-1-ol **(5d)** acquired in $CDCl_3$

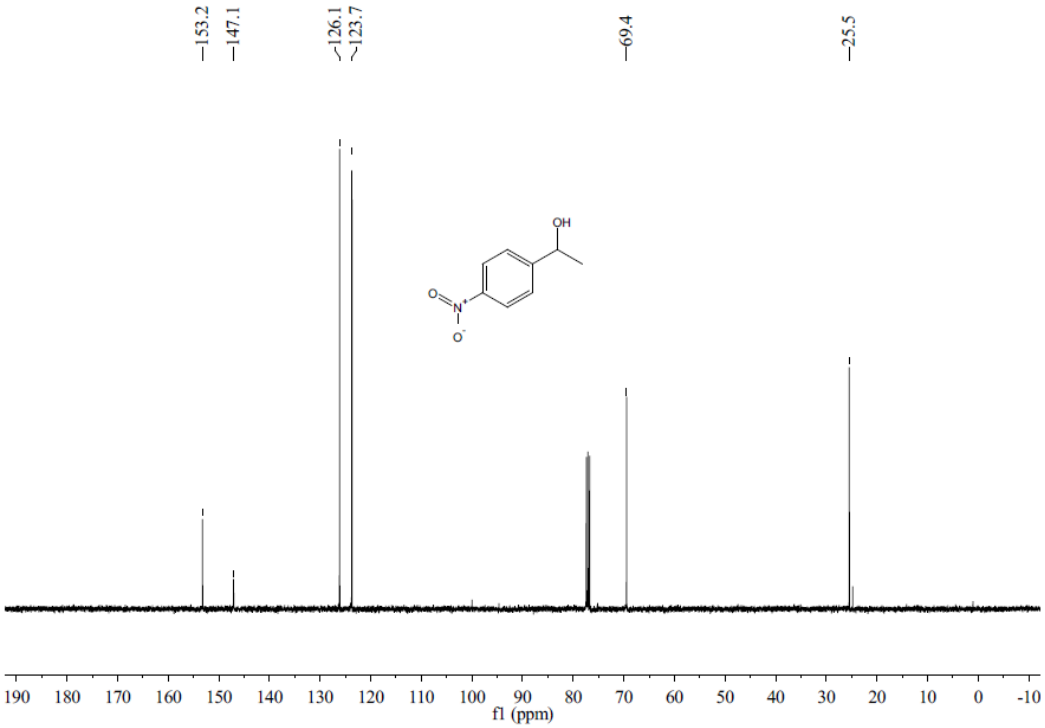


Figure S37.[13]C NMR spectrum of 1-(4-nitrophenyl)ethan-1-ol **(5d)** acquired in $CDCl_3$

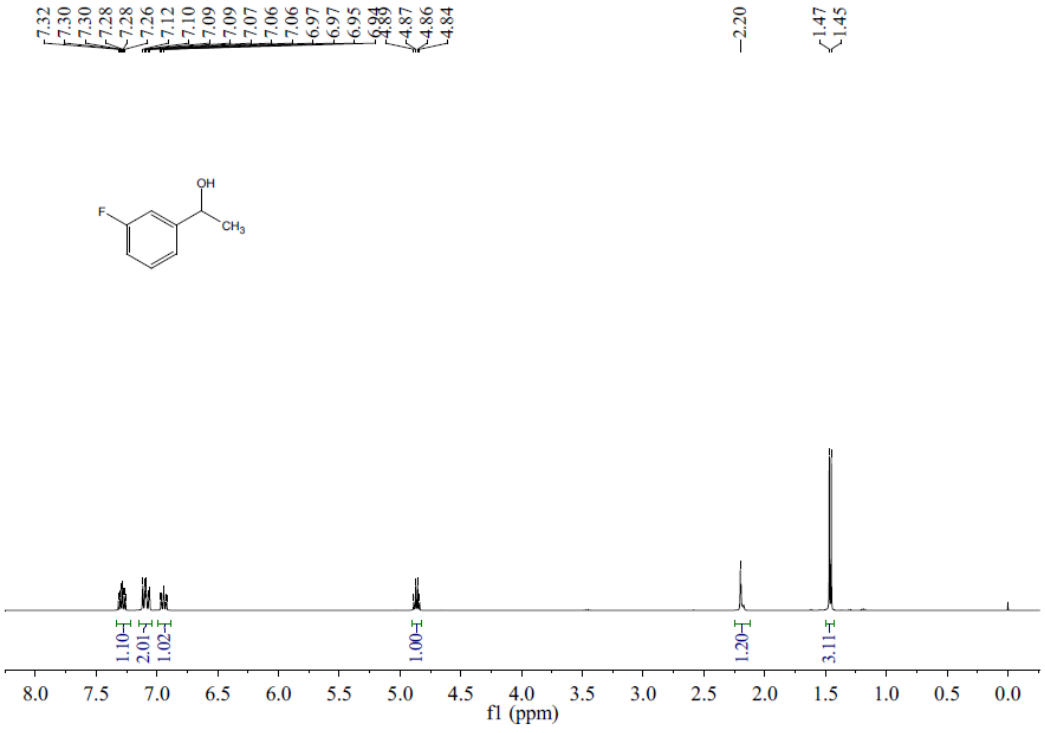


Figure S38.[1]H NMR spectrum of 1-(3-fluorophenyl)ethan-1-ol **(5e)** acquired in $CDCl_3$

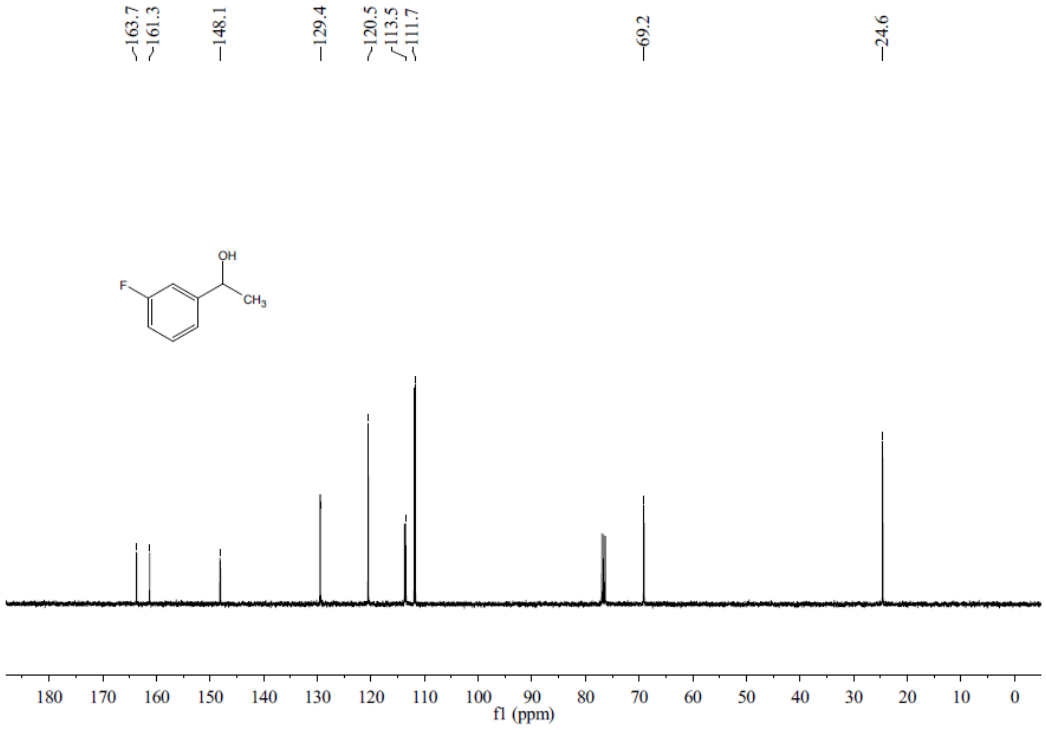


Figure S39. ^{13}C NMR spectrum of 1-(3-fluorophenyl)ethan-1-ol **(5e)** acquired in $CDCl_3$

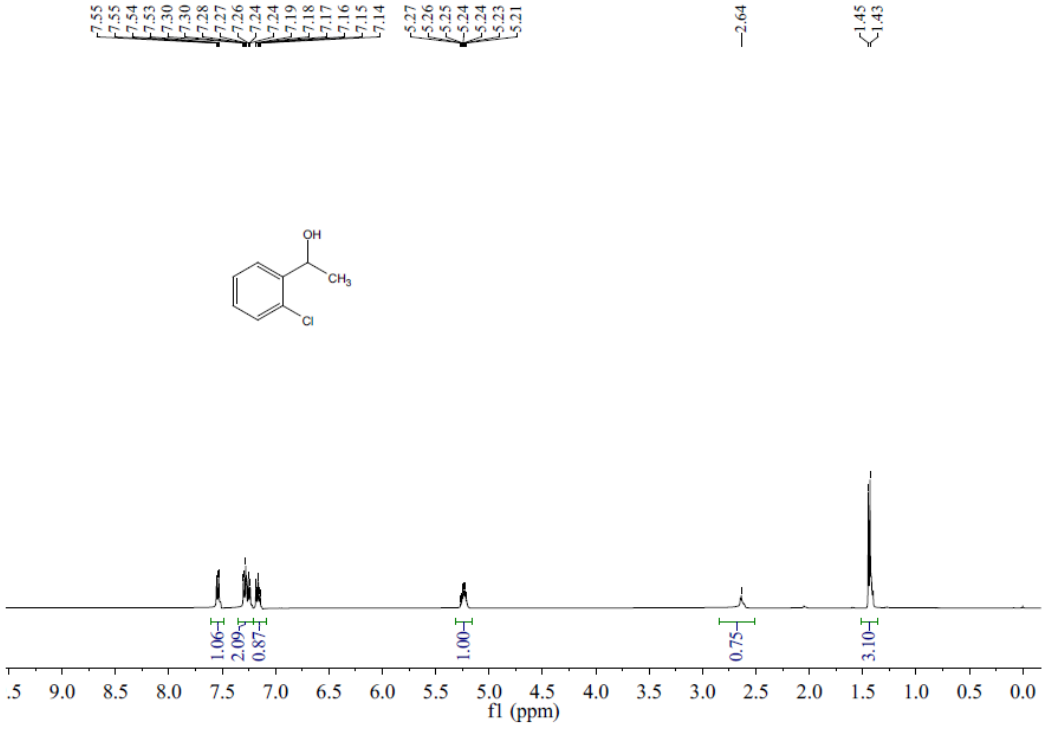


Figure S40. ^{1}H NMR spectrum of 1-(2-chlorophenyl)ethan-1-ol **(5f)** acquired in $CDCl_3$

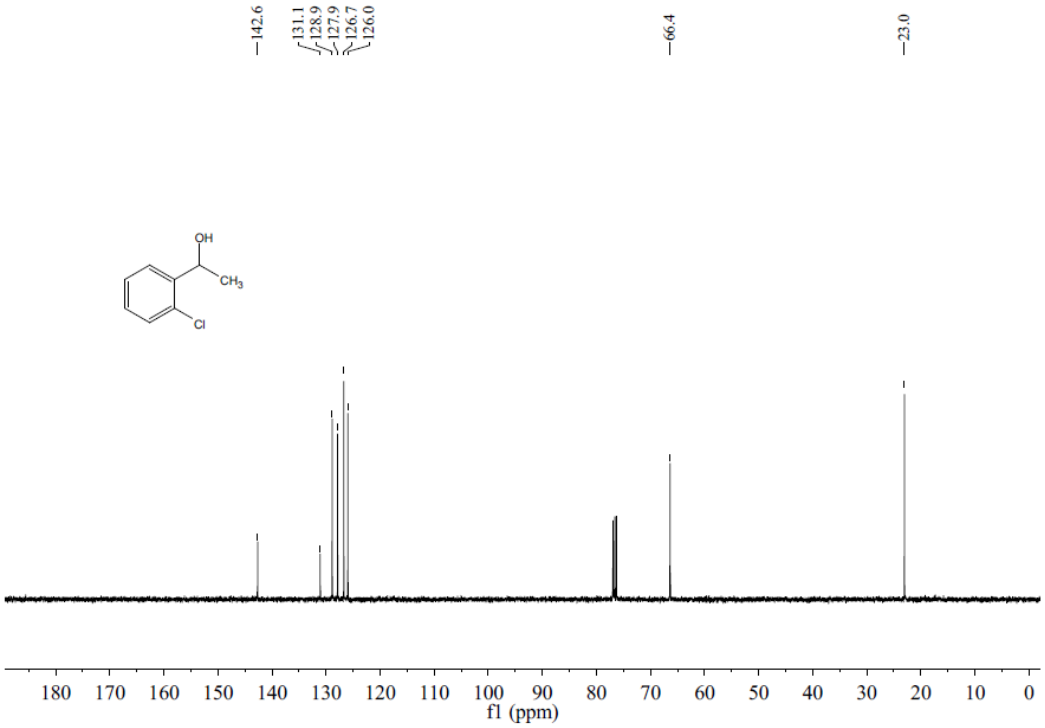


Figure S41. ^{13}C NMR spectrum of 1-(2-chlorophenyl)ethan-1-ol **(5f)** acquired in $CDCl_3$

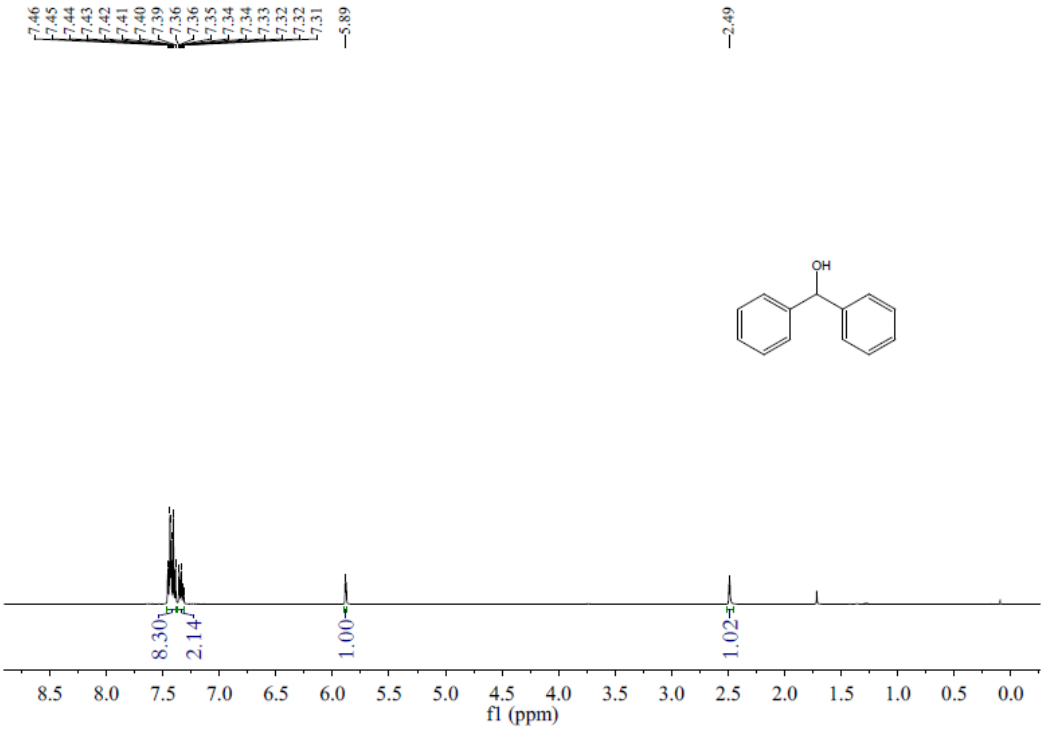


Figure S42. ^{1}H NMR spectrum of diphenylmethanol **(5g)** acquired in $CDCl_3$

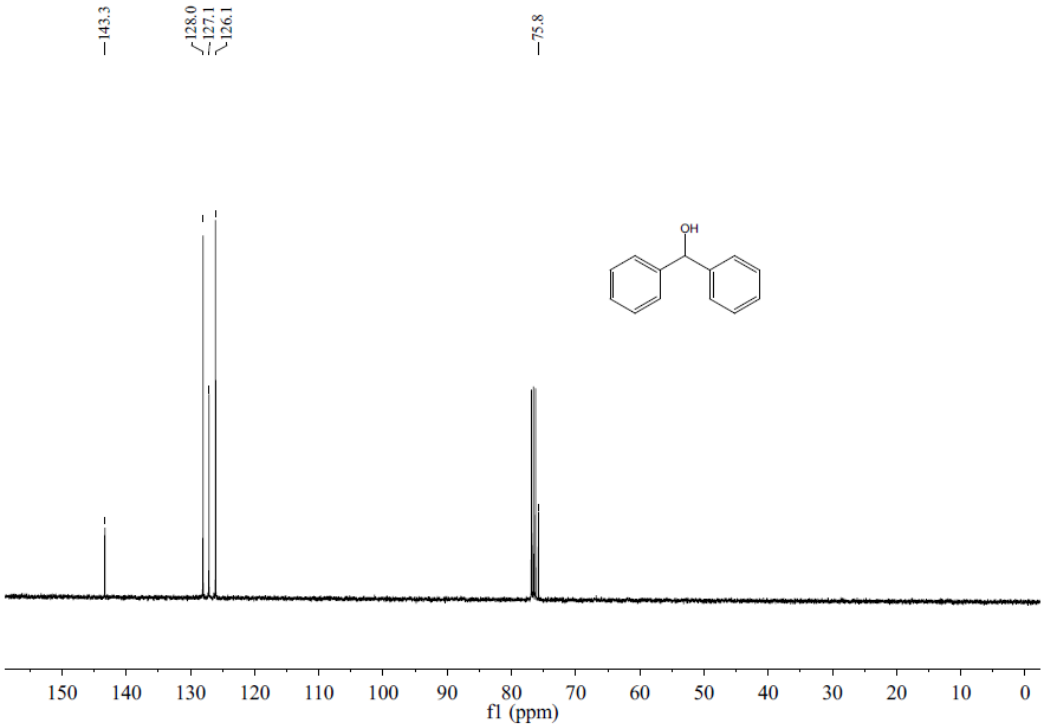


Figure S43. ^{13}C NMR spectrum of diphenylmethanol **(5g)** acquired in $CDCl_3$

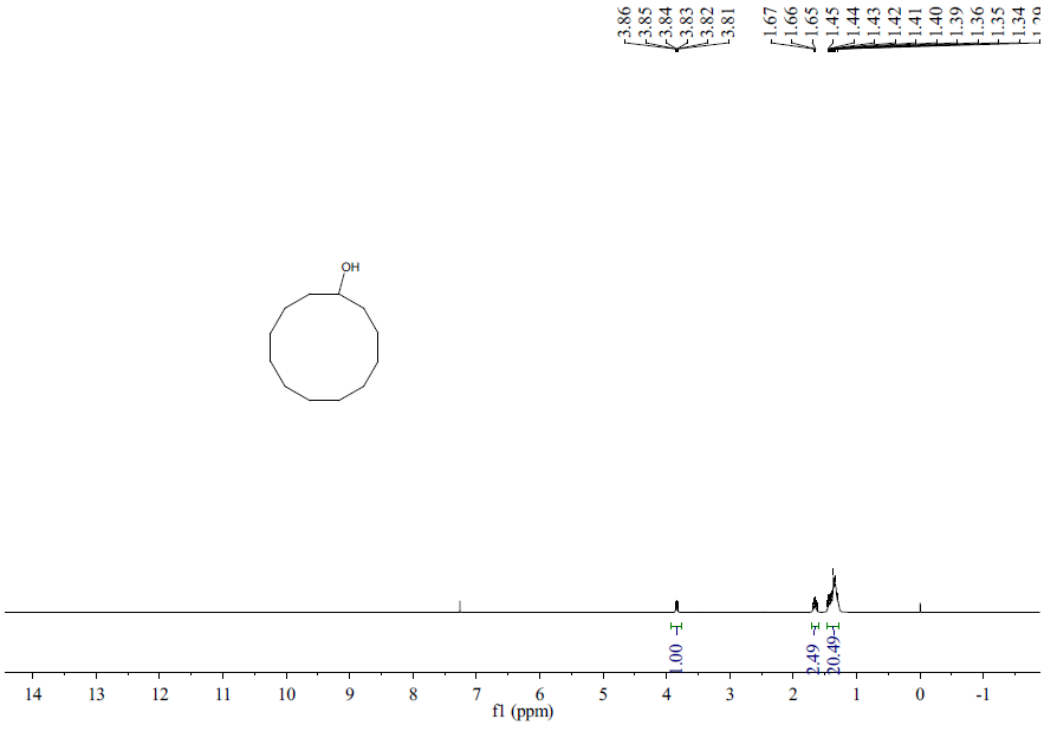


Figure S44. ^{1}H NMR spectrum of cyclododecanol **(5h)** acquired in $CDCl_3$

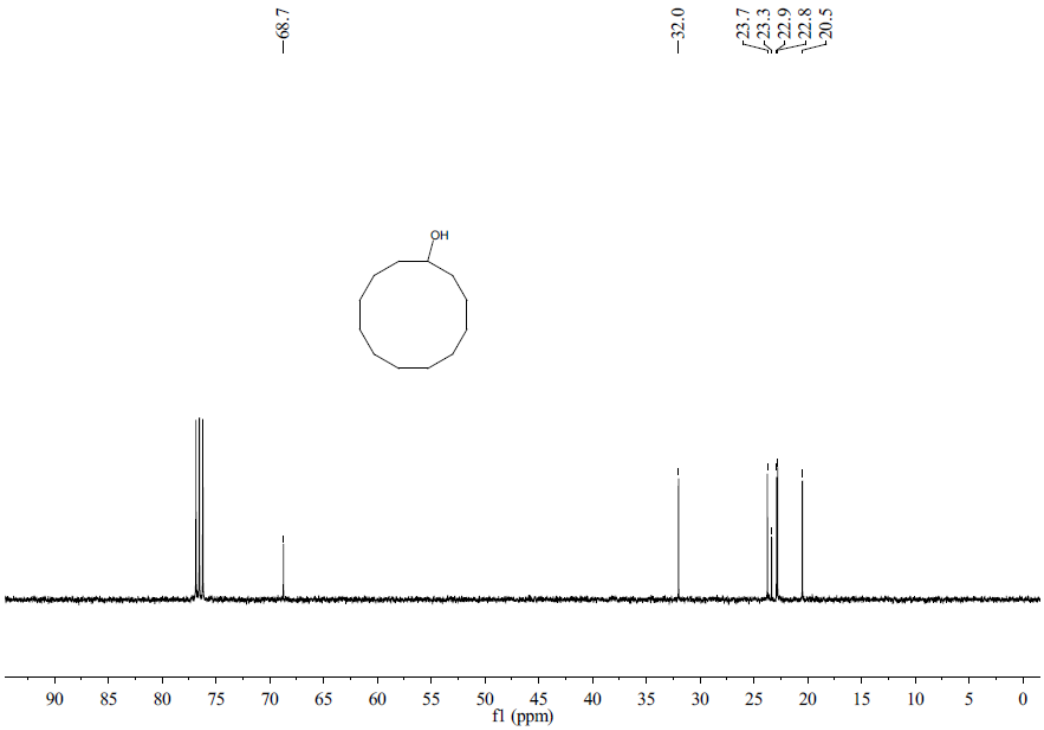


Figure S45. ^{13}C NMR spectrum of cyclododecanol **(5h)** acquired in $CDCl_3$

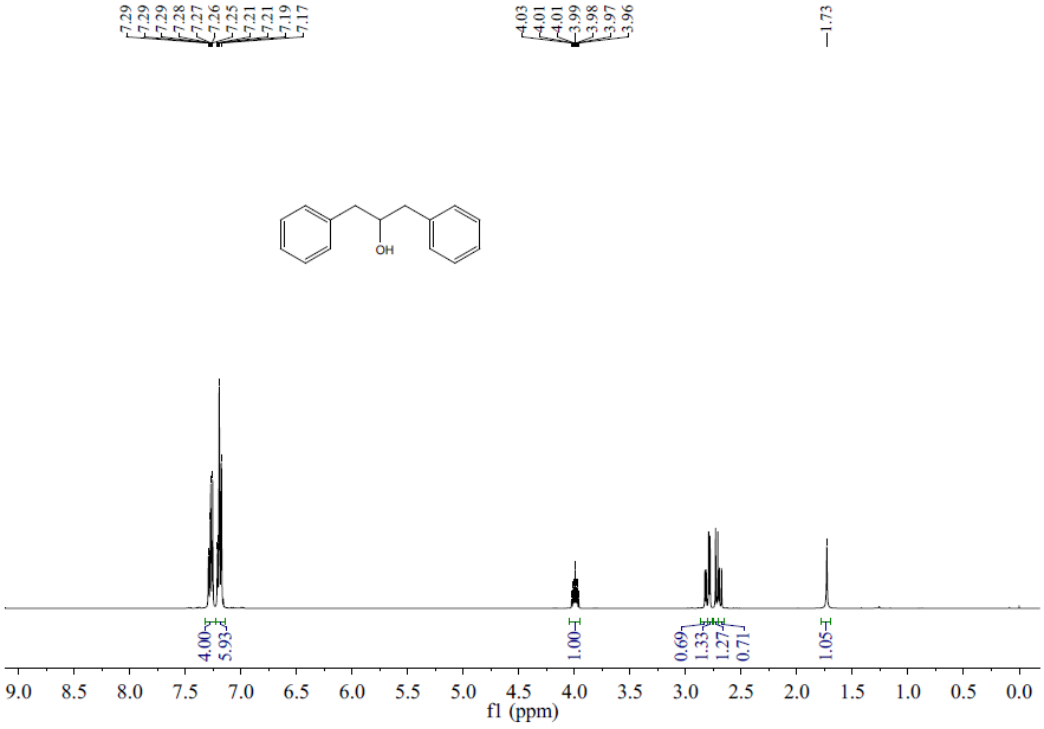


Figure S46. ^{1}H NMR spectrum of 1,3-diphenylpropan-2-ol **(5i)** acquired in $CDCl_3$

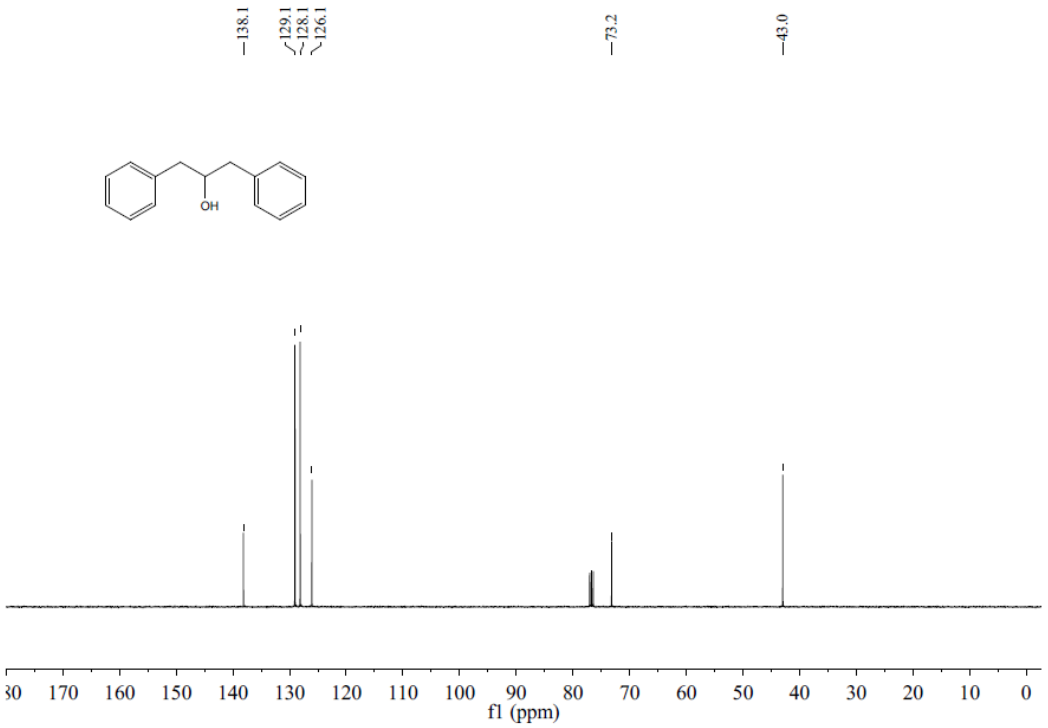


Figure S47. ^{13}C NMR spectrum of 1,3-diphenylpropan-2-ol **(5i)** acquired in $CDCl_3$

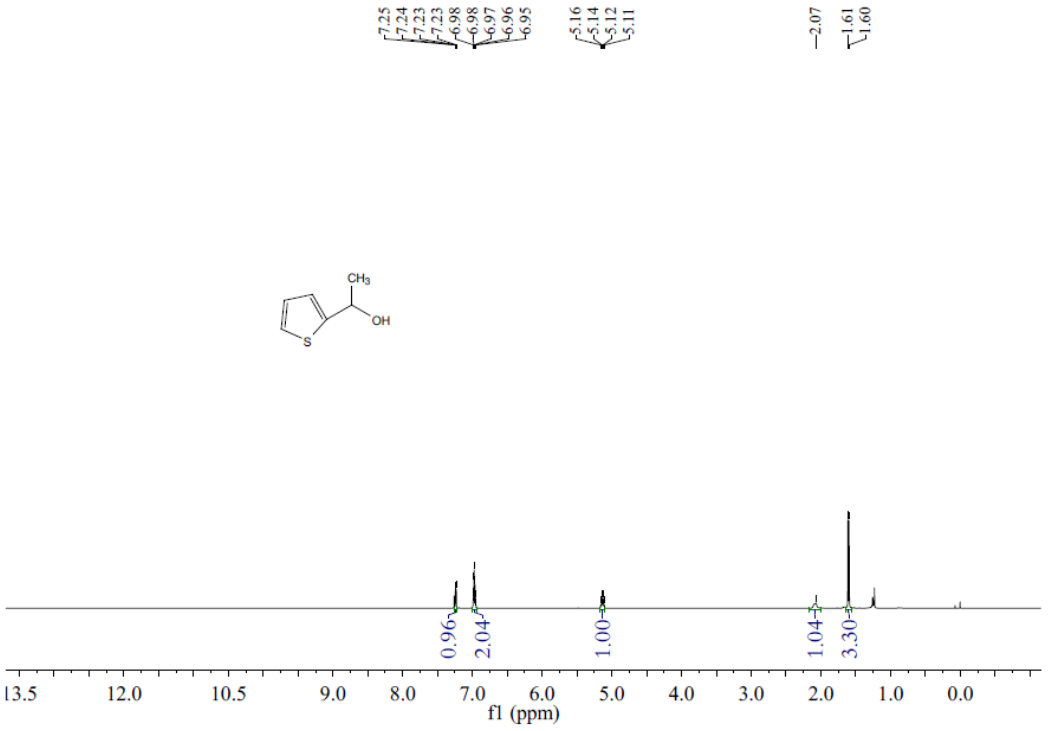


Figure S48. ^{1}H NMR spectrum of 1-(thiophen-2-yl)ethan-1-ol **(5j)** acquired in $CDCl_3$

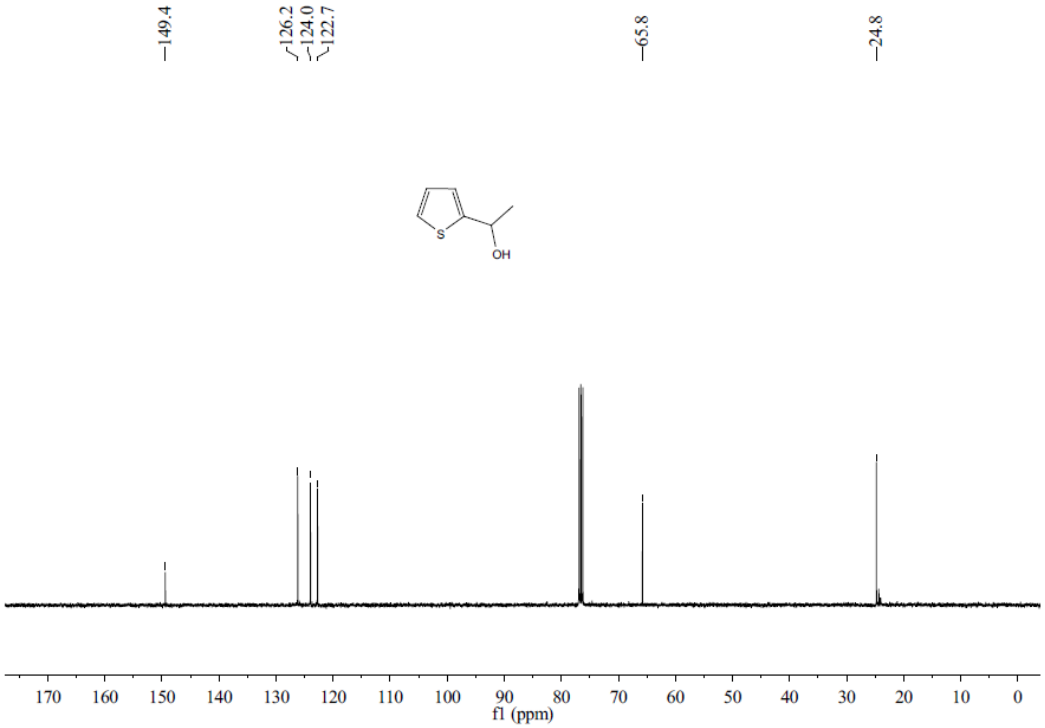


Figure S49. ^{13}C NMR spectrum of 1-(thiophen-2-yl)ethan-1-ol **(5j)** acquired in $CDCl_3$

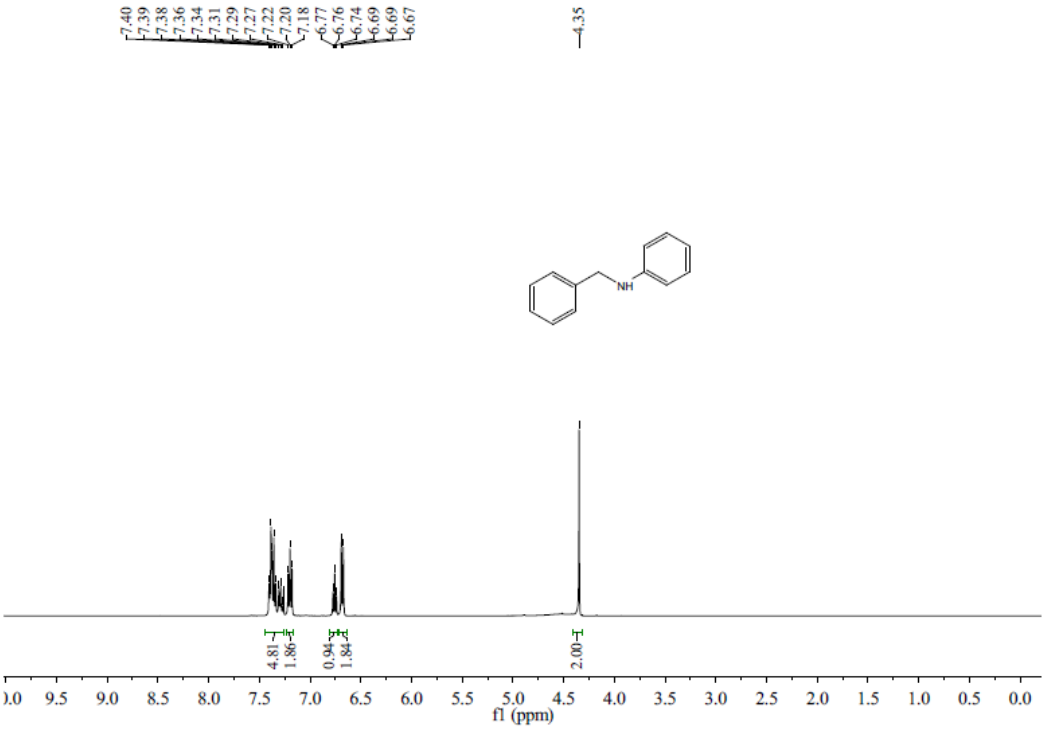


Figure S50. ^{1}H NMR spectrum of N-benzylaniline **(6a)** acquired in $CDCl_3$

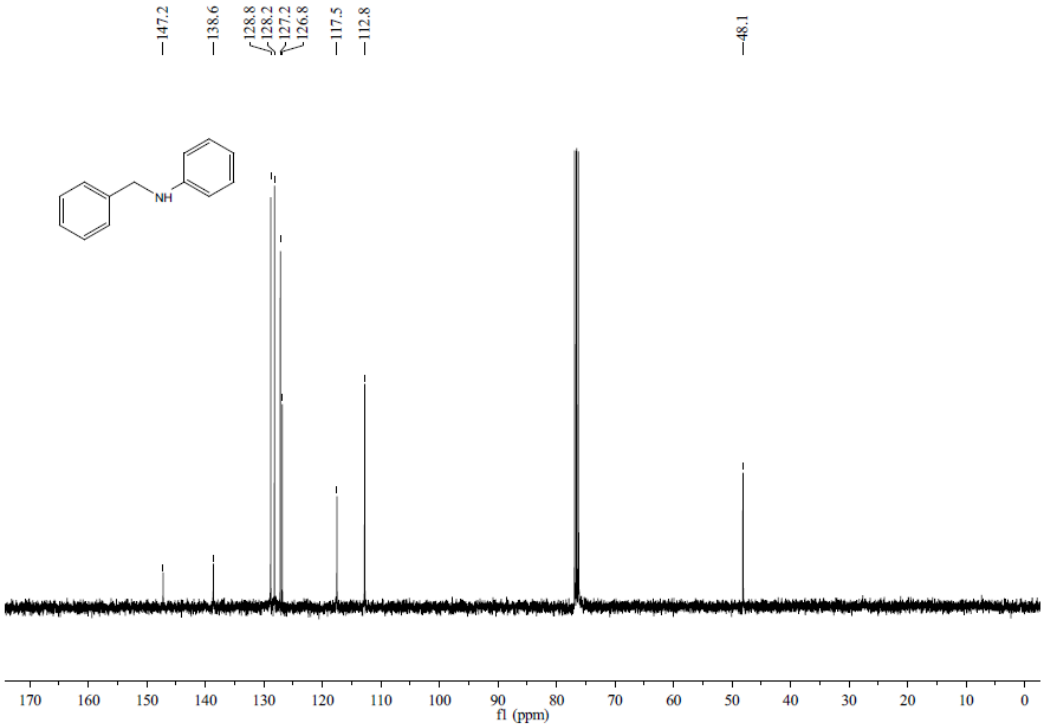


Figure S51. ^{13}C NMR spectrum of N-benzylaniline **(6a)** acquired in $CDCl_3$

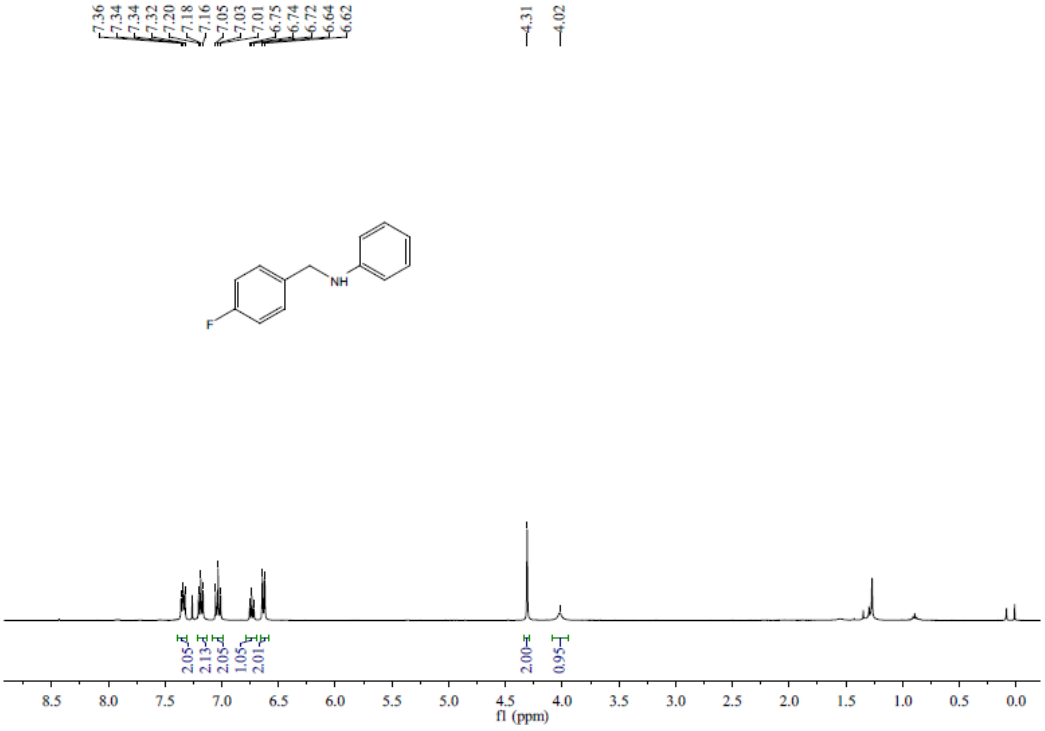


Figure S52. ^{1}H NMR spectrum of N-(4-fluorobenzyl)aniline **(6b)** acquired in $CDCl_3$

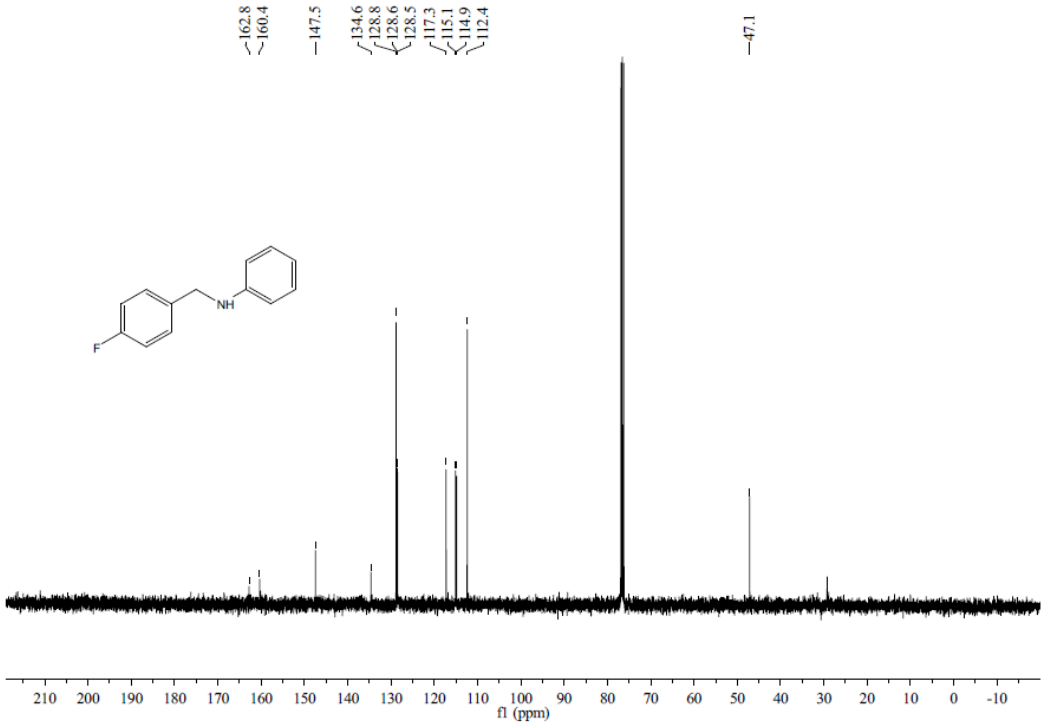


Figure S53. ^{13}C NMR spectrum of N-(4-fluorobenzyl)aniline **(6b)** acquired in $CDCl_3$

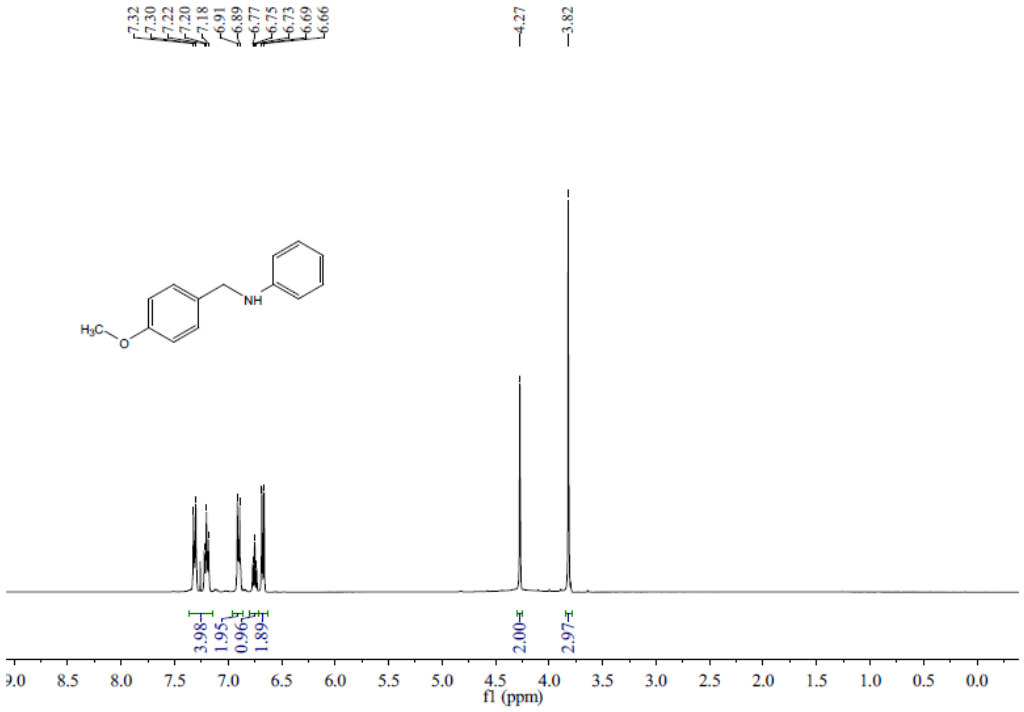


Figure S54. ^{1}H NMR spectrum of N-(4-methoxybenzyl)-4,4,5,5-tetramethyl-N-phenyl-1,3,2-dioxaborolan-2-amine **(6c)** acquired in $CDCl_3$

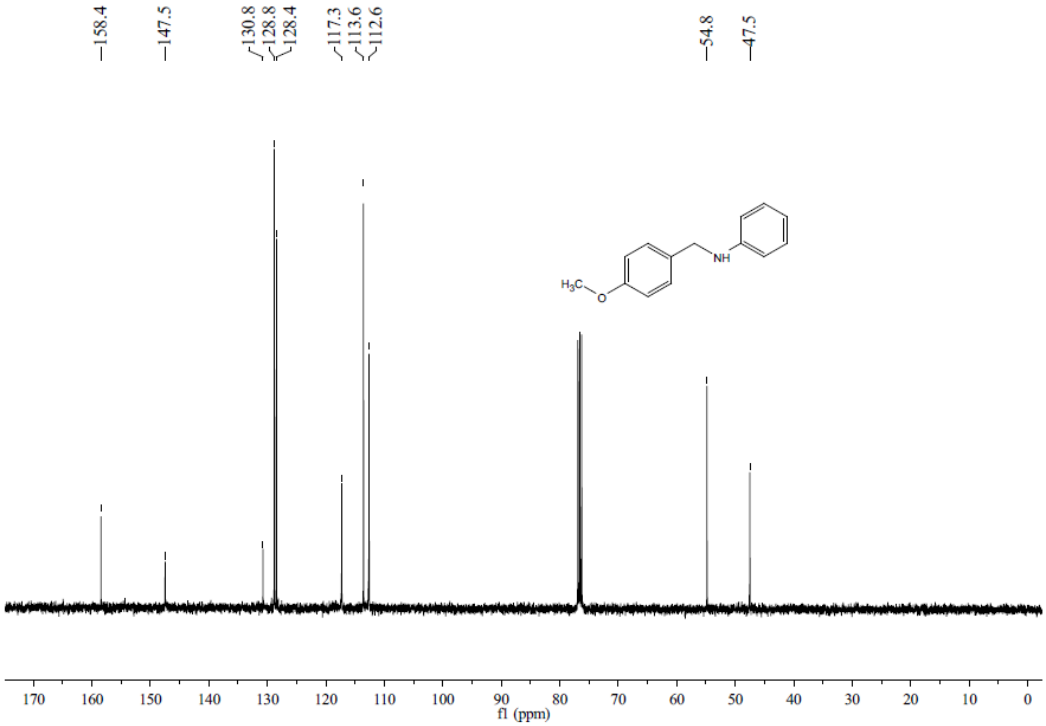
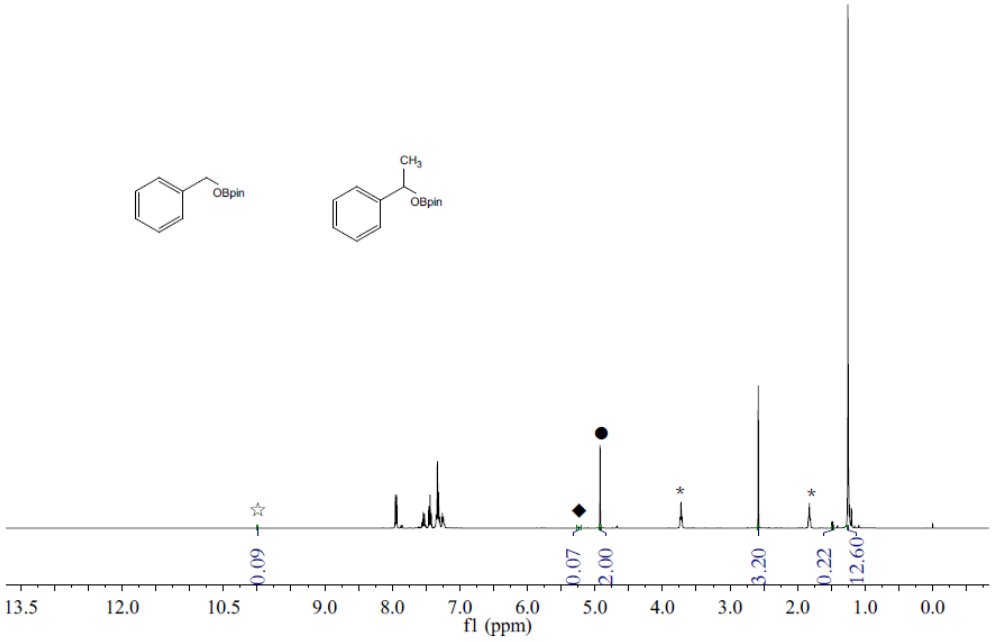


Figure S55. ^{13}C NMR spectrum of N-(4-methoxybenzyl)-4,4,5,5-tetramethyl-N-phenyl-1,3,2-dioxaborolan-2-amine **(6c)** acquired in $CDCl_3$

(NMR spectrum from reaction mixture of intermolecular hydroboration reaction after 20min(◆: ketone product peak ●: aldehyde product peak)



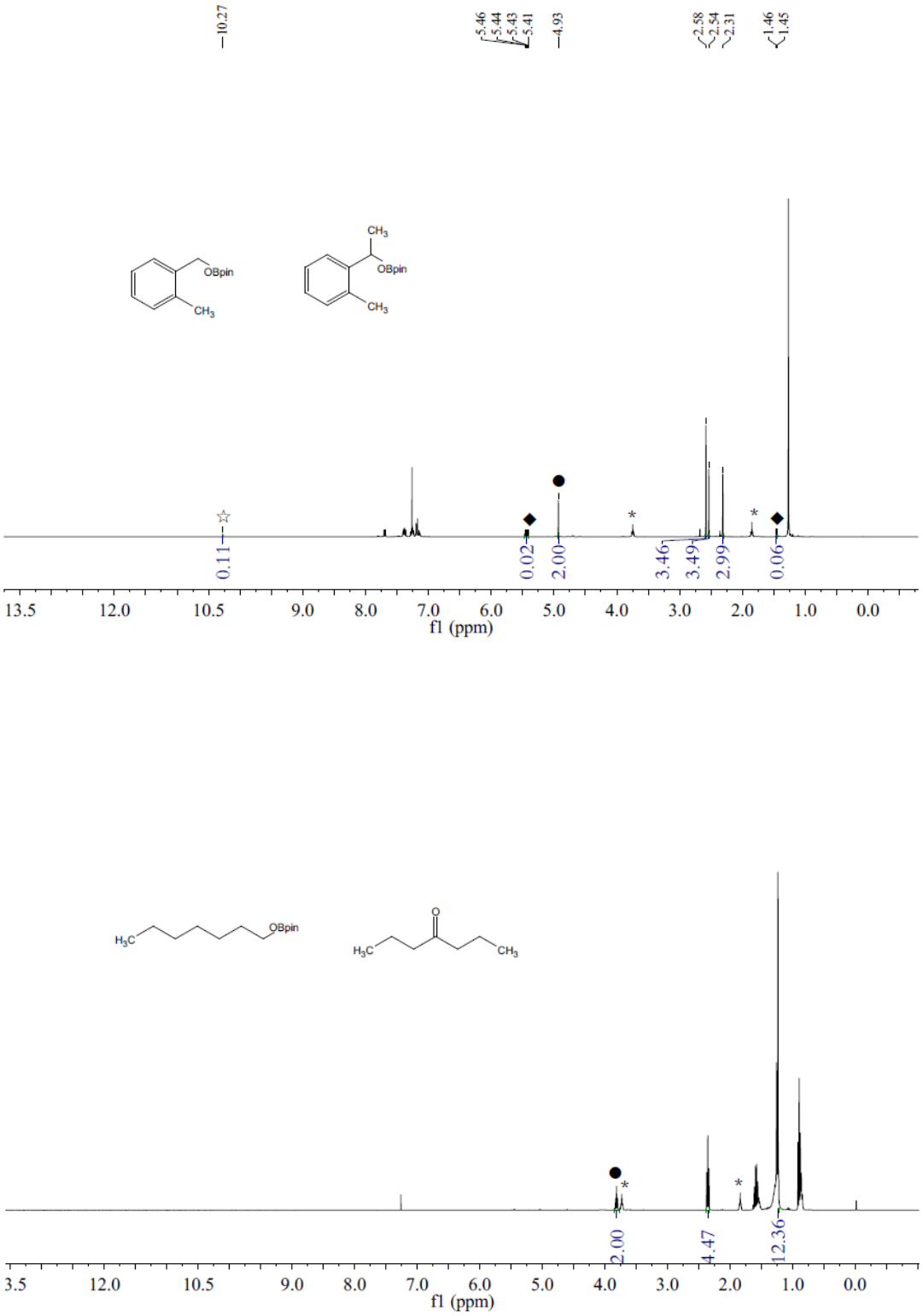


Figure S56. ^{1}H NMR spectrum of intermolecular chemoselective reaction acquired in $CDCl_3$

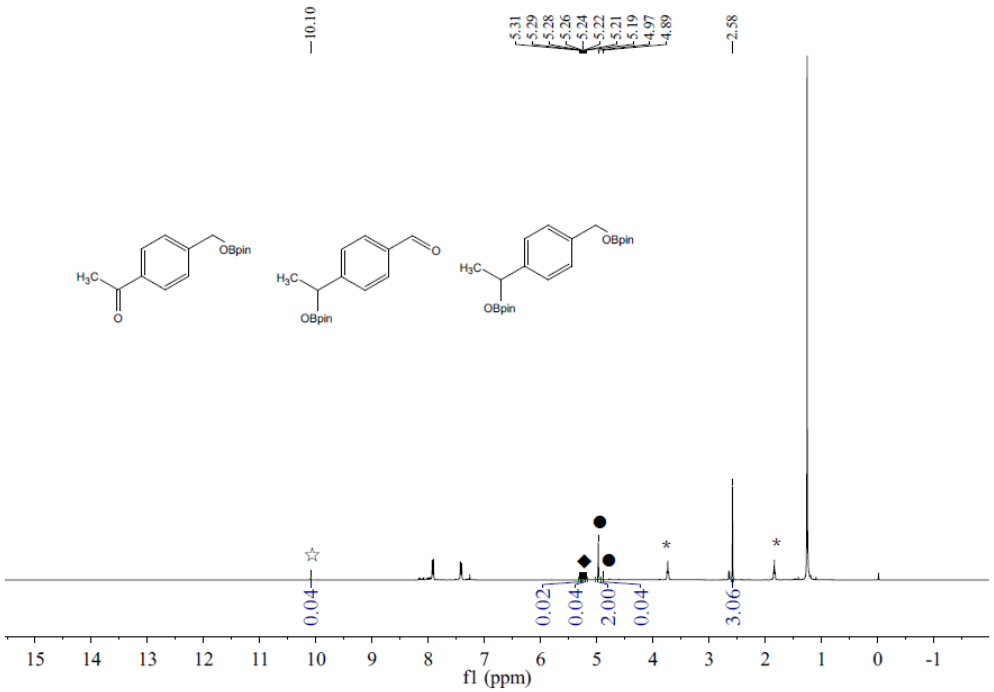


Figure S57. ^{1}H NMR spectrum of intramolecular chemoselective reaction acquired in $CDCl_3$

$(MeCp)_3La$ NMR

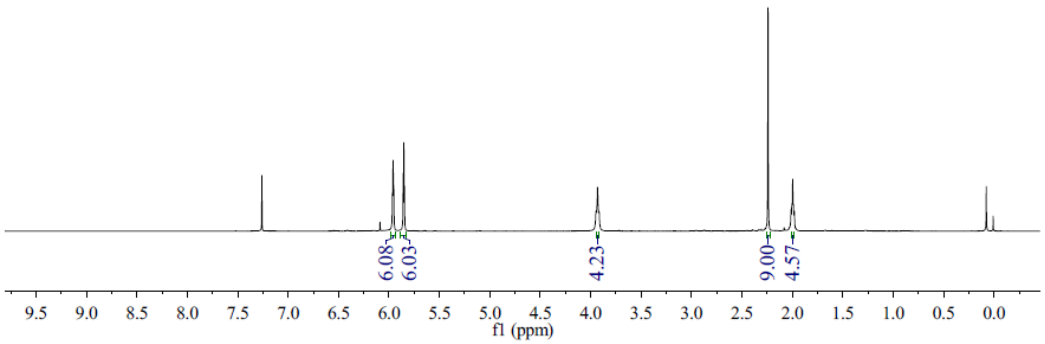


Figure S58. ^{1}H NMR spectrum of $(MeCp)_3La$ **(7a)** acquired in $CDCl_3$

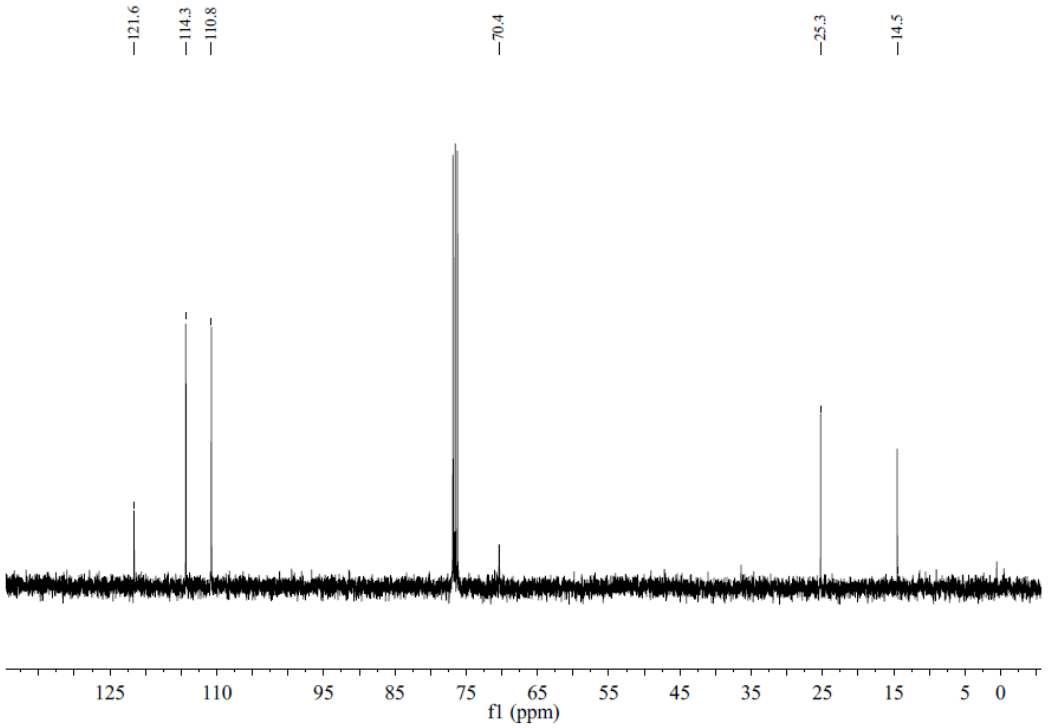


Figure S59. ^{13}C NMR spectrum of $(MeCp)_3La$ **(7a)** acquired in $CDCl_3$

7. Computational method

In this work, all the DFT[13] studies were performed with Gaussian 09 program[14] with B3PW91 method[15]. For the La atom, the SDD[16] basisset was used; and for the other atoms in the geometry optimizations, the 6-31G(d,p) basis set[17] was used. Vibrational frequency was calculated to characterize all stationary points to be minima or transition states which have been checked by intrinsic reaction coordinate (IRC)[18]. The solvation effect was estimated by the single-point energy computations on the optimized gas-phase geometries using the SMD[19] model with tetrahydrofuran as solvent. All the single-point energy calculations on stationary points were confirmed with B3PW91/BSII[20] level (BSII:SDD for La and 6–311++G(d,p) for other atoms). The enthalpy and Gibbs energy of solvation was determined by adding the solvation single-point energy and thermal correction to enthalpy and the Gibbs energy. The translational entropy in solution was corrected using the method proposed by Whitesides *et al.*[21]

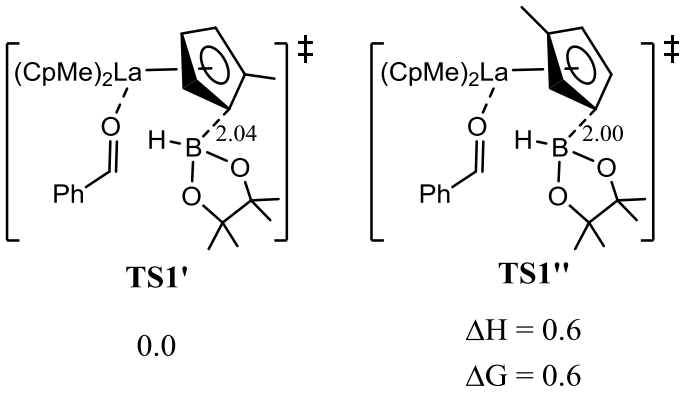


Figure S60. Energy (in kcal/mol) comparison of HBpin attack to the methyl substituted cyclopentadienyl group at different positions. Bond lengths are shown in Å.

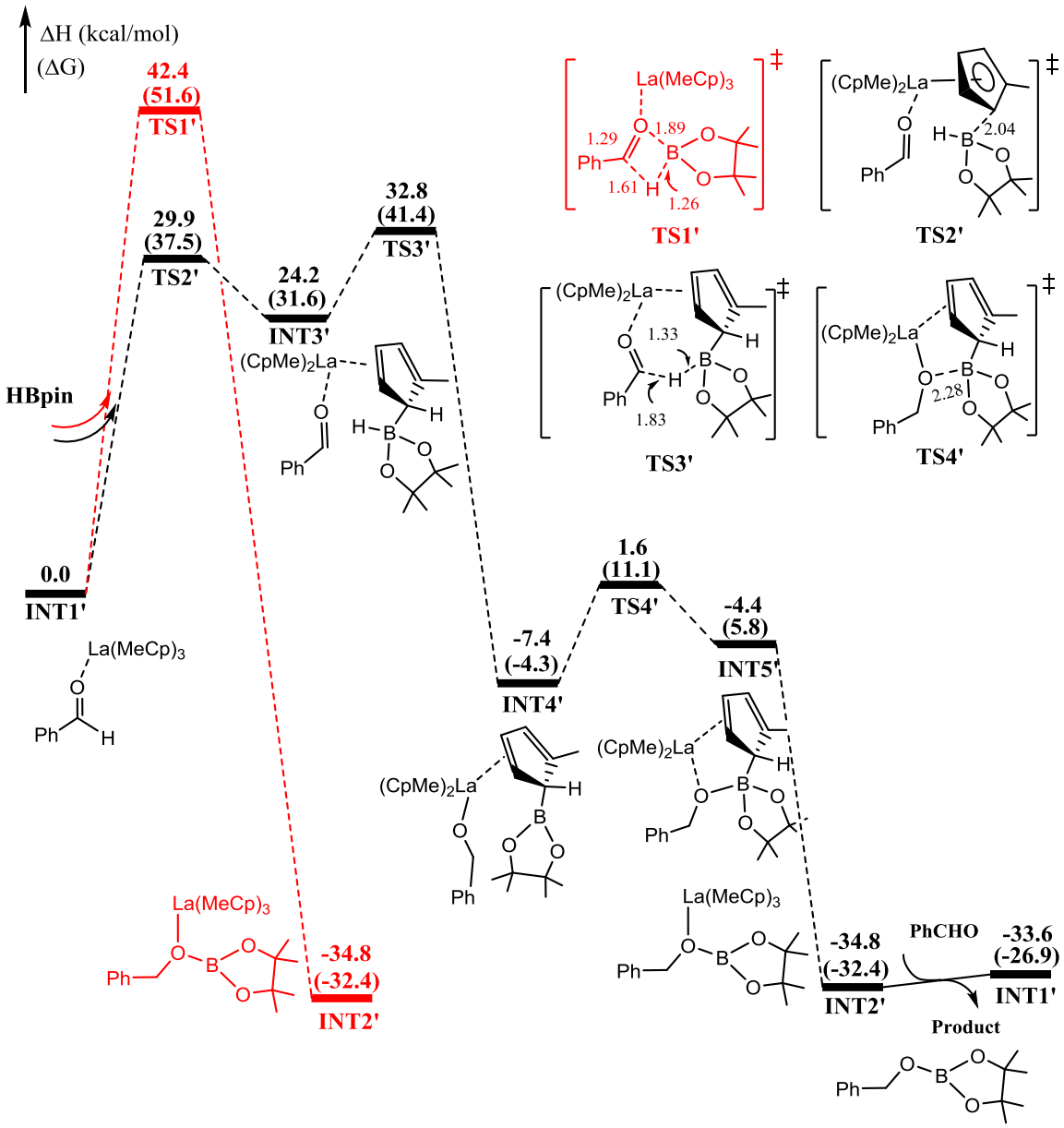


Figure S61. Energy profile (in kcal/mol) for the $(MeCp)_3La$ catalyzed hydroboration of aldehyde with pinacolborane. Bond lengths are shown in Å.

8. Cartesian coordinates and energies

Benzaldehyde

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.733417	1.058364	-0.000076
2	6	0	-0.360940	1.290686	0.000252
3	6	0	0.532634	0.214871	0.000441
4	6	0	0.046641	-1.098997	0.000254
5	6	0	-1.322581	-1.329750	-0.000079
6	6	0	-2.212095	-0.251450	-0.000245
7	1	0	-2.428701	1.892663	-0.000208
8	1	0	0.024991	2.308073	0.000383
9	1	0	0.763167	-1.914961	0.000404
10	1	0	-1.703773	-2.346858	-0.000208
11	1	0	-3.283055	-0.434709	-0.000511
12	6	0	1.988592	0.469116	0.000876
13	1	0	2.269501	1.546587	-0.000980
14	8	0	2.840608	-0.395979	-0.000927

Zero-point correction= 0.110251 (Hartree/Particle)
Thermal correction to Energy= 0.116565
Thermal correction to Enthalpy= 0.117509
Thermal correction to Gibbs Free Energy= 0.079706
Sum of electronic and zero-point Energies= -345.336909
Sum of electronic and thermal Energies= -345.330595
Sum of electronic and thermal Enthalpies= -345.329651
Sum of electronic and thermal Free Energies= -345.367454
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -345.53869484

HBpin

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000017	1.935672	-0.000006
2	8	0	-1.077254	1.191895	-0.389882
3	8	0	1.077231	1.191919	0.389882
4	6	0	-0.785010	-0.188982	-0.048475
5	6	0	0.785014	-0.188965	0.048485
6	6	0	1.473858	-0.460756	-1.289081
7	1	0	2.540453	-0.242382	-1.188315
8	1	0	1.362956	-1.504864	-1.596014
9	1	0	1.072214	0.179579	-2.079616
10	6	0	-1.366193	-1.087534	-1.130801
11	1	0	-1.121855	-2.137303	-0.938338
12	1	0	-2.455432	-0.990498	-1.140603
13	1	0	-0.995632	-0.818285	-2.121596
14	6	0	-1.473871	-0.460778	1.289082
15	1	0	-1.072249	0.179566	2.079621
16	1	0	-2.540469	-0.242421	1.188303
17	1	0	-1.362958	-1.504882	1.596022
18	6	0	1.366235	-1.087510	1.130799
19	1	0	1.121915	-2.137284	0.938339
20	1	0	2.455472	-0.990452	1.140576
21	1	0	0.995694	-0.818271	2.121603
22	1	0	-0.000037	3.125776	-0.000005

Zero-point correction= 0.191079 (Hartree/Particle)

Thermal correction to Energy= 0.200614
Thermal correction to Enthalpy= 0.201558
Thermal correction to Gibbs Free Energy= 0.157973
Sum of electronic and zero-point Energies= -411.539321
Sum of electronic and thermal Energies= -411.529786
Sum of electronic and thermal Enthalpies= -411.528842
Sum of electronic and thermal Free Energies= -411.572426
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -411.83166129

Cp_3La

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-0.000639	-0.000741	-0.002842
2	6	0	1.443049	2.322187	-0.706256
3	6	0	0.119048	2.587533	-1.141545
4	6	0	1.444951	2.319336	0.705394
5	1	0	2.304455	2.168906	-1.345350
6	6	0	-0.690787	2.763199	0.003311
7	1	0	-0.205112	2.686921	-2.171881
8	6	0	0.122153	2.582688	1.145333
9	1	0	2.308050	2.163085	1.341463
10	1	0	-1.747478	2.997806	0.005221
11	1	0	-0.199264	2.677813	2.176924
12	6	0	-2.047116	-1.979653	-0.000710
13	6	0	-2.297238	-1.189791	1.144371
14	6	0	-2.302980	-1.186917	-1.142568
15	1	0	-1.721411	-3.011980	-0.002704
16	6	0	-2.731733	0.088723	0.709402
17	1	0	-2.216863	-1.518930	2.174766
18	6	0	-2.735254	0.090522	-0.702256
19	1	0	-2.228040	-1.513500	-2.174203
20	1	0	-3.027848	0.911670	1.348921
21	1	0	-3.034690	0.915039	-1.338195
22	6	0	2.738245	-0.779938	-0.012330
23	6	0	2.186712	-1.383190	1.140685
24	6	0	2.173217	-1.407180	-1.145996
25	1	0	3.467719	0.019629	-0.024964
26	6	0	1.295522	-2.403314	0.718847
27	1	0	2.437091	-1.140503	2.167798
28	6	0	1.287495	-2.418251	-0.692622
29	1	0	2.411818	-1.186328	-2.180840
30	1	0	0.735726	-3.067404	1.366612
31	1	0	0.720567	-3.095684	-1.319928

Zero-point correction= 0.250593 (Hartree/Particle)
Thermal correction to Energy= 0.265810
Thermal correction to Enthalpy= 0.266755
Thermal correction to Gibbs Free Energy= 0.205388
Sum of electronic and zero-point Energies= -1015.979583
Sum of electronic and thermal Energies= -1015.964366
Sum of electronic and thermal Enthalpies= -1015.963421
Sum of electronic and thermal Free Energies= -1016.024788
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy=-1016.40542865

$Cp_3La^{\cdots}HBpin$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	1.159441	-0.033839	-0.002359

2	6	0	2.543028	-1.023035	2.262357
3	6	0	2.467796	0.373443	2.478582
4	6	0	1.244570	-1.561548	2.420888
5	1	0	3.445148	-1.585302	2.052920
6	6	0	1.122255	0.700973	2.761808
7	1	0	3.300552	1.065578	2.449810
8	6	0	0.368773	-0.496401	2.727726
9	1	0	0.974941	-2.607231	2.342613
10	1	0	0.740945	1.688257	2.993047
11	1	0	-0.688524	-0.586683	2.948010
12	6	0	2.261351	1.814287	-1.878654
13	6	0	0.911821	2.206896	-1.781555
14	6	0	2.897064	2.112007	-0.648619
15	1	0	2.732687	1.367422	-2.744199
16	6	0	0.716300	2.776243	-0.493258
17	1	0	0.170565	2.127009	-2.568190
18	6	0	1.943937	2.728809	0.196346
19	1	0	3.943677	1.949359	-0.416359
20	1	0	-0.193991	3.236225	-0.125646
21	1	0	2.126697	3.102635	1.195246
22	6	0	1.024639	-2.774553	-0.817071
23	6	0	0.376459	-2.075912	-1.864023
24	6	0	2.396577	-2.440646	-0.857778
25	1	0	0.559177	-3.468954	-0.128805
26	6	0	1.344900	-1.310990	-2.549707
27	1	0	-0.675558	-2.139617	-2.116892
28	6	0	2.595040	-1.529876	-1.922897
29	1	0	3.166332	-2.832943	-0.204859
30	1	0	1.164230	-0.677592	-3.409253
31	1	0	3.544745	-1.105447	-2.226768
32	5	0	-2.185551	-1.377000	0.528874
33	8	0	-1.719910	-0.191063	-0.009331
34	8	0	-3.533618	-1.427347	0.653178
35	6	0	-2.873552	0.724639	-0.065995
36	6	0	-4.083972	-0.277140	-0.041515
37	6	0	-4.499551	-0.769595	-1.427833
38	1	0	-5.194562	-1.604867	-1.308678
39	1	0	-4.999974	0.014680	-2.002521
40	1	0	-3.639919	-1.127441	-2.001733
41	6	0	-2.787013	1.565845	-1.327801
42	1	0	-3.694052	2.168986	-1.437793
43	1	0	-1.936417	2.247060	-1.271161
44	1	0	-2.671678	0.948278	-2.220193
45	6	0	-2.789018	1.603602	1.178643
46	1	0	-2.868283	1.012308	2.094993
47	1	0	-1.825181	2.118947	1.190318
48	1	0	-3.579887	2.358862	1.182522
49	6	0	-5.301149	0.213697	0.728971
50	1	0	-5.712796	1.119035	0.271462
51	1	0	-6.077038	-0.556337	0.710965
52	1	0	-5.061695	0.426032	1.772301
53	1	0	-1.463816	-2.261628	0.846442

Zero-point correction= 0.443133 (Hartree/Particle)
Thermal correction to Energy= 0.469699
Thermal correction to Enthalpy= 0.470643
Thermal correction to Gibbs Free Energy= 0.385647
Sum of electronic and zero-point Energies= -1427.519798
Sum of electronic and thermal Energies= -1427.493232
Sum of electronic and thermal Enthalpies= -1427.492288
Sum of electronic and thermal Free Energies= -1427.577284
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1428.22275711

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.072419	-0.957227	-0.018645
2	6	0	-4.741590	-1.360044	-0.004723
3	6	0	-3.719159	-0.400516	-0.006852
4	6	0	-4.035337	0.967658	-0.021836
5	6	0	-5.364712	1.364871	-0.035292
6	6	0	-6.380962	0.403665	-0.034004
7	1	0	-6.867159	-1.696889	-0.017588
8	1	0	-4.487013	-2.417458	0.007284
9	1	0	-3.227092	1.692346	-0.021777
10	1	0	-5.617177	2.420939	-0.046919
11	1	0	-7.420380	0.719834	-0.044962
12	6	0	-2.328061	-0.846671	0.004619
13	8	0	-1.363622	-0.088087	-0.003215
14	1	0	-2.167275	-1.940199	0.021165
15	57	0	1.241983	0.030092	0.003974
16	6	0	1.378113	0.282513	2.853320
17	6	0	2.550576	0.904528	2.362242
18	6	0	0.274901	1.083362	2.488225
19	1	0	1.335202	-0.641405	3.416397
20	6	0	2.168741	2.101439	1.707125
21	1	0	3.565876	0.549914	2.499893
22	6	0	0.762766	2.209180	1.779182
23	1	0	-0.763132	0.885390	2.728183
24	1	0	2.839478	2.815200	1.244351
25	1	0	0.163899	3.019122	1.380300
26	6	0	1.015088	0.421706	-2.811647
27	6	0	0.325311	1.529252	-2.259184
28	6	0	2.390343	0.584262	-2.533409
29	1	0	0.568665	-0.394480	-3.367309
30	6	0	1.273101	2.373555	-1.640933
31	1	0	-0.742052	1.706848	-2.319085
32	6	0	2.550345	1.786110	-1.801212
33	1	0	3.186693	-0.083435	-2.839472
34	1	0	1.062378	3.309316	-1.138664
35	1	0	3.491224	2.202820	-1.460080
36	6	0	2.384696	-2.369847	1.029148
37	6	0	1.016825	-2.686082	0.888966
38	6	0	2.938481	-2.229399	-0.266785
39	1	0	2.920159	-2.259397	1.963743
40	6	0	0.727641	-2.759274	-0.498862
41	1	0	0.320924	-2.871234	1.699506
42	6	0	1.914819	-2.487446	-1.209367
43	1	0	3.975969	-2.013115	-0.496478
44	1	0	-0.224815	-3.026858	-0.943519
45	1	0	2.024513	-2.481388	-2.286206

Zero-point correction= 0.361926 (Hartree/Particle)
Thermal correction to Energy= 0.385456
Thermal correction to Enthalpy= 0.386400
Thermal correction to Gibbs Free Energy= 0.304486
Sum of electronic and zero-point Energies= -1361.330052
Sum of electronic and thermal Energies= -1361.306522
Sum of electronic and thermal Enthalpies= -1361.305578
Sum of electronic and thermal Free Energies= -1361.387492
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1361.94019694

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	2.530774	-0.012441	-0.756704
2	8	0	2.679293	-1.216171	-1.411018
3	8	0	3.218275	0.087343	0.439686
4	6	0	3.368740	-2.089465	-0.471724
5	6	0	4.104846	-1.059404	0.466538
6	6	0	5.451777	-0.598787	-0.093296
7	1	0	5.803354	0.255477	0.491828
8	1	0	6.206438	-1.388918	-0.037241
9	1	0	5.360156	-0.280740	-1.136091
10	6	0	4.291361	-2.998330	-1.271550
11	1	0	4.891962	-3.623897	-0.603016
12	1	0	3.695098	-3.659331	-1.906874
13	1	0	4.963550	-2.428314	-1.916018
14	6	0	2.316044	-2.916715	0.259233
15	1	0	1.626774	-2.277455	0.815905
16	1	0	1.736077	-3.483420	-0.473450
17	1	0	2.777152	-3.626116	0.952998
18	6	0	4.262228	-1.507769	1.912370
19	1	0	4.883479	-2.407218	1.975539
20	1	0	4.752566	-0.718435	2.489492
21	1	0	3.296771	-1.716755	2.376558
22	1	0	2.557982	0.991918	-1.521324
23	6	0	1.557025	5.115519	-0.921801
24	6	0	1.330725	3.838469	-1.422990
25	6	0	1.308968	2.741204	-0.552601
26	6	0	1.525362	2.920751	0.820160
27	6	0	1.752752	4.198993	1.314999
28	6	0	1.767163	5.293548	0.446482
29	1	0	1.565860	5.969912	-1.591627
30	1	0	1.163151	3.688705	-2.487263
31	1	0	1.516603	2.052877	1.470609
32	1	0	1.919728	4.347110	2.377700
33	1	0	1.942425	6.291306	0.839092
34	6	0	1.045103	1.398052	-1.093004
35	8	0	0.747361	0.391723	-0.336961
36	1	0	0.762719	1.366575	-2.156508
37	57	0	-1.785435	-0.424827	0.070894
38	6	0	-3.338861	1.366492	-1.565928
39	6	0	-4.073240	1.198885	-0.368834
40	6	0	-2.180634	2.111919	-1.265015
41	1	0	-3.619262	0.993434	-2.542254
42	6	0	-3.381768	1.877450	0.666103
43	1	0	-5.025066	0.688441	-0.271783
44	6	0	-2.207916	2.430372	0.120497
45	1	0	-1.448406	2.457328	-1.985668
46	1	0	-3.702484	1.958973	1.696498
47	1	0	-1.474382	3.022598	0.653728
48	6	0	-0.932557	-2.041252	2.279108
49	6	0	-0.422417	-0.755466	2.574301
50	6	0	-2.341514	-1.986379	2.382776
51	1	0	-0.348417	-2.921428	2.042520
52	6	0	-1.514457	0.094188	2.863661
53	1	0	0.624082	-0.473161	2.584000
54	6	0	-2.701418	-0.666876	2.745674
55	1	0	-3.022956	-2.817043	2.243529
56	1	0	-1.453449	1.140566	3.137178
57	1	0	-3.708621	-0.311611	2.928907

58	6	0	-3.043453	-1.911476	-1.998657
59	6	0	-1.818938	-1.493511	-2.568665
60	6	0	-2.755280	-2.868576	-0.997411
61	1	0	-4.031612	-1.575654	-2.288942
62	6	0	-0.772877	-2.198335	-1.925570
63	1	0	-1.703635	-0.777103	-3.373664
64	6	0	-1.352066	-3.049074	-0.957672
65	1	0	-3.484101	-3.399931	-0.396547
66	1	0	0.285750	-2.099068	-2.134875
67	1	0	-0.820981	-3.731986	-0.307127

Zero-point correction= 0.553515 (Hartree/Particle)
Thermal correction to Energy= 0.587151
Thermal correction to Enthalpy= 0.588095
Thermal correction to Gibbs Free Energy= 0.486349
Sum of electronic and zero-point Energies= -1772.809031
Sum of electronic and thermal Energies= -1772.775395
Sum of electronic and thermal Enthalpies= -1772.774450
Sum of electronic and thermal Free Energies= -1772.876197
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.70959548

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.824907	-0.648869	0.096138
2	8	0	-2.910147	-0.715084	0.927274
3	8	0	-1.761952	-1.644664	-0.836969
4	6	0	-3.551590	-1.991298	0.659175
5	6	0	-3.051847	-2.314832	-0.797161
6	6	0	-3.912232	-1.669638	-1.883678
7	1	0	-3.396847	-1.761500	-2.843585
8	1	0	-4.886681	-2.159084	-1.968896
9	1	0	-4.073281	-0.605721	-1.686015
10	6	0	-5.055935	-1.814160	0.799560
11	1	0	-5.580834	-2.736471	0.530807
12	1	0	-5.302942	-1.575893	1.837975
13	1	0	-5.426561	-1.002965	0.170390
14	6	0	-3.029850	-2.974975	1.705965
15	1	0	-1.949090	-3.117862	1.614686
16	1	0	-3.235951	-2.575806	2.702861
17	1	0	-3.516791	-3.950588	1.619948
18	6	0	-2.843928	-3.791708	-1.093542
19	1	0	-3.790172	-4.336878	-1.016035
20	1	0	-2.466236	-3.913018	-2.112451
21	1	0	-2.122943	-4.245304	-0.411215
22	1	0	-1.571478	1.080710	1.999425
23	6	0	-4.014098	3.975603	0.658481
24	6	0	-3.108081	3.076652	1.216488
25	6	0	-2.211571	2.374513	0.405600
26	6	0	-2.242430	2.580485	-0.977665
27	6	0	-3.155934	3.472782	-1.536968
28	6	0	-4.041414	4.175147	-0.721251
29	1	0	-4.706169	4.512803	1.301125
30	1	0	-3.101405	2.913981	2.291945
31	1	0	-1.554120	2.033885	-1.615652
32	1	0	-3.171587	3.622115	-2.613132
33	1	0	-4.751140	4.871943	-1.158254
34	6	0	-1.200354	1.451897	1.039549
35	8	0	-0.863093	0.336881	0.188083
36	1	0	-0.259678	1.981102	1.220072

37	57	0	1.994244	-0.025760	-0.003939
38	6	0	2.542544	2.772473	0.397489
39	6	0	3.744045	2.201073	-0.084244
40	6	0	1.604131	2.764051	-0.659022
41	1	0	2.381190	3.165156	1.394087
42	6	0	3.549365	1.852600	-1.442700
43	1	0	4.665751	2.088735	0.474509
44	6	0	2.225293	2.193517	-1.796391
45	1	0	0.602003	3.176099	-0.628596
46	1	0	4.292028	1.415338	-2.098748
47	1	0	1.772844	2.069548	-2.772801
48	6	0	1.420224	-2.539985	-1.161205
49	6	0	1.165418	-1.615307	-2.207471
50	6	0	2.812998	-2.572344	-0.939152
51	1	0	0.672205	-3.124548	-0.640999
52	6	0	2.400291	-1.081396	-2.628255
53	1	0	0.188949	-1.380842	-2.612066
54	6	0	3.420616	-1.655114	-1.831418
55	1	0	3.331104	-3.193250	-0.218954
56	1	0	2.545690	-0.358284	-3.420611
57	1	0	4.484407	-1.466591	-1.923745
58	6	0	3.143351	0.125113	2.594136
59	6	0	1.773763	0.373768	2.831288
60	6	0	3.282711	-1.229111	2.206823
61	1	0	3.948334	0.840501	2.707137
62	6	0	1.066793	-0.834422	2.605590
63	1	0	1.348300	1.310294	3.171780
64	6	0	1.997494	-1.823563	2.225434
65	1	0	4.214879	-1.733241	1.978964
66	1	0	0.000957	-0.983078	2.736563
67	1	0	1.770763	-2.856596	1.993480

Zero-point correction= 0.559103 (Hartree/Particle)
Thermal correction to Energy= 0.592814
Thermal correction to Enthalpy= 0.593758
Thermal correction to Gibbs Free Energy= 0.489921
Sum of electronic and zero-point Energies= -1772.912545
Sum of electronic and thermal Energies= -1772.878834
Sum of electronic and thermal Enthalpies= -1772.877890
Sum of electronic and thermal Free Energies= -1772.981726
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.81700237

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	1.761162	-0.048804	0.038779
2	6	0	1.729608	-1.191487	-2.723952
3	6	0	2.340310	-2.150410	-1.843544
4	6	0	0.359754	-1.230874	-2.529096
5	1	0	2.255877	-0.553021	-3.421057
6	6	0	1.330210	-2.782897	-1.125394
7	1	0	3.402371	-2.362423	-1.777957
8	6	0	0.060125	-2.213004	-1.508214
9	1	0	-0.383764	-0.648688	-3.060884
10	1	0	1.457131	-3.589953	-0.414592
11	1	0	-0.786554	-2.877101	-1.642781
12	6	0	3.268291	-0.592670	2.361924
13	6	0	2.208005	0.226055	2.815564
14	6	0	2.724467	-1.845673	1.991409
15	1	0	4.314902	-0.318379	2.330516

16	6	0	1.012808	-0.526487	2.732909
17	1	0	2.299387	1.239554	3.187748
18	6	0	1.328711	-1.806094	2.225331
19	1	0	3.285966	-2.697047	1.623134
20	1	0	0.023660	-0.184867	3.013913
21	1	0	0.616054	-2.599685	2.038758
22	6	0	2.822475	1.857226	-1.834465
23	6	0	2.638971	2.586655	-0.637106
24	6	0	3.885066	0.946496	-1.627167
25	1	0	2.267316	1.994750	-2.754914
26	6	0	3.573100	2.117412	0.312915
27	1	0	1.909439	3.370162	-0.476994
28	6	0	4.345759	1.102754	-0.301888
29	1	0	4.297262	0.265888	-2.361850
30	1	0	3.696734	2.488003	1.322670
31	1	0	5.170749	0.565559	0.149575
32	6	0	-4.065506	4.431805	-0.504113
33	6	0	-3.332168	3.258239	-0.646173
34	6	0	-2.050267	3.160547	-0.086519
35	6	0	-1.506295	4.245262	0.619093
36	6	0	-2.241875	5.413374	0.760824
37	6	0	-3.519463	5.506236	0.198903
38	1	0	-5.057717	4.511694	-0.937901
39	1	0	-3.743009	2.412752	-1.192805
40	1	0	-0.513549	4.146018	1.047070
41	1	0	-1.827314	6.255537	1.306986
42	1	0	-4.091649	6.423076	0.311292
43	6	0	-1.294999	1.918510	-0.258589
44	1	0	-1.806571	1.090396	-0.779468
45	8	0	-0.146707	1.767787	0.160653
46	5	0	-1.164973	-1.576091	-0.108850
47	8	0	-2.336678	-1.145474	-0.808151
48	8	0	-1.494669	-2.665055	0.731715
49	6	0	-3.463696	-1.778476	-0.179809
50	6	0	-2.832870	-3.082009	0.433143
51	6	0	-2.792310	-4.253030	-0.557242
52	1	0	-2.116749	-5.019796	-0.167491
53	1	0	-3.782183	-4.702380	-0.687318
54	1	0	-2.434059	-3.955432	-1.546744
55	6	0	-4.540992	-2.018434	-1.231636
56	1	0	-5.392033	-2.561708	-0.807122
57	1	0	-4.910082	-1.059421	-1.608846
58	1	0	-4.154006	-2.584370	-2.081479
59	6	0	-3.996273	-0.829082	0.899415
60	1	0	-3.242307	-0.651517	1.671686
61	1	0	-4.245873	0.132391	0.439932
62	1	0	-4.899873	-1.217610	1.379539
63	6	0	-3.477254	-3.559695	1.731665
64	1	0	-4.535000	-3.803887	1.584759
65	1	0	-2.968131	-4.463252	2.080423
66	1	0	-3.394598	-2.807072	2.518043
67	1	0	-0.530919	-0.695429	0.445126

Zero-point correction= 0.553820 (Hartree/Particle)
Thermal correction to Energy= 0.587555
Thermal correction to Enthalpy= 0.588499
Thermal correction to Gibbs Free Energy= 0.486086
Sum of electronic and zero-point Energies= -1772.825981
Sum of electronic and thermal Energies= -1772.792246
Sum of electronic and thermal Enthalpies= -1772.791302
Sum of electronic and thermal Free Energies= -1772.893715
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.72226146

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-1.842170	-0.110274	-0.100928
2	6	0	-1.129062	-0.849707	2.921208
3	6	0	-1.749403	-1.950383	2.201645
4	6	0	0.231048	-1.006897	2.855772
5	1	0	-1.660687	-0.066605	3.448225
6	6	0	-0.752403	-2.756906	1.701704
7	1	0	-2.818929	-2.136096	2.135092
8	6	0	0.549534	-2.169039	2.025815
9	1	0	0.973987	-0.356664	3.303189
10	1	0	-0.885000	-3.667578	1.129532
11	1	0	1.329316	-2.846801	2.376728
12	6	0	-3.243381	-1.191606	-2.246669
13	6	0	-2.385270	-0.227530	-2.826614
14	6	0	-2.441324	-2.263216	-1.781921
15	1	0	-4.323540	-1.132112	-2.193027
16	6	0	-1.057049	-0.709594	-2.721796
17	1	0	-2.692619	0.701613	-3.292339
18	6	0	-1.089262	-1.967601	-2.079308
19	1	0	-2.804401	-3.167376	-1.305799
20	1	0	-0.167985	-0.201878	-3.077518
21	1	0	-0.226324	-2.572169	-1.824997
22	6	0	-2.999828	1.867678	1.591683
23	6	0	-3.155186	2.366363	0.275808
24	6	0	-3.856525	0.752317	1.735546
25	1	0	-2.356141	2.283574	2.358047
26	6	0	-4.103073	1.558703	-0.391369
27	1	0	-2.641088	3.222402	-0.143758
28	6	0	-4.532987	0.555042	0.508548
29	1	0	-3.998679	0.168722	2.637226
30	1	0	-4.451853	1.693667	-1.407604
31	1	0	-5.278760	-0.205191	0.307075
32	6	0	3.788355	4.393954	0.510977
33	6	0	3.055635	3.212314	0.554825
34	6	0	1.779656	3.158308	-0.025968
35	6	0	1.240285	4.293237	-0.652155
36	6	0	1.976247	5.468612	-0.695914
37	6	0	3.247959	5.518070	-0.114418
38	1	0	4.775730	4.441339	0.960152
39	1	0	3.457338	2.324329	1.036961
40	1	0	0.251616	4.227519	-1.095728
41	1	0	1.567403	6.350493	-1.180224
42	1	0	3.820002	6.441186	-0.150954
43	6	0	1.036281	1.902892	0.050729
44	1	0	1.552243	1.046071	0.518717
45	8	0	-0.111472	1.771813	-0.390830
46	5	0	1.266091	-1.622926	0.547029
47	8	0	2.509987	-0.910844	0.815162
48	8	0	1.582860	-2.722780	-0.334281
49	6	0	3.476265	-1.368645	-0.134791
50	6	0	3.000765	-2.836829	-0.422157
51	6	0	3.492652	-3.827674	0.642495
52	1	0	2.928827	-4.759803	0.541398
53	1	0	4.557654	-4.057011	0.529265
54	1	0	3.334492	-3.439890	1.652517
55	6	0	4.864426	-1.254693	0.487512
56	1	0	5.629949	-1.681661	-0.169664

57	1	0	5.115473	-0.201285	0.651257
58	1	0	4.908333	-1.762625	1.452897
59	6	0	3.400578	-0.490144	-1.390158
60	1	0	2.415783	-0.568904	-1.859623
61	1	0	3.569863	0.555486	-1.113198
62	1	0	4.159025	-0.764164	-2.130413
63	6	0	3.360342	-3.370325	-1.806241
64	1	0	4.445428	-3.386583	-1.957953
65	1	0	2.990716	-4.395204	-1.911683
66	1	0	2.903881	-2.769421	-2.595633
67	1	0	0.409544	-0.862853	0.020447

Zero-point correction= 0.553562 (Hartree/Particle)
Thermal correction to Energy= 0.587773
Thermal correction to Enthalpy= 0.588717
Thermal correction to Gibbs Free Energy= 0.484852
Sum of electronic and zero-point Energies= -1772.828494
Sum of electronic and thermal Energies= -1772.794283
Sum of electronic and thermal Enthalpies= -1772.793339
Sum of electronic and thermal Free Energies= -1772.897205
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.72978116

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-1.792917	-0.455675	-0.096797
2	6	0	-0.656853	1.167913	2.569302
3	6	0	-0.924983	-0.256017	2.740774
4	6	0	0.654103	1.320560	2.225076
5	1	0	-1.379192	1.959986	2.728893
6	6	0	0.224324	-0.950365	2.474433
7	1	0	-1.862260	-0.681365	3.089977
8	6	0	1.289263	-0.004094	2.082242
9	1	0	1.161175	2.260012	2.040252
10	1	0	0.361585	-2.021961	2.544663
11	1	0	2.210007	-0.121714	2.667242
12	6	0	-2.860318	-2.868799	-1.036548
13	6	0	-1.994219	-2.420900	-2.062357
14	6	0	-2.066957	-3.244530	0.073018
15	1	0	-3.939502	-2.931829	-1.097293
16	6	0	-0.664143	-2.535773	-1.589319
17	1	0	-2.295793	-2.074659	-3.044521
18	6	0	-0.707237	-3.044098	-0.273573
19	1	0	-2.435506	-3.650129	1.009048
20	1	0	0.235881	-2.277027	-2.132639
21	1	0	0.161465	-3.228588	0.342947
22	6	0	-3.544169	1.718759	0.532066
23	6	0	-3.860856	1.343410	-0.793052
24	6	0	-3.949439	0.670114	1.391964
25	1	0	-3.090913	2.653717	0.838801
26	6	0	-4.454423	0.060866	-0.755225
27	1	0	-3.677304	1.930983	-1.684555
28	6	0	-4.509512	-0.356913	0.597584
29	1	0	-3.882086	0.672398	2.473399
30	1	0	-4.824693	-0.492456	-1.609412
31	1	0	-4.936609	-1.283875	0.961453
32	6	0	2.475967	4.271496	-0.435415
33	6	0	2.151207	2.999711	-0.897288
34	6	0	0.807323	2.627821	-1.037082
35	6	0	-0.203829	3.549622	-0.726910

36	6	0	0.125301	4.822167	-0.276478
37	6	0	1.466256	5.183850	-0.126926
38	1	0	3.518368	4.551895	-0.314852
39	1	0	2.928543	2.271294	-1.096637
40	1	0	-1.239156	3.253962	-0.862049
41	1	0	-0.659830	5.536845	-0.046140
42	1	0	1.723329	6.178780	0.226507
43	6	0	0.440053	1.302058	-1.572403
44	1	0	1.210424	0.781102	-2.154950
45	8	0	-0.775240	0.976992	-1.718871
46	5	0	1.921120	-0.337215	0.539350
47	8	0	3.182381	0.306572	0.299433
48	8	0	2.088708	-1.739713	0.280890
49	6	0	4.053072	-0.633956	-0.339846
50	6	0	3.486305	-2.012278	0.147875
51	6	0	4.029843	-2.420960	1.523207
52	1	0	3.434365	-3.256692	1.902563
53	1	0	5.075312	-2.742183	1.471811
54	1	0	3.960673	-1.599988	2.242180
55	6	0	5.484756	-0.334742	0.095284
56	1	0	6.182463	-1.082695	-0.296812
57	1	0	5.791117	0.643650	-0.288109
58	1	0	5.573732	-0.308265	1.183175
59	6	0	3.941286	-0.472166	-1.860798
60	1	0	2.931634	-0.709338	-2.208945
61	1	0	4.169823	0.562036	-2.137206
62	1	0	4.644797	-1.120481	-2.392751
63	6	0	3.672569	-3.170876	-0.827197
64	1	0	4.734603	-3.359745	-1.018382
65	1	0	3.241307	-4.082693	-0.402784
66	1	0	3.174283	-2.979894	-1.779627
67	1	0	0.993724	0.186379	-0.280603

Zero-point correction= 0.551651 (Hartree/Particle)
Thermal correction to Energy= 0.584938
Thermal correction to Enthalpy= 0.585883
Thermal correction to Gibbs Free Energy= 0.484098
Sum of electronic and zero-point Energies= -1772.814258
Sum of electronic and thermal Energies= -1772.780971
Sum of electronic and thermal Enthalpies= -1772.780026
Sum of electronic and thermal Free Energies= -1772.881811
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy=-1773.71234134

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-1.412961	-1.106820	-0.171371
2	6	0	0.425892	-1.219818	3.062875
3	6	0	0.371967	-2.314557	2.092804
4	6	0	1.648234	-0.644513	3.006406
5	1	0	-0.387174	-0.936091	3.721082
6	6	0	1.557384	-2.386268	1.431621
7	1	0	-0.459748	-3.008444	1.989344
8	6	0	2.480393	-1.344107	1.975457
9	1	0	2.005896	0.188256	3.599144
10	1	0	1.839076	-3.112471	0.679626
11	1	0	3.302773	-1.871880	2.498916
12	6	0	-1.473256	-2.981053	-2.312710
13	6	0	-1.612485	-1.702041	-2.907083
14	6	0	-0.159670	-3.084114	-1.807862

15	1	0	-2.237783	-3.746755	-2.262782
16	6	0	-0.371081	-1.028110	-2.789982
17	1	0	-2.498105	-1.324796	-3.406493
18	6	0	0.524384	-1.874448	-2.102106
19	1	0	0.263074	-3.953064	-1.315039
20	1	0	-0.154239	-0.030595	-3.153398
21	1	0	1.551437	-1.643435	-1.845128
22	6	0	-3.669849	-0.598238	1.502943
23	6	0	-4.196779	-0.852103	0.214406
24	6	0	-3.155514	-1.813297	2.007303
25	1	0	-3.657781	0.360071	2.008077
26	6	0	-4.022533	-2.229917	-0.069058
27	1	0	-4.689557	-0.130408	-0.427709
28	6	0	-3.375534	-2.824383	1.036046
29	1	0	-2.720479	-1.959299	2.989577
30	1	0	-4.349258	-2.739089	-0.967389
31	1	0	-3.126998	-3.875221	1.137917
32	6	0	-2.268025	5.682710	-0.068411
33	6	0	-1.277825	4.704867	-0.081038
34	6	0	-1.611539	3.345177	-0.100808
35	6	0	-2.958407	2.986926	-0.106565
36	6	0	-3.954737	3.964554	-0.092567
37	6	0	-3.614722	5.314904	-0.073946
38	1	0	-1.990458	6.733722	-0.052210
39	1	0	-0.229541	5.000433	-0.074298
40	1	0	-3.216156	1.932854	-0.117257
41	1	0	-5.000756	3.667972	-0.095001
42	1	0	-4.389936	6.076315	-0.062269
43	6	0	-0.505133	2.303885	-0.124693
44	1	0	0.088234	2.472008	-1.043153
45	8	0	-0.933956	0.990407	-0.060055
46	5	0	3.282531	-0.421152	0.966651
47	8	0	4.020057	0.644458	1.398990
48	8	0	3.395020	-0.663775	-0.373525
49	6	0	4.540005	1.315336	0.218653
50	6	0	4.470580	0.181767	-0.871515
51	6	0	5.721469	-0.695335	-0.914852
52	1	0	5.521306	-1.568451	-1.541917
53	1	0	6.575344	-0.157831	-1.337008
54	1	0	5.994903	-1.050305	0.083274
55	6	0	5.941152	1.820917	0.531256
56	1	0	6.393870	2.279053	-0.353954
57	1	0	5.890010	2.581042	1.315848
58	1	0	6.593391	1.018485	0.881293
59	6	0	3.605145	2.488679	-0.066281
60	1	0	2.592252	2.145026	-0.291482
61	1	0	3.556196	3.125480	0.821301
62	1	0	3.962298	3.094543	-0.904180
63	6	0	4.108977	0.655016	-2.271242
64	1	0	4.870719	1.340842	-2.656068
65	1	0	4.054753	-0.202239	-2.948077
66	1	0	3.142172	1.160988	-2.289645
67	1	0	0.176442	2.524451	0.716348

Zero-point correction= 0.555892 (Hartree/Particle)
Thermal correction to Energy= 0.590510
Thermal correction to Enthalpy= 0.591454
Thermal correction to Gibbs Free Energy= 0.483449
Sum of electronic and zero-point Energies= -1772.866681
Sum of electronic and thermal Energies= -1772.832064
Sum of electronic and thermal Enthalpies= -1772.831120
Sum of electronic and thermal Free Energies= -1772.939125

B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.78153723

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.736931	5.152627	-0.716570
2	6	0	0.221221	4.004512	-1.311427
3	6	0	-0.005205	2.843759	-0.560583
4	6	0	0.298922	2.866760	0.803119
5	6	0	0.820049	4.014897	1.403258
6	6	0	1.041376	5.162137	0.646137
7	1	0	0.910416	6.040985	-1.318439
8	1	0	-0.002665	4.003408	-2.376638
9	1	0	0.109657	1.979190	1.402054
10	1	0	1.050309	4.010742	2.465657
11	1	0	1.449504	6.055915	1.109753
12	6	0	-0.581312	1.610806	-1.234188
13	1	0	-1.654501	1.778436	-1.416988
14	8	0	-0.413575	0.429592	-0.502618
15	5	0	-2.220454	-0.926007	-0.668182
16	8	0	-3.110277	-0.034710	-1.242991
17	8	0	-2.533022	-1.210147	0.649120
18	6	0	-4.199472	0.151298	-0.310426
19	6	0	-3.566158	-0.286410	1.064473
20	6	0	-4.516576	-1.028426	1.997107
21	1	0	-3.983790	-1.316985	2.907993
22	1	0	-5.356705	-0.388970	2.288003
23	1	0	-4.911348	-1.936283	1.536899
24	6	0	-5.328979	-0.772174	-0.774602
25	1	0	-6.230905	-0.652809	-0.166732
26	1	0	-5.578529	-0.530347	-1.811603
27	1	0	-5.023948	-1.822193	-0.737309
28	6	0	-4.661097	1.601348	-0.374285
29	1	0	-3.846517	2.296033	-0.161160
30	1	0	-5.040256	1.820433	-1.376878
31	1	0	-5.470841	1.785035	0.339675
32	6	0	-2.901580	0.865042	1.815532
33	1	0	-3.641043	1.576230	2.196012
34	1	0	-2.350935	0.458341	2.668443
35	1	0	-2.192728	1.392875	1.176194
36	1	0	-0.120163	1.522687	-2.233165
37	6	0	2.908866	0.300863	-2.076827
38	6	0	3.231297	1.176912	-1.017273
39	6	0	4.010310	0.457765	-0.075791
40	6	0	4.177143	-0.860352	-0.561417
41	6	0	3.492048	-0.959368	-1.795212
42	1	0	2.330097	0.552019	-2.957571
43	1	0	2.942889	2.218633	-0.942161
44	1	0	4.434048	0.857674	0.837769
45	1	0	4.748193	-1.647907	-0.084162
46	1	0	3.463582	-1.832025	-2.437102
47	57	0	1.452017	-0.667986	0.176818
48	6	0	-1.509509	-2.055608	-1.562848
49	6	0	-0.897154	-1.634337	-2.852903
50	6	0	-0.448963	-2.897915	-0.934603
51	6	0	0.350388	-2.151872	-2.959379
52	1	0	-1.397948	-0.995468	-3.570288
53	6	0	0.628991	-2.949418	-1.767848
54	1	0	-0.575928	-3.437757	-0.003928
55	1	0	1.039521	-2.014592	-3.784579

56	1	0	1.532049	-3.532807	-1.608718
57	6	0	2.232366	-0.629172	2.892469
58	6	0	0.813926	-0.617021	2.926172
59	6	0	2.646262	-1.908038	2.453338
60	1	0	2.884637	0.181272	3.196873
61	6	0	0.352601	-1.878752	2.493064
62	1	0	0.192328	0.208895	3.252220
63	6	0	1.487378	-2.675411	2.194348
64	1	0	3.671106	-2.241342	2.343521
65	1	0	-0.685343	-2.170680	2.391132
66	1	0	1.471878	-3.709020	1.865317
67	1	0	-2.378284	-2.708927	-1.772893

Zero-point correction= 0.556596 (Hartree/Particle)
Thermal correction to Energy= 0.589617
Thermal correction to Enthalpy= 0.590561
Thermal correction to Gibbs Free Energy= 0.490649
Sum of electronic and zero-point Energies= -1772.863956
Sum of electronic and thermal Energies= -1772.830934
Sum of electronic and thermal Enthalpies= -1772.829990
Sum of electronic and thermal Free Energies= -1772.929902
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.76937117

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.004586	4.408278	-0.620734
2	6	0	1.101774	3.562358	-1.259593
3	6	0	0.381662	2.605728	-0.533946
4	6	0	0.589756	2.516854	0.848582
5	6	0	1.508055	3.353623	1.487983
6	6	0	2.217572	4.302171	0.755706
7	1	0	2.554389	5.145333	-1.199691
8	1	0	0.954802	3.641207	-2.334392
9	1	0	-0.005334	1.815937	1.429790
10	1	0	1.655213	3.270893	2.561386
11	1	0	2.929201	4.956800	1.250458
12	6	0	-0.622967	1.716359	-1.227313
13	1	0	-1.608122	2.196927	-1.256184
14	8	0	-0.746323	0.474118	-0.554048
15	5	0	-2.091859	-0.287524	-0.638084
16	8	0	-3.113588	0.576570	-1.162353
17	8	0	-2.522902	-0.732704	0.665780
18	6	0	-4.254538	0.503052	-0.305466
19	6	0	-3.622534	0.084773	1.070709
20	6	0	-4.537344	-0.739876	1.971526
21	1	0	-4.013221	-0.991620	2.899103
22	1	0	-5.441157	-0.181184	2.238757
23	1	0	-4.832791	-1.674524	1.490647
24	6	0	-5.214880	-0.557687	-0.858846
25	1	0	-6.168055	-0.568270	-0.320153
26	1	0	-5.416972	-0.333854	-1.910519
27	1	0	-4.781798	-1.559916	-0.800036
28	6	0	-4.953367	1.859617	-0.308572
29	1	0	-4.265623	2.666107	-0.044573
30	1	0	-5.346725	2.068306	-1.308445
31	1	0	-5.793638	1.874170	0.394102
32	6	0	-3.090523	1.288178	1.858815
33	1	0	-3.899287	1.898531	2.274126
34	1	0	-2.480958	0.921343	2.690442

35	1	0	-2.463739	1.927433	1.231654
36	1	0	-0.316651	1.555421	-2.271800
37	6	0	3.004627	0.261575	-1.934486
38	6	0	3.487654	0.877524	-0.755222
39	6	0	4.085420	-0.122010	0.048464
40	6	0	3.973281	-1.356683	-0.633346
41	6	0	3.308557	-1.117984	-1.859237
42	1	0	2.509771	0.760752	-2.759097
43	1	0	3.419888	1.931903	-0.515108
44	1	0	4.565207	0.034914	1.006720
45	1	0	4.359733	-2.310632	-0.294363
46	1	0	3.102736	-1.858050	-2.622463
47	57	0	1.342183	-0.686255	0.148803
48	6	0	-1.806770	-1.665764	-1.628840
49	6	0	-1.157852	-1.299359	-2.896503
50	6	0	-0.864154	-2.605960	-1.003393
51	6	0	0.087118	-1.854487	-2.953875
52	1	0	-1.599409	-0.636417	-3.632123
53	6	0	0.271606	-2.684112	-1.773761
54	1	0	-1.065236	-3.154243	-0.091059
55	1	0	0.818567	-1.723260	-3.743244
56	1	0	1.132301	-3.322240	-1.583505
57	6	0	2.083728	-0.864654	2.841702
58	6	0	0.675643	-0.691594	2.881826
59	6	0	2.346509	-2.151169	2.318258
60	1	0	2.825201	-0.157428	3.194641
61	6	0	0.070742	-1.860468	2.374001
62	1	0	0.150786	0.176180	3.264023
63	6	0	1.104819	-2.761934	2.018824
64	1	0	3.324985	-2.596082	2.186186
65	1	0	-0.992953	-2.004979	2.235772
66	1	0	0.969696	-3.761248	1.619909
67	1	0	-2.832520	-2.036005	-1.706900

Zero-point correction= 0.557577 (Hartree/Particle)
Thermal correction to Energy= 0.590587
Thermal correction to Enthalpy= 0.591531
Thermal correction to Gibbs Free Energy= 0.492965
Sum of electronic and zero-point Energies= -1772.876674
Sum of electronic and thermal Energies= -1772.843665
Sum of electronic and thermal Enthalpies= -1772.842721
Sum of electronic and thermal Free Energies= -1772.941287
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1773.77936745

$(MeCp)_3La$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	0.002478	0.003436	-0.318702
2	6	0	-1.911642	-1.887403	-1.129996
3	6	0	-0.674206	-2.452458	-1.522950
4	6	0	-1.972974	-1.920273	0.281272
5	1	0	-2.679123	-1.505846	-1.792830
6	6	0	0.014321	-2.847035	-0.351311
7	1	0	-0.330925	-2.595210	-2.541887
8	6	0	-0.780443	-2.518008	0.772885
9	1	0	-2.802861	-1.581404	0.891516
10	1	0	0.982507	-3.331914	-0.315566
11	6	0	2.457921	1.445140	-0.317057
12	6	0	2.569252	0.572269	0.791933
13	6	0	2.469052	0.673041	-1.502891

14	1	0	2.387284	2.524806	-0.261759
15	6	0	2.657040	-0.749708	0.276392
16	6	0	2.603052	-0.687608	-1.134133
17	1	0	2.423243	1.060009	-2.515148
18	1	0	2.782139	-1.648075	0.870455
19	1	0	2.663810	-1.530761	-1.812019
20	6	0	-2.474294	1.408632	-0.343430
21	6	0	-1.797449	1.921044	0.789146
22	6	0	-1.786267	1.824453	-1.507856
23	1	0	-3.374593	0.806526	-0.318142
24	6	0	-0.685507	2.666434	0.309909
25	6	0	-0.682675	2.613526	-1.102054
26	1	0	0.017907	3.212722	0.928551
27	1	0	0.031754	3.098103	-1.756769
28	6	0	2.689618	0.973886	2.235373
29	1	0	2.262850	0.222534	2.909303
30	1	0	3.741083	1.096255	2.524716
31	1	0	2.190605	1.927685	2.435274
32	6	0	-0.475019	-2.844870	2.208045
33	1	0	-0.881680	-3.826016	2.484124
34	1	0	0.602877	-2.881596	2.396776
35	1	0	-0.913573	-2.116363	2.899232
36	6	0	-2.235371	1.799146	2.221867
37	1	0	-2.899436	2.626182	2.503415
38	1	0	-2.787763	0.870977	2.401507
39	1	0	-1.387029	1.825729	2.914784
40	1	0	-2.076765	1.608556	-2.530363

Zero-point correction= 0.333297 (Hartree/Particle)
Thermal correction to Energy= 0.353927
Thermal correction to Enthalpy= 0.354872
Thermal correction to Gibbs Free Energy= 0.281607
Sum of electronic and zero-point Energies= -1133.811244
Sum of electronic and thermal Energies= -1133.790614
Sum of electronic and thermal Enthalpies= -1133.789669
Sum of electronic and thermal Free Energies= -1133.862934
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1134.34014584

$(MeCp)_3La^{\cdots}HBpin$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	1.165303	0.020622	-0.072442
2	6	0	2.582142	-1.025109	2.190313
3	6	0	2.503364	0.374151	2.381930
4	6	0	1.296146	-1.585959	2.394404
5	6	0	1.160119	0.697892	2.673547
6	1	0	3.334325	1.065599	2.329113
7	6	0	0.418676	-0.510421	2.674232
8	1	0	0.772847	1.685972	2.892397
9	6	0	2.057159	1.867088	-2.046945
10	6	0	0.861440	2.475410	-1.612032
11	6	0	2.993731	1.944547	-0.990556
12	1	0	2.228410	1.421818	-3.017201
13	6	0	1.061924	2.978839	-0.293828
14	1	0	-0.028534	2.617997	-2.215538
15	6	0	2.379836	2.641663	0.079013
16	1	0	2.851872	2.916836	1.013708
17	6	0	0.970004	-2.711057	-0.955250
18	6	0	0.371569	-2.023371	-2.042298
19	6	0	2.345253	-2.382080	-0.920076

20	1	0	0.467643	-3.418409	-0.306949
21	6	0	1.382121	-1.248718	-2.656133
22	6	0	2.600116	-1.468837	-1.968741
23	1	0	3.076614	-2.773015	-0.224056
24	1	0	1.245978	-0.629792	-3.534852
25	5	0	-2.214297	-1.323900	0.501744
26	8	0	-1.776896	-0.107523	0.012725
27	8	0	-3.556056	-1.394189	0.680064
28	6	0	-2.936108	0.799936	0.072473
29	6	0	-4.141949	-0.206708	0.083833
30	6	0	-4.619492	-0.609807	-1.310800
31	1	0	-5.309839	-1.452049	-1.214879
32	1	0	-5.145132	0.209567	-1.809160
33	1	0	-3.787022	-0.928018	-1.943878
34	6	0	-2.904213	1.726528	-1.129457
35	1	0	-3.804049	2.349678	-1.149447
36	1	0	-2.037752	2.387739	-1.069747
37	1	0	-2.844650	1.171867	-2.067517
38	6	0	-2.798251	1.585104	1.373554
39	1	0	-2.848181	0.926981	2.245354
40	1	0	-1.831281	2.092461	1.387883
41	1	0	-3.582296	2.342113	1.464983
42	6	0	-5.325473	0.227517	0.936921
43	1	0	-5.758201	1.158013	0.555681
44	1	0	-6.099585	-0.543795	0.902579
45	1	0	-5.042458	0.374122	1.980574
46	1	0	-1.475931	-2.218569	0.741189
47	1	0	-0.631689	-0.609308	2.926100
48	1	0	3.488120	-1.586974	1.992283
49	1	0	4.016326	1.584315	-1.013493
50	1	0	3.560910	-1.034718	-2.218809
51	6	0	-1.019852	-2.221557	-2.567925
52	1	0	-1.446844	-1.293784	-2.964143
53	1	0	-1.024386	-2.950758	-3.388248
54	1	0	-1.696608	-2.611136	-1.800791
55	6	0	0.151502	3.899507	0.467929
56	1	0	0.163346	3.701156	1.545300
57	1	0	0.458383	4.945238	0.336076
58	1	0	-0.885975	3.835355	0.126327
59	6	0	0.981373	-3.049624	2.495065
60	1	0	1.628332	-3.651945	1.849998
61	1	0	1.130658	-3.406830	3.522422
62	1	0	-0.057338	-3.269623	2.229843

Zero-point correction= 0.526165 (Hartree/Particle)
Thermal correction to Energy= 0.557895
Thermal correction to Enthalpy= 0.558839
Thermal correction to Gibbs Free Energy= 0.463144
Sum of electronic and zero-point Energies= -1545.342965
Sum of electronic and thermal Energies= -1545.311235
Sum of electronic and thermal Enthalpies= -1545.310291
Sum of electronic and thermal Free Energies= -1545.405987
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1546.15096562

INT1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.968945	0.915367	-0.067560
2	6	0	-4.626597	1.274051	-0.122198
3	6	0	-3.632829	0.299131	0.047057

4	6	0	-3.990354	-1.039927	0.272474
5	6	0	-5.331207	-1.393246	0.325167
6	6	0	-6.318491	-0.417120	0.155126
7	1	0	-6.740930	1.667473	-0.198525
8	1	0	-4.340825	2.308850	-0.297026
9	1	0	-3.205078	-1.777800	0.402116
10	1	0	-5.614844	-2.427086	0.498116
11	1	0	-7.366977	-0.698957	0.196631
12	6	0	-2.230118	0.701905	-0.021855
13	8	0	-1.280752	-0.065172	0.118697
14	1	0	-2.043566	1.773590	-0.215347
15	57	0	1.323568	0.003231	-0.064129
16	6	0	1.230301	1.002149	-2.767269
17	6	0	2.501128	0.403701	-2.589741
18	6	0	0.252074	-0.019060	-2.795881
19	1	0	1.036278	2.061075	-2.892815
20	6	0	2.313016	-0.996537	-2.508076
21	1	0	3.451245	0.924502	-2.550926
22	6	0	0.928799	-1.255078	-2.617644
23	1	0	3.092009	-1.739488	-2.389195
24	1	0	0.460240	-2.232856	-2.617356
25	6	0	1.454468	-1.587134	2.302916
26	6	0	0.786420	-2.450037	1.394984
27	6	0	2.792365	-1.431515	1.872079
28	1	0	1.017682	-1.156795	3.197471
29	6	0	1.718644	-2.805324	0.392283
30	6	0	2.954882	-2.178819	0.683268
31	1	0	3.559313	-0.848699	2.367423
32	1	0	1.521997	-3.467922	-0.442489
33	1	0	3.870831	-2.278443	0.112230
34	6	0	2.131716	2.729758	-0.041245
35	6	0	0.798332	2.798850	0.417682
36	6	0	2.903512	2.099641	0.961832
37	1	0	2.498438	3.093479	-0.992472
38	6	0	0.740253	2.240984	1.726266
39	1	0	-0.028551	3.266617	-0.107635
40	6	0	2.044855	1.810336	2.051168
41	1	0	3.970793	1.910722	0.923347
42	1	0	2.337821	1.354709	2.989236
43	6	0	-1.200249	0.153824	-3.128853
44	1	0	-1.361414	0.121130	-4.214158
45	1	0	-1.818634	-0.635084	-2.689226
46	1	0	-1.587172	1.120425	-2.785229
47	6	0	-0.437994	2.251716	2.657611
48	1	0	-0.455008	1.370817	3.307883
49	1	0	-0.416179	3.133466	3.311155
50	1	0	-1.391873	2.285673	2.120680
51	6	0	-0.602572	-2.997717	1.549049
52	1	0	-0.599342	-3.918995	2.146134
53	1	0	-1.264262	-2.287185	2.054595
54	1	0	-1.047788	-3.245420	0.579304

Zero-point correction= 0.444900 (Hartree/Particle)
Thermal correction to Energy= 0.473520
Thermal correction to Enthalpy= 0.474464
Thermal correction to Gibbs Free Energy= 0.382105
Sum of electronic and zero-point Energies= -1479.158487
Sum of electronic and thermal Energies= -1479.129867
Sum of electronic and thermal Enthalpies= -1479.128923
Sum of electronic and thermal Free Energies= -1479.221282
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1479.87193917

TS1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	2.625976	-0.078771	-0.817513
2	8	0	2.764686	-1.300447	-1.439171
3	8	0	3.394647	0.078222	0.322345
4	6	0	3.578023	-2.111096	-0.544424
5	6	0	4.343575	-1.019524	0.291941
6	6	0	5.602122	-0.503657	-0.409213
7	1	0	5.957633	0.387032	0.116022
8	1	0	6.403100	-1.248871	-0.404792
9	1	0	5.394111	-0.225052	-1.446601
10	6	0	4.466646	-3.001004	-1.402109
11	1	0	5.156267	-3.576787	-0.776105
12	1	0	3.847557	-3.708849	-1.960351
13	1	0	5.047242	-2.421360	-2.122274
14	6	0	2.639495	-2.966090	0.302094
15	1	0	1.977752	-2.347114	0.912745
16	1	0	2.021812	-3.576707	-0.360998
17	1	0	3.197361	-3.638565	0.961013
18	6	0	4.668018	-1.418145	1.723897
19	1	0	5.335363	-2.286057	1.742061
20	1	0	5.176698	-0.591688	2.228470
21	1	0	3.766662	-1.656327	2.290416
22	1	0	2.584666	0.895465	-1.616832
23	6	0	1.824032	5.004314	-1.045361
24	6	0	1.520070	3.725266	-1.496350
25	6	0	1.455790	2.659600	-0.588348
26	6	0	1.707043	2.875477	0.771528
27	6	0	2.008458	4.157340	1.217841
28	6	0	2.066743	5.218901	0.312763
29	1	0	1.867954	5.832552	-1.746058
30	1	0	1.325365	3.548574	-2.552067
31	1	0	1.665255	2.035876	1.455742
32	1	0	2.200486	4.331666	2.272318
33	1	0	2.301436	6.218785	0.667024
34	6	0	1.121802	1.312422	-1.090141
35	8	0	0.845132	0.315271	-0.312183
36	1	0	0.771062	1.284671	-2.132953
37	57	0	-1.818911	-0.318367	0.269740
38	6	0	-3.813447	0.846808	-1.438190
39	6	0	-3.914722	1.502780	-0.185873
40	6	0	-2.631068	1.275762	-2.081425
41	1	0	-4.537431	0.153101	-1.848299
42	6	0	-2.795483	2.353710	-0.050130
43	1	0	-4.724458	1.388925	0.525587
44	6	0	-2.000452	2.203980	-1.207102
45	1	0	-2.581337	3.004310	0.788053
46	1	0	-1.121067	2.791185	-1.440781
47	6	0	-1.456417	-1.279282	2.958165
48	6	0	-0.492825	-0.250995	2.891052
49	6	0	-2.748903	-0.699519	2.888333
50	1	0	-1.233502	-2.332698	3.079455
51	6	0	-1.199087	0.977351	2.764498
52	6	0	-2.584047	0.700470	2.792412
53	1	0	-3.691700	-1.231227	2.948008
54	1	0	-0.751589	1.964172	2.719568
55	1	0	-3.379935	1.433040	2.750111
56	6	0	-3.416045	-2.512463	-0.474235
57	6	0	-2.730838	-2.223168	-1.680891

58	6	0	-2.478244	-3.062933	0.427705
59	1	0	-4.477305	-2.381183	-0.294821
60	6	0	-1.370387	-2.562624	-1.527757
61	1	0	-3.178268	-1.834555	-2.587156
62	6	0	-1.216043	-3.068956	-0.205003
63	1	0	-2.691190	-3.412279	1.429468
64	1	0	-0.296676	-3.451950	0.221550
65	6	0	0.987524	-0.427277	3.070178
66	1	0	1.345725	0.130350	3.944731
67	1	0	1.227619	-1.481409	3.244289
68	1	0	1.573768	-0.094185	2.207332
69	6	0	-2.220020	0.967472	-3.492235
70	1	0	-2.608851	1.720458	-4.190549
71	1	0	-1.131044	0.952701	-3.619894
72	1	0	-2.599068	-0.002896	-3.825242
73	6	0	-0.330012	-2.535468	-2.611216
74	1	0	0.647818	-2.201140	-2.253133
75	1	0	-0.192753	-3.535879	-3.043305
76	1	0	-0.632027	-1.876367	-3.431699

Zero-point correction= 0.636784 (Hartree/Particle)
Thermal correction to Energy= 0.675441
Thermal correction to Enthalpy= 0.676385
Thermal correction to Gibbs Free Energy= 0.565676
Sum of electronic and zero-point Energies= -1890.631420
Sum of electronic and thermal Energies= -1890.592763
Sum of electronic and thermal Enthalpies= -1890.591818
Sum of electronic and thermal Free Energies= -1890.702528

B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.63617870

INT2'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	3.058001	-0.681982	-0.542378
2	8	0	2.439725	-1.726196	0.107403
3	8	0	4.421817	-0.841845	-0.669284
4	6	0	3.496814	-2.552939	0.653648
5	6	0	4.709494	-2.210208	-0.287936
6	6	0	4.720691	-3.036328	-1.574682
7	1	0	5.445879	-2.601942	-2.268443
8	1	0	5.005273	-4.075615	-1.386191
9	1	0	3.739826	-3.027393	-2.059312
10	6	0	3.049362	-4.006747	0.616295
11	1	0	3.851416	-4.668524	0.959092
12	1	0	2.191550	-4.145365	1.280457
13	1	0	2.750526	-4.310328	-0.388575
14	6	0	3.718398	-2.103834	2.098503
15	1	0	4.044031	-1.060562	2.144458
16	1	0	2.774977	-2.187258	2.644596
17	1	0	4.463687	-2.724106	2.605239
18	6	0	6.076246	-2.252319	0.379196
19	1	0	6.299205	-3.259824	0.744964
20	1	0	6.848437	-1.978632	-0.345611
21	1	0	6.137547	-1.555495	1.217307
22	1	0	3.962106	1.052844	-2.138959
23	6	0	2.774029	4.803949	0.063806
24	6	0	2.511629	3.736184	-0.793909
25	6	0	3.326333	2.600588	-0.788253
26	6	0	4.414491	2.551731	0.091338
27	6	0	4.677402	3.615613	0.950404

28	6	0	3.856983	4.744219	0.938771
29	1	0	2.133842	5.681737	0.047037
30	1	0	1.668910	3.787442	-1.479864
31	1	0	5.053729	1.672378	0.094809
32	1	0	5.526928	3.568235	1.626499
33	1	0	4.064271	5.575642	1.606884
34	6	0	3.034195	1.436498	-1.701003
35	8	0	2.355409	0.380008	-1.009603
36	1	0	2.372269	1.751178	-2.513261
37	57	0	-2.767907	0.009250	0.149426
38	6	0	-3.396288	1.027299	-2.441369
39	6	0	-4.101062	1.852035	-1.529922
40	6	0	-2.011343	1.268683	-2.293682
41	1	0	-3.842636	0.335988	-3.145713
42	6	0	-3.151693	2.630813	-0.828226
43	1	0	-5.179189	1.910557	-1.425951
44	6	0	-1.866596	2.261130	-1.282651
45	1	0	-3.371335	3.372619	-0.070649
46	1	0	-0.925461	2.680089	-0.942437
47	6	0	-2.017081	-0.383761	2.853709
48	6	0	-1.183537	0.685643	2.430351
49	6	0	-3.352559	0.076378	2.900092
50	1	0	-1.676158	-1.375573	3.126037
51	6	0	-2.021898	1.806565	2.216072
52	6	0	-3.357910	1.434206	2.497104
53	1	0	-4.215237	-0.501753	3.209781
54	1	0	-1.684624	2.786733	1.900713
55	1	0	-4.225362	2.082899	2.446305
56	6	0	-4.477031	-2.027069	-0.764368
57	6	0	-3.320619	-2.194295	-1.563103
58	6	0	-4.146703	-2.413339	0.557394
59	1	0	-5.450229	-1.698411	-1.111767
60	6	0	-2.267484	-2.669926	-0.745019
61	1	0	-3.249508	-2.013941	-2.628972
62	6	0	-2.787615	-2.801162	0.570081
63	1	0	-4.820145	-2.426763	1.406261
64	1	0	-2.239675	-3.169652	1.429155
65	6	0	0.315262	0.664344	2.324014
66	1	0	0.779113	0.794127	3.310442
67	1	0	0.692868	-0.277706	1.912994
68	1	0	0.686184	1.471001	1.685139
69	6	0	-0.905502	0.666797	-3.114179
70	1	0	-0.603204	1.342633	-3.925041
71	1	0	-0.010373	0.460376	-2.516601
72	1	0	-1.220220	-0.271439	-3.581783
73	6	0	-0.892259	-3.059352	-1.211307
74	1	0	-0.096365	-2.703773	-0.547814
75	1	0	-0.794416	-4.150999	-1.270981
76	1	0	-0.688259	-2.662851	-2.210738

Zero-point correction= 0.641506 (Hartree/Particle)
Thermal correction to Energy= 0.680976
Thermal correction to Enthalpy= 0.681920
Thermal correction to Gibbs Free Energy= 0.560633
Sum of electronic and zero-point Energies= -1890.737538
Sum of electronic and thermal Energies= -1890.698068
Sum of electronic and thermal Enthalpies= -1890.697124
Sum of electronic and thermal Free Energies= -1890.818411
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.76494996

TS2'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-1.695124	-0.456767	-0.171367
2	6	0	-1.561935	-1.695820	2.546267
3	6	0	-1.898946	-2.691508	1.567882
4	6	0	-0.190102	-1.471633	2.512944
5	1	0	-2.253274	-1.227684	3.235093
6	6	0	-0.724637	-3.076684	0.926818
7	1	0	-2.891827	-3.090346	1.385485
8	6	0	0.367045	-2.304583	1.464635
9	1	0	-0.627841	-3.837480	0.162644
10	1	0	1.336891	-2.768351	1.601718
11	6	0	-2.931978	-1.244426	-2.554376
12	6	0	-2.035905	-0.230847	-2.970435
13	6	0	-2.166376	-2.365734	-2.163726
14	1	0	-4.012430	-1.176444	-2.550150
15	6	0	-0.712323	-0.730830	-2.866435
16	1	0	-2.311501	0.746637	-3.350723
17	6	0	-0.798911	-2.047189	-2.354276
18	1	0	-2.558316	-3.311180	-1.806037
19	1	0	0.050448	-2.688140	-2.150957
20	6	0	-3.177646	1.357774	1.568817
21	6	0	-3.180211	1.950809	0.278922
22	6	0	-3.974514	0.190689	1.484863
23	6	0	-3.971458	1.161915	-0.583029
24	1	0	-2.675868	2.872027	0.013005
25	6	0	-4.456660	0.061845	0.161783
26	1	0	-4.211483	-0.472797	2.307765
27	1	0	-4.177208	1.368576	-1.625304
28	1	0	-5.112810	-0.720171	-0.202201
29	6	0	3.042867	5.173682	0.419054
30	6	0	2.564032	3.876653	0.572364
31	6	0	1.351536	3.501773	-0.023335
32	6	0	0.620354	4.433369	-0.777089
33	6	0	1.103185	5.725331	-0.930870
34	6	0	2.312320	6.094666	-0.332509
35	1	0	3.980462	5.468016	0.880864
36	1	0	3.120872	3.147785	1.156301
37	1	0	-0.314440	4.120564	-1.231821
38	1	0	0.543578	6.450072	-1.514798
39	1	0	2.686022	7.107588	-0.454758
40	6	0	0.866153	2.133360	0.161870
41	1	0	1.524789	1.444480	0.718809
42	8	0	-0.211456	1.733594	-0.279702
43	5	0	1.531259	-1.320258	0.113357
44	8	0	2.550068	-0.693698	0.886419
45	8	0	2.108679	-2.280454	-0.741934
46	6	0	3.822580	-1.100212	0.351919
47	6	0	3.485336	-2.453991	-0.378886
48	6	0	3.617796	-3.684949	0.526612
49	1	0	3.136941	-4.534931	0.034392
50	1	0	4.667494	-3.939784	0.703998
51	1	0	3.143205	-3.547174	1.501533
52	6	0	4.820855	-1.221859	1.498215
53	1	0	5.787845	-1.591388	1.140684
54	1	0	4.984440	-0.239284	1.951782
55	1	0	4.457376	-1.893688	2.278173
56	6	0	4.284325	-0.005995	-0.616483
57	1	0	3.581937	0.109314	-1.446797
58	1	0	4.332582	0.946468	-0.079713
59	1	0	5.277641	-0.211362	-1.027519

60	6	0	4.280196	-2.704901	-1.657819
61	1	0	5.353933	-2.769465	-1.451034
62	1	0	3.964529	-3.654096	-2.100849
63	1	0	4.110723	-1.919809	-2.397020
64	1	0	0.728983	-0.581309	-0.417832
65	6	0	-2.571346	1.947766	2.809130
66	1	0	-1.641833	2.486430	2.594025
67	1	0	-3.253417	2.667370	3.280847
68	1	0	-2.347727	1.182499	3.558804
69	6	0	0.541466	-0.041511	-3.319134
70	1	0	1.420909	-0.497782	-2.856852
71	1	0	0.660725	-0.123218	-4.407301
72	1	0	0.537268	1.026323	-3.075524
73	6	0	0.598362	-0.626422	3.466983
74	1	0	-0.021940	0.148480	3.927877
75	1	0	1.004842	-1.241447	4.281118
76	1	0	1.452168	-0.157031	2.971074

Zero-point correction= 0.637029 (Hartree/Particle)
Thermal correction to Energy= 0.675996
Thermal correction to Enthalpy= 0.676941
Thermal correction to Gibbs Free Energy= 0.563845
Sum of electronic and zero-point Energies= -1890.657193
Sum of electronic and thermal Energies= -1890.618225
Sum of electronic and thermal Enthalpies= -1890.617281
Sum of electronic and thermal Free Energies= -1890.730377
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy=-1891.65686425

INT3'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	1.786941	-0.493967	0.147750
2	6	0	0.869402	-1.067216	-2.905390
3	6	0	1.321587	-2.225603	-2.153187
4	6	0	-0.504025	-1.028969	-2.880277
5	1	0	1.505625	-0.391429	-3.464982
6	6	0	0.218138	-2.875793	-1.654897
7	1	0	2.355591	-2.554859	-2.067472
8	6	0	-0.983787	-2.110432	-2.006170
9	1	0	0.213034	-3.776463	-1.052669
10	1	0	-1.851467	-2.678428	-2.345846
11	6	0	2.964475	-2.044282	2.105855
12	6	0	2.507781	-0.900493	2.805564
13	6	0	1.826893	-2.789980	1.716563
14	1	0	3.999185	-2.308178	1.922325
15	6	0	1.090259	-0.939948	2.859863
16	1	0	3.132285	-0.141301	3.263287
17	6	0	0.673230	-2.108065	2.173376
18	1	0	1.834909	-3.727237	1.171811
19	1	0	-0.352391	-2.415914	2.001461
20	6	0	3.236339	1.468426	-1.372985
21	6	0	3.612922	1.651656	-0.015541
22	6	0	3.774346	0.225160	-1.784093
23	6	0	4.388358	0.543962	0.394999
24	1	0	3.367929	2.517281	0.590086
25	6	0	4.478028	-0.348916	-0.695711
26	1	0	3.704166	-0.195429	-2.780233
27	1	0	4.836422	0.406465	1.370639
28	1	0	5.021966	-1.286750	-0.711737
29	6	0	-2.973692	4.951659	-0.211159

30	6	0	-2.471106	3.656994	-0.290874
31	6	0	-1.214784	3.359306	0.257477
32	6	0	-0.463607	4.364216	0.887841
33	6	0	-0.970828	5.653229	0.968182
34	6	0	-2.223835	5.945598	0.418481
35	1	0	-3.944578	5.187717	-0.636048
36	1	0	-3.038147	2.868070	-0.778870
37	1	0	0.505642	4.110202	1.305615
38	1	0	-0.397253	6.435589	1.456382
39	1	0	-2.616327	6.956770	0.483010
40	6	0	-0.712887	1.991923	0.141336
41	1	0	-1.388398	1.249171	-0.318534
42	8	0	0.407504	1.650089	0.537149
43	5	0	-1.583422	-1.434543	-0.527076
44	8	0	-2.697356	-0.520603	-0.774649
45	8	0	-2.071544	-2.457688	0.369623
46	6	0	-3.754992	-0.852687	0.128977
47	6	0	-3.491644	-2.372188	0.427213
48	6	0	-4.099603	-3.291938	-0.641843
49	1	0	-3.669829	-4.291632	-0.529204
50	1	0	-5.187270	-3.372650	-0.542525
51	1	0	-3.877722	-2.937114	-1.651662
52	6	0	-5.089923	-0.552693	-0.547104
53	1	0	-5.931343	-0.871348	0.078031
54	1	0	-5.189009	0.525131	-0.714530
55	1	0	-5.166528	-1.049364	-1.516513
56	6	0	-3.617530	0.009776	1.389521
57	1	0	-2.674275	-0.200825	1.901280
58	1	0	-3.629484	1.068205	1.110015
59	1	0	-4.437157	-0.156726	2.095862
60	6	0	-3.949079	-2.845908	1.804552
61	1	0	-5.029836	-2.718921	1.933254
62	1	0	-3.719772	-3.909975	1.918827
63	1	0	-3.434240	-2.307669	2.603086
64	1	0	-0.600107	-0.826725	-0.020005
65	6	0	2.510005	2.464759	-2.230496
66	1	0	1.912357	3.152306	-1.624349
67	1	0	3.214115	3.074205	-2.811228
68	1	0	1.837726	1.981846	-2.947465
69	6	0	0.211578	0.022561	3.605649
70	1	0	-0.761908	0.144075	3.122042
71	1	0	0.021853	-0.332756	4.626411
72	1	0	0.671864	1.012379	3.687437
73	6	0	-1.392180	-0.079711	-3.616699
74	1	0	-0.830462	0.763031	-4.031772
75	1	0	-1.890467	-0.587301	-4.453289
76	1	0	-2.183110	0.294575	-2.959441

Zero-point correction= 0.636790 (Hartree/Particle)
Thermal correction to Energy= 0.676034
Thermal correction to Enthalpy= 0.676979
Thermal correction to Gibbs Free Energy= 0.563707
Sum of electronic and zero-point Energies= -1890.661888
Sum of electronic and thermal Energies= -1890.622644
Sum of electronic and thermal Enthalpies= -1890.621700
Sum of electronic and thermal Free Energies= -1890.734971
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.66603980

TS3'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	57	0	-1.777691	-0.431919	0.200230
2	6	0	-0.176446	1.010643	2.850418
3	6	0	-0.608750	-0.380456	2.893676
4	6	0	1.131277	1.056106	2.449530
5	1	0	-0.781196	1.861063	3.147209
6	6	0	0.425097	-1.174142	2.475678
7	1	0	-1.568378	-0.726285	3.271478
8	6	0	1.571868	-0.317843	2.109237
9	1	0	0.432726	-2.255688	2.430192
10	1	0	2.505493	-0.614948	2.601163
11	6	0	-3.054913	-2.747198	-0.697713
12	6	0	-2.345723	-2.282447	-1.834819
13	6	0	-2.119518	-3.198139	0.266094
14	1	0	-4.133798	-2.778495	-0.600354
15	6	0	-0.963745	-2.452648	-1.557076
16	6	0	-0.822484	-3.021542	-0.272531
17	1	0	-2.360938	-3.628650	1.232149
18	1	0	-0.147541	-2.201899	-2.224962
19	1	0	0.125051	-3.244076	0.199916
20	6	0	-3.287995	1.877949	0.959185
21	6	0	-3.835951	1.491973	-0.291175
22	6	0	-3.609557	0.888563	1.918343
23	1	0	-2.751356	2.799558	1.156208
24	6	0	-4.472055	0.241831	-0.095225
25	6	0	-4.334888	-0.133301	1.265678
26	1	0	-3.366005	0.925142	2.973360
27	1	0	-5.013762	-0.308508	-0.855733
28	1	0	-4.746313	-1.024042	1.726200
29	6	0	2.992920	3.941839	-1.311413
30	6	0	2.421024	2.695799	-1.547999
31	6	0	1.079229	2.464723	-1.221064
32	6	0	0.313397	3.497058	-0.659881
33	6	0	0.886177	4.740667	-0.426979
34	6	0	2.227118	4.964154	-0.750941
35	1	0	4.034558	4.116847	-1.564131
36	1	0	3.009293	1.893024	-1.976296
37	1	0	-0.728003	3.306779	-0.422168
38	1	0	0.290453	5.541209	0.002403
39	1	0	2.673094	5.938218	-0.569270
40	6	0	0.455327	1.170668	-1.538888
41	1	0	1.037817	0.491080	-2.174880
42	8	0	-0.794087	1.006750	-1.437067
43	5	0	2.059704	-0.534920	0.486879
44	8	0	3.343597	0.051298	0.214974
45	8	0	2.122968	-1.920675	0.107316
46	6	0	4.163576	-0.911297	-0.453999
47	6	0	3.492490	-2.281974	-0.071608
48	6	0	4.024264	-2.857473	1.248335
49	1	0	3.372183	-3.677856	1.562619
50	1	0	5.040622	-3.250481	1.141743
51	1	0	4.032747	-2.108942	2.044941
52	6	0	5.599314	-0.742309	0.038775
53	1	0	6.262874	-1.494952	-0.401223
54	1	0	5.971961	0.245718	-0.249251
55	1	0	5.659462	-0.815908	1.126212
56	6	0	4.124698	-0.649296	-1.964063
57	1	0	3.107678	-0.740082	-2.356885
58	1	0	4.489476	0.362898	-2.163574
59	1	0	4.765610	-1.344328	-2.515567
60	6	0	3.572740	-3.363541	-1.146296
61	1	0	4.612680	-3.621476	-1.374847

62	1	0	3.072504	-4.269903	-0.791608
63	1	0	3.078101	-3.050734	-2.068086
64	1	0	1.118251	0.093041	-0.212351
65	6	0	-2.941676	-1.805795	-3.128614
66	1	0	-3.006432	-2.624848	-3.856183
67	1	0	-3.955864	-1.419013	-2.988988
68	1	0	-2.340514	-1.013696	-3.586842
69	6	0	-3.831460	2.294029	-1.560606
70	1	0	-4.499350	3.160245	-1.478203
71	1	0	-2.833363	2.666788	-1.809876
72	1	0	-4.179333	1.694062	-2.406738
73	6	0	2.019888	2.254306	2.384861
74	1	0	2.764615	2.220062	3.190999
75	1	0	2.578702	2.284757	1.445227
76	1	0	1.454764	3.183871	2.493215

Zero-point correction= 0.635174 (Hartree/Particle)
Thermal correction to Energy= 0.673529
Thermal correction to Enthalpy= 0.674474
Thermal correction to Gibbs Free Energy= 0.562908
Sum of electronic and zero-point Energies= -1890.647304
Sum of electronic and thermal Energies= -1890.608949
Sum of electronic and thermal Enthalpies= -1890.608005
Sum of electronic and thermal Free Energies= -1890.719570
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.64970487

INT4'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	-1.792401	-0.460839	0.072514
2	6	0	-0.040271	-0.364618	3.203455
3	6	0	-0.566165	-1.621452	2.673715
4	6	0	1.302435	-0.311427	3.006730
5	1	0	-0.635231	0.391406	3.703863
6	6	0	0.450449	-2.340877	2.133718
7	1	0	-1.597765	-1.951464	2.769879
8	6	0	1.726755	-1.578603	2.306033
9	1	0	0.387820	-3.325044	1.687565
10	1	0	2.378256	-2.150777	2.994639
11	6	0	-3.186884	-2.526023	-1.279383
12	6	0	-2.636503	-1.733967	-2.321888
13	6	0	-2.131816	-3.187516	-0.611174
14	1	0	-4.243753	-2.623234	-1.058750
15	6	0	-1.231028	-1.921782	-2.288220
16	6	0	-0.916345	-2.810437	-1.236281
17	1	0	-2.238788	-3.877499	0.219235
18	1	0	-0.521372	-1.456840	-2.963127
19	1	0	0.079348	-3.139771	-0.963807
20	6	0	-3.058454	1.428055	1.820890
21	6	0	-3.572448	1.722911	0.536026
22	6	0	-3.569515	0.170571	2.235832
23	1	0	-2.416244	2.080979	2.402207
24	6	0	-4.378788	0.621035	0.148867
25	6	0	-4.388929	-0.328700	1.202691
26	1	0	-3.396158	-0.300789	3.196968
27	1	0	-4.939403	0.549323	-0.776995
28	1	0	-4.938272	-1.262505	1.214572
29	6	0	2.046805	5.147812	-1.409333
30	6	0	1.306933	4.098778	-1.947202
31	6	0	0.740315	3.121497	-1.119428

32	6	0	0.932654	3.217178	0.258859
33	6	0	1.674608	4.268179	0.801633
34	6	0	2.234198	5.236516	-0.028556
35	1	0	2.478619	5.898349	-2.066709
36	1	0	1.165000	4.036670	-3.025165
37	1	0	0.495545	2.455572	0.896873
38	1	0	1.813886	4.330645	1.878160
39	1	0	2.810700	6.055314	0.393552
40	6	0	-0.071955	1.992936	-1.732766
41	1	0	-0.926483	2.451461	-2.262522
42	8	0	-0.510552	1.044521	-0.824470
43	5	0	2.635705	-1.440697	1.012288
44	8	0	3.694335	-0.582745	0.928517
45	8	0	2.482884	-2.238544	-0.087876
46	6	0	4.178093	-0.639857	-0.444314
47	6	0	3.664870	-2.047947	-0.916666
48	6	0	4.621664	-3.189655	-0.573023
49	1	0	4.111276	-4.142678	-0.737375
50	1	0	5.516804	-3.167303	-1.201349
51	1	0	4.933419	-3.148360	0.474989
52	6	0	5.690397	-0.475134	-0.427343
53	1	0	6.101349	-0.571021	-1.437520
54	1	0	5.945017	0.520617	-0.053922
55	1	0	6.173063	-1.212002	0.217691
56	6	0	3.519549	0.520155	-1.186483
57	1	0	2.430548	0.423040	-1.186998
58	1	0	3.767143	1.457669	-0.682689
59	1	0	3.869272	0.584079	-2.221047
60	6	0	3.251378	-2.126098	-2.377992
61	1	0	4.105693	-1.923731	-3.032078
62	1	0	2.883528	-3.130768	-2.604654
63	1	0	2.457442	-1.414316	-2.609028
64	1	0	0.545196	1.524463	-2.521785
65	6	0	-3.404957	-0.960497	-3.356000
66	1	0	-3.585622	-1.570330	-4.250738
67	1	0	-4.383297	-0.643818	-2.981614
68	1	0	-2.865151	-0.065386	-3.683188
69	6	0	-3.369131	2.995452	-0.233786
70	1	0	-4.089325	3.763238	0.077059
71	1	0	-2.366438	3.405594	-0.081012
72	1	0	-3.508375	2.842757	-1.309035
73	6	0	2.242763	0.766097	3.432134
74	1	0	3.010860	0.377366	4.112253
75	1	0	2.773396	1.190715	2.573921
76	1	0	1.709437	1.568351	3.949101

Zero-point correction= 0.638774 (Hartree/Particle)
Thermal correction to Energy= 0.678649
Thermal correction to Enthalpy= 0.679593
Thermal correction to Gibbs Free Energy= 0.559376
Sum of electronic and zero-point Energies= -1890.703515
Sum of electronic and thermal Energies= -1890.663640
Sum of electronic and thermal Enthalpies= -1890.662696
Sum of electronic and thermal Free Energies= -1890.782913
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.71891753

TS4'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.370094	4.811449	1.298152

2	6	0	-0.577342	3.736901	1.694897
3	6	0	-0.216493	2.733643	0.787224
4	6	0	-0.668837	2.839617	-0.531809
5	6	0	-1.465537	3.913391	-0.933400
6	6	0	-1.820976	4.902903	-0.019464
7	1	0	-1.644012	5.575813	2.020764
8	1	0	-0.235463	3.671119	2.726137
9	1	0	-0.375423	2.081004	-1.254308
10	1	0	-1.802195	3.979303	-1.964878
11	1	0	-2.443644	5.737689	-0.328760
12	6	0	0.668028	1.583126	1.233854
13	1	0	1.717418	1.918653	1.207182
14	8	0	0.525193	0.426001	0.462739
15	5	0	2.481076	-0.723464	0.281657
16	8	0	3.323153	0.202835	0.877097
17	8	0	2.692425	-0.817553	-1.083750
18	6	0	4.297590	0.603628	-0.112395
19	6	0	3.583953	0.251907	-1.471093
20	6	0	4.511008	-0.275357	-2.560795
21	1	0	3.927512	-0.508299	-3.456320
22	1	0	5.259506	0.475865	-2.833726
23	1	0	5.026459	-1.186204	-2.250039
24	6	0	5.549416	-0.239964	0.144323
25	1	0	6.372406	0.037700	-0.521024
26	1	0	5.874436	-0.084726	1.176982
27	1	0	5.342828	-1.306033	0.011866
28	6	0	4.624673	2.078420	0.081879
29	1	0	3.733362	2.705214	0.016327
30	1	0	5.072635	2.227190	1.068874
31	1	0	5.344822	2.419301	-0.669387
32	6	0	2.740889	1.398441	-2.026392
33	1	0	3.366925	2.222061	-2.383371
34	1	0	2.155539	1.026886	-2.872049
35	1	0	2.045415	1.777959	-1.276193
36	1	0	0.452461	1.380540	2.295881
37	6	0	-2.741129	-0.186002	2.195842
38	6	0	-3.323225	0.593902	1.167814
39	6	0	-3.979633	-0.271878	0.255957
40	6	0	-3.797732	-1.596446	0.710805
41	6	0	-3.025321	-1.544257	1.896863
42	1	0	-3.294165	1.676665	1.111341
43	1	0	-4.542683	0.033087	-0.617121
44	1	0	-4.191014	-2.492682	0.244565
45	1	0	-2.756753	-2.392739	2.515756
46	57	0	-1.282625	-0.766935	-0.244504
47	6	0	1.983947	-2.035067	1.063074
48	6	0	1.493261	-1.908286	2.474305
49	6	0	0.936360	-2.864787	0.392270
50	6	0	0.310442	-2.569147	2.583465
51	6	0	-0.033000	-3.168105	1.299863
52	1	0	1.007688	-3.219529	-0.628571
53	1	0	-0.281924	-2.663633	3.487084
54	1	0	-0.895157	-3.806587	1.125026
55	6	0	-2.269296	-0.442544	-2.920074
56	6	0	-0.858364	-0.275864	-2.996970
57	6	0	-2.507735	-1.804163	-2.615201
58	6	0	-0.239060	-1.520604	-2.749333
59	1	0	-0.347710	0.644994	-3.257589
60	6	0	-1.262625	-2.467779	-2.501741
61	1	0	-3.486198	-2.258782	-2.507946
62	1	0	0.828911	-1.699460	-2.726790
63	1	0	-1.122106	-3.524137	-2.298205

64	1	0	2.921758	-2.622952	1.071036
65	6	0	-2.065963	0.337624	3.430225
66	1	0	-2.714672	0.228152	4.308734
67	1	0	-1.131629	-0.189554	3.650814
68	1	0	-1.836400	1.402082	3.328266
69	6	0	-3.307958	0.592807	-3.249050
70	1	0	-3.288251	0.842108	-4.317345
71	1	0	-4.314067	0.228927	-3.021590
72	1	0	-3.162944	1.529812	-2.699212
73	6	0	2.239275	-1.202109	3.557125
74	1	0	3.206311	-1.684893	3.747047
75	1	0	2.462493	-0.168532	3.275540
76	1	0	1.674447	-1.203399	4.493624

Zero-point correction= 0.639717 (Hartree/Particle)
Thermal correction to Energy= 0.677829
Thermal correction to Enthalpy= 0.678773
Thermal correction to Gibbs Free Energy= 0.568768
Sum of electronic and zero-point Energies= -1890.696745
Sum of electronic and thermal Energies= -1890.658633
Sum of electronic and thermal Enthalpies= -1890.657688
Sum of electronic and thermal Free Energies= -1890.767693
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.70372896

INT5'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.789431	3.709539	-2.544637
2	6	0	0.834034	2.706469	-2.686773
3	6	0	0.227670	2.129345	-1.564202
4	6	0	0.596526	2.591309	-0.294624
5	6	0	1.564199	3.589426	-0.149949
6	6	0	2.166113	4.149249	-1.273879
7	1	0	2.248646	4.145146	-3.427907
8	1	0	0.551799	2.366767	-3.680715
9	1	0	0.081858	2.203054	0.581816
10	1	0	1.829270	3.941491	0.843207
11	1	0	2.916272	4.926997	-1.164224
12	6	0	-0.832030	1.066024	-1.731187
13	1	0	-1.822275	1.524847	-1.836121
14	8	0	-0.857240	0.180726	-0.623121
15	5	0	-2.219179	-0.403693	-0.153403
16	8	0	-3.286805	0.156725	-0.941766
17	8	0	-2.488874	-0.070379	1.228775
18	6	0	-4.325999	0.591683	-0.063172
19	6	0	-3.546437	0.887147	1.269954
20	6	0	-4.356107	0.664596	2.545077
21	1	0	-3.738114	0.892806	3.419359
22	1	0	-5.236262	1.316301	2.577885
23	1	0	-4.685539	-0.372684	2.631670
24	6	0	-5.348989	-0.541449	0.089543
25	1	0	-6.234068	-0.219046	0.647522
26	1	0	-5.669695	-0.862421	-0.905951
27	1	0	-4.920235	-1.404719	0.605022
28	6	0	-5.016789	1.800603	-0.688591
29	1	0	-4.303902	2.592493	-0.928984
30	1	0	-5.511442	1.500801	-1.617836
31	1	0	-5.779912	2.210871	-0.018252
32	6	0	-2.947570	2.298810	1.299269
33	1	0	-3.714828	3.069482	1.428466

34	1	0	-2.253503	2.367607	2.142686
35	1	0	-2.392910	2.518447	0.383240
36	1	0	-0.644201	0.507086	-2.658577
37	6	0	2.654391	-0.944891	-2.085663
38	6	0	3.278099	0.150697	-1.438737
39	6	0	3.954882	-0.325331	-0.288390
40	6	0	3.746584	-1.720797	-0.211280
41	6	0	2.938799	-2.098967	-1.310527
42	1	0	3.263175	1.177115	-1.788501
43	1	0	4.552063	0.271187	0.389402
44	1	0	4.150568	-2.388551	0.540422
45	1	0	2.636404	-3.110237	-1.555352
46	57	0	1.280397	-0.566688	0.421242
47	6	0	-2.080005	-2.099823	-0.290246
48	6	0	-1.637770	-2.553177	-1.629894
49	6	0	-1.055126	-2.626014	0.631234
50	6	0	-0.417263	-3.156795	-1.507564
51	6	0	-0.054075	-3.211202	-0.101537
52	1	0	-1.123897	-2.567305	1.710163
53	1	0	0.176188	-3.564519	-2.319244
54	1	0	0.824779	-3.713053	0.298454
55	6	0	2.408252	0.486233	2.825976
56	6	0	1.018361	0.786344	2.884052
57	6	0	2.528471	-0.920000	2.930001
58	6	0	0.295422	-0.417188	3.035628
59	1	0	0.590738	1.783294	2.880095
60	6	0	1.231716	-1.478391	3.052138
61	1	0	3.463581	-1.467868	2.948753
62	1	0	-0.783604	-0.499958	3.072882
63	1	0	1.003926	-2.531949	3.171043
64	1	0	-3.099916	-2.395870	-0.025081
65	6	0	1.939752	-0.911589	-3.405673
66	1	0	2.533504	-1.406283	-4.184369
67	1	0	0.970478	-1.419683	-3.366648
68	1	0	1.771639	0.118001	-3.733210
69	6	0	3.536167	1.478674	2.830336
70	1	0	3.604240	1.985538	3.801066
71	1	0	4.497630	0.987214	2.656061
72	1	0	3.418354	2.258008	2.069280
73	6	0	-2.429728	-2.353591	-2.881538
74	1	0	-3.297737	-3.025876	-2.902846
75	1	0	-2.828522	-1.335615	-2.933869
76	1	0	-1.833807	-2.557450	-3.776527

Zero-point correction= 0.640969 (Hartree/Particle)
Thermal correction to Energy= 0.679032
Thermal correction to Enthalpy= 0.679977
Thermal correction to Gibbs Free Energy= 0.571111
Sum of electronic and zero-point Energies= -1890.708792
Sum of electronic and thermal Energies= -1890.670729
Sum of electronic and thermal Enthalpies= -1890.669784
Sum of electronic and thermal Free Energies= -1890.778650
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.71459656

Product

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.756829	-0.326326	-0.638229
2	8	0	-1.173469	0.948751	-0.323901
3	8	0	-1.671708	-1.302137	-0.327093

4	6	0	-2.373184	0.798170	0.473716
5	6	0	-2.895689	-0.616273	0.021796
6	6	0	-3.752948	-0.559721	-1.243716
7	1	0	-3.895742	-1.576953	-1.618188
8	1	0	-4.736567	-0.122216	-1.048849
9	1	0	-3.262465	0.023110	-2.029040
10	6	0	-3.307253	1.959807	0.169028
11	1	0	-4.254916	1.848318	0.705784
12	1	0	-2.845366	2.897309	0.491717
13	1	0	-3.517389	2.037481	-0.899346
14	6	0	-1.939320	0.834606	1.939382
15	1	0	-1.272894	-0.000367	2.175044
16	1	0	-1.394580	1.764344	2.124996
17	1	0	-2.797040	0.796400	2.617306
18	6	0	-3.606997	-1.415274	1.104205
19	1	0	-4.507447	-0.894596	1.445917
20	1	0	-3.909580	-2.386588	0.702857
21	1	0	-2.957410	-1.593908	1.962980
22	1	0	1.693215	0.339395	-2.478411
23	6	0	4.752498	0.953714	0.311469
24	6	0	3.593069	1.155402	-0.432107
25	6	0	2.647729	0.133698	-0.569276
26	6	0	2.880388	-1.092879	0.054555
27	6	0	4.039091	-1.293411	0.803970
28	6	0	4.979034	-0.273690	0.933930
29	1	0	5.476500	1.757899	0.411466
30	1	0	3.418832	2.118555	-0.908066
31	1	0	2.145218	-1.884240	-0.049446
32	1	0	4.206923	-2.252285	1.287216
33	1	0	5.881094	-0.431431	1.518532
34	6	0	1.417396	0.368562	-1.415769
35	8	0	0.433278	-0.632685	-1.213778
36	1	0	1.006072	1.363687	-1.210243

Zero-point correction= 0.306895 (Hartree/Particle)
Thermal correction to Energy= 0.322639
Thermal correction to Enthalpy= 0.323583
Thermal correction to Gibbs Free Energy= 0.263657
Sum of electronic and zero-point Energies= -756.935750
Sum of electronic and thermal Energies= -756.920007
Sum of electronic and thermal Enthalpies= -756.919063
Sum of electronic and thermal Free Energies= -756.978989
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -757.42844760

TS1”

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	57	0	1.375259	0.354931	0.021507
2	6	0	1.676184	-0.835042	-2.713901
3	6	0	2.474328	-1.656775	-1.840670
4	6	0	0.335847	-1.103688	-2.486361
5	1	0	2.067975	-0.136349	-3.442398
6	6	0	1.590622	-2.418226	-1.074918
7	6	0	0.231887	-2.092877	-1.438690
8	1	0	-0.505795	-0.672312	-3.016107
9	1	0	1.871327	-3.186315	-0.363797
10	1	0	-0.480880	-2.902857	-1.542828
11	6	0	2.829104	0.366093	2.446613
12	6	0	1.559457	0.903871	2.765402

13	6	0	2.680864	-1.020252	2.185224
14	1	0	3.768376	0.904661	2.451190
15	6	0	0.618514	-0.147055	2.693930
16	1	0	1.350621	1.934208	3.028195
17	6	0	1.303598	-1.327977	2.327713
18	1	0	-0.445949	-0.065973	2.877423
19	1	0	0.845925	-2.300126	2.187537
20	6	0	1.871911	2.447978	-1.844568
21	6	0	1.589596	3.115339	-0.630959
22	6	0	3.143708	1.843102	-1.714824
23	1	0	1.240488	2.425677	-2.725325
24	6	0	2.680543	2.910401	0.242747
25	1	0	0.697134	3.685686	-0.409337
26	6	0	3.656608	2.129430	-0.425359
27	1	0	3.674764	1.305629	-2.491359
28	1	0	2.779753	3.313309	1.243765
29	6	0	-5.260192	3.536022	-0.573983
30	6	0	-4.292223	2.551466	-0.744704
31	6	0	-3.039813	2.684806	-0.129003
32	6	0	-2.762056	3.809935	0.662696
33	6	0	-3.731255	4.788607	0.833325
34	6	0	-4.978180	4.651887	0.214638
35	1	0	-6.230379	3.436722	-1.051466
36	1	0	-4.496593	1.676560	-1.357374
37	1	0	-1.787210	3.890609	1.133645
38	1	0	-3.522994	5.660474	1.446448
39	1	0	-5.733759	5.420919	0.350072
40	6	0	-2.034188	1.640186	-0.334540
41	1	0	-2.345393	0.756608	-0.917585
42	8	0	-0.893835	1.705820	0.123759
43	5	0	-1.165415	-1.716396	-0.060139
44	8	0	-2.365910	-1.557047	-0.816013
45	8	0	-1.285940	-2.835759	0.791140
46	6	0	-3.357310	-2.416845	-0.229827
47	6	0	-2.489857	-3.537349	0.454266
48	6	0	-2.150779	-4.699511	-0.488353
49	1	0	-1.348773	-5.292195	-0.039405
50	1	0	-3.014656	-5.353387	-0.644974
51	1	0	-1.812440	-4.360616	-1.471500
52	6	0	-4.292021	-2.908416	-1.329340
53	1	0	-5.026755	-3.618555	-0.934844
54	1	0	-4.839778	-2.061344	-1.754151
55	1	0	-3.741443	-3.389331	-2.140412
56	6	0	-4.148596	-1.587686	0.788151
57	1	0	-3.498176	-1.224954	1.589311
58	1	0	-4.579795	-0.718460	0.282060
59	1	0	-4.968467	-2.157101	1.236909
60	6	0	-3.081615	-4.106644	1.740635
61	1	0	-4.057827	-4.568507	1.556526
62	1	0	-2.414574	-4.876169	2.140870
63	1	0	-3.194614	-3.334800	2.504186
64	1	0	-0.731866	-0.721158	0.481111
65	6	0	3.971980	-1.769942	-1.861583
66	1	0	4.312453	-2.183013	-2.819187
67	1	0	4.473556	-0.804003	-1.738855
68	1	0	4.327725	-2.436650	-1.071824
69	6	0	5.039498	1.813399	0.071475
70	1	0	5.278039	0.743557	0.036011
71	1	0	5.798283	2.327858	-0.531135
72	1	0	5.172998	2.144296	1.105395
73	6	0	3.799841	-2.000758	1.981280
74	1	0	4.646482	-1.555792	1.447667

75	1	0	4.184183	-2.356321	2.946207
76	1	0	3.474764	-2.884571	1.423964

Zero-point correction= 0.636565 (Hartree/Particle)
Thermal correction to Energy= 0.675627
Thermal correction to Enthalpy= 0.676571
Thermal correction to Gibbs Free Energy= 0.562926
Sum of electronic and zero-point Energies= -1890.653527
Sum of electronic and thermal Energies= -1890.614465
Sum of electronic and thermal Enthalpies= -1890.613521
Sum of electronic and thermal Free Energies= -1890.727166
B3PW91/6-311++G(d,p)-SDD /SMD//B3PW91/6-31G(d,p)-SDD energy= -1891.65559968

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