Supplementary Information

for

Controlled reduction of isocyanates to formamides using monomeric magnesium

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Contents:

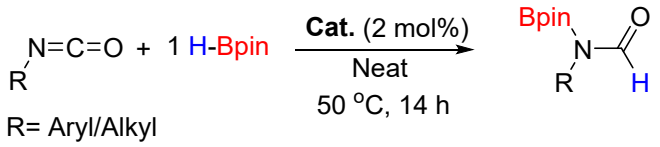
❖ General experimental information:

All reactions were carried out under argon atmosphere using Schlenk techniques or inside a MBraun glove box. Catalysts **1** was prepared according to our previous paper.[S1]

Pinacolborane (HBpin), isocyanates were purchased from Sigma-Aldrich, TCI Chemicals and used without further purification. C_6D_6, toluene-d_8, CD_3CN and $CDCl_3$ were purchased from Sigma-Aldrich, were degassed by three freeze-pump-thaw cycles and stored over molecular sieves. ^1H, $^{13}C\{^1H\}$ and ^{11}B NMR spectra were recorded on Bruker AV–200 MHz, AV-400 MHz and

AV-500 MHz and referenced to the resonances of the internal standard with respect to the solvent used. HRMS spectra were obtained using Thermo scientific Q-Exactive instrument.

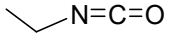
❖ General catalytic procedure for the synthesis of N-boryl formamide:

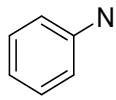
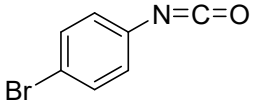
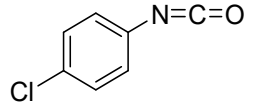
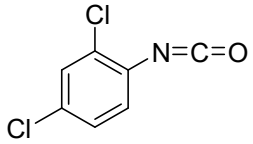
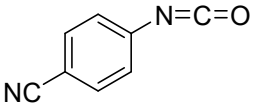
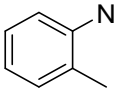
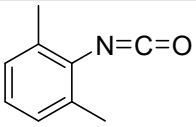
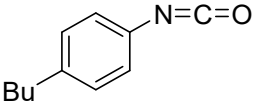
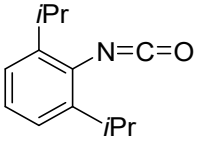
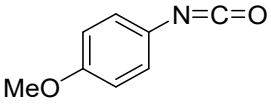
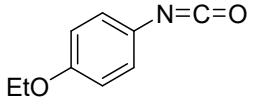


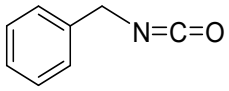
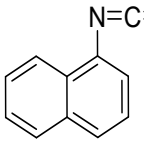
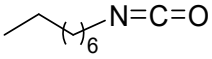
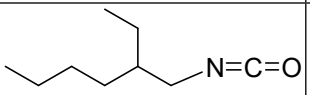
Scheme S1. General catalytic procedure for the synthesis of N-borylated formamide from phenyl isocyanate.

Ethyl isocyanate (0.250 mmol), pinacolborane (1.1 equiv., 0.275 mmol), catalyst (**1**, 2.0 mol%) were charged in a Schlenk tube/ nmr tube inside the glove box. The reaction mixture was allowed to heat at 50 °C for 14 h. Upon completion of the reaction, the volatiles were removed using vacuum in a Schlenk line and mesitylene (0.25 mmol) was added as the internal standard, while making the NMR in appropriate deuterated solvent. The progress of the reaction was monitored by the ^{1}H NMR spectroscopy, which indicated the completion of the reaction by the appearance of a new formamide -NC*H*O resonance.

❖ Table S1. Isocyanate substrate scope for N-boryl formamide:

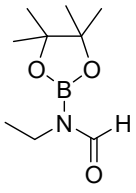
Entry	Substrate	Temperature (°C)	Time (h)	Catalyst **1** (mol%)	NMR Yield (%)	Product	Selectivity (Formamide: dihydroborated:amine)
1.		50	14	2	93	**2a**	100:0:0

2.		50	14	2	20	**2b**	20:0:15
3.		50	14	2	58	**2c**	100:0:0
4.		50	14	2	55	**2d**	100:0:0
5.		50	14	2	30	**2e**	100:0:0
6.		50	14	2	41	**2f**	41:8:7
7.		50	14	2	69	**2g**	100:0:0
8.		50	14	2	43	**2h**	100:0:0
9.		50	14	2	62	**2i**	100:0:0
10.		50	14	2	26	**2j**	26:24:0
11.		50	14	2	52	**2k**	100:0:0
12.		50	14	2	56	**2l**	100:0:0

13.		50	14	2	59	**2m**	59:18:0
14.		50	14	2	70	**2n**	100:0:0
15.		50	14	2	59	**2o**	100:0:0
16.		50	14	2	53	**2p**	100:0:0

❖ **Analytical data of N-boryl formamide of corresponding isocyanates with their NMR spectra:**

N-ethyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2a): ^{1}H NMR (400 MHz, CHLOROFORM-*d*) δ 8.66 (s, 1H, NC*H*O), 3.34-3.30 (t, 2H, NCH_2CH$_3$), 1.52-1.47 (q, 3H, NCH$_2$CH_3), 1.30 (s, 12H, CH_3) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.92 (s, 1 C), 84.01 (s, 1 C), 39.93 (s, 1 C), 29.51 (s, 1 C), 26.53 (s, 1 C), 24.79 (s, 1 C), 24.46 (s, 1 C), 24.41 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data.[S2]

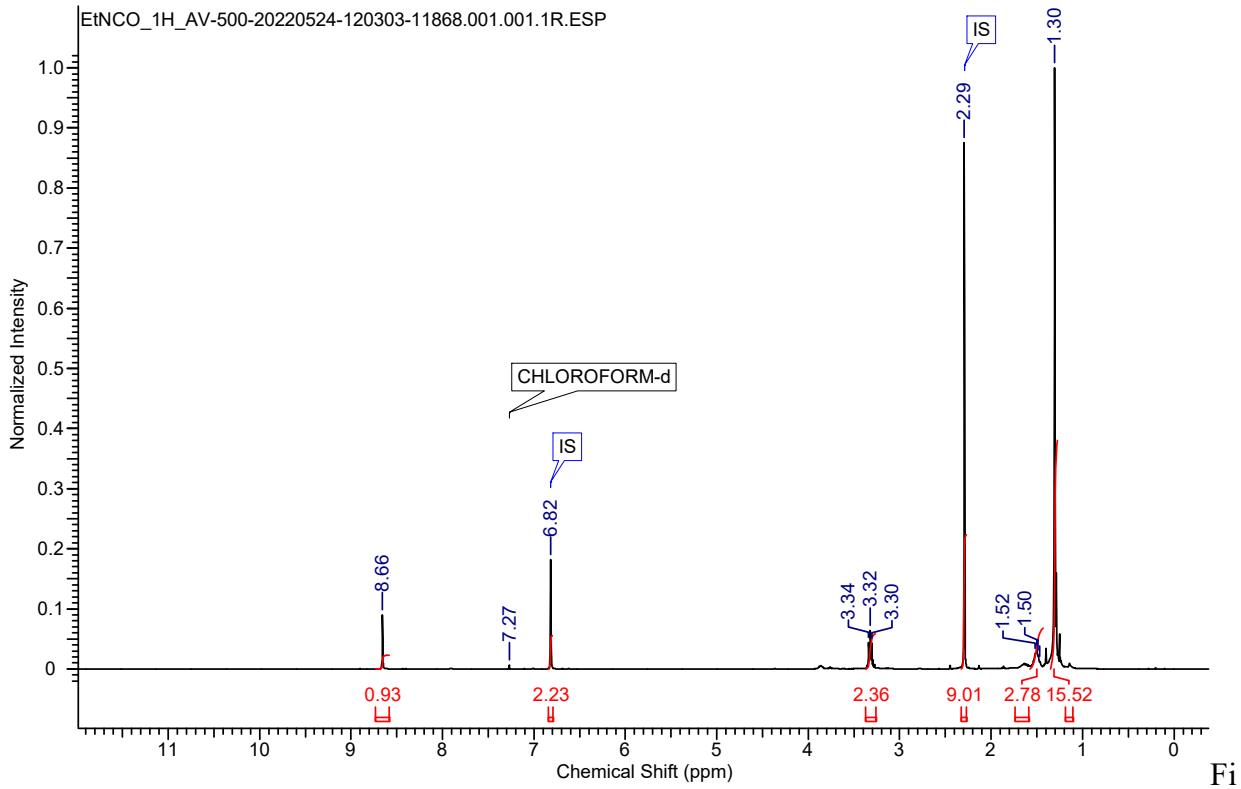


Figure S1. ^{1}H NMR spectrum of **2a** ($CDCl_3$, 500 MHz, 298 K).

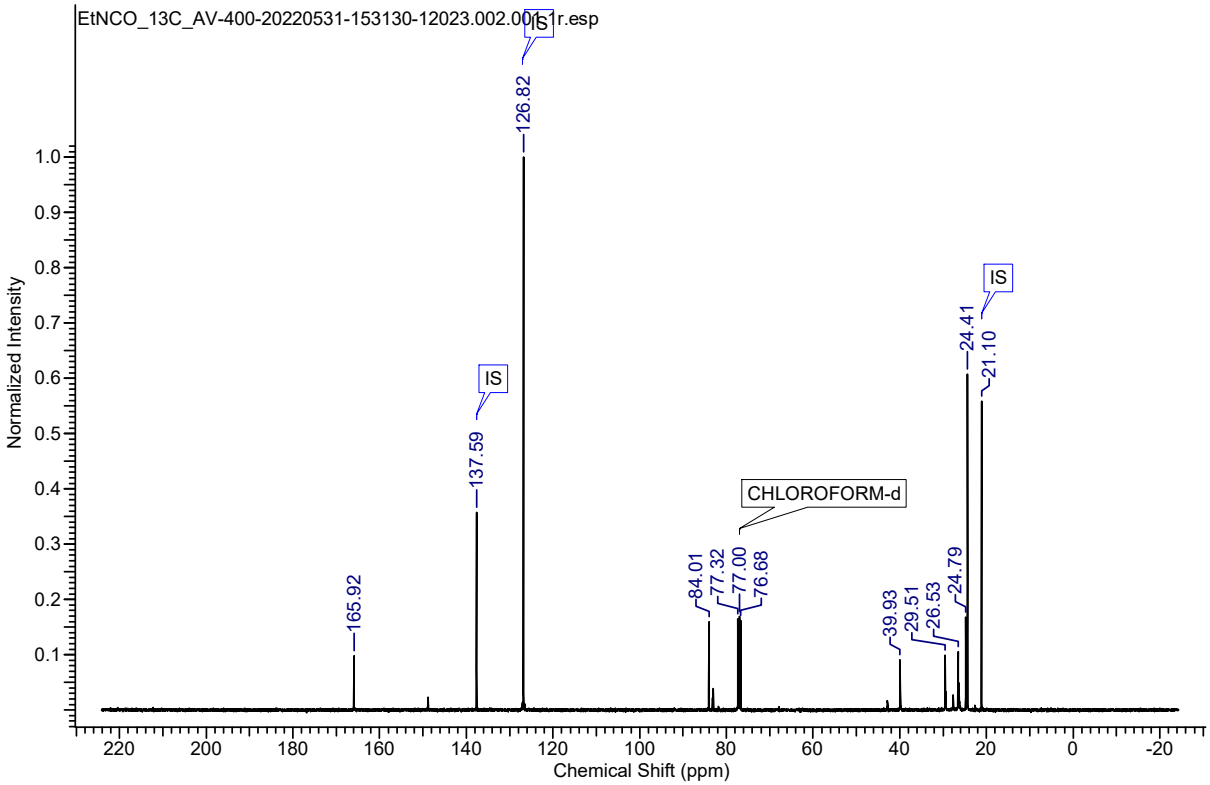
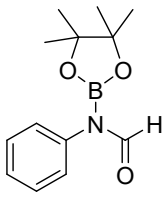


Figure S2. ^{13}C NMR spectrum of **2a** ($CDCl_3$, 101 MHz, 298 K).

N-phenyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2b): ^{1}H NMR (400 MHz, CHLOROFORM-*d*) δ 8.71 (s, 1 H, NC*H*O), 7.29-7.20 (m, 5H, Ph*H*), 2.87 (s, 3H, NCH_3), 1.08 (s, 12H) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.31 (s, 1 C), 148.58 (s, 1 C), 147.40 (s, 1 C), 133.58 (s, 1 C), 129.20 (s, 1 C), 128.84 (s, 1 C), 128.69 (s, 1 C), 128.40 (s, 1 C), 128.34 (s, 1 C), 128.24 (s, 1 C), 127.27 (s, 1 C), 127.05 (s, 1 C), 126.97 (s, 1 C), 120.51 (s, 1 C), 119.68 (s, 1 C), 118.74 (s, 1 C), 84.43 (s, 1 C), 82.98 (s, 1 C), 82.57 (s, 1 C), 81.78 (s, 1 C), 34.19 (s, 1 C), 24.55 (s, 1 C), 24.42 (s, 1 C), 24.34 (s, 1 C), 24.09 (s, 1 C), 22.60 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

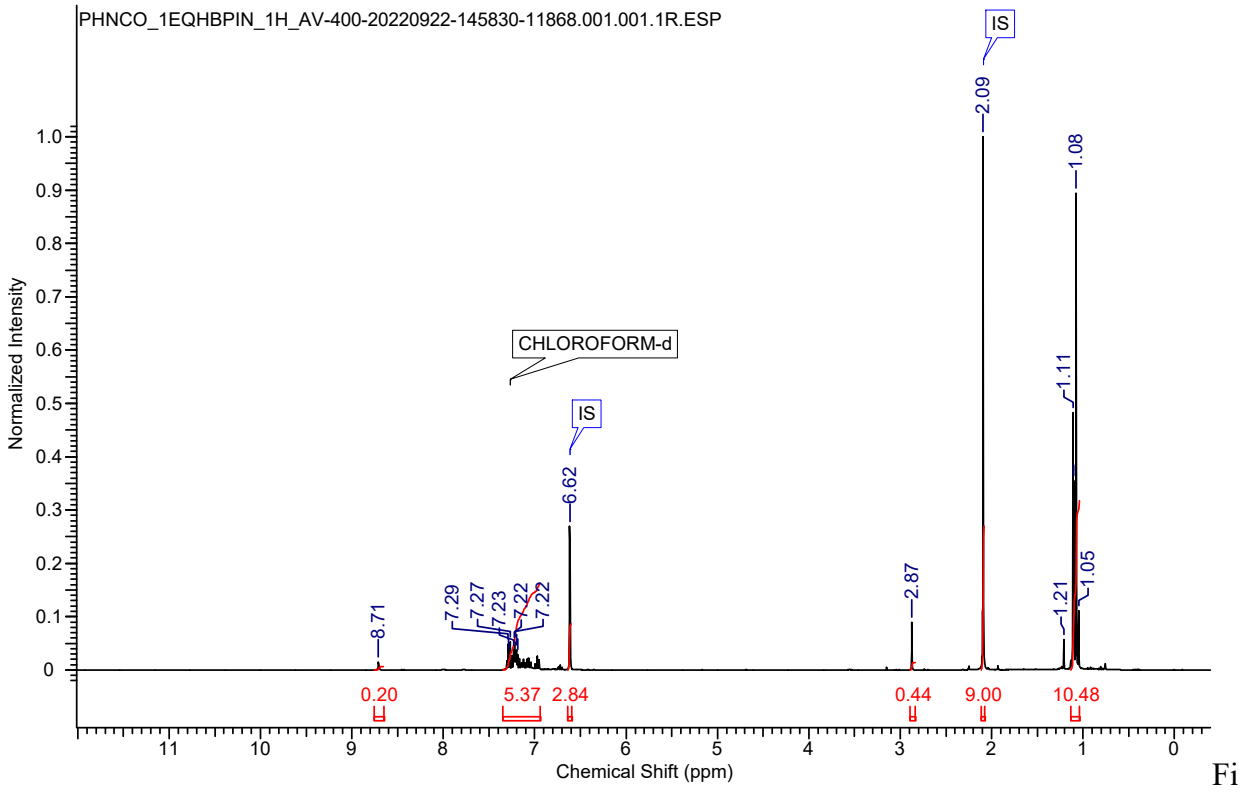


Figure S3. ^{1}H NMR spectrum of **2b** ($CDCl_3$, 400 MHz, 298 K).

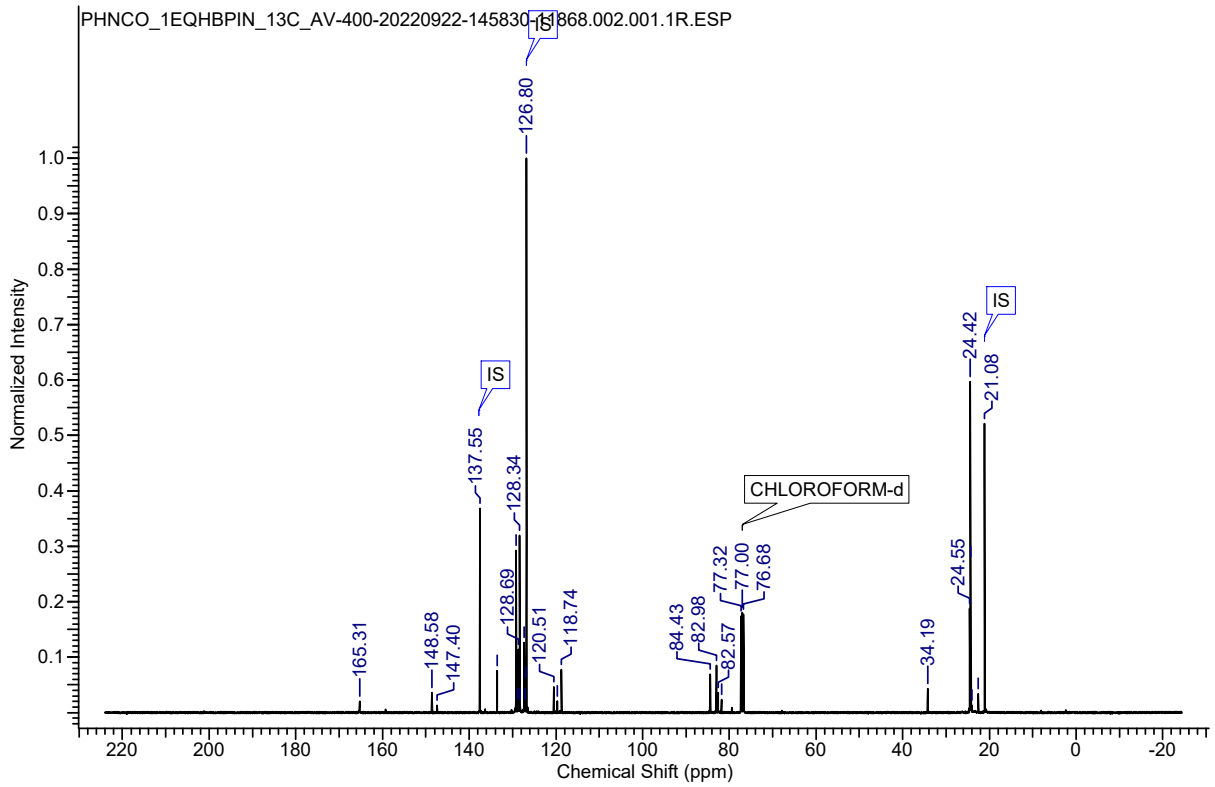
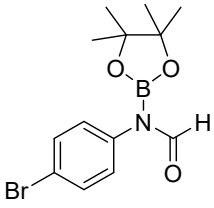


Figure S4. ^{13}C NMR spectrum of **2b** ($CDCl_3$, 101 MHz, 298 K).



N-(4-bromophenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2c): ^1H NMR ($CDCl_3$, 400 MHz, 298 K): δ 8.89 (s, 1H, NC*H*O), 7.53-7.51 (d, 2H, Ph*H*), 7.08-7.06 (d, 2H, Ph*H*), 1.34 (s, 12H, CH_3) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 50.28 MHz, 298 K): δ 165.05 (s, 1 C), 132.51 (s, 1 C), 131.86 (s, 1 C), 131.69 (s, 1 C), 130.03 (s, 1 C), 128.97 (s, 1 C), 120.67 (s, 1 C), 120.32 (s, 1 C), 84.70 (s, 1 C), 83.04 (s, 1 C), 24.56 (s, 1 C), 24.44 (s, 1 C), 24.39 (s, 1 C) ppm.

The spectroscopic data is consistent with the literature data. [S2]

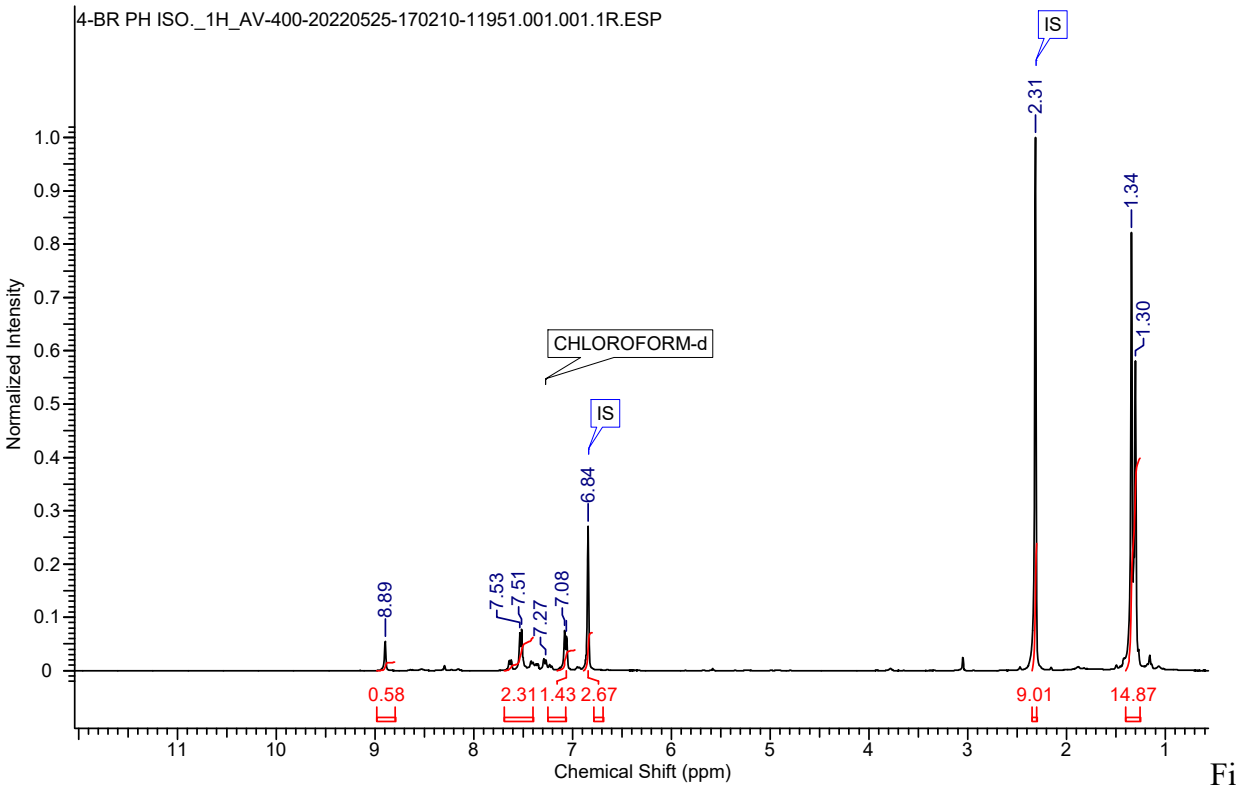


Figure S5. ^{1}H NMR spectrum of **2c** ($CDCl_3$, 400 MHz, 298 K).

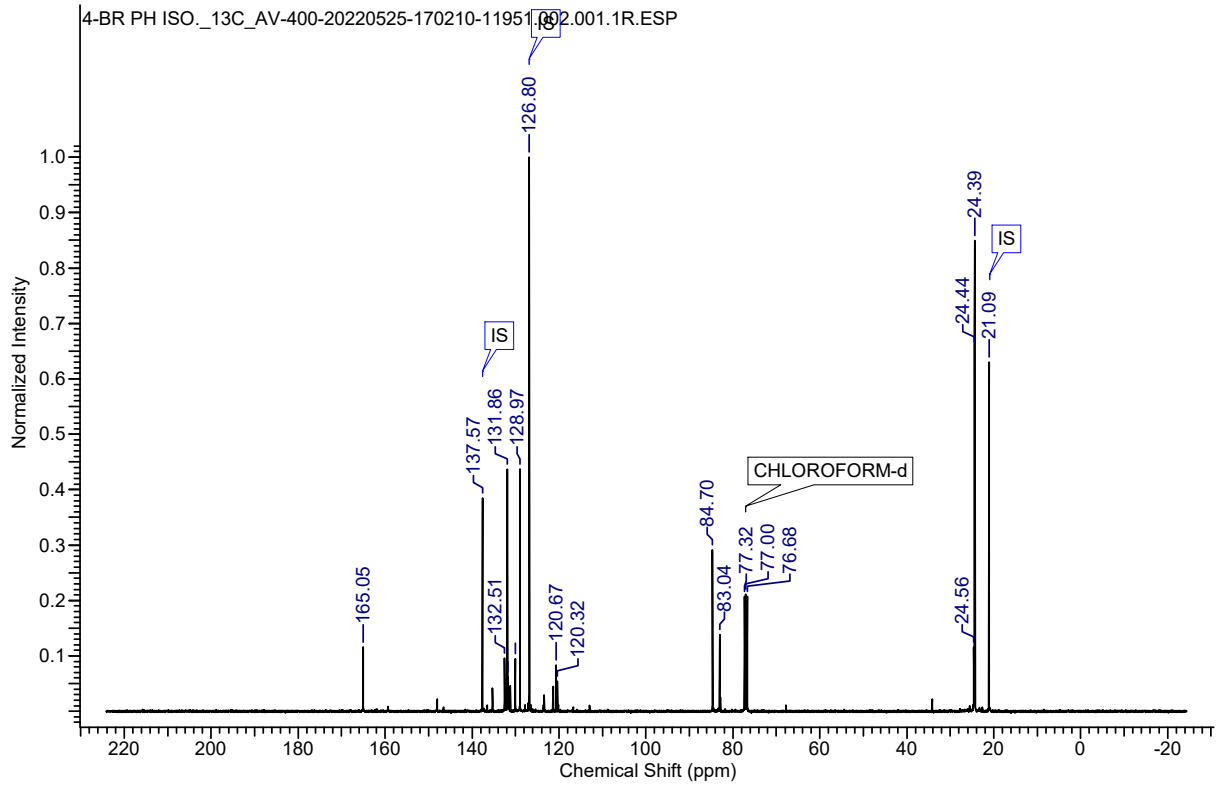
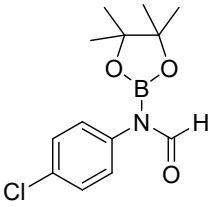


Figure S6. ^{13}C NMR spectrum of **2c** ($CDCl_3$, 101 MHz, 298 K).

N-(4-chlorophenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2d): ^{1}H NMR ($CDCl_3$, 200 MHz, 298 K): δ 8.84 (s, 1H, NC*H*O), 7.33-7.30 (d, 2H, Ph*H*), 7.08-7.06 (d, 2H, Ph*H*), 1.29 (s, 12H, CH_3) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.10 (s, 1 C), 129.72 (s, 1 C), 129.51 (s, 1 C), 128.88 (s, 1 C), 128.60 (s, 1 C), 84.67 (s, 1 C), 83.01 (s, 1 C), 24.44 (s, 1 C), 24.37 (s, 1 C), 24.28 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

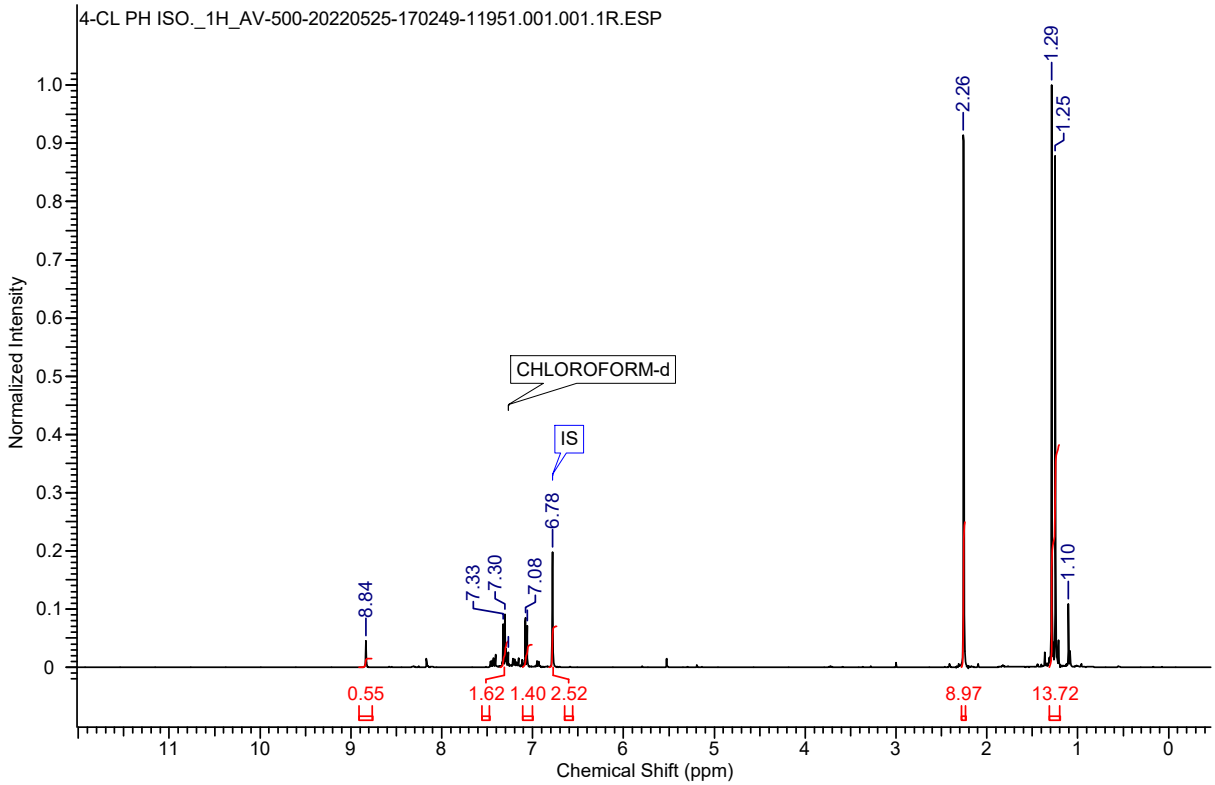


Figure S7. ^{1}H NMR spectrum of **2d** ($CDCl_3$, 500 MHz, 298 K).

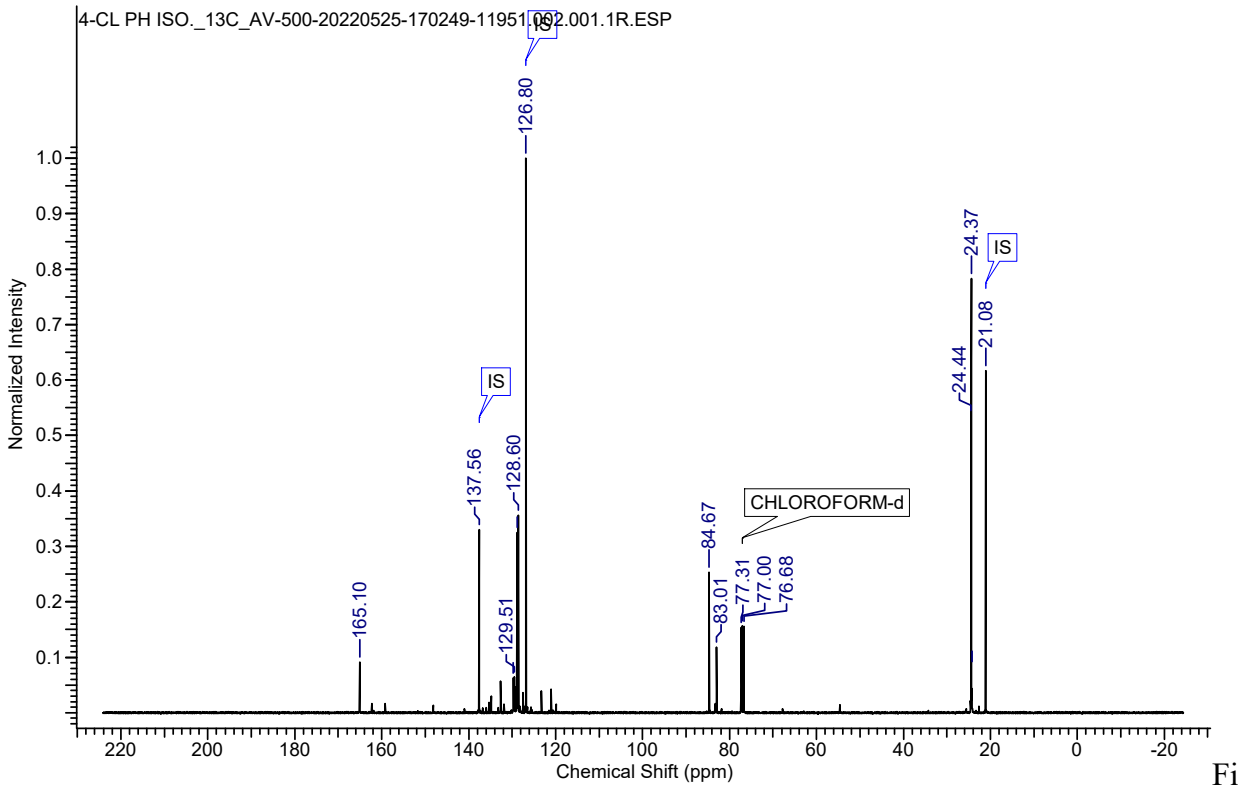
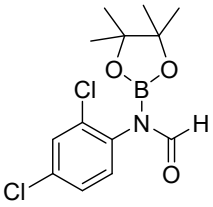


Figure S8. ^{13}C NMR spectrum of **2d** ($CDCl_3$, 101 MHz, 298 K).

N-(2,4-dichlorophenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2e): ^{1}H NMR ($CDCl_3$, 200 MHz, 298 K): δ 8.91 (s, 1H, NC*H*O), 7.53-7.32 (m, 3H, Ph*H*), 1.37 (s, 12H, CH_3) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.10 (s, 1 C), 129.72 (s, 1 C), 129.51 (s, 1 C), 128.88 (s, 1 C), 128.60 (s, 1 C), 84.67 (s, 1 C), 83.01 (s, 1 C), 24.44 (s, 1 C), 24.37 (s, 1 C), 24.28 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

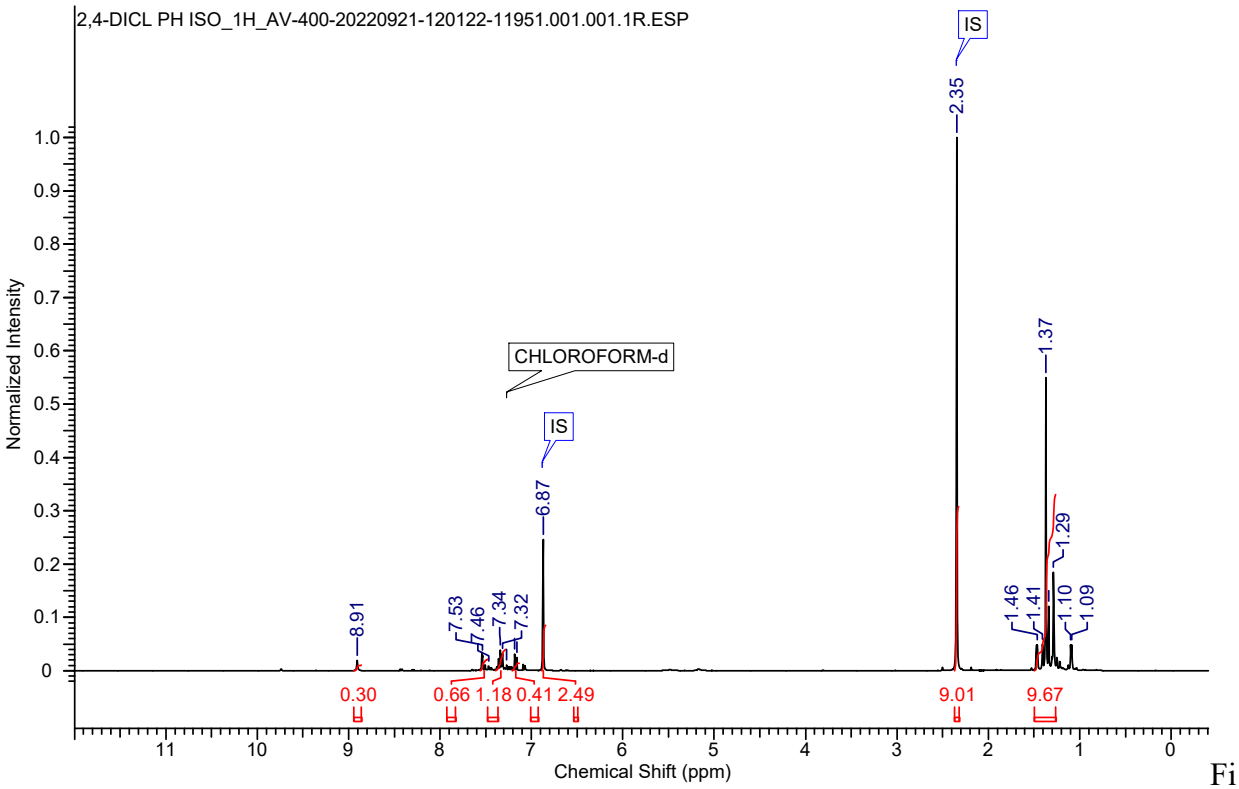


Figure S9. ^{1}H NMR spectrum of **2e** ($CDCl_3$, 400 MHz, 298 K).

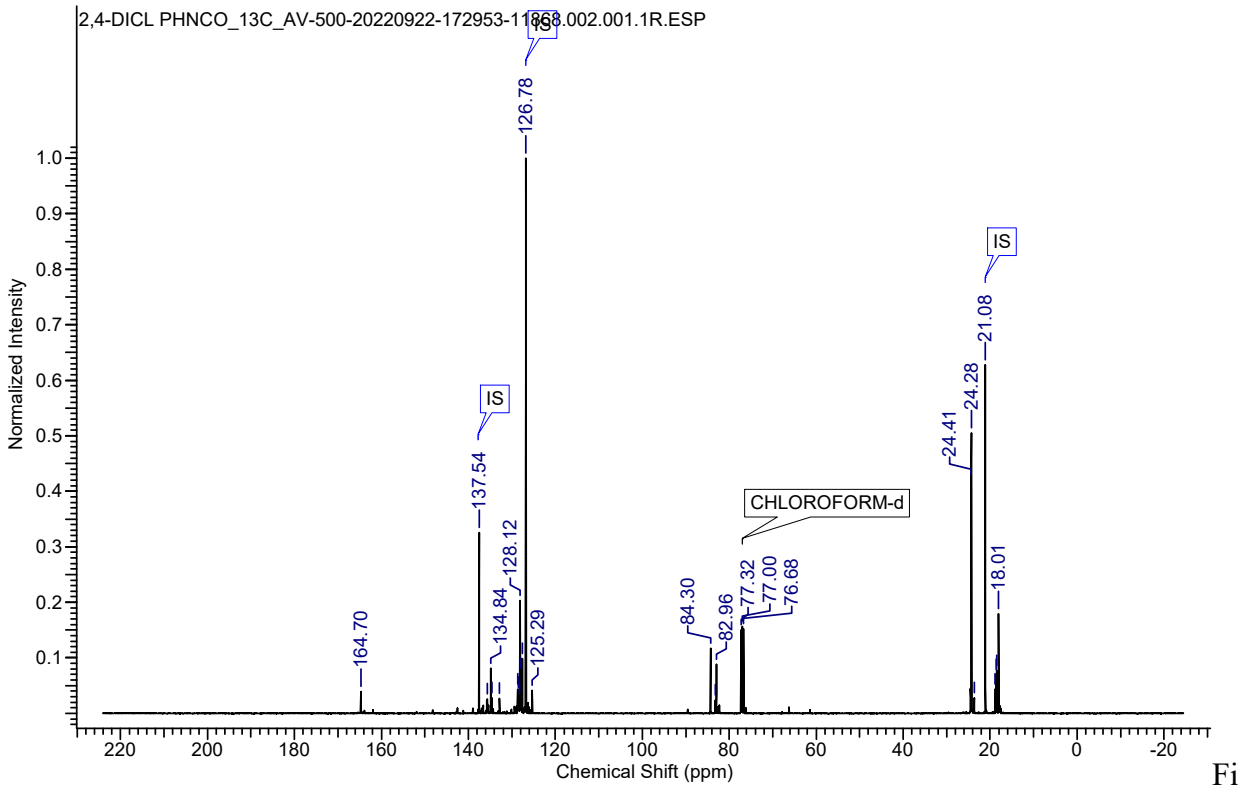
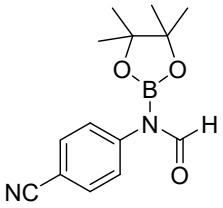


Figure S10. ^{13}C NMR spectrum of **2e** ($CDCl_3$, 101 MHz, 298 K).



N-(4-cyanophenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2f): ^1H NMR ($CDCl_3$, 500 MHz, 298 K): δ 8.74 (s, 1H, NC*H*O), 7.52-7.50 (d, 2H, Ph*H*), 7.18-7.16 (d, 2H, Ph*H*), 5.57 (s, 2H, NCH_2-OBpin), 2.92 (s, 3H, NCH_3), 1.13 (s, 12H, CH_3) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ 164.54 (s, 1 C), 140.55 (s, 1 C), 128.05 (s, 1 C), 125.56 (s, 1 C), 120.95 (s, 1 C), 119.65 (s, 1 C), 118.32 (s, 1 C), 117.98 (s, 1 C), 110.51 (s, 1 C), 84.95 (s, 1 C), 83.93 (s, 1 C), 83.29 (s, 1 C), 82.98 (s, 1 C), 24.50 (s, 1 C), 24.38 (s, 1 C), 24.34 (s, 1 C) ppm.

The spectroscopic data is consistent with the literature data. [S2]

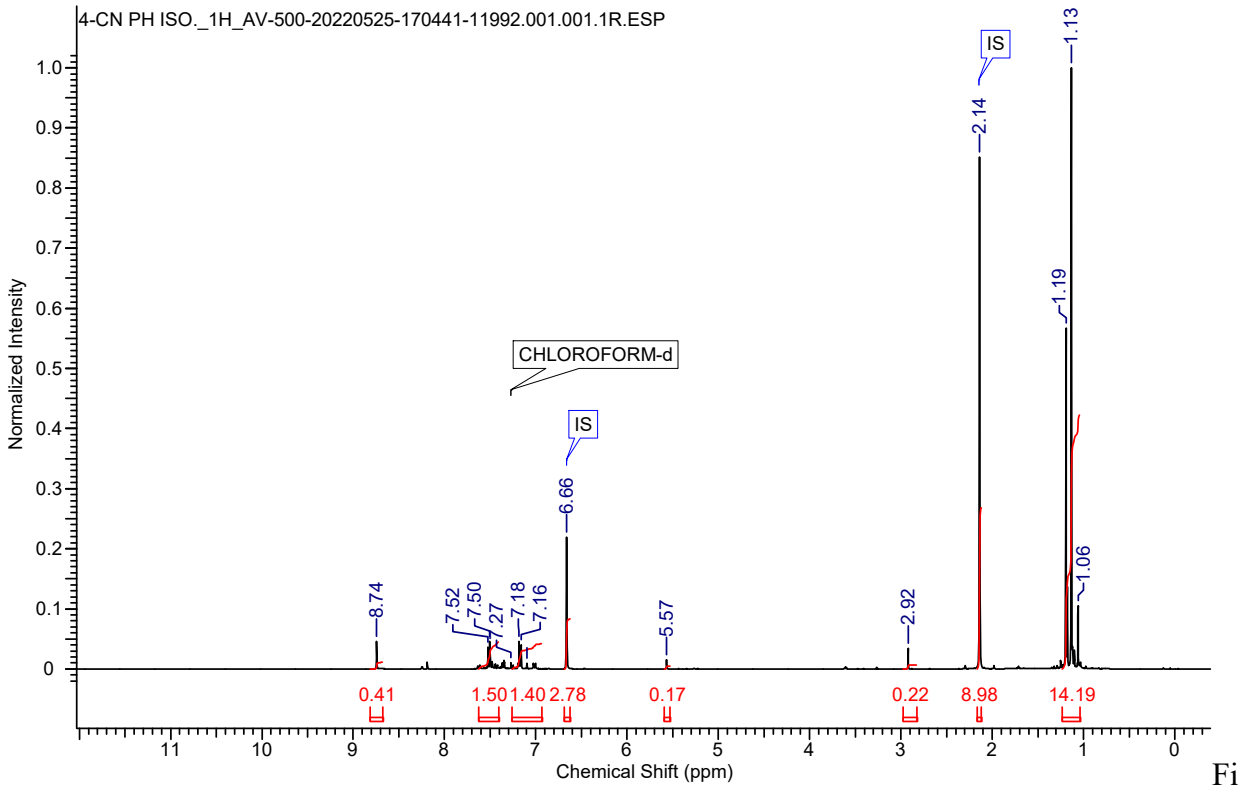


Figure S11. ^{1}H NMR spectrum of **2f** ($CDCl_3$, 500 MHz, 298 K).

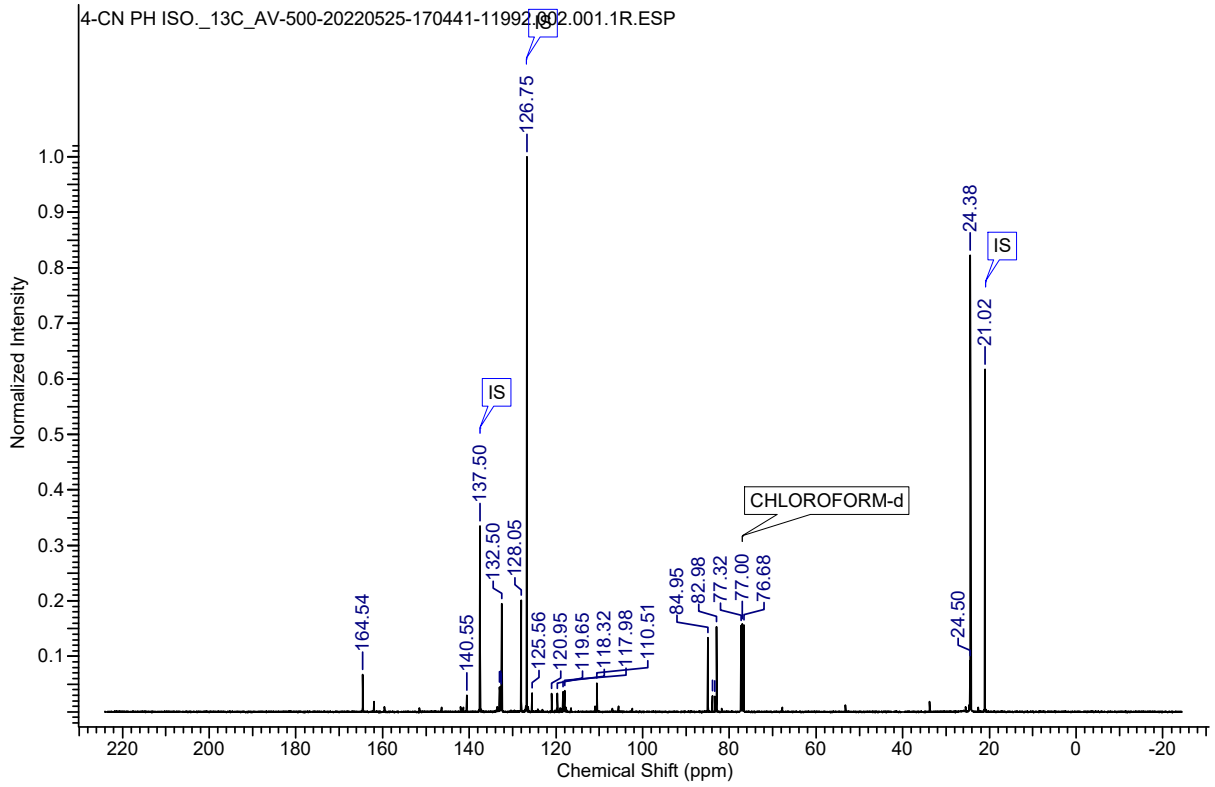
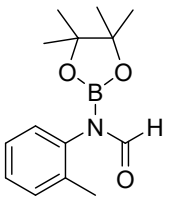


Figure S12. ^{13}C NMR spectrum of **2f** ($CDCl_3$, 101 MHz, 298 K).

N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-N-(o-tolyl)formamide (2g): ^1H NMR ($CDCl_3$, 400 MHz, 298 K): δ 8.96 (s, 1H, NC*H*O), 7.31-7.28 (m, 3H, Ph*H*), 7.08-7.06 (m, 1H, Ph*H*), 2.24 (s, 3H, NCH_3), 1.35 (s, 12H, CH_3) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.01 (s, 1 C), 134.90 (s, 1 C), 130.61 (s, 1 C), 128.12 (s, 1 C), 127.74 (s, 1 C), 126.52 (s, 1 C), 84.35 (s, 1 C), 82.99 (s, 1 C), 24.41 (s, 1 C), 24.25 (s, 1 C), 17.72 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

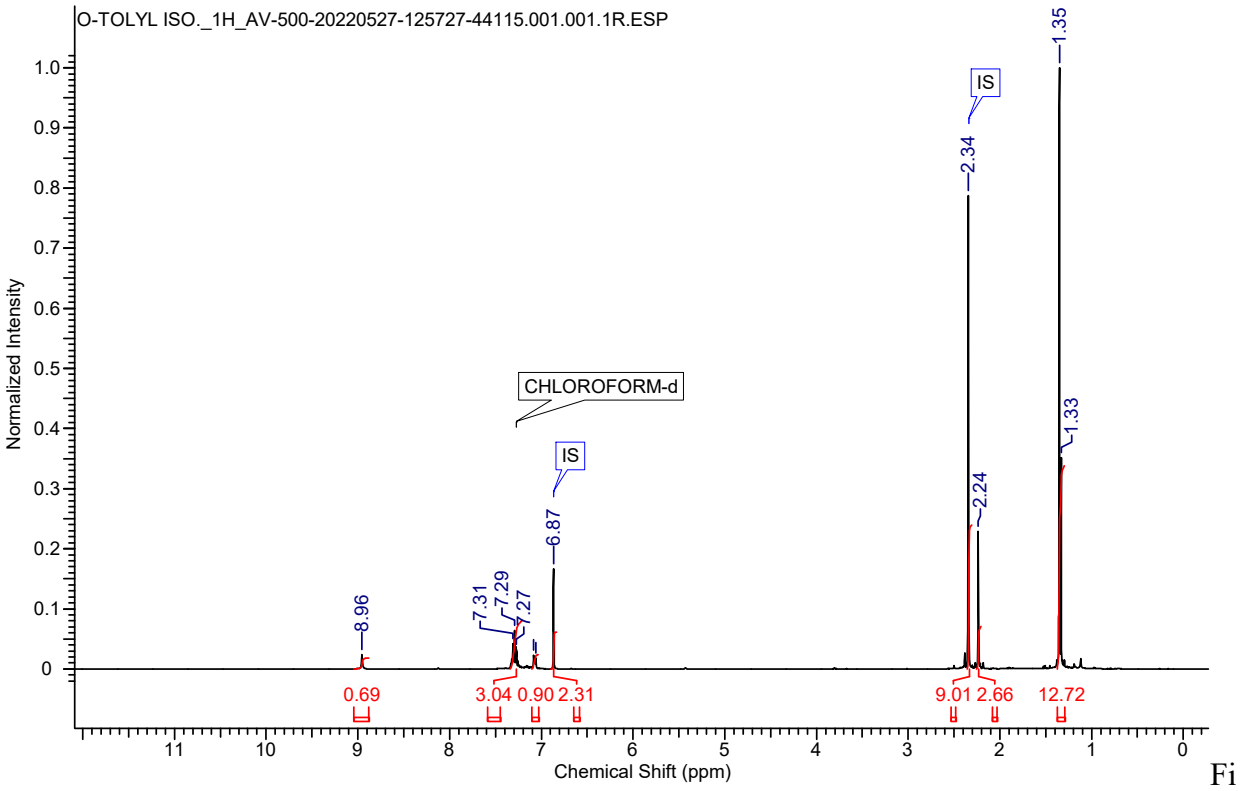


Figure S13. ^{1}H NMR spectrum of **2g** ($CDCl_3$, 500 MHz, 298 K).

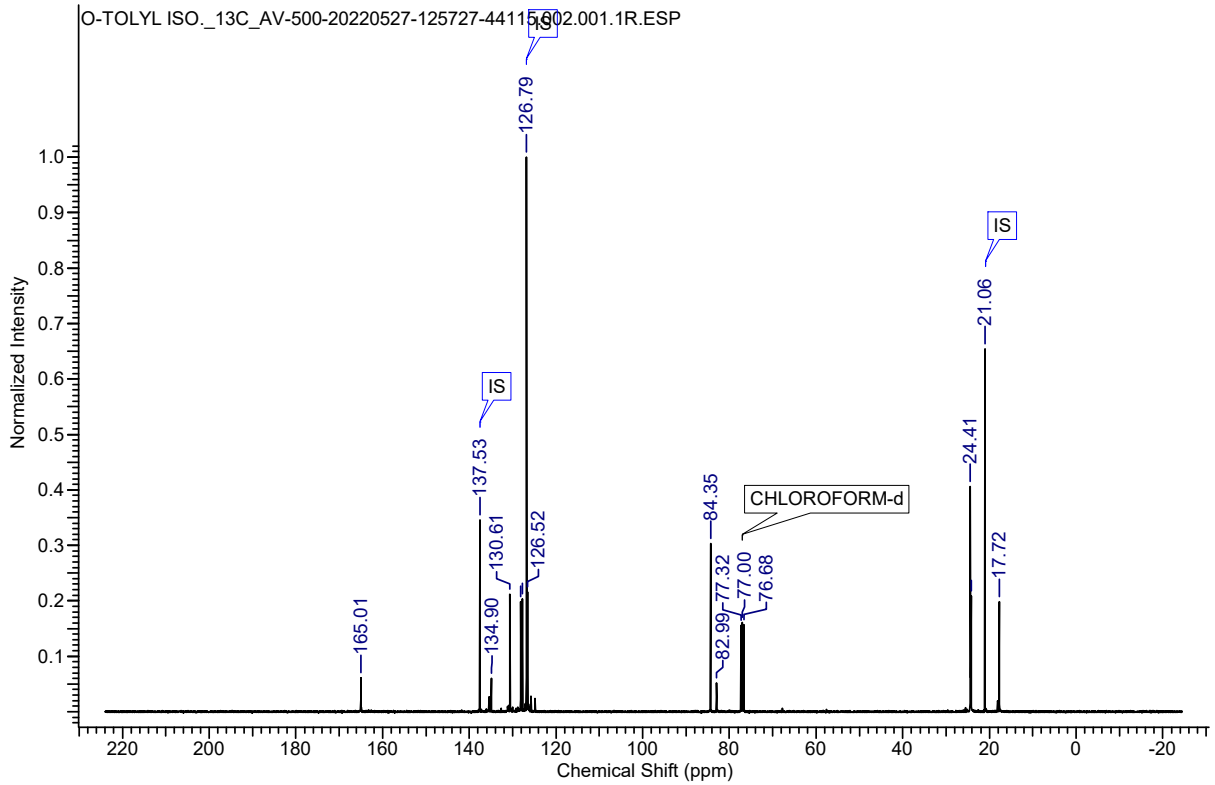


Figure S14. ^{13}C NMR spectrum of **2g** ($CDCl_3$, 101 MHz, 298 K).

N-(2,6-dimethylphenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2h): ^{1}H NMR ($CDCl_3$, 500 MHz, 298 K): δ 8.99 (s, 1H, NC*H*O), 7.20-7.07 (m, 3H, Ph*H*), 2.41 (s, 3H, PhCH_3), 2.23 (s, 3H, PhCH_3), 1.37 (s, 12H, CH_3) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ 164.70 (s, 1 C), 134.84 (s, 1 C), 128.12 (s, 1 C), 127.94 (s, 1 C), 127.59 (s, 1 C), 84.30 (s, 1 C), 82.96 (s, 1 C), 24.41 (s, 1 C), 24.28 (s, 1 C), 18.59 (s, 1 C), 18.41 (s, 1 C), 18.01 (s, 1 C) ppm.

The spectroscopic data is consistent with the literature data. [S2]

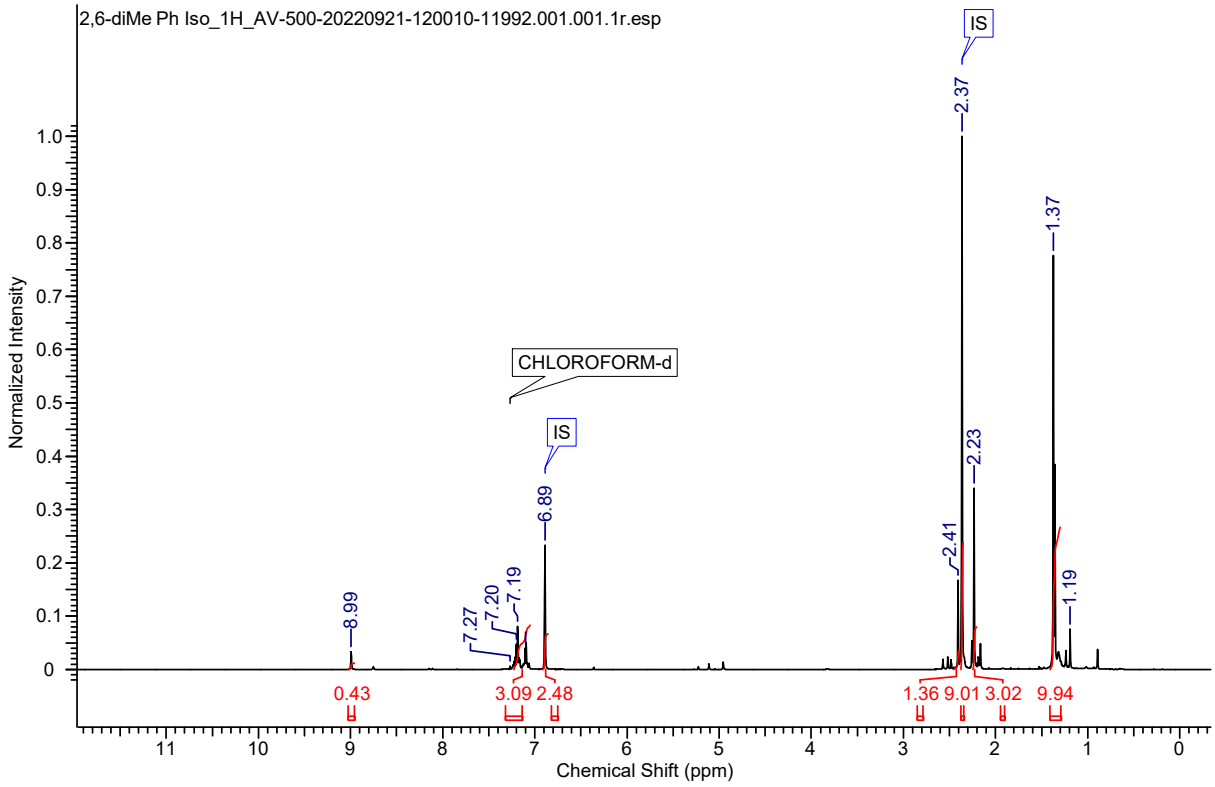


Figure S15. ^{1}H NMR spectrum of **2h** ($CDCl_3$, 500 MHz, 298 K).

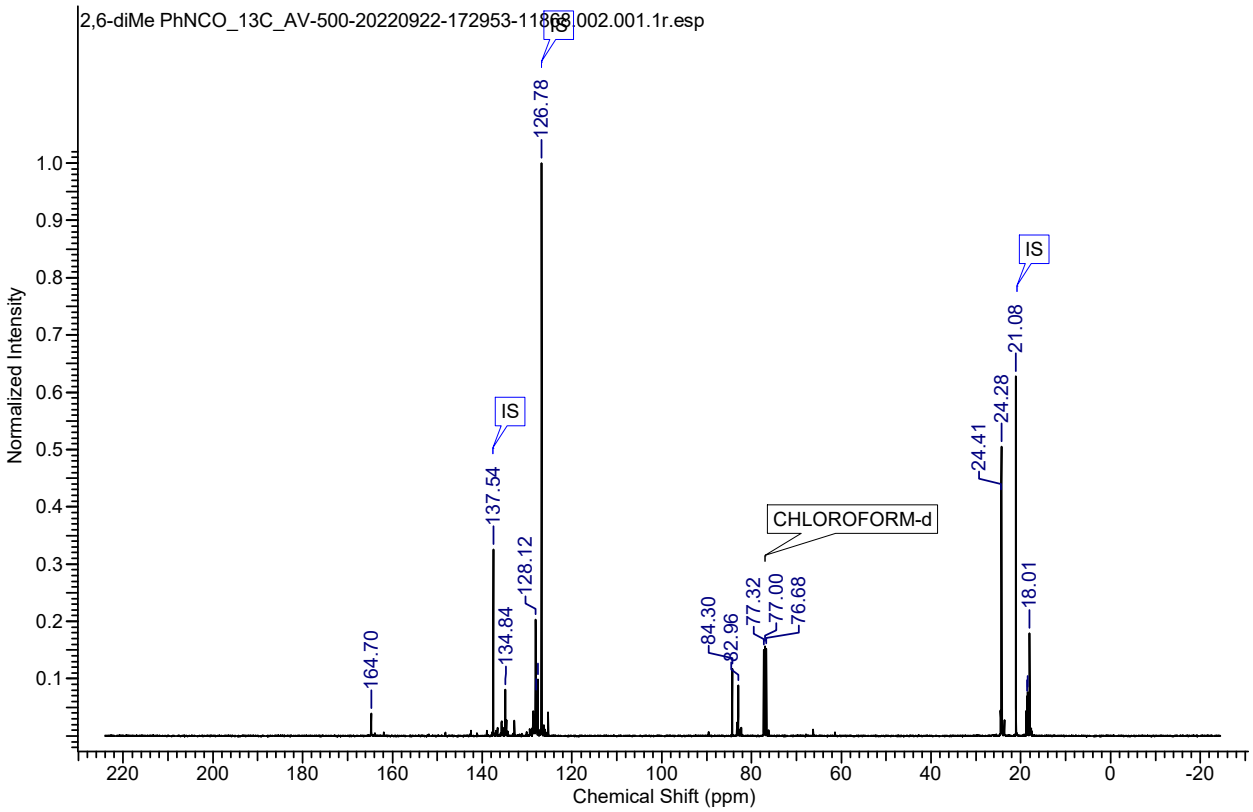
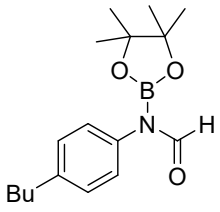
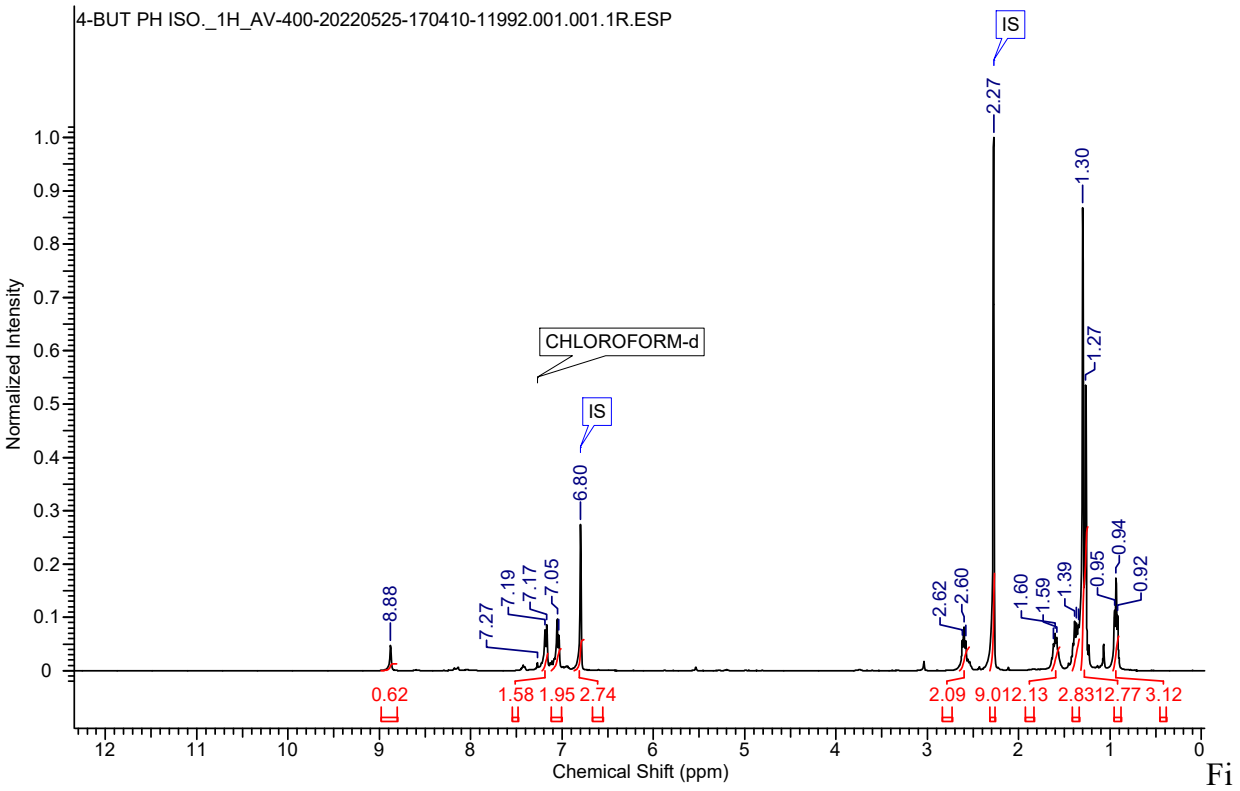


Figure S16. ^{13}C NMR spectrum of **2h** ($CDCl_3$, 101 MHz, 298 K).

N-(4-butylphenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2i): ^1H NMR ($CDCl_3$, 100 MHz, 298 K): δ ppm 8.88 (s, 1H, NC*H*O), 7.19-7.17 (d, 2H, Ph*H*), 7.05-7.03 (d, 2H, Ph*H*), 2.62-2.58 (t, 2H, *Bu*), 1.62-1.59 (t, 2H, *Bu*), 1.39-1.35 (t, 2H, *Bu*), 1.30 (s, 12H, CH_3) 0.95-0.92 (t, 3H, *Bu*) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.48 (s, 1 C), 141.51 (s, 1 C), 128.67 (s, 1 C), 126.90 (s, 1 C), 84.36 (s, 1 C), 82.98 (s, 1 C), 35.16 (s, 1 C), 33.28 (s, 1 C), 24.54 (s, 1 C), 24.41 (s, 1 C), 24.34 (s, 1 C), 22.34 (s, 1 C), 13.83 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]



Fi

gure S17. ^{1}H NMR spectrum of **2i** ($CDCl_3$, 400 MHz, 298 K).

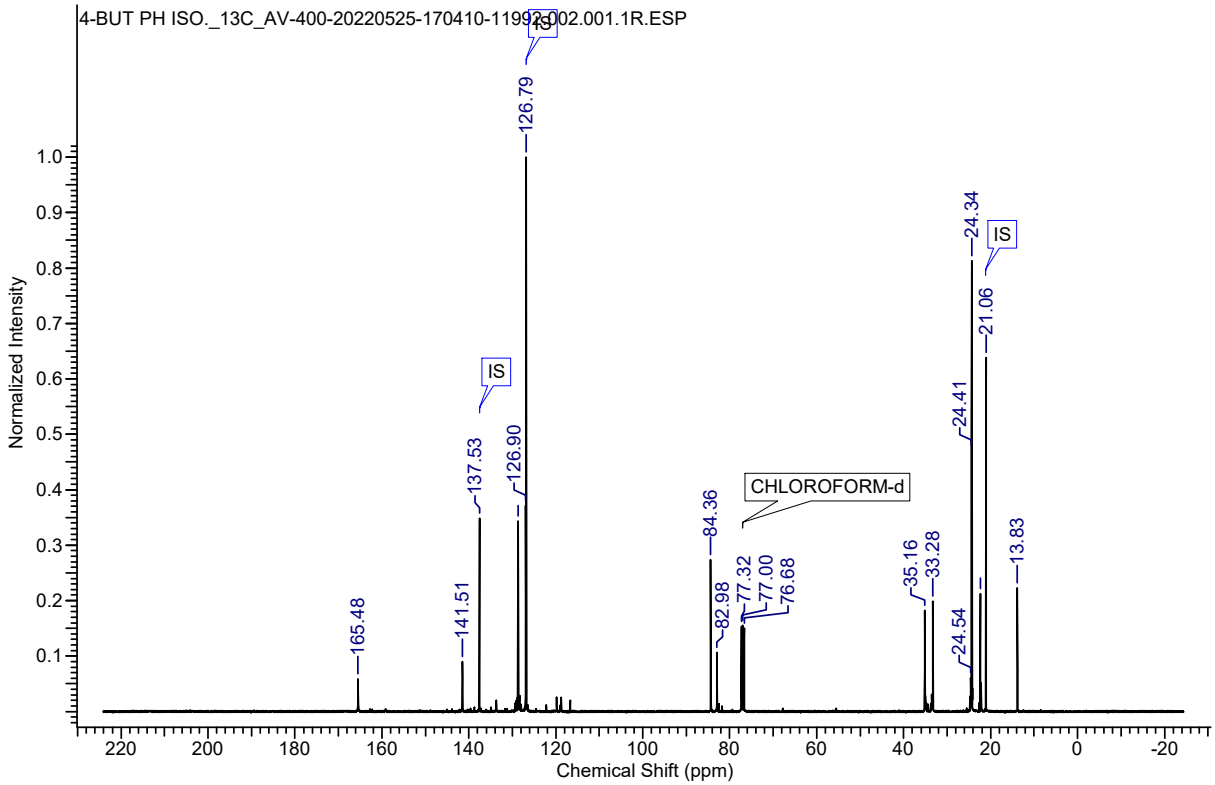
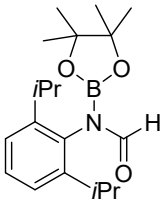


Figure S18. ^{13}C NMR spectrum of **2i** ($CDCl_3$, 101 MHz, 298 K).

N-(2,6-diisopropylphenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2j):



^{1}H NMR ($CDCl_3$, 500 MHz, 298 K): δ 8.91 (s, 1H, NC*H*O), 7.15-7.08 (m, 3H, Ph*H*), 4.97 (s, 2H, NCH_2), 3.27-3.22 {q, 1H, C*H*-$(CH_3)_2$}, 2.83-2.78 (q, 1H, C*H*-$(CH_3)_2$), 1.22 (s, 12H, CH_3), 1.15-1.13 {d, 6H, CH-(CH_3)$_2$}, 1.04-1.02 {d, 6H, CH-(CH_3)$_2$} ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.45 (s, 1 C), 147.31 (s, 1 C), 145.22 (s, 1 C), 142.92 (s, 1 C), 128.37 (s, 1 C), 126.90 (s, 1 C), 123.46 (s, 1 C), 123.35 (s, 1 C), 123.28 (s, 1 C), 84.39 (s, 1 C), 82.73 (s, 1 C), 82.21 (s, 1 C), 77.07 (s, 1 C), 28.65 (s, 1 C), 27.98 (s, 1 C), 24.81 (s, 1 C), 24.45 (s, 1 C), 24.34 (s, 1 C), 24.33 (s, 1 C), 23.78 (s, 1 C), 23.57 (s, 1 C), 22.76 (s, 1 C) ppm.

The spectroscopic data is consistent with the literature data. [S2]

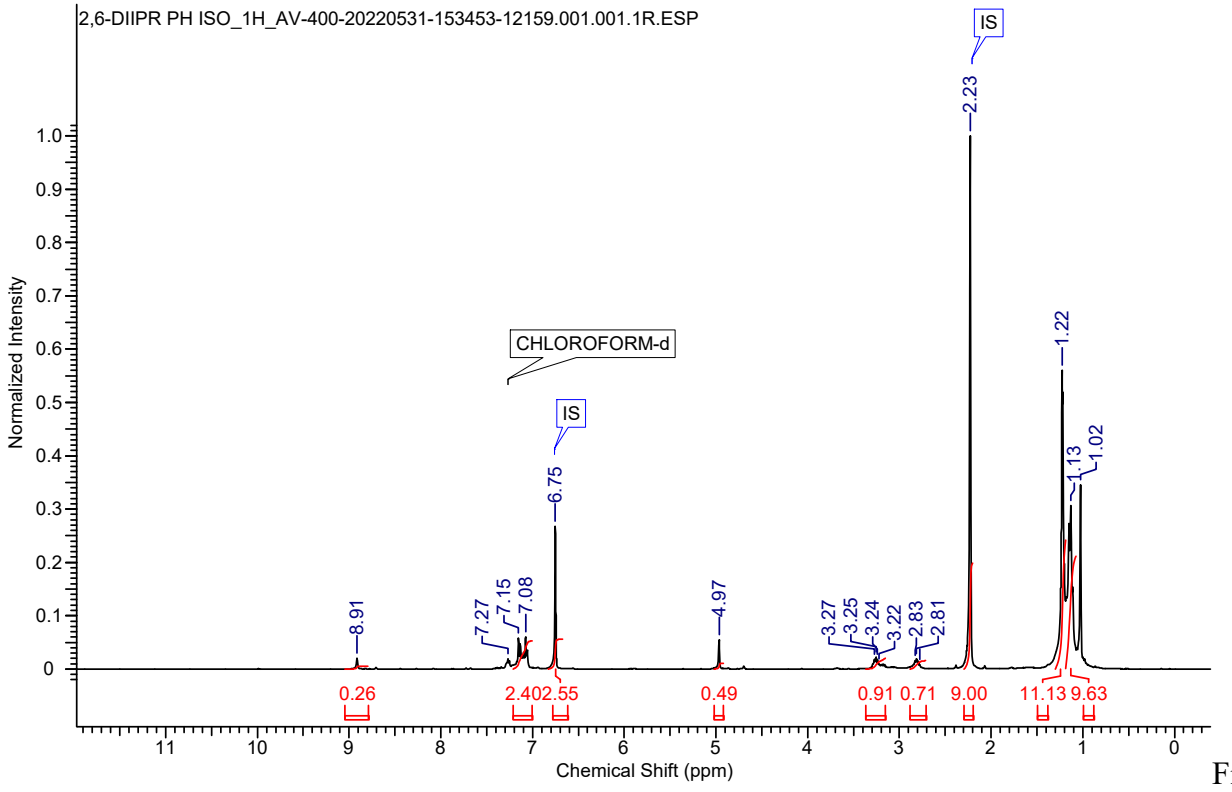


Figure S19. ^{1}H NMR spectrum of **2j** ($CDCl_3$, 400 MHz, 298 K).

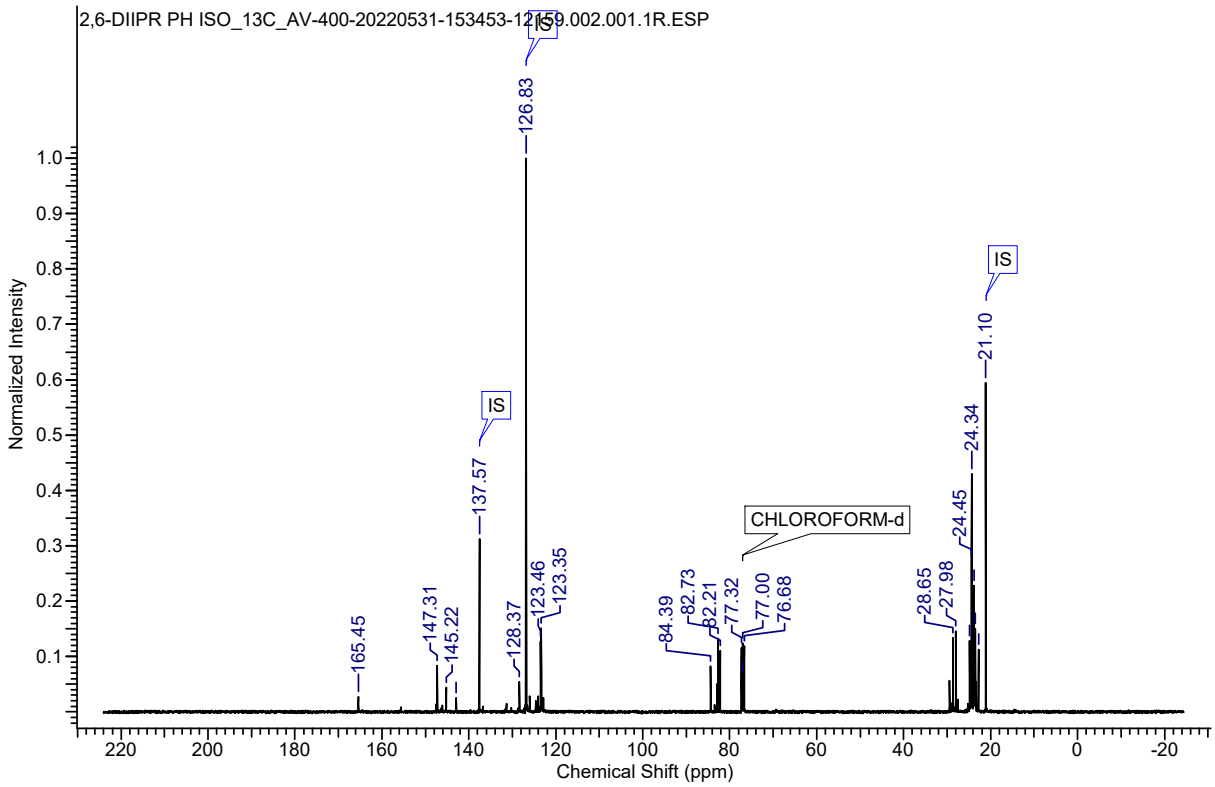
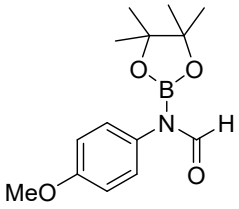


Figure S20. ^{13}C NMR spectrum of **2j** ($CDCl_3$, 101 MHz, 298 K).

N-(4-methoxyphenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2k): ^{1}H NMR ($CDCl_3$, 500 MHz, 298 K): δ 8.94 (s, 1H, NC*H*O), 6.99-6.96 (d, 2H, Ph*H*), 6.82-6.80 (d, 2H, Ph*H*), 3.69 (s, 3H, PhCH_3), 1.22 (s, 12H, CH_3) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.56 (s, 1 C), 158.25 (s, 1 C), 128.18 (s, 1 C), 125.45 (s, 1 C), 124.04 (s, 1 C), 114.02 (s, 1 C), 84.37 (s, 1 C), 82.95 (s, 1 C), 55.16 (s, 1 C), 24.41 (s, 1 C), 24.34 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

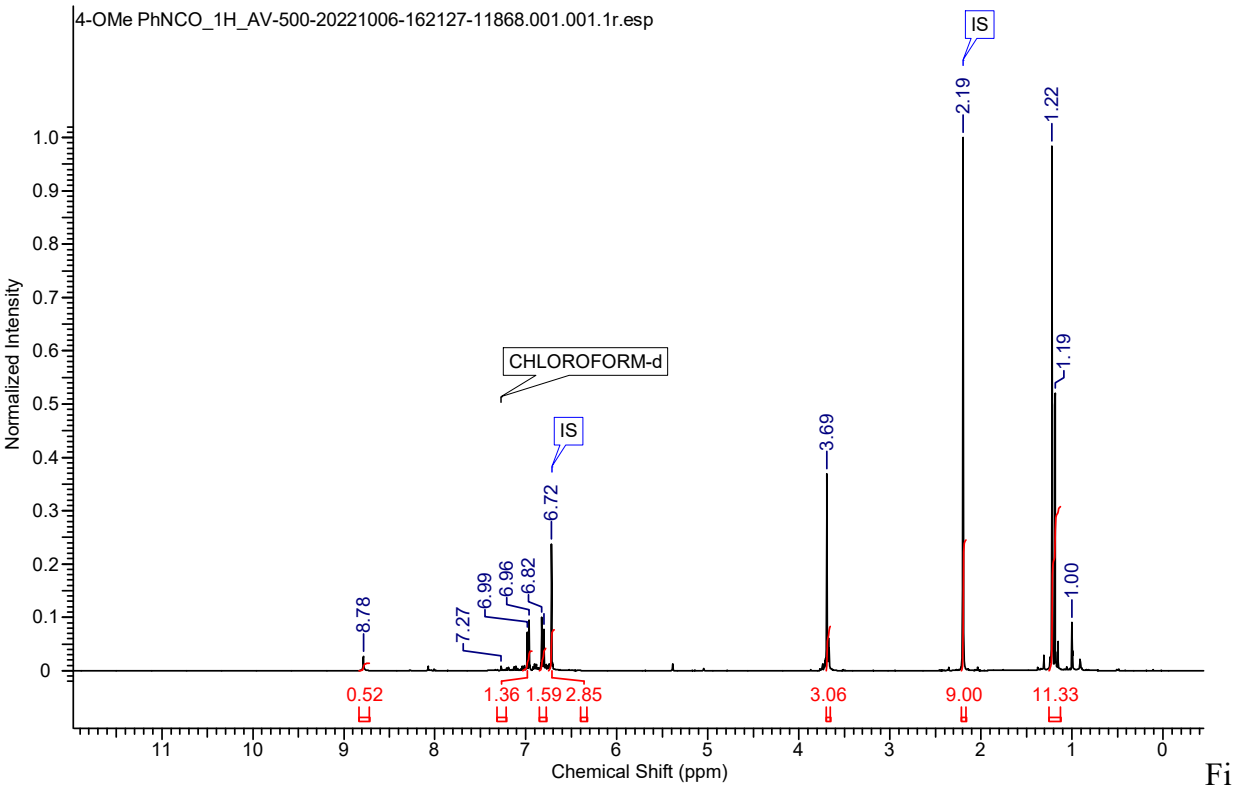


Figure S21. ^{1}H NMR spectrum of **2k** ($CDCl_3$, 400 MHz, 298 K).

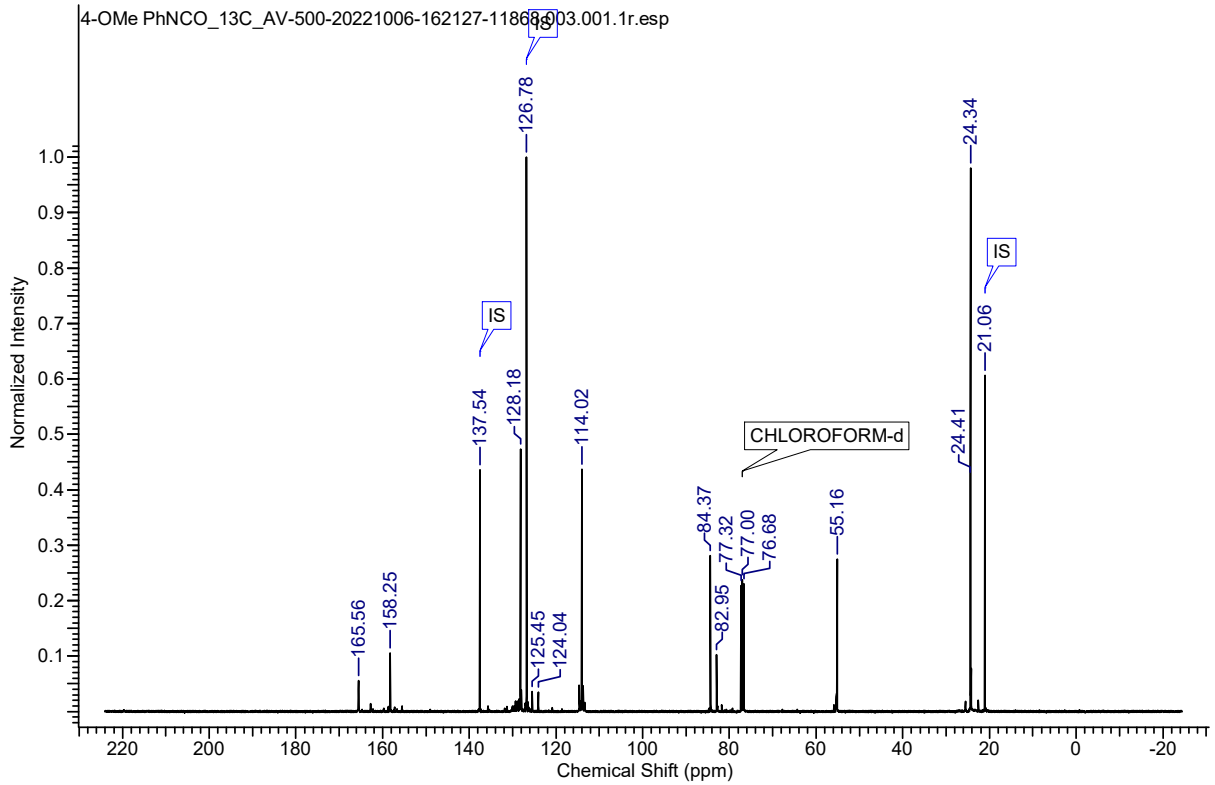
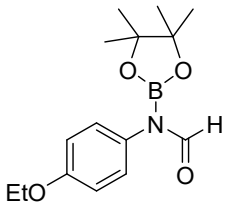


Figure S22. ^{13}C NMR spectrum of **2k** ($CDCl_3$, 101 MHz, 298 K).

N-(4-ethoxyphenyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2l): ^{1}H NMR ($CDCl_3$, 500 MHz, 298 K): δ 8.93 (s, 1H, NC*H*O), 7.11-7.09 (d, 2H, Ph*H*), 6.95-6.93 (d, 2H, Ph*H*), 4.08-4.03 (q, 2H, Ph-OCH_2CH$_3$), 1.47-1.44 (t, 3H, Ph-OCH$_2$CH_3), 1.36 (s, 12H, CH_3) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ ppm 165.58 (s, 1 C), 157.67 (s, 1 C), 129.30 (s, 1 C), 128.14 (s, 1 C), 118.66 (s, 1 C), 115.12 (s, 1 C), 114.86 (s, 1 C), 114.51 (s, 1 C), 84.35 (s, 1 C), 82.98 (s, 1 C), 63.59 (s, 1 C), 63.54 (s, 1 C), 63.36 (s, 1 C), 24.75 (s, 1 C), 24.53 (s, 1 C), 24.40 (s, 1 C), 24.34 (s, 1 C), 24.25 (s, 1 C), 14.71 (s, 1 C), 14.63 (s, 1 C), 14.59 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

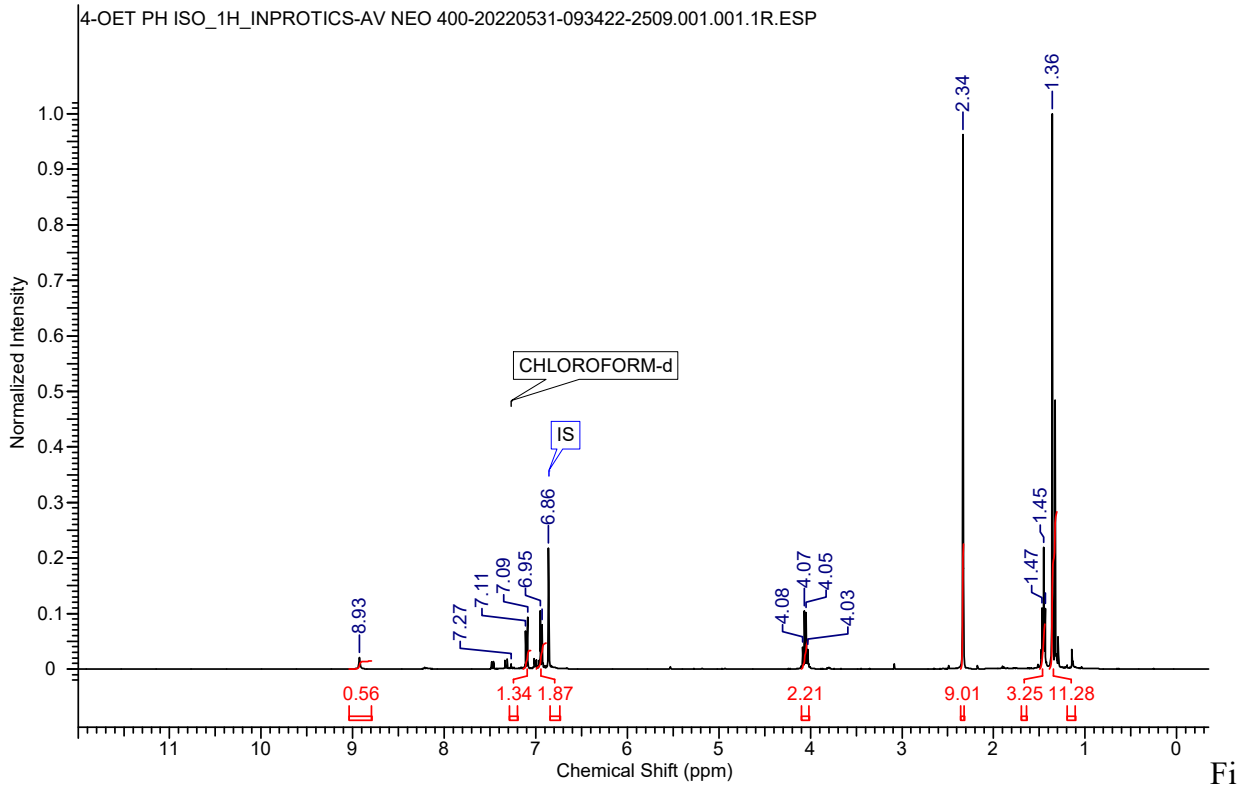


Figure S23. ^{1}H NMR spectrum of **2l** ($CDCl_3$, 500 MHz, 298 K).

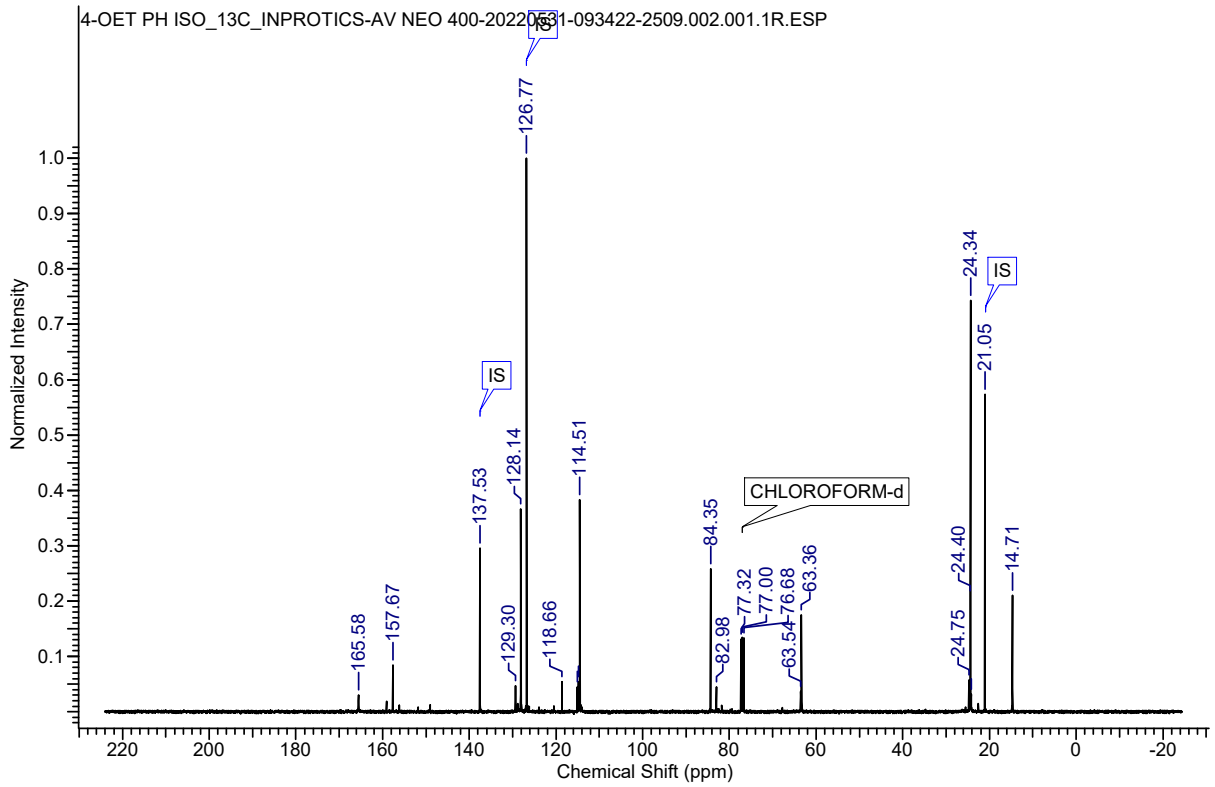
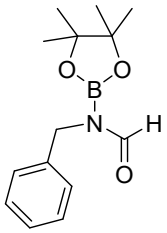


Figure S24. ^{13}C NMR spectrum of **2l** ($CDCl_3$, 100.28 MHz, 298 K).

N-benzyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2l): ^{1}H NMR ($CDCl_3$, 500 MHz, 298 K): δ 8.79 (s, 1H, NC*H*O), 7.43-7.29 (m, 5H, Ph*H*), 5.10 (s, 2H, NCH_2), 4.58 (s, 2H, PhCH_2), 1.35 (s, 12H, CH_3) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ 165.61 (s, 1 C), 148.98 (s, 1 C), 138.76 (s, 1 C), 135.71 (s, 1 C), 128.99 (s, 1 C), 128.79 (s, 1 C), 128.72 (s, 1 C), 128.57 (s, 1 C), 128.50 (s, 1 C), 128.33 (s, 1 C), 128.18 (s, 1 C), 128.09 (s, 1 C), 128.05 (s, 1 C), 127.83 (s, 1 C), 127.75 (s, 1 C), 127.19 (s, 1 C), 126.96 (s, 1 C), 126.60 (s, 1 C), 84.28 (s, 1 C), 82.99 (s, 1 C), 46.12 (s, 1 C), 44.29 (s, 1 C), 43.41 (s, 1 C), 24.53 (s, 1 C), 24.42 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]

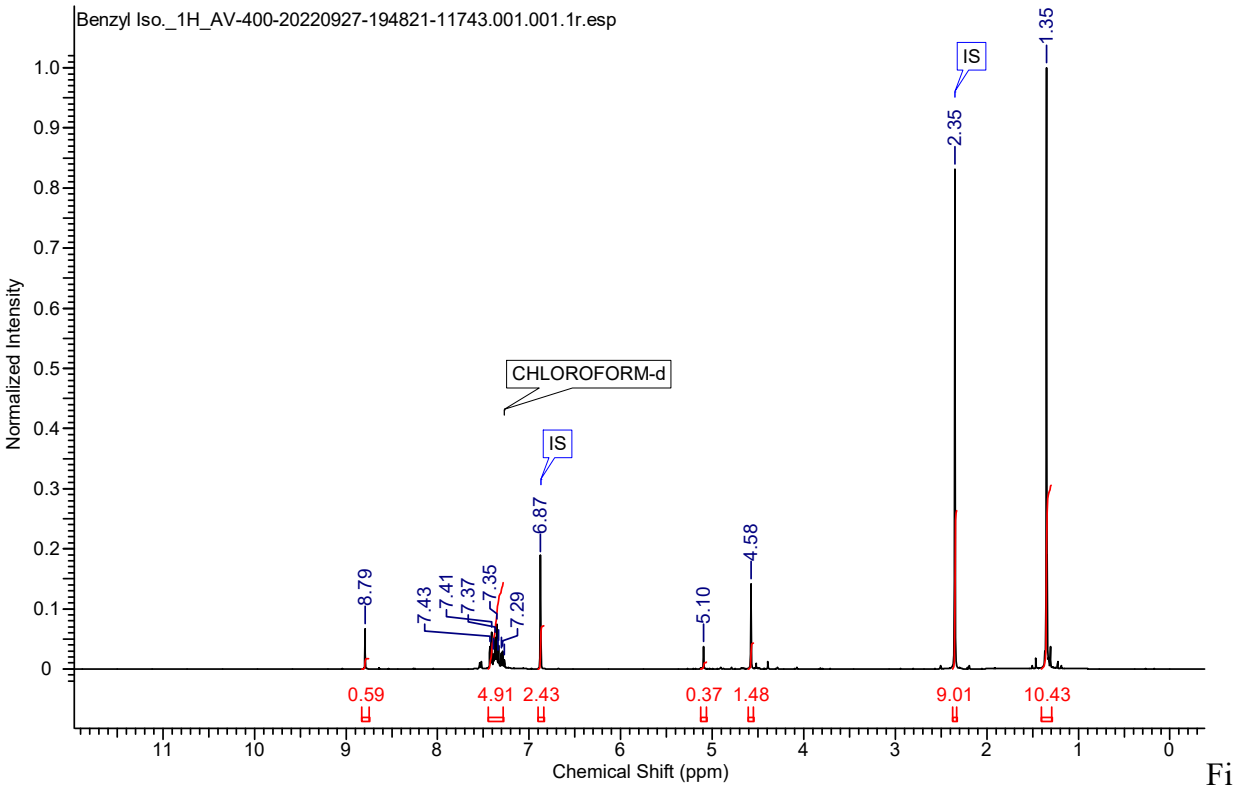


Figure S25. ^{1}H NMR spectrum of **2m** ($CDCl_3$, 500 MHz, 298 K).

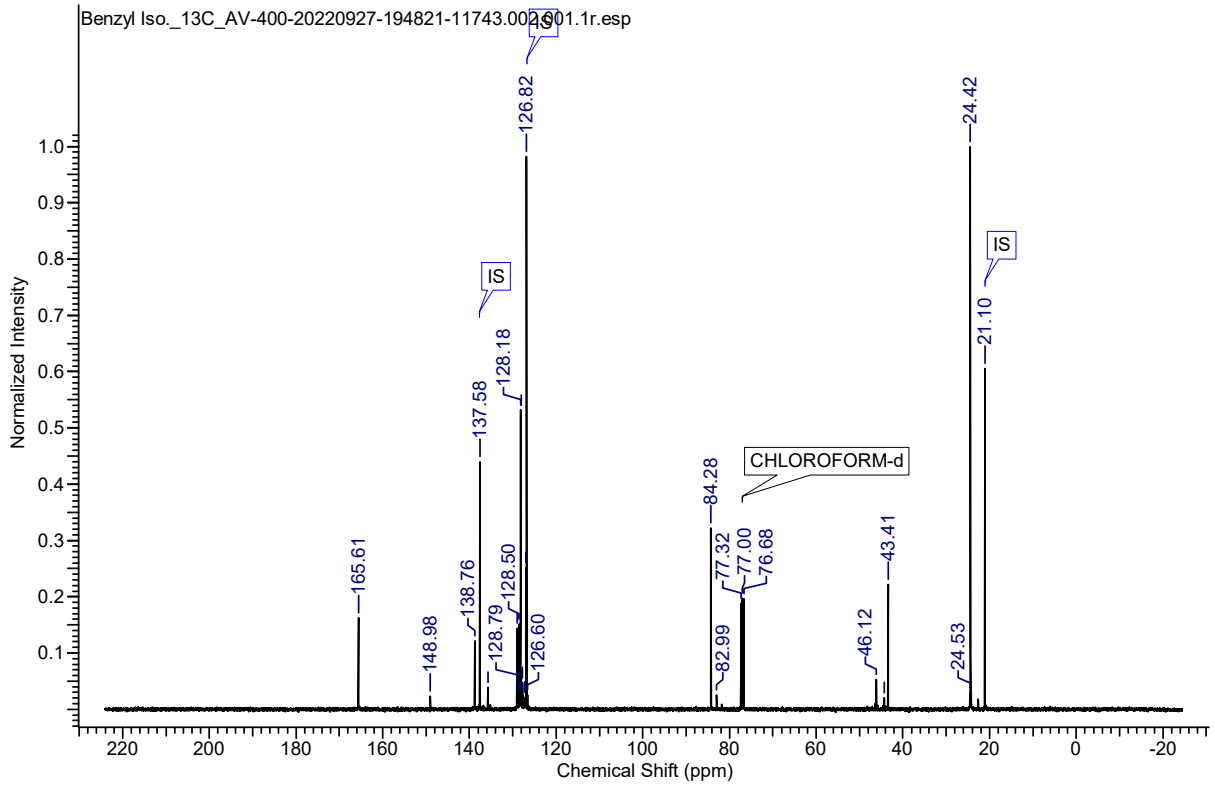
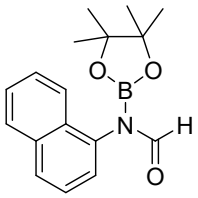


Figure S26. ^{13}C NMR spectrum of **2m** ($CDCl_3$, 101 MHz, 298 K).

N-(naphthalen-1-yl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide(2n):



^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ ppm 9.20 (s, 1 H), 7.96-7.90 (m, 2 H), 7.81-7.79 (d, 1H), 7.60-7.55 (m, 3H), 7.37-7.35 (d, 1H), 1.36 (s, 12 H) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ ppm 165.49 (s, 1 C), 134.27 (s, 1 C), 133.14 (s, 1 C), 130.07 (s, 1 C), 128.35 (s, 1 C), 128.18 (s, 1 C), 126.43 (s, 1 C), 125.96 (s, 1 C), 125.57 (s, 1 C), 125.37 (s, 1 C), 122.26 (s, 1 C), 84.46 (s, 1 C), 82.99 (s, 1 C), 24.43 (s, 1 C), 24.12 (s, 1 C) ppm.

The spectroscopic data is consistent with the literature data. [S2]

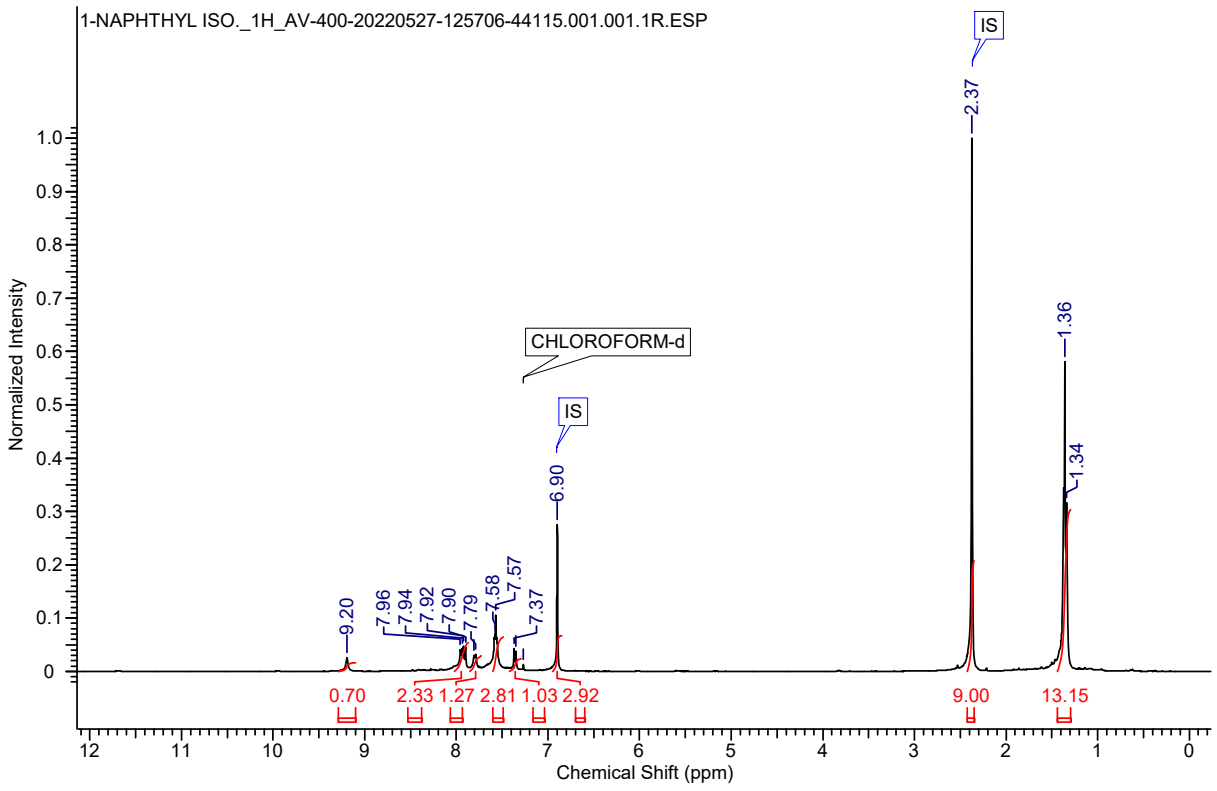


Figure S27. ^{1}H NMR spectrum of **2n** ($CDCl_3$, 400 MHz, 298 K).

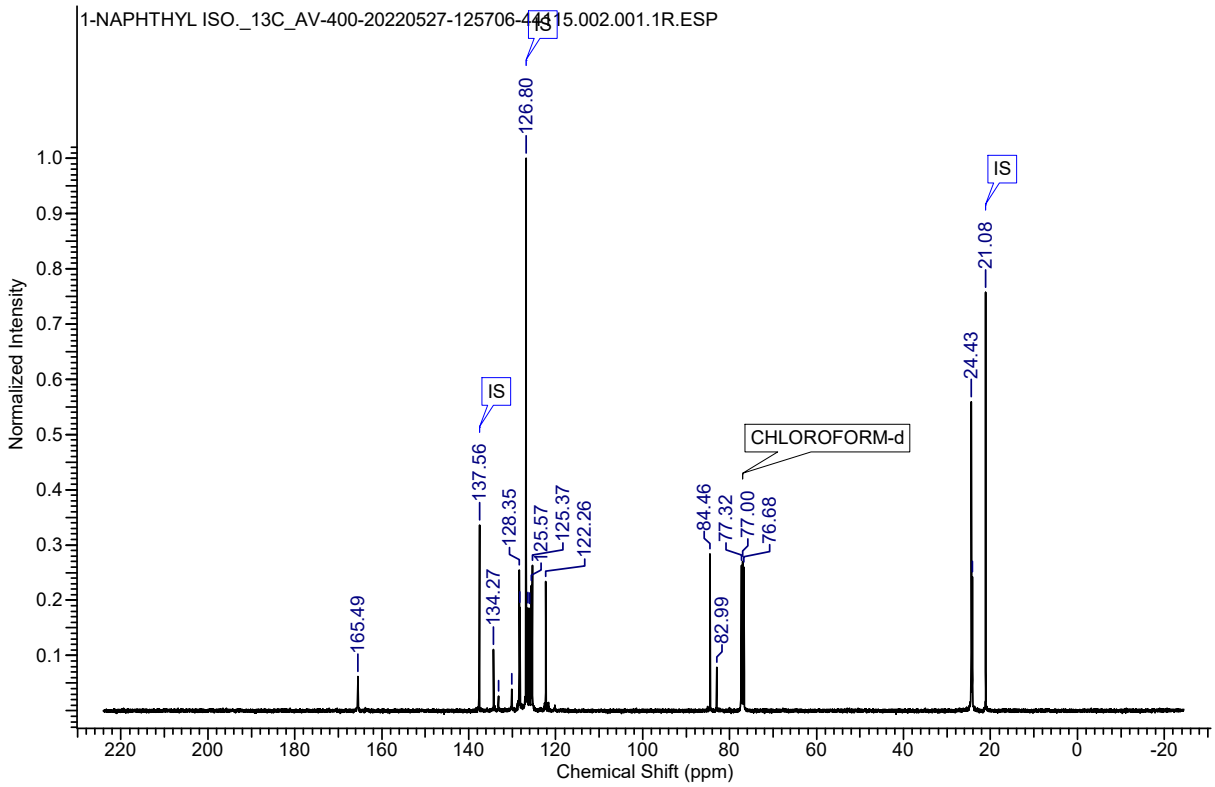
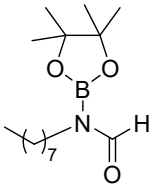
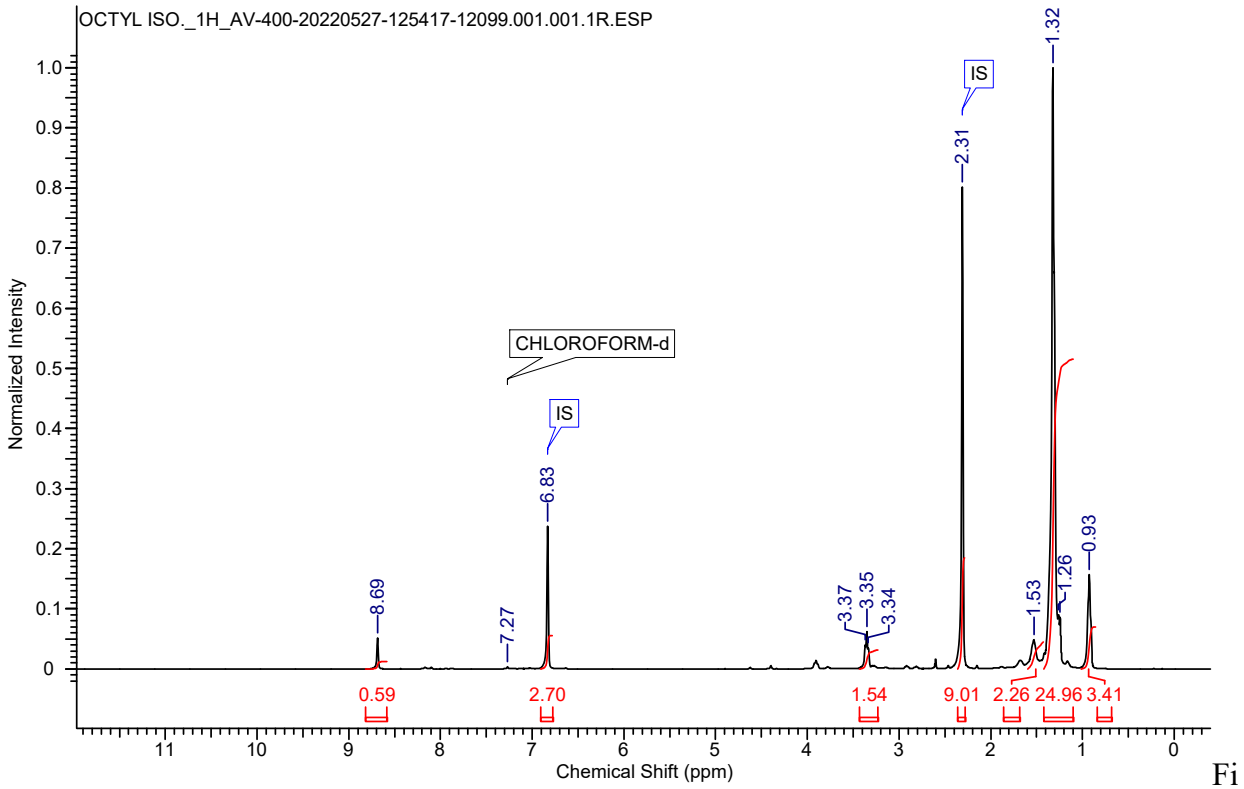


Figure S28. ^{13}C NMR spectrum of **2n** ($CDCl_3$, 101 MHz, 298 K).

N-octyl-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2o): ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ 8.69 (s, 1H, NC*H*O), 3.37-3.34 (t, 2H, *Octyl*), 1.53 (bs, 2H, *Octyl*), 1.32 (s, 12H, CH_3) 1.29-1.25 (m, 12H, *Octyl*), 0.93 (t, 3H, *Octyl*) ppm; $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz, 298 K): δ ppm 165.91 (s, 1 C), 83.93 (s, 1 C), 82.93 (s, 1 C), 48.29 (s, 1 C), 42.86 (s, 1 C), 39.96 (s, 1 C), 31.71 (s, 1 C), 31.65 (s, 1 C), 29.49 (s, 1 C), 29.17 (s, 1 C), 29.14 (s, 1 C), 29.07 (s, 1 C), 26.73 (s, 1 C), 26.61 (s, 1 C), 24.43 (s, 1 C), 24.40 (s, 1 C), 24.34 (s, 1 C), 22.54 (s, 1 C), 22.51 (s, 1 C), 13.96 (s, 1 C) ppm.



The spectroscopic data is consistent with the literature data. [S2]



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gure S29. ^{1}H NMR spectrum of **2o** ($CDCl_3$, 400 MHz, 298 K).

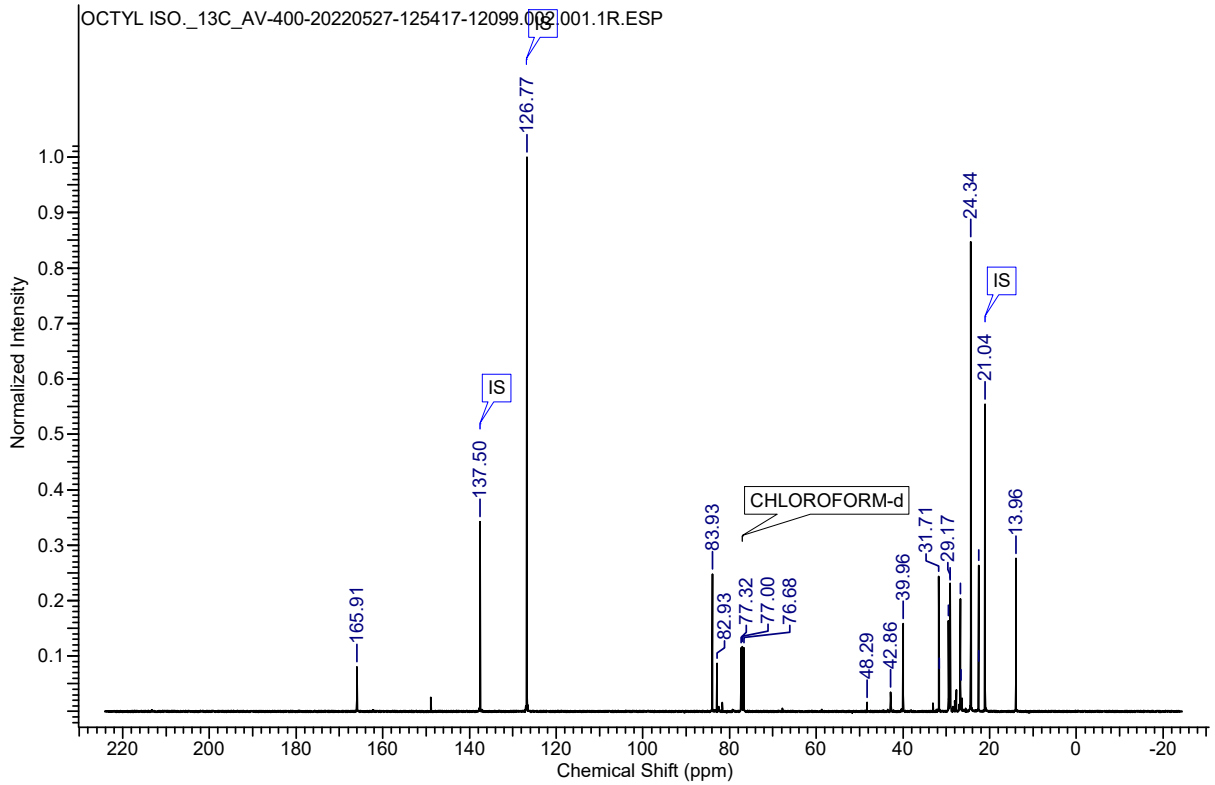
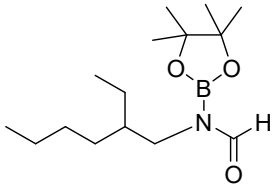


Figure S30. ^{13}C NMR spectrum of **2o** ($CDCl_3$, 101 MHz, 298 K).

N-(2-ethylhexyl)-N-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)formamide (2p): ^{1}H NMR



($CDCl_3$, 400 MHz, 298 K): δ 8.70 (s, 1H, NC*H*O), 3.25-3.23 (t, 2H, NCH_2), 1.31 (s, 12H, CH_3) 1.29 (bs, 8H, CH_2), 0.94-0.89 (m, 7H, CH_2CH_3) ppm; ^{13}C{^{1}H} NMR ($CDCl_3$, 101 MHz, 298 K): δ 166.16 (s, 1 C), 83.95 (s, 1 C), 82.95 (s, 1 C), 43.76 (s, 1 C), 40.71 (s, 1 C), 39.09 (s, 1 C), 38.27 (s, 1 C), 30.72 (s, 1 C), 30.35 (s, 1 C), 28.69 (s, 1 C), 28.42 (s, 1 C), 24.39 (s, 1 C), 24.33 (s, 1 C), 24.30 (s, 1 C), 23.92 (s, 1 C), 23.51 (s, 1 C), 22.98 (s, 1 C), 22.89 (s, 1 C), 13.97 (s, 1 C), 13.94 (s, 1 C), 10.65 (s, 1 C), 10.35 (s, 1 C) ppm.

The spectroscopic data is consistent with the literature data. [S2]

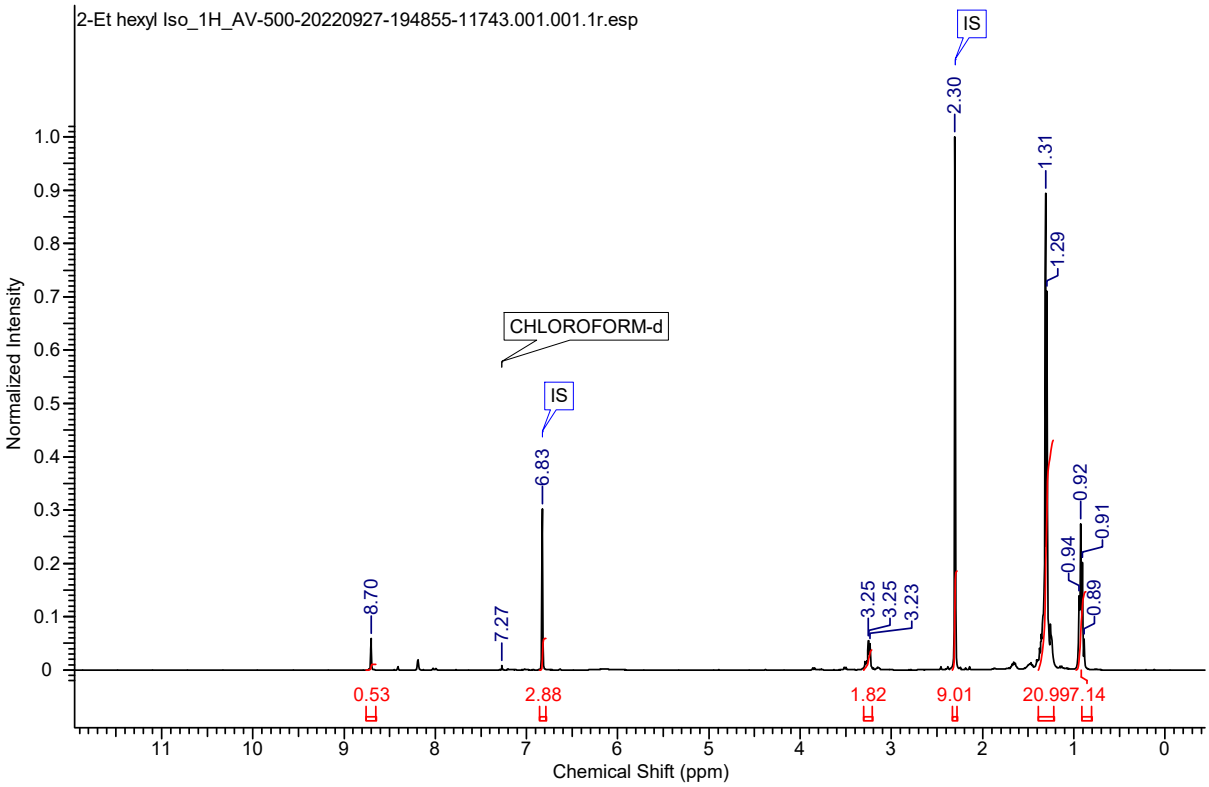


Figure S31. ^{1}H NMR spectrum of **2p** ($CDCl_3$, 400 MHz, 298 K).

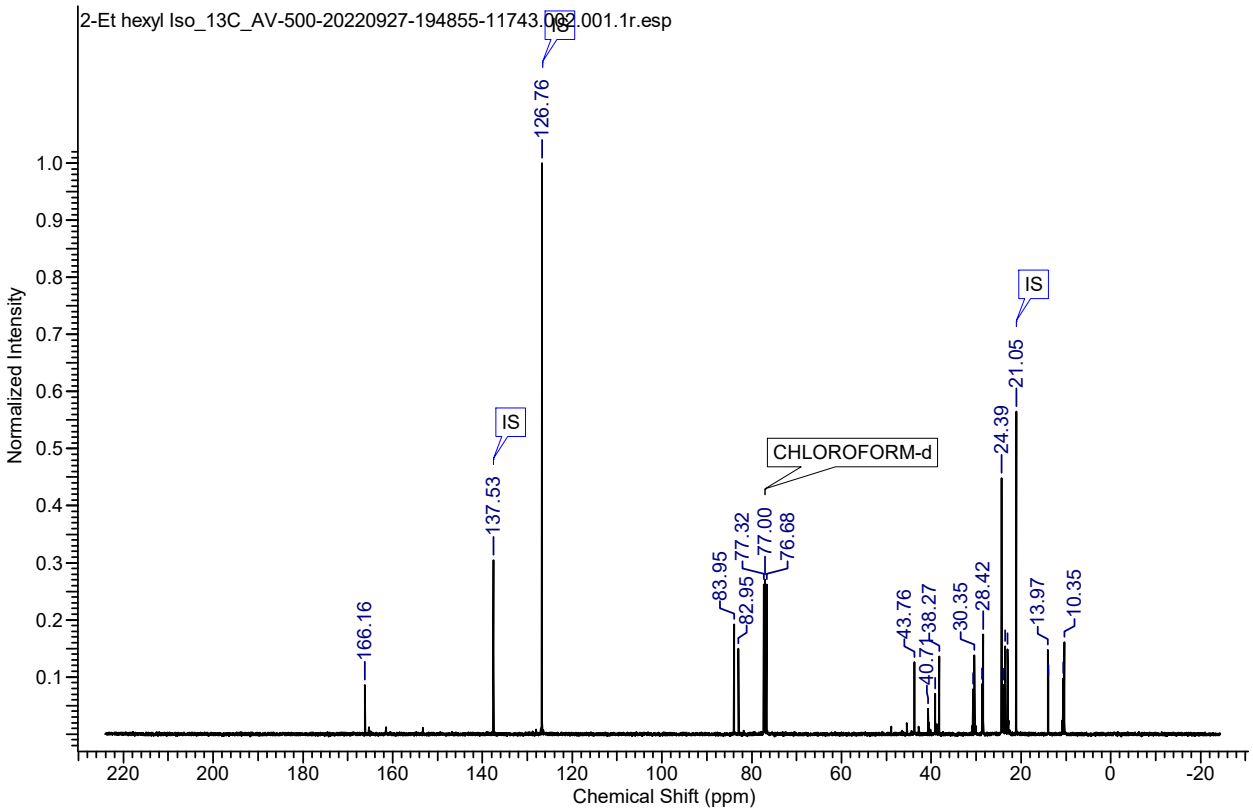
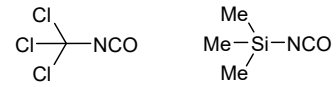


Figure S32. ^{13}C NMR spectrum of **2p** ($CDCl_3$, 101 MHz, 298 K).

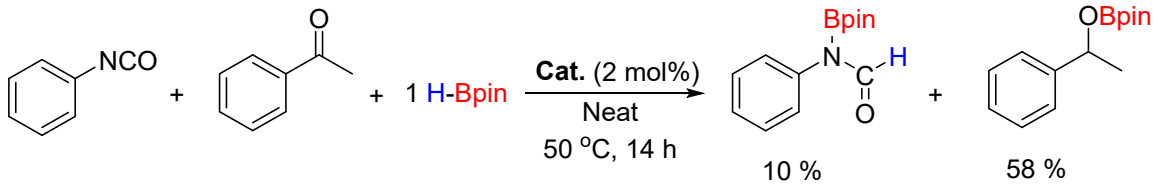
❖ List of unsuccessful substrates for catalytic hydroboration:



Very less yield due to unidentified side reactions

❖ **Competitive experiment for alkene/alkyne/nitrile/ketone/ester hydroboration- a selectivity study:**

1. Hydroboration of phenyl isocyanate and acetophenone in presence of 1 equiv. HBpin:



Scheme S2. Hydroboration of phenyl isocyanate and 4-fluoro acetophenone.

Phenyl isocyanate (0.25 mmol), acetophenone (0.25 mmol), pinacolborane (32 mg, 0.25 mmol), catalyst (2.0 mol% for **1**) were charged in a Schlenk tube inside the glove box. The reaction mixture was stirred for 14 hours at 50 °C after in neat conditions. Upon completion of the reaction, the progress of the reaction was monitored by ^{1}H NMR after addition of mesitylene (0.25 mmol) as an internal standard in $CDCl_3$. A sharp singlet resonance at $\delta = 8.89$ ppm indicates for the formation of hydroboration product from phenyl isocyanate and a quartet resonance at 5.29-5.24 ppm indicates the hydroboration product from acetophenone.

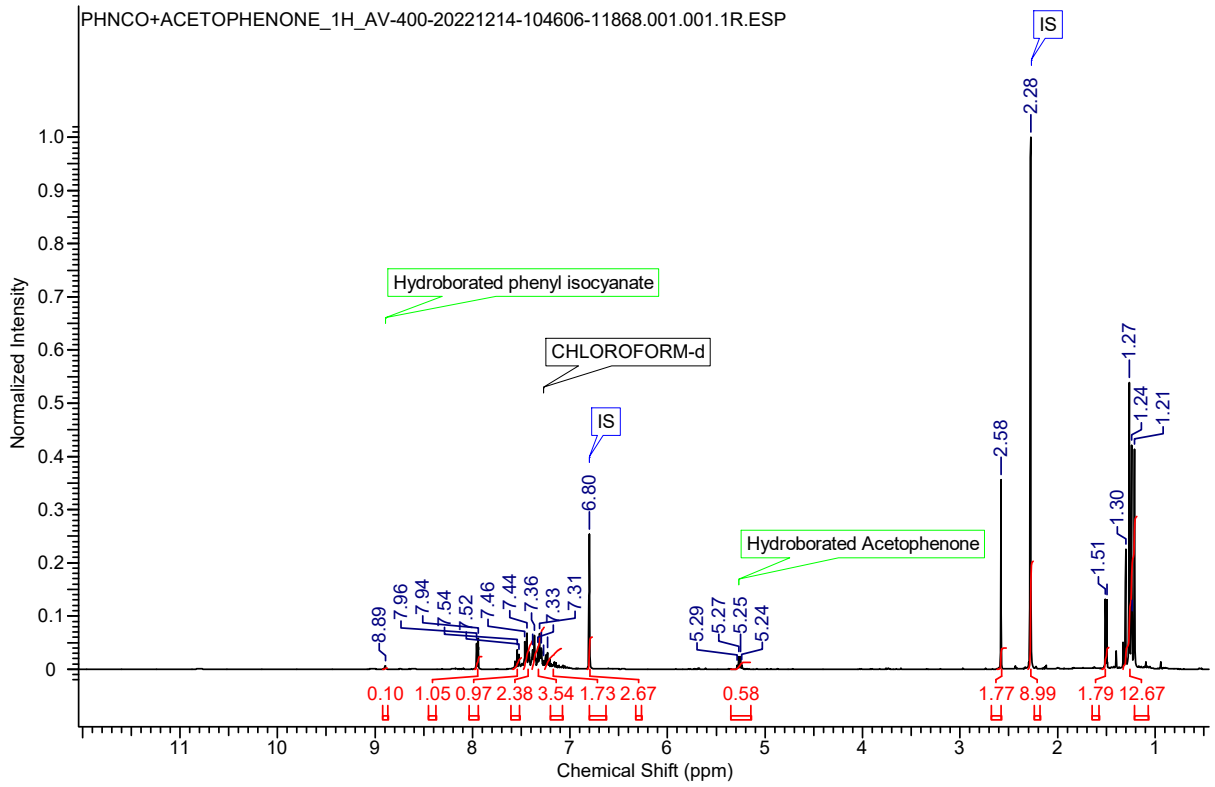
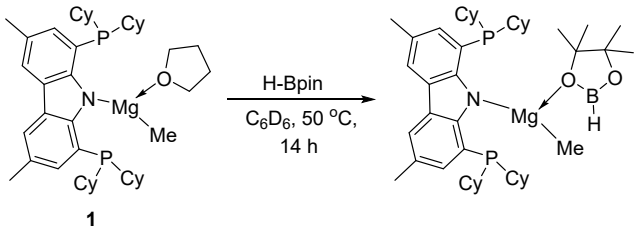


Figure S33. ^{1}H NMR spectrum of the reaction of phenyl isocyanate and acetophenone in presence of one equiv. HBpin ($CDCl_3$, 400 MHz, 298 K).

❖ **Mechanistic investigation:**

Stoichiometric reaction of catalyst 1 and HBpin:



1

Scheme S3. Stoichiometric reaction of **1** with HBpin and the tentative product formation.

A solution of HBpin (20 mg, 0.14 mmol) in C_6D_6 was added drop by drop to the C_6D_6 solution of **1** (90 mg, 0.14 mmol) at room temperature or inside the glove box. The reaction mixture was stirred/heated for 14 hours at 50 °C. After that the reaction mixture was subjected for characterization. ^{1}H NMR (C_6D_6, 400 MHz, 298 K): ^{1}H NMR spectra shows a new peak at 2.29 ppm which can be a proton peak for HBPin. This supports the formation of O-coordinated magnesium methyl complex. The ^{11}B NMR also indicates that the Bpin moiety is coordinated to the Mg centre through one of the O-atoms. ^{11}B NMR (C_6D_6, 128 MHz, 298 K): δ 33.96 (s, Me-Bpin), 28.90 (d, for unreacted HBpin), 21.92 (s, Bpin coordinated catalyst) ppm.

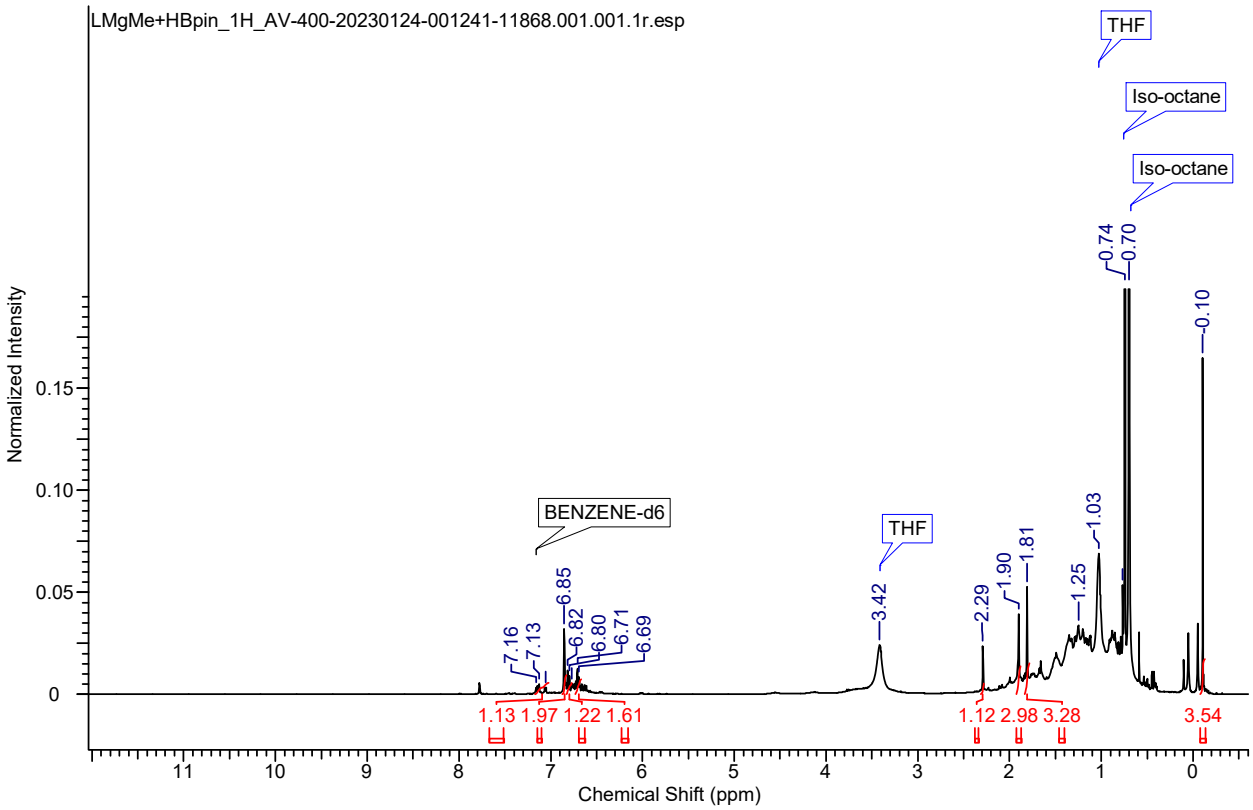


Figure S34. ^{1}H NMR spectrum of the reaction of **1** with HBpin (C_6D_6, 400 MHz, 298 K).

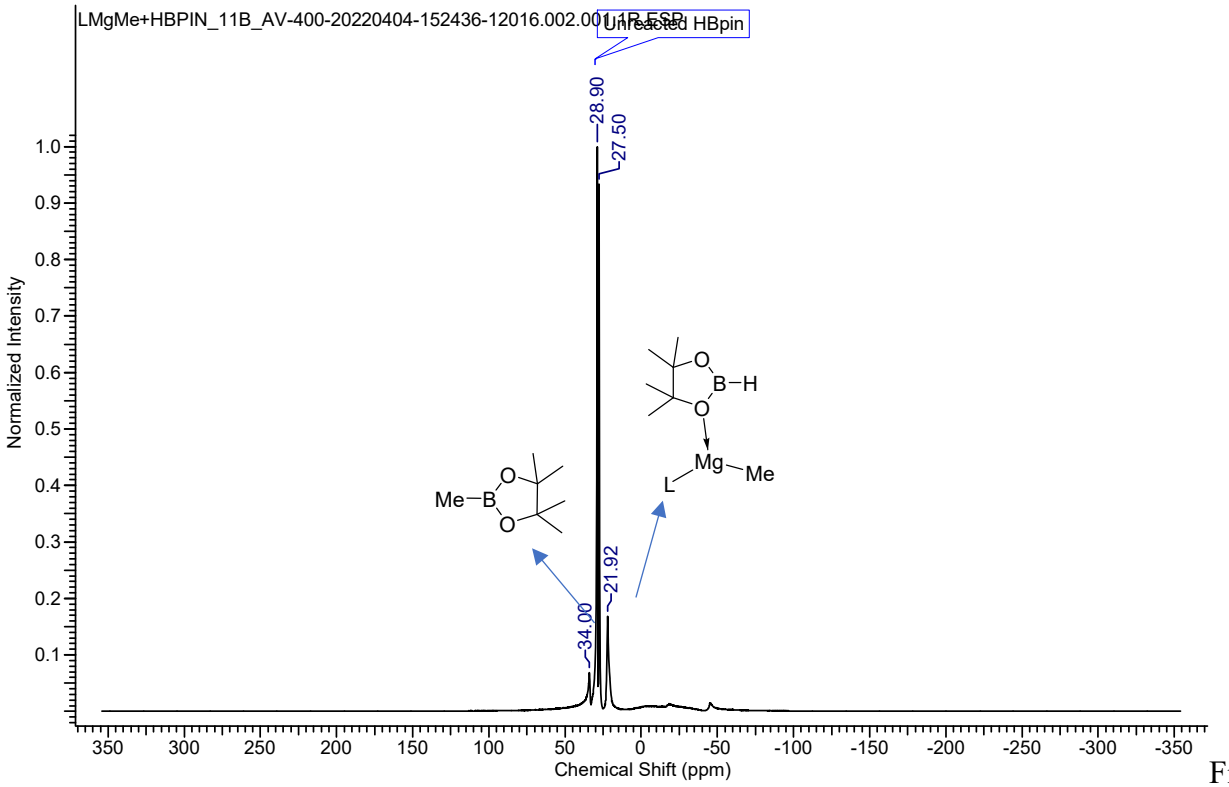


Figure S35. ^{11}B NMR spectrum of the reaction of **1** with HBpin (C_6D_6, 128 MHz, 298 K).

Heating of the catalyst at 70 °C for 8 hours under vacuum:

We have heated the catalyst under vacuum at 70 °C for 8 hours but we did not observe the removal of THF confirmed by ^1H NMR.

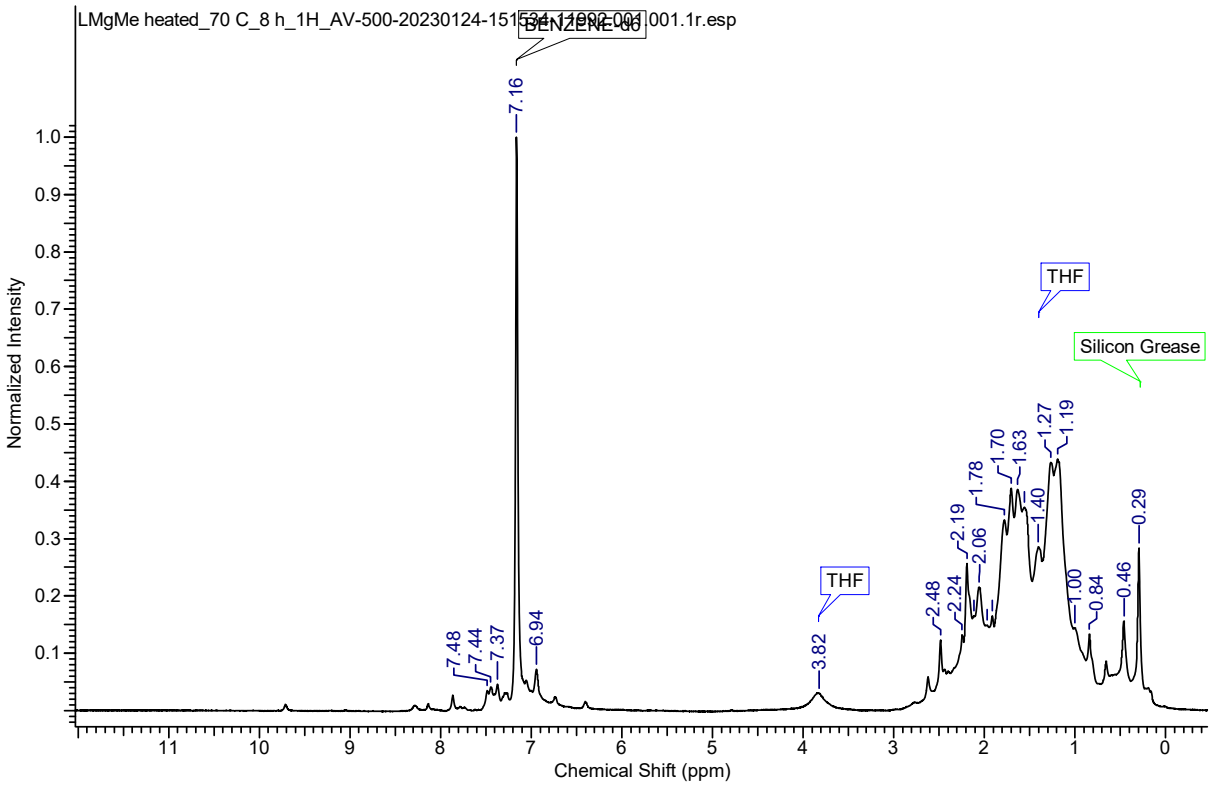
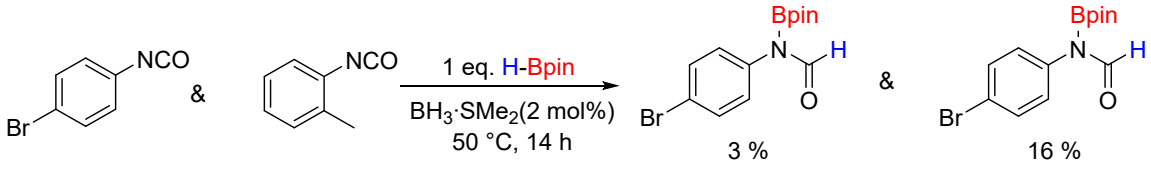


Figure S36. ^{1}H NMR spectrum heating of the catalyst at 70 °C for 8 hours under vacuum (C_6D_6, 128 MHz, 298 K).

Stoichiometric reaction of 1 with phenyl isocyanate or ethyl isocyanate:

No reaction was observed when an equimolar amount of **1** was treated separately with phenyl isocyanate or ethyl isocyanate in THF/toluene solvent at room temperature and at 60-100 °C. Further heating at 80-100 °C overnight in neat conditions also does not indicate any appreciable changes in the ^{1}H NMR spectra.

Hydroboration of 4-bromo phenyl isocyanate and o-tolyl isocyanate with $BH_3{\cdot}SMe_2$:



Scheme S4. Synthetic scheme for the reaction of 4-bromo phenyl isocyanate and o-tolyl isocyanate with $BH_3{\cdot}SMe_2$.

To identify whether the BH_3 is behaving as hidden catalyst in the hydroboration of phenyl isocyanate or not, we performed the reaction with $BH_3{\cdot}SMe_2$. A Screw cap NMR tube was charged with $BH_3{\cdot}SMe_2$ (2 mol%) inside the argon-filled glovebox. Subsequently 4- bromo phenyl isocyanate (0.25 mmol, 1.0 equiv) and 2-methyl phenyl isocyanate were added to the reaction mixture in separate NMR tubes and heated at 50 ºC up to 14 hours in an oil bath. After completion of the reaction 0.25 mmol mesitylene was added as an internal standard prior to the NMR measurement in $CDCl_3$ solvent. The ^1H NMR suggests that there is very less product formation in both the reactions, i.e., N-boryl formamide was observed (Figure S35 and S36), which clearly suggest very less influence of BH_3 as an active catalyst for the hydroboration of isocyanate.

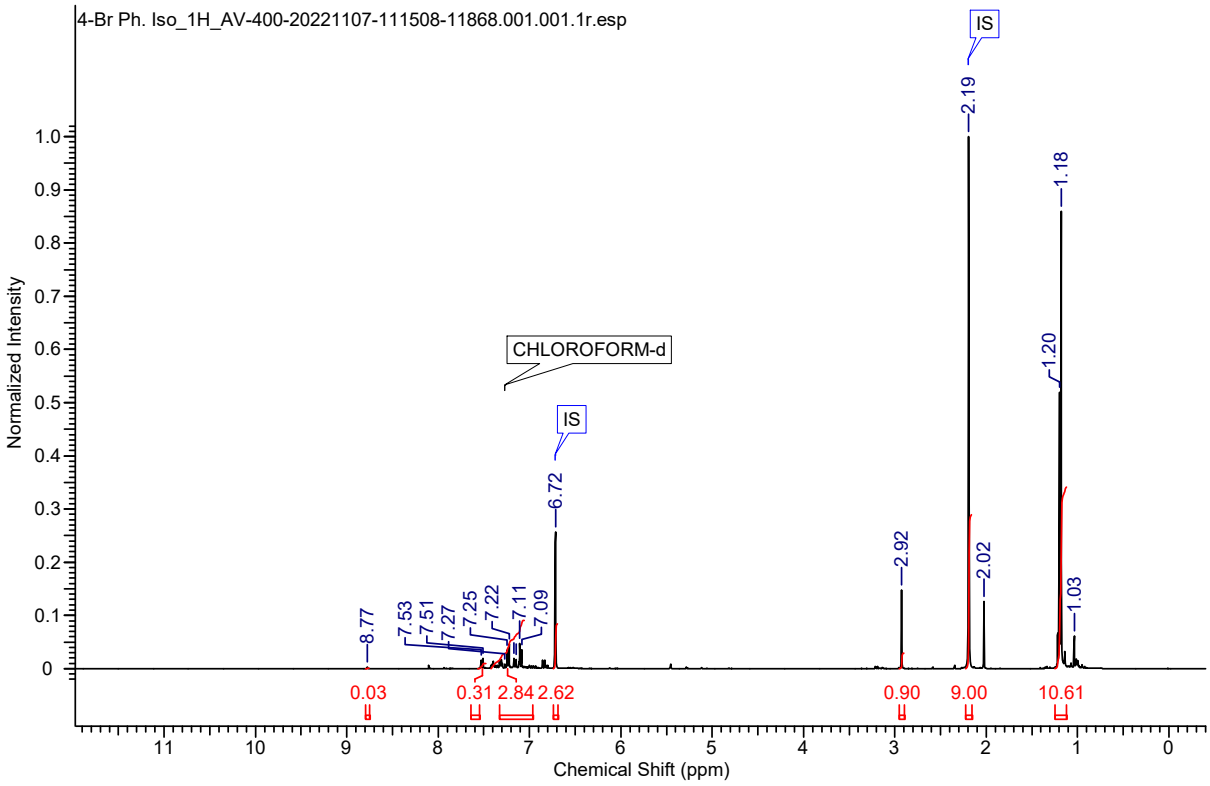


Figure S37. ^1H NMR spectrum of reaction of 4-bromo phenyl isocyanate with $BH_3{\cdot}SMe_2$ at 50 ºC ($CDCl_3$, 400 MHz, 298 K).

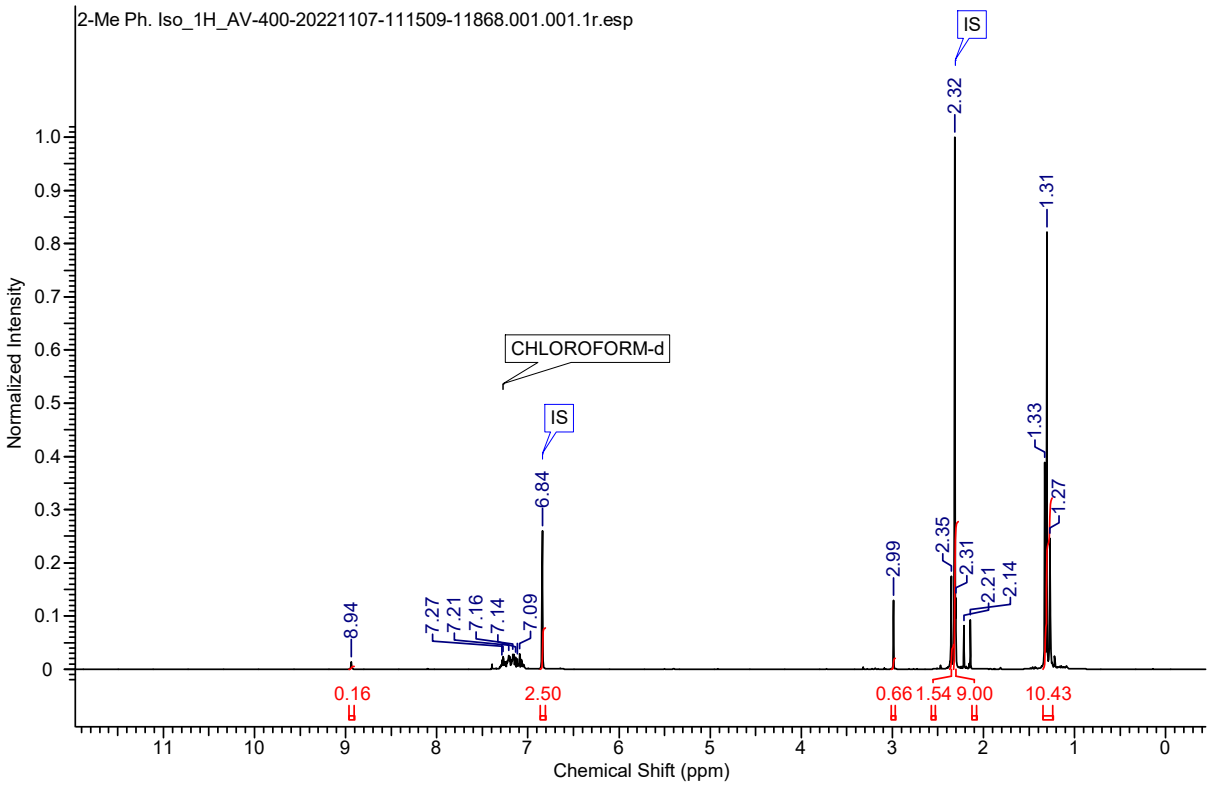


Figure S38. ^{1}H NMR spectrum of reaction of 2-methyl phenyl isocyanate with $BH_3 \cdot SMe_2$ at 50 ºC ($CDCl_3$, 400 MHz, 298 K).

❖ Details of the theoretical calculations:

Full quantum calculations have been carried out with Density Functional theory(DFT)[S3] using Turbomole 7.4. [S4] The TZVP basis set have been employed in all the calculations. [S5] Geometry optimizations were performed using the Perdew, Burke, and Ernzerhof functional (PBE).[S6] Dispersion corrections [S7] have been included in all the calculations. The resolution of identity (RI) [S8] along with the multipole accelerated RI (marij) [S9] approximations have been used for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent corrections have also been included in all the calculations using the cosmo model, [S10] with epsilon (∈) = 2.48, to model the HBpin which has been employed to study the reaction involved. Necessary care was taken to ensure that the obtained transition state structures possessed only one imaginary frequency corresponding to the correct normal mode, in order to obtain more reliable energy values for the investigated potential energy surface. In addition, intrinsic reaction coordinate (IRC)[S11] calculations were done with all the transition states in order to further confirm that they were the

correct transition states, yielding the correct reactant and product structures. The values reported here are ΔG values, with zero-point energy, internal energy, and entropic contributions, with the temperature taken to be 323.15 K. This is because this is the temperature at which the experiments were done. The translational entropy term has been corrected by a free volume correction introduced by Mammen and co-workers.[S12] The efficiency of the catalytic cycle for the reaction mechanism investigated has been calculated with the AUTOF [S13-S14] program by employing the "Energetic Span Model" (ESM), developed by Shaik and co-workers. [S14-S16] This has been done for all the free energy profiles discussed in the manuscript. The turnover frequency (TOF) calculations take into account the principal rate-determining transition state, as well as the potentially rate-influencing transition states and intermediates during the catalysis process. In most cases, the TOF is calculated from the TOF-determining transition state (TDTS), the TOF-determining intermediate (TDI), and from the reaction energy, ΔGr as shown below:

$$\text{TOF} = \frac{KbT}{h} e^{-\delta E/RT}$$

δE =TDTS – TDI if TDTS appears after TDI

δE =TDTS – TDI -ΔGr if TDTS appears before TDI

δE =TDTS – TDI -ΔGr if TDTS appears before TDI

This model has been employed to calculate the TOFs for the free energy profiles obtained for the mechanisms in the solvent phase discussed in the manuscript.

Discarded Mechanisms

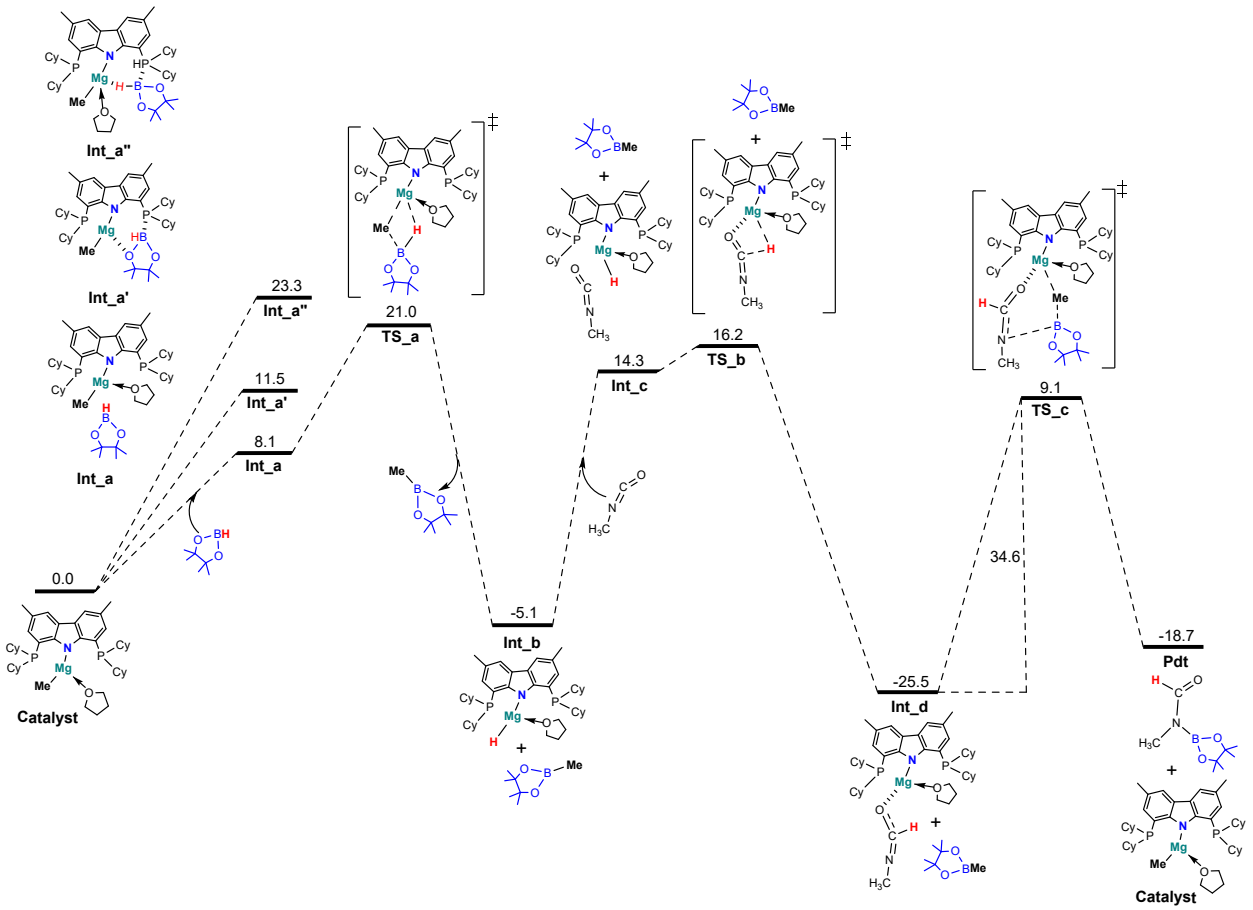


Figure S39. Reaction mechanism with DFT studies considering magnesium methyl as catalyst.

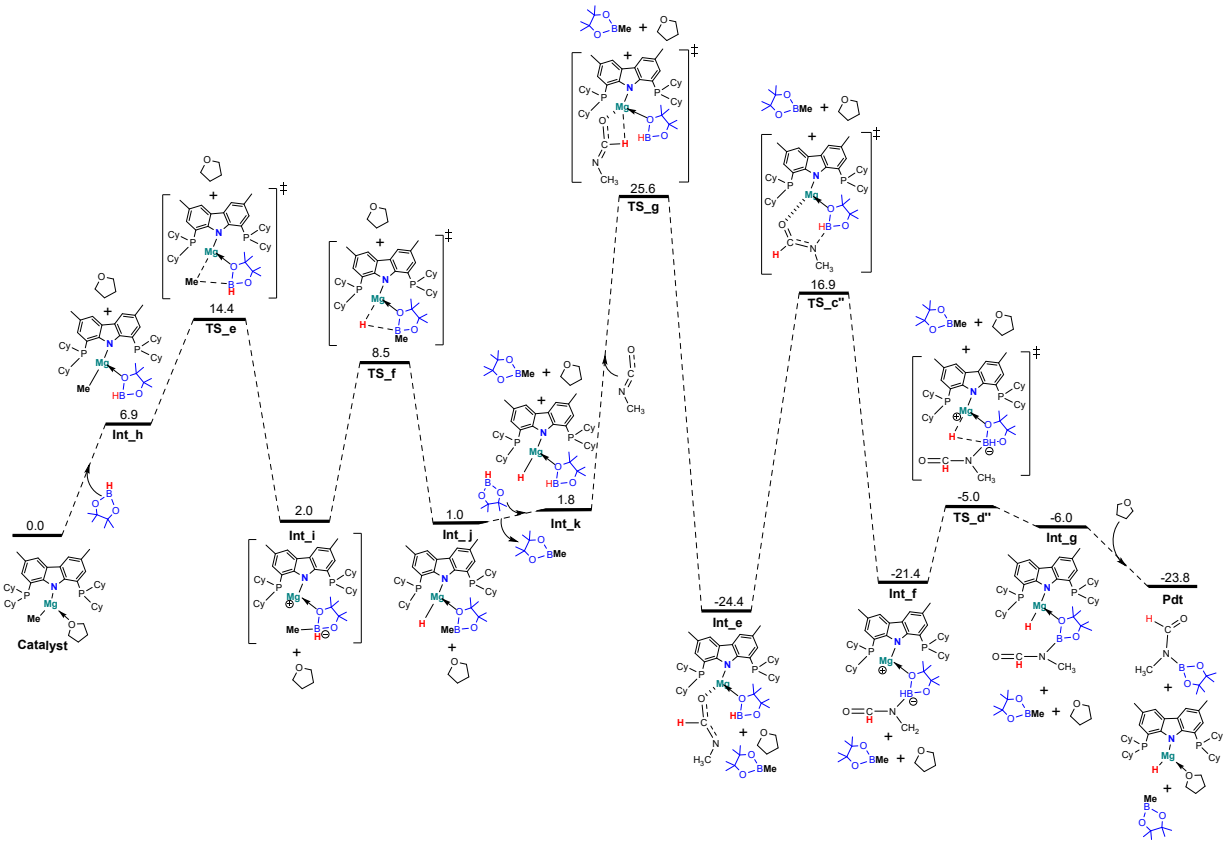


Figure S40. Mechanism via the formation of magnesium hydride

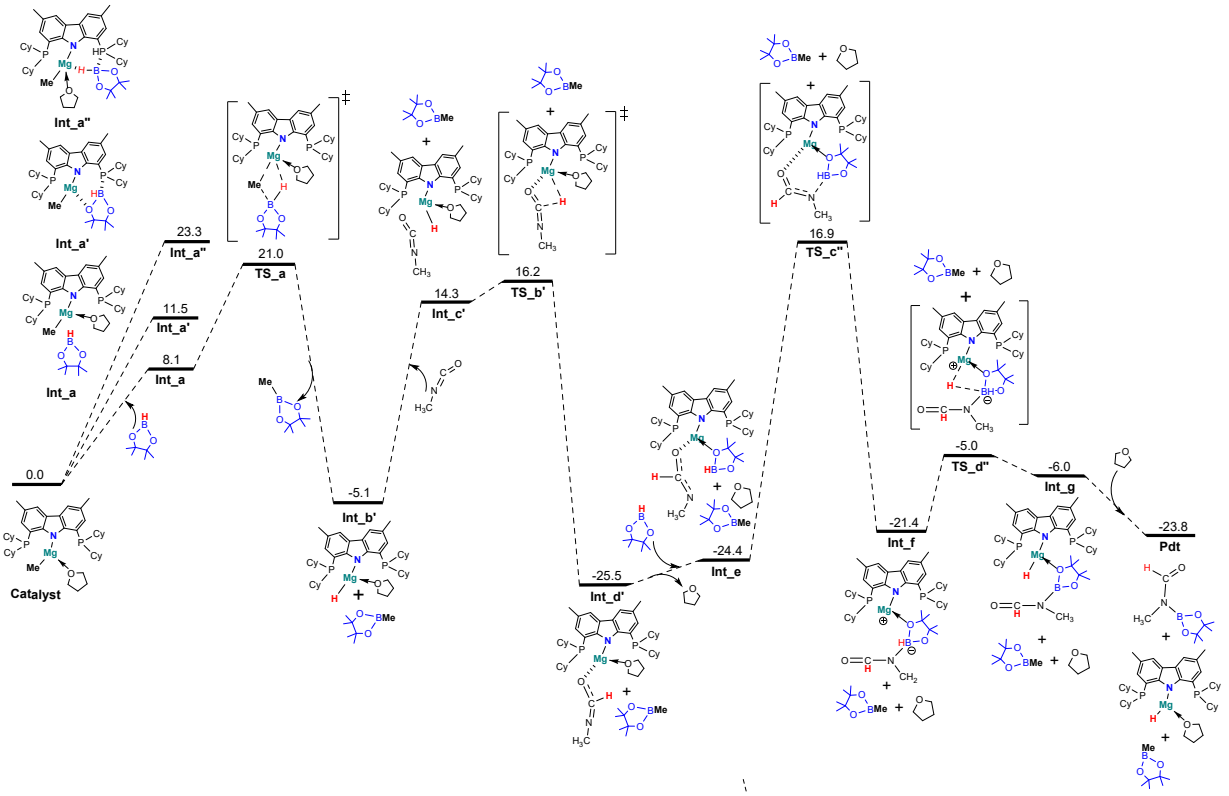


Figure S41. Alternative mechanism via the formation of magnesium hydride.

❖ References:

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❖ The XYZ coordinates of the optimized structures discussed in the manuscript

The optimized geometries of the structures reported in the manuscript (the atomic symbol followed by the three Cartesian coordinates, in Å).

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Int_2

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C	-0.3574153	4.3406024	8.5451690
H	-1.0706182	3.5494159	8.8260732
H	0.2344181	3.9506365	7.6976131
C	0.5859967	4.6479736	9.7150850
H	1.1470058	3.7450465	10.0057604
H	-0.0108539	4.9479479	10.5954160
C	1.5661079	5.7766674	9.3613718
H	2.2281804	5.4414527	8.5442571
H	2.2145740	5.9955175	10.2252484
C	3.0221035	8.8103040	9.9101213
H	3.7774158	8.0029345	9.9720962
C	2.2645117	8.8474422	11.2466448
H	1.4890433	9.6302291	11.2076753
H	1.7453979	7.8947992	11.4313157
C	3.2205624	9.1586813	12.4095061
H	3.9508163	8.3350777	12.5080898
H	2.6578306	9.1957107	13.3561040
C	3.9705692	10.4768413	12.1802405
H	3.2447936	11.3103378	12.1812409
H	4.6725162	10.6689358	13.0069909
C	4.7160553	10.4621344	10.8403323
H	5.2094401	11.4311014	10.6602248
H	5.5190046	9.7034936	10.8829801
C	3.7684376	10.1349505	9.6783865
H	4.3205975	10.0985720	8.7251409
H	3.0255909	10.9433495	9.5707840
H	5.6712364	7.1631667	8.1760899
H	6.4416268	9.1872730	8.7684412
O	4.9437297	8.7802617	6.1836766
H	5.2631873	6.1476389	6.7733236
C	6.0158269	6.8310523	7.1894760
B	5.2749053	10.1316656	6.1588459
C	7.4115494	9.1278190	8.2585888
H	7.9427356	8.2372210	8.6206566
C	6.2206568	8.0010840	6.2398439
H	6.9580992	6.2776875	7.3118223
H	7.9961470	10.0165042	8.5320683
C	7.2462863	9.0935232	6.7398734
O	6.6011665	10.3692886	6.3654646
H	5.6211816	6.9049810	4.4893042
C	6.4803618	7.5054533	4.8200215
H	6.6126420	8.3372767	4.1160324
C	8.6053331	9.0337104	6.0564042
H	7.3773094	6.8727542	4.7882916
H	9.0934776	8.0684629	6.2550513
H	9.2486354	9.8302736	6.4540915
H	8.5203026	9.1689803	4.9717399
C	2.9536171	5.7960638	5.4981114
N	3.2382693	13.8399806	6.2264752
H	2.6638631	13.9586317	8.2159193
C	3.0755364	13.2214877	7.5152052
H	2.3847440	12.3689007	7.4568390
H	4.0463054	12.8769442	7.9022780
C	3.5078916	13.6036340	5.0772434
O	3.7701509	13.5231691	3.9216159
H	1.9791065	5.4441850	5.1124941
H	3.1091192	5.2652447	6.4550515
H	3.7126068	5.4087566	4.7924705
H	4.4568533	10.9782040	5.9829143

TS_1

P	1.6811986	9.4868652	5.0714655
P	3.8413383	7.5604577	9.7289483
Mg	3.4891269	8.3360939	7.0219821
N	2.0890601	9.4781187	8.1113705
C	0.8507153	10.6283073	6.2608130
C	-0.0756023	11.6405399	5.9928415
H	-0.3769470	11.8338019	4.9621511
C	-0.6530147	12.4417549	7.0078269
C	-0.3135166	12.2044789	8.3428787
H	-0.7660838	12.8109994	9.1331603
C	0.6048672	11.1934981	8.6616681
C	1.2018751	10.4135286	7.6157096
C	2.0671460	9.6390810	9.4816817
C	1.1742252	10.6879620	9.8854399
C	1.0419838	11.0063990	11.2451079
H	0.3696212	11.8097228	11.5615726
C	1.7636282	10.2903007	12.2068764
C	2.6151690	9.2381361	11.7901810
H	3.1461451	8.6754695	12.5607591
C	2.7892999	8.8941438	10.4449499
C	-1.6065378	13.5504848	6.6307180
H	-1.0712888	14.4039880	6.1821862
H	-2.1500001	13.9259327	7.5092111
H	-2.3496034	13.2125253	5.8919001
C	1.6460083	10.6193912	13.6764886
H	0.8605856	11.3670865	13.8555766
H	2.5891923	11.0247369	14.0784359
H	1.4005143	9.7261140	14.2725768
C	0.3423610	8.1925570	4.7559892
H	-0.5407159	8.7146371	4.3462649
C	0.8423165	7.1516649	3.7388764
H	1.0791375	7.6314160	2.7750854
H	1.7819556	6.7138002	4.1149857
C	-0.1885044	6.0332953	3.5219803
H	-1.0933152	6.4579829	3.0507687
H	0.2149827	5.2881579	2.8172175
C	-0.5769704	5.3642469	4.8462303
H	0.3095129	4.8581598	5.2695594
H	-1.3362041	4.5847384	4.6736713
C	-1.0899489	6.4008769	5.8527539
H	-1.3272669	5.9192391	6.8158079
H	-2.0320293	6.8397369	5.4780811
C	-0.0624790	7.5179930	6.0765499
H	-0.4524275	8.2662301	6.7827048
H	0.8376239	7.0848657	6.5438904
C	1.8481771	10.3612656	3.4018902
H	2.4846332	9.6481513	2.8429972
C	2.6503179	11.6656381	3.5439178
H	2.0717646	12.3857487	4.1472257
H	3.5814471	11.4762794	4.1002324
C	2.9729260	12.2806078	2.1753275
H	3.5092540	13.2334087	2.3127759
H	3.6594605	11.6077353	1.6300157
C	1.7062270	12.4927252	1.3392576
H	1.0687450	13.2494454	1.8317343
H	1.9639379	12.8954466	0.3465046
C	0.9158172	11.1870390	1.1977506
H	1.5153616	10.4581586	0.6228000
H	-0.0100197	11.3554490	0.6239875
C	0.5741828	10.5852845	2.5695192
H	-0.1059871	11.2726601	3.0972384
H	0.0230811	9.6428567	2.4343971
C	2.8613111	5.9951207	10.1002452
H	2.7222417	5.9296187	11.1939753
C	1.4806611	6.0854383	9.4293637
H	1.6256741	6.2562498	8.3489515
H	0.9264551	6.9555155	9.8125912
C	0.6688120	4.7985395	9.6252846
H	0.4363255	4.6721775	10.6981232
H	-0.2969730	4.8880573	9.1016159
C	1.4388459	3.5712745	9.1244211
H	0.8570074	2.6524364	9.3011855
H	1.5796288	3.6540574	8.0318832
C	2.8120404	3.4723271	9.8003345

H	3.3748506	2.6109751	9.4056147
H	2.6732211	3.2914398	10.8817185
C	3.6287896	4.7584754	9.6020959
H	3.8482509	4.8880659	8.5284732
H	4.5995993	4.6681468	10.1156198
C	5.3996253	7.4086490	10.7792990
H	6.0329093	6.7528330	10.1515290
C	5.3064775	6.7597270	12.1704241
H	4.6830189	7.3813930	12.8330149
H	4.8219683	5.7732555	12.1142096
C	6.7074344	6.6194517	12.7893060
H	7.3010920	5.9176555	12.1764309
H	6.6302592	6.1732259	13.7938338
C	7.4339891	7.9696711	12.8600290
H	6.8931418	8.6330512	13.5586882
H	8.4475673	7.8376330	13.2710590
C	7.4998619	8.6437810	11.4827062
H	7.9708139	9.6371256	11.5619553
H	8.1386484	8.0436583	10.8100179
C	6.1015604	8.7729855	10.8652445
H	6.1560057	9.2250682	9.8627822
H	5.4893336	9.4518015	11.4830476
H	6.9902853	8.1750176	7.8880231
H	7.2249644	10.4155540	8.6464539
O	5.0957247	9.7591567	6.9184669
H	6.2225860	7.2740204	6.5579400
C	6.8925286	8.1105942	6.7975258
B	4.9952531	11.2225046	6.8474117
C	7.9378308	10.6322358	7.8405558
H	8.7390471	9.8801266	7.8749386
C	6.3463159	9.4038384	6.2082607
H	7.8814542	7.8923725	6.3678725
H	8.3813686	11.6191966	8.0316907
C	7.2389871	10.6676140	6.4757176
O	6.2768367	11.7489107	6.4869325
H	5.2116597	8.4565317	4.6378182
C	5.9990158	9.2190388	4.7284803
H	5.6301003	10.1546537	4.2859814
C	8.2642764	10.9389739	5.3780387
H	6.8726270	8.8776886	4.1560753
H	8.9588148	10.0922473	5.2719492
H	8.8508112	11.8311358	5.6383716
H	7.7762396	11.1200591	4.4128499
C	3.7564412	6.4004485	6.0844093
H	4.0739477	11.6560947	6.0588455
N	4.3350410	11.9001963	8.1321779
H	4.3577781	11.0779687	10.0623298
C	4.6383785	12.0162894	9.5698577
H	5.7152955	12.1977984	9.6768170
H	4.0743651	12.8428242	10.0160152
C	3.4892561	12.6111534	7.4976207
O	2.7033806	13.4161443	7.1802616
H	2.8463430	5.7797420	6.1820466
H	4.5727223	5.8111848	6.5415186
H	3.9719408	6.4573916	5.0017787
Int_3			
B	5.3953022	10.9754141	7.3593221
H	3.1668902	11.9321497	6.5133944
C	3.4549146	12.5061691	7.4167462
N	4.5953500	12.0169951	8.0074394
H	6.1973164	12.7275057	9.1946090
C	5.1005547	12.6902296	9.2140107
Mg_Catalyst			
P	4.8514862	9.6339260	3.4611660
P	1.1771719	9.6324486	7.5001443
Mg	3.2934492	8.9557077	5.7286529
N	2.2501972	10.5392298	4.7868621
C	3.6175649	10.7803228	2.7134254
C	3.6540947	11.3701229	1.4454755
H	4.5031643	11.1746836	0.7845736
C	2.6214660	12.2169836	0.9729481
C	1.5138708	12.4718494	1.7920798
H	0.7118724	13.1208624	1.4270278
C	1.4306785	11.8901967	3.0661437
C	2.4938361	11.0431426	3.5271606
C	1.0164961	11.0396767	5.1468333
C	0.4572556	11.8861475	4.1322776
C	-0.8078637	12.4591974	4.3311226
H	-1.2488311	13.1051161	3.5657190
C	-1.5208911	12.1984025	5.5077985
H	4.6954113	13.7088114	9.2433011
H	4.7661272	12.1526418	10.1131434
H	7.9733187	9.7368324	8.3576553
C	8.3560360	9.8328734	7.3336385
H	9.0088721	10.7151888	7.2960310
H	8.9581500	8.9446560	7.1020000
H	8.2482500	9.2185503	4.5916031
H	8.5735677	10.9370177	4.9163774
C	7.7925170	10.1645321	4.9176511
H	7.0216491	10.4510769	4.1926879
H	7.3451902	7.2000604	6.4717436
C	7.2244788	10.0191128	6.3234526
O	5.0911565	9.6107092	7.3562525
O	6.5482910	11.2726519	6.6856110
C	6.0767688	8.9379272	6.4391258
C	6.5331485	7.6339711	7.0725604
H	6.8961796	7.7847522	8.0966399
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C	5.3158412	8.6763076	5.1433667
H	4.9853587	9.6091888	4.6669820
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H	5.9381595	8.1181984	4.4311014
O	2.8221221	13.4842303	7.7986767
C	6.9649261	10.1931444	11.0204889
H	6.3977831	10.9616487	11.5719841
H	6.7219367	10.3401013	9.9557806
C	8.4672498	10.3906529	11.2637162
H	9.0354964	9.6852252	10.6299875
H	8.7678792	11.4045980	10.9543669
C	8.8288023	10.1482194	12.7349284
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H	9.9163365	10.2447223	12.8830352
C	8.3453221	8.7706498	13.2056437
H	8.8961564	7.9838558	12.6591776
H	8.5712184	8.6290157	14.2747206
C	6.8377545	8.5887574	12.9636780
H	6.2901684	9.3201709	13.5792906
H	6.5211445	7.5905752	13.3006229
H	7.0635323	8.0517795	10.8966917
C	6.4968563	8.8039203	11.4794275
P	4.7207387	8.4979214	10.9069934
C	4.1543898	7.0086361	11.9096103
H	4.2830122	7.2490289	12.9805341
C	4.9984668	5.7726890	11.5556043
H	4.9430843	5.6083091	10.4658460
H	6.0599388	5.9430579	11.7977681
C	4.4923556	4.5180761	12.2828509
H	5.0939930	3.6455641	11.9807194
H	4.6403440	4.6435054	13.3707645
C	3.0057728	4.2693188	12.0001679
H	2.8748512	4.0502488	10.9252951
H	2.6542785	3.3822050	12.5512226
H	2.2164125	5.6628750	13.4589172
C	2.1641245	5.4974766	12.3676296
H	1.1029951	5.3246942	12.1249617
H	2.0686035	7.6327639	11.9331999
H	2.5141205	6.6185614	10.5528518
C	2.6611120	6.7530088	11.6391135
C	2.9601573	12.0939871	14.5994632
H	2.0382707	12.6141473	14.8962381
H	3.1826993	11.3367805	15.3666918
H	3.7781337	12.8334880	14.6285956
C	-0.9485958	11.3582648	6.4942664
H	-1.5267120	11.1623843	7.4018684
C	0.3131400	10.7746667	6.3418899
C	2.7215059	12.8197047	-0.4087976
H	3.6891797	13.3232128	-0.5609267
H	1.9277375	13.5608509	-0.5774583
H	2.6308635	12.0518496	-1.1949511
C	-2.8933391	12.7882699	5.7323916
H	-3.1524227	13.5050315	4.9405646
H	-2.9540876	13.3163601	6.6970634
H	-3.6733559	12.0088934	5.7433897
C	5.4959775	8.6380479	2.0066909
H	5.8069331	9.3344299	1.2082206
C	6.7115210	7.7932164	2.4248488
H	7.5355965	8.4426106	2.7593116
H	6.4337262	7.1657704	3.2914730
C	7.1921188	6.8937313	1.2767592
H	7.5724109	7.5283920	0.4562637
C	2.8215059	11.4712675	13.2299363
C	3.7166141	10.4536791	12.8254897
H	4.4616650	10.1142456	13.5480164
C	3.6658555	9.8611168	11.5568206
H	4.3549755	5.7346591	8.3619854
C	3.5107218	6.2779751	7.9017320
Mg	3.4767438	8.4006271	8.3404032
N	2.3946432	9.8378434	9.3963031
C	2.6561700	10.3022082	10.6700443
C	1.7214123	11.3145632	11.0719230
C	1.8227756	11.8934456	12.3433878
H	1.1166634	12.6693664	12.6542917
H	3.5433413	6.0679145	6.8161869
H	2.5951666	5.7828569	8.2741765
C	1.2873439	10.5442114	8.9635300
C	0.8239330	11.4693537	9.9549804
C	-0.3086802	12.2538334	9.7052372
H	-0.6706328	12.9584885	10.4599746
C	-0.9930878	12.1278489	8.4915350
C	-2.2149957	12.9648300	8.1963073
H	-1.9948041	13.7571889	7.4622011
H	-3.0311644	12.3544973	7.7787372
H	-2.5918077	13.4527848	9.1062973
C	-0.5305751	11.1977959	7.5314403
H	-1.1057585	11.0907181	6.6103255
C	0.6042626	10.4033436	7.7327960
P	1.2434753	9.0505918	6.6563854
H	1.4796291	11.6509550	5.0613365
C	1.9125084	10.7858442	4.5299831
H	2.9345251	10.6479291	4.9185114
C	1.9643272	11.0844532	3.0258159
H	2.5392665	12.0079092	2.8498949
H	2.5068789	10.2692308	2.5140784
C	0.5563764	11.2063740	2.4316608
H	0.6121555	11.3761354	1.3446279
H	1.1871514	6.1052958	6.2740688
H	0.1654070	9.0851840	2.2274368
C	-0.2805391	9.9581766	2.7375694
H	-0.6173677	4.5268385	5.6219083
C	-0.8664753	5.4123093	6.2291925
H	-1.8448156	5.7783030	5.8684506
C	-0.9847593	5.0316669	7.7099685
H	-0.0353802	4.5736685	8.0418087
H	-1.3006724	10.0712366	2.3368205
H	-1.7690915	4.2700309	7.8479622
C	-1.2770809	6.2641604	8.5732625
H	-2.2727410	6.6655319	8.3105264
H	-1.3207937	5.9874200	9.6391985
H	-0.4704577	8.2496062	8.9630060
C	-0.2217486	7.3584079	8.3672974
H	0.7535071	6.9959421	8.7342822
C	-0.0933138	7.7388483	6.8822194
H	-1.0476554	8.1958187	6.5630866
C	0.1920808	6.5038482	6.0129768
C	-0.3435446	9.6822965	4.2481481
C	1.0698631	9.5380945	4.8366604
H	1.5556013	8.6815204	4.3301501
H	-0.9436336	8.7803788	4.4397563
H	0.2296181	6.7786647	4.9463338
H	-0.8633852	10.5212127	4.7366140
H	0.0571824	12.0912940	2.8655668
H	8.0395557	6.2762984	1.6161167
C	6.0616862	6.0062180	0.7434471
H	5.7516539	5.3010355	1.5358636
H	6.4190806	5.3947355	-0.1006206
C	4.8523267	6.8487694	0.3198531
H	4.0297487	6.1993665	-0.0215153
H	5.1321001	7.4814725	-0.5414213
C	4.3665710	7.7446357	1.4665654
H	3.5200612	8.3671931	1.1370458
H	3.9937387	7.1108184	2.2917828
C	6.2766737	10.7615396	3.9650621
H	7.0321388	10.0662520	4.3770352
C	5.7975057	11.6688822	5.1136936
H	4.9668074	12.2997344	4.7524665
H	5.3931418	11.0529336	5.9330655
C	6.9289363	12.5630777	5.6360587
H	6.5434619	13.2269134	6.4273526
H	7.7040357	11.9305458	6.1050886

C	7.5603237	13.3838038	4.5057958
H	6.8084608	14.0890558	4.1074396
H	8.3930963	13.9936396	4.8913790
C	8.0466076	12.4749494	3.3701532
H	8.8669069	11.8347866	3.7423250
H	8.4650101	13.0772523	2.5474047
C	6.9124558	11.5847653	2.8390661
H	6.1361272	12.2213732	2.3812775
H	7.2938929	10.9254454	2.0426363
C	-0.2095353	8.6650590	8.3138284
H	-0.9630351	9.3739379	8.7011992
C	-0.8748212	7.7661489	7.2572536
H	-0.0978995	7.1241320	6.8035224
H	-1.2872959	8.3838239	6.4443404
C	-1.9675981	6.8813917	7.8687327
H	-2.7915201	7.5208755	8.2329866
H	-2.3978130	6.2276361	7.0924450
C	-1.4215074	6.0456821	9.0323478
H	-2.2250638	5.4410995	9.4824949
H	-0.6695044	5.3336772	8.6450417
C	-0.7676229	6.9389791	10.0925147
H	-0.3441042	6.3266477	10.9049773
H	-1.5404145	7.5812945	10.5521498
C	0.3278039	7.8278242	9.4866588
H	1.1583040	7.1928372	9.1266774
H	0.7496615	8.4825267	10.2652969
C	1.8505756	10.7708408	8.8454616
H	2.3123944	10.0783809	9.5746021
C	0.8126850	11.6409779	9.5645449
H	0.2929332	12.2656556	8.8178367
H	0.0441670	11.0125797	10.0433244
C	1.4715853	12.5505945	10.6125234
H	1.9079032	11.9269762	11.4138448
H	0.7073347	13.1861123	11.0890309
C	2.5740512	13.4146518	9.9891063
H	2.1205516	14.1044637	9.2542084
H	3.0515738	14.0418393	10.7590488
C	3.6207934	12.5452171	9.2829869
H	4.3867041	13.1755018	8.8019007
H	4.1469502	11.9263654	10.0320297
C	2.9747515	11.6290505	8.2363483
H	3.7389462	10.9746321	7.7845530
H	2.5585982	12.2418502	7.4177532
O	2.2388714	7.4094826	4.7713406
C	1.1880892	7.6220093	3.7741765
C	4.7877020	8.2276476	7.0905986
C	2.3906939	5.9869759	5.0518164
C	0.8886251	6.2353578	3.2172726
H	1.5702410	8.3362976	3.0338907
C	1.1690354	5.3247702	4.4231355
H	2.4621021	5.8662139	6.1417903
H	3.3315058	5.6420980	4.5918305
H	0.3202861	8.0674671	4.2848199
H	1.5717704	5.9973511	2.3872915
H	-0.1424744	6.1547431	2.8485288
H	0.3185836	5.3406206	5.1224487
H	1.3628935	4.2813617	4.1413306
H	4.3464194	7.8277842	8.0216852
H	5.5220533	8.9957735	7.3951757
H	5.3733682	7.4091144	6.6308301

HBpin

O	0.7535016	2.1134698	-0.7440536
C	2.2111757	2.3543998	-0.7642582
C	2.9205241	1.0612633	-0.3888722
B	0.1713852	3.2716149	-0.2826452
O	1.0623491	4.1989140	0.2062589
C	2.3756868	3.5267809	0.2757450
C	2.5343477	3.0401851	1.7177124
C	3.4580583	4.5410427	-0.0684062
C	2.5593024	2.7635403	-2.1972291
H	-1.0106619	3.4569356	-0.3042528
H	3.6432317	2.8943794	-2.3231105
H	2.2232804	1.9738932	-2.8833178
H	2.0566834	3.6996482	-2.4791893
H	3.4856590	5.3256612	0.7008136
H	4.4441689	4.0546266	-0.0957087
H	3.2736125	5.0179556	-1.0387277
H	2.7336745	0.3011716	-1.1603115
H	4.0066583	1.2240693	-0.3253823
H	2.5668545	0.6700016	0.5724599
H	3.5211928	2.5841254	1.8793653
H	2.4351018	3.8998233	2.3947908
H	1.7594234	2.3063284	1.9796697

Methyl Isocyanate

C	17.2736936	10.5062113	16.2340583
N	18.0558240	10.1763869	17.0876533
O	16.5125855	10.9598867	15.4438212
C	18.7457983	9.0248329	17.6074988
H	18.0548964	8.1813759	17.7521357
H	19.1934301	9.2823486	18.5751690
H	19.5508820	8.7151477	16.9245237

THF

O	-3.1411902	1.3550951	2.1278148
C	-4.2814500	1.4152382	1.2380810
C	-2.6916830	-0.0161296	2.2323940
C	-4.3638320	0.0514156	0.5489340
H	-4.1330159	2.2497732	0.5355099
C	-3.8049398	-0.8787189	1.6360421
H	-2.4878870	-0.2354758	3.2917748
H	-1.7505852	-0.1360081	1.6638743
H	-5.1927740	1.6163540	1.8309689
H	-3.7180402	0.0293402	-0.3424436
H	-5.3868136	-0.2045750	0.2409240
H	-4.5759754	-1.0908771	2.3925873
H	-3.4334837	-1.8345817	1.2418585

MeBpin

H	16.9017969	-5.4546332	9.7499799
H	17.9680656	-3.4279764	10.1149146
O	16.9998025	-4.0805523	7.4757290
H	16.5226378	-6.5855621	8.4305312
C	17.3305550	-6.0162222	8.9109334
B	17.6926515	-2.9004727	7.2603250
C	18.9726349	-3.8344394	9.9289679
H	19.1265685	-4.7024043	10.5851834
C	17.9823338	-5.0923421	7.8914068
H	18.0654633	-6.7334477	9.3056884
H	19.7093533	-3.0640554	10.1947683
C	19.1565762	-4.2080188	8.4556719
O	19.0107316	-2.9649298	7.6842511
H	17.4559476	-6.2910484	6.1817974
C	18.3667806	-5.8724837	6.6315621
H	18.8465312	-5.2193025	5.8887380
C	20.5523984	-4.7687848	8.2199629
H	19.0506321	-6.7002522	6.8655005
H	20.6666989	-5.7409693	8.7217684
H	21.3013688	-4.0804938	8.6360049
H	20.7620116	-4.8982038	7.1510532
C	17.0518829	-1.6172868	6.6309466
H	16.2069077	-1.8557339	5.9703798
H	17.7927699	-1.0326218	6.0668796
H	16.6694295	-0.9603124	7.4298959

Int_a

B	2.8491632	3.5830579	-1.9374078
H	2.6302764	2.8982224	-2.8942744
Mg	-0.0836016	0.4212731	0.3596591
C	0.0800729	1.7393671	2.0531825
O	2.2563070	4.8106024	-1.7536100
O	3.7178001	3.2152912	-0.9408151
C	2.6130428	5.2543888	-0.3870023
C	2.8411628	6.7588066	-0.4172949
H	3.5885204	7.0428074	-1.1680791
H	3.1777715	7.1143208	0.5674829
H	1.8980127	7.2685181	-0.6590826
C	1.4244490	4.9069829	0.5081592
H	1.2410384	3.8247949	0.5441147
H	0.5235188	5.3978957	0.1143297
H	1.5843293	5.2595965	1.5363666
H	3.1558005	3.2932072	1.6560672
H	4.9281529	3.3336320	1.4966436
C	4.0082269	3.9211068	1.3697042
H	4.0576826	4.7821953	2.0524208
C	3.8985185	4.3949855	-0.0728121
H	5.1416345	5.3970514	-1.5653163
C	5.2018191	5.0589624	-0.5211538
H	6.0170540	4.3261177	-0.4447978
H	5.4498111	5.9206898	0.1140640
H	-0.4518895	2.6925050	1.8795974
H	-0.3543087	1.3105948	2.9742495
H	1.1303391	1.9897095	2.2920267
C	0.2179256	-2.5183964	-0.6520100
C	-0.4478547	-3.6136677	-1.2949569
H	-0.2012179	-5.5564046	-2.2335755
C	1.6844288	-4.7462490	-1.5592094
C	0.2966310	-4.7165292	-1.7393497
H	1.8722563	-6.6976964	-2.4797616
C	2.5087406	-5.9177317	-2.0384887
H	3.2410905	-5.6121364	-2.8032223
H	3.0774824	-6.3769935	-1.2140519
C	2.3210644	-3.6559190	-0.9186967
H	3.4067280	-3.6956858	-0.7936291
C	1.6160590	-2.5416948	-0.4523732
C	-1.8399074	-3.2402669	-1.3330263
C	-3.0104935	-3.8382956	-1.8231494
H	-2.9701092	-4.8205812	-2.3033050
C	-4.2384219	-3.1789501	-1.7011965
C	-5.5139908	-3.8013323	-2.2188862
H	-6.2341401	-3.9862288	-1.4053517
H	-6.0161019	-3.1477867	-2.9503159
H	-5.3151485	-4.7634871	-2.7118758
C	-4.2813803	-1.9119922	-1.0701507
H	-5.2525657	-1.4173735	-0.9794158
C	-3.1395010	-1.2808344	-0.5663127
C	-1.9027350	-1.9491137	-0.7104943
N	-0.6587262	-1.5102696	-0.2981775
O	0.1341929	1.3789977	-1.5159489
C	-0.8841900	1.0283025	-3.6127123
H	-0.7138790	0.8104783	-4.6753556
H	-1.8053995	0.5197532	-3.2910813
H	-1.4990630	2.6118930	-1.1766477
C	-0.9511308	2.5337722	-3.3114596
H	-1.9351401	2.9720003	-3.5271379
H	0.0286326	3.4678724	-1.5721823
C	-0.6069381	2.6098142	-1.8221275
H	-0.2007082	3.0761819	-3.9054626
C	0.2795958	0.5906904	-2.7395506
H	1.2520711	0.8352985	-3.1963355
P	-3.0648025	0.3517601	0.2856687
H	0.2622470	-0.4662232	-2.4478143
C	-4.5585124	1.2808395	-0.3861503
H	-5.4537995	0.6559038	-0.2231262
C	-4.4206679	1.5337353	-1.8958613
C	-4.7481111	2.6052909	0.3727049
H	-4.8893085	2.4192354	1.4492871
H	-3.8272550	3.2095585	0.2785734
H	-3.4991060	2.1126645	-2.0788624
C	-5.9402892	3.4005046	-0.1787393
H	-6.8704442	2.8382890	0.0203029
H	-6.0303474	4.3586210	0.3577859
H	-4.3080834	0.5795644	-2.4324090
C	-5.6178918	2.3211674	-2.4439322
H	-6.5311097	1.7073136	-2.3458579
H	-5.4803025	2.5096795	-3.5210706
C	-5.8103237	3.6409650	-1.6878592
H	-4.9395411	4.2950028	-1.8763347
H	-6.6947244	4.1772669	-2.0675659
H	-5.7487331	0.1089004	1.8452212
H	-5.1199678	-1.5323947	1.6234431
C	-5.0112227	-0.6146897	2.2269715
C	-5.3229506	-0.9328252	3.6983958
H	-5.3124206	0.0061487	4.2806350
H	-6.3421576	-1.3443563	3.7819181
H	-4.5240395	-2.0912501	5.3595255
H	-4.3839063	-2.8804605	3.7804432
C	-4.3007774	-1.9068415	4.2961894
C	-2.8736657	-1.3730453	4.1308725
H	-2.1414361	-2.1002254	4.5186259
H	-2.7542681	-0.4535307	4.7314876
H	-2.5710753	-1.9959840	2.0775907
C	-2.5616093	-1.0606724	2.6622858
H	-1.5467166	-0.6462450	2.5737697
C	-3.5829996	-0.0801405	2.0600822
H	-3.4894979	0.8798006	2.6010797
H	0.6519228	-1.0121113	2.7809464
C	1.2888150	-1.9083058	2.8404293
H	0.7603162	-2.7115737	2.2981020

C	1.4787878	-2.3187969	4.3069778
H	1.8914061	-1.4635077	4.8716713
H	0.4992498	-2.5499058	4.7568415
H	1.9653376	-4.3982059	3.9590485
H	2.5783277	-3.7735780	5.4983318
C	2.4273658	-3.5161791	4.4375174
H	4.4347169	-4.1052396	3.8274827
C	3.7726230	-3.2267238	3.7609678
H	4.2808661	-2.4058339	4.2985686
H	3.1662056	-3.6829770	1.7314803
C	3.5860878	-2.8276670	2.2884160
H	4.5654982	-2.6019019	1.8365698
H	3.0890404	-0.7494818	2.6351353
C	2.6347802	-1.6324213	2.1485618
P	2.3145926	-1.0538237	0.3776493
C	4.0267762	-0.8726919	-0.3699526
H	4.5309044	-1.8532417	-0.3075422
H	4.9720550	-0.1471429	1.4608651
C	4.8576079	0.1603859	0.4091011
H	4.3205291	1.1221588	0.4053528
C	6.2431028	0.3519016	-0.2268766
H	6.8210624	-0.5845715	-0.1248340
H	6.8000571	1.1262423	0.3263155
C	6.1402943	0.7287487	-1.7102704
H	7.1461205	0.8110135	-2.1534955
H	5.1900318	0.0185267	-3.5367180
H	5.6647193	1.7204760	-1.7917316
C	5.2991212	-0.2935730	-2.4852047
H	5.8210514	-1.2675528	-2.4971990
C	3.9127333	-0.4743042	-1.8512003
H	3.3337808	-1.2318655	-2.4026701
H	3.3547133	0.4745925	-1.9192516

Int_a´

P	5.3434134	10.0433247	3.2464127
P	1.1382869	9.0139977	7.2634468
Mg	2.5912857	8.2164869	5.1974425
N	2.3200202	10.2485155	4.6767243
C	3.8339075	10.9785018	2.7867302
C	3.8773198	11.8074719	1.6521388
H	4.7466181	11.7591597	0.9946177
C	2.8629982	12.7289727	1.3247816
C	1.7687574	12.8520081	2.1894106
H	0.9940691	13.5963949	1.9831210
C	1.6635822	12.0192005	3.3065204
C	2.6660677	11.0187884	3.5891485
C	1.1355566	10.7932451	5.1532609
C	0.6785606	11.8822912	4.3483296
C	-0.5113142	12.5463085	4.6756184
H	-0.8682814	13.3763667	4.0585754
C	-1.2477106	12.1559425	5.8002459
C	-0.7683659	11.0920348	6.5994601
H	-1.3479872	10.8063495	7.4820331
C	0.4113356	10.4016613	6.3021863
C	2.9688661	13.5616616	0.0696183
H	4.0110269	13.8460282	-0.1400450
H	2.3759432	14.4837498	0.1513834
H	2.5984430	13.0111041	-0.8111392
C	-2.5439286	12.8412575	6.1602898
H	-2.6552654	13.7925811	5.6211133
H	-2.6019833	13.0548398	7.2386701
H	-3.4148730	12.2139433	5.9080511
C	5.6050952	8.7924149	1.8858101
H	5.6228530	9.3717022	0.9441296
C	6.9356062	8.0322161	2.0311554
H	7.7872278	8.7286355	1.9959703
H	6.9771321	7.5584740	3.0237627
C	7.0831032	6.9690328	0.9331377
H	7.1668623	7.4712412	-0.0475401
H	8.0220549	6.4125749	1.0834082
C	5.8875331	6.0095059	0.9063254
H	5.8609869	5.4331571	1.8481253
H	6.0053740	5.2772491	0.0918242
C	4.5681961	6.7747803	0.7485151
H	3.7124924	6.0816221	0.7762913
H	4.5466080	7.2669814	-0.2402431
C	4.4015341	7.8343875	1.8446091
H	3.4712045	8.4027820	1.6899162
H	4.3016624	7.3298357	2.8195531
C	6.8003192	11.2339525	3.2029776
H	7.5633395	10.6482554	3.7485070
C	6.4975891	12.5017365	4.0237950
H	5.7196286	13.0862608	3.5034461
H	6.0893882	12.2338908	5.0085466
C	7.7638041	13.3535728	4.1892915
H	7.5195551	14.2728511	4.7454860
H	8.4935428	12.7967540	4.8038215
C	8.3974215	13.7000785	2.8371847
H	7.7141399	14.3636408	2.2769226
H	9.3328997	14.2633133	2.9843350
C	8.6605088	12.4387382	2.0067988
H	9.4243870	11.8188517	2.5096361
H	9.0692751	12.7056873	1.0190589
C	7.3782685	11.6109670	1.8284613
H	6.6491279	12.2179071	1.2685063
H	7.5881489	10.7191223	1.2198517
C	-0.3107042	8.0451275	7.9368435
H	-0.9565854	8.7316852	8.5125170
C	-1.1265048	7.4533750	6.7727103
H	-0.4588029	6.8394912	6.1432035
H	-1.5083245	8.2623130	6.1311216
C	-2.2834354	6.5871364	7.2892616
H	-3.0018803	7.2262263	7.8335254
H	-2.8294570	6.1524355	6.4369666
C	-1.7809605	5.4799198	8.2240918
H	-2.6269714	4.8902572	8.6116616
H	-1.1454604	4.7831068	7.6489020
C	-0.9648400	6.0637996	9.3841277
H	-0.5710054	5.2574325	10.0235197
H	-1.6252035	6.6790878	10.0208939
C	0.1938618	6.9344602	8.8763583
H	0.9125766	6.3007761	8.3252336
H	0.7403830	7.3659712	9.7301376
C	1.9750339	9.8211321	8.7406329
H	2.4527192	8.9741349	9.2679590
C	1.0445622	10.5517855	9.7164061
H	0.5187398	11.3558881	9.1735621
H	0.2723466	9.8701397	10.1073966
C	1.8420556	11.1592149	10.8818013
H	2.2851086	10.3418595	11.4795430
H	1.1615454	11.7067898	11.5535664
C	2.9608004	12.0825487	10.3830378
H	2.5105699	12.9556433	9.8776710
H	3.5399077	12.4741352	11.2347029
C	3.8817789	11.3550225	9.3963141
H	4.6509556	12.0412719	9.0064067
H	4.4188764	10.5467819	9.9255283
C	3.0861163	10.7553946	8.2310372
H	3.7517266	10.2221470	7.5348815
H	2.6258100	11.5693386	7.6443482
H	4.4431211	7.5961394	8.1601439
H	5.9124854	9.3976093	7.8852402
O	4.5685466	8.2829047	5.6207311
H	3.7200651	6.2561609	7.2337561
C	4.6678973	6.7539944	7.4939736
B	5.4630639	9.4116457	5.2051672
C	6.7789171	8.7283934	7.7926643
H	6.7968894	8.0543042	8.6608346
C	5.3769731	7.2186008	6.2228927
H	5.2864112	6.0262093	8.0391889
H	7.6866238	9.3473094	7.8139667
C	6.7514059	7.9532027	6.4653150
O	6.8133778	8.8947113	5.3755351
H	4.4561510	5.7455637	4.9459915
C	5.4705645	6.0582074	5.2314125
H	6.0054188	6.3547639	4.3212713
C	7.9659005	7.0340725	6.3800789
H	5.9876334	5.1960961	5.6762404
H	7.9094380	6.2342918	7.1338026
H	8.8785119	7.6171042	6.5680050
H	8.0506886	6.5765940	5.3865963
H	5.1721713	10.4470162	5.7923037
C	1.8023753	6.4381498	4.2982003
H	0.7829707	6.6102207	3.9069207
H	1.7152762	5.6150956	5.0321176
H	2.3975353	6.0467192	3.4542755

Int_a″

P	5.4250382	10.0247552	3.2357446
P	1.3117192	9.0175230	7.3797141
Mg	2.8061559	8.1183250	5.3289260
N	2.4919981	10.2399061	4.7954933
C	3.8559315	10.8210445	2.7428199
C	3.7954784	11.5356728	1.5343603
H	4.6016836	11.4156801	0.8085993
C	2.7610185	12.4389107	1.2183838
C	1.7674849	12.6720714	2.1766314
H	0.9891930	13.4162645	1.9822910
C	1.7619696	11.9450811	3.3701270
C	2.7624912	10.9393681	3.6404610
C	1.3561057	10.8398214	5.3213008
C	0.8666848	11.9031098	4.4947500
C	-0.3011328	12.5936108	4.8447888
H	-0.6784507	13.3979232	4.2056757
C	-0.9961357	12.2539032	6.0107012
C	-0.5116489	11.1914349	6.8081219
H	-1.0803708	10.9146719	7.7007826
C	0.6467118	10.4754605	6.4883115
C	2.7481206	13.1445554	-0.1163108
H	3.7651631	13.4078530	-0.4446272
H	2.1567625	14.0702433	-0.0725756
H	2.3075926	12.5109837	-0.9042623
C	-2.2339452	13.0094797	6.4304531
H	-2.6470598	13.5940954	5.5961294
H	-2.0180756	13.7140535	7.2507221
H	-3.0205773	12.3281301	6.7890434
C	5.7366582	8.6032792	2.0670175
H	5.6534358	9.0244315	1.0477016
C	7.1392029	7.9950183	2.2434339
H	7.9176122	8.7480348	2.0513434
H	7.2710580	7.6857081	3.2921582
C	7.3366207	6.7912641	1.3110783
H	7.3293076	7.1410143	0.2629122
H	8.3293920	6.3471681	1.4879926
C	6.2373504	5.7387570	1.4983436
H	6.3082728	5.3145441	2.5158879
H	6.3861686	4.9024359	0.7970426
C	4.8457316	6.3539612	1.3082382
H	4.0631959	5.5995757	1.4866078
H	4.7321169	6.6887867	0.2610542
C	4.6326752	7.5475647	2.2465868
H	3.6465405	8.0057606	2.0771942
H	4.6409277	7.1849447	3.2889714
C	6.8198195	11.2557520	2.9613142
H	7.6438406	10.7518014	3.4995082
C	6.5343162	12.5864226	3.6829363
H	5.6892792	13.0904312	3.1829789
H	6.2267273	12.4001118	4.7212282
C	7.7735424	13.4927956	3.6533847
H	7.5396221	14.4542424	4.1381226
H	8.5737246	13.0230490	4.2528431
C	8.2799785	13.7241672	2.2248560
H	7.5254010	14.3030463	1.6621009
H	9.1991997	14.3313148	2.2365936
C	8.5286039	12.3950511	1.5019132
H	9.3544140	11.8544655	1.9980295
H	8.8461195	12.5743947	0.4620856
C	7.2697556	11.5136600	1.5140043
H	6.4740312	12.0404357	0.9642580
H	7.4625607	10.5723623	0.9777464
C	-0.1939443	8.0334965	7.8950817
H	-0.8533183	8.6689295	8.5123620
C	-0.9583777	7.6024904	6.6295663
H	-0.2590935	7.0714408	5.9598515
H	-1.3076455	8.4920987	6.0827800
C	-2.1388078	6.6823213	6.9645959
H	-2.8912766	7.2486719	7.5422801
H	-2.6338008	6.3602900	6.0335754
C	-1.6862416	5.4651818	7.7801350
H	-2.5502425	4.8319410	8.0381781
H	-1.0108776	4.8465294	7.1625753
C	-0.9449785	5.8994406	9.0506682
H	-0.5940499	5.0185451	9.6118603
H	-1.6447418	6.4398558	9.7135250
C	0.2456806	6.8109633	8.7205360
H	0.9925383	6.2413315	8.1400922
H	0.7422655	7.1335730	9.6500412
C	2.0773858	9.7129219	8.9497718
H	2.5884632	8.8441026	9.4045005
C	1.1060544	10.3062757	9.9771110

H	0.5560618	11.1419725	9.5108197
H	0.3571823	9.5601010	10.2858437
C	1.8666691	10.8231661	11.2098202
H	2.3353929	9.9666486	11.7273063
H	1.1581357	11.2732309	11.9241402
C	2.9533990	11.8350348	10.8234327
H	2.4733595	12.7386706	10.4069576
H	3.5096627	12.1569906	11.7185594
C	3.9111589	11.2523145	9.7770211
H	4.6528463	12.0072150	9.4707729
H	4.4788566	10.4161362	10.2243819
C	3.1463225	10.7455945	8.5486916
H	3.8305007	10.3192430	7.7981800
H	2.6470561	11.5956021	8.0526790
H	4.8161779	8.2609004	8.4617552
H	6.0129428	10.1912272	7.8843244
O	4.8312103	8.5315344	5.8138727
H	4.2689616	6.7161994	7.7695104
C	5.1432717	7.3615474	7.9269724
B	5.5730367	9.7047017	5.2556196
C	6.9539993	9.6269180	7.8919754
H	7.0440463	9.1054223	8.8555845
C	5.7791485	7.7114941	6.5839304
H	5.8623375	6.8193236	8.5594589
H	7.7797590	10.3478508	7.8088334
C	7.0377625	8.6583689	6.7012337
O	6.9855462	9.4188302	5.4819315
H	5.1251004	5.9287010	5.5719886
C	6.0719744	6.4335980	5.7980203
H	6.5796263	6.6583296	4.8517409
C	8.3690487	7.9126047	6.7497302
H	6.7052104	5.7473102	6.3780157
H	8.4133118	7.2381119	7.6178748
H	9.1888665	8.6394556	6.8403336
H	8.5322599	7.3249974	5.8375989
H	5.1401441	10.7651495	5.6913908
C	2.6173618	5.9504516	5.5565509
H	1.5531489	5.6538831	5.4816822
H	2.9446967	5.6144767	6.5581215
H	3.1651424	5.3157303	4.8341998
H	1.8395013	5.8684139	3.2012384
C	1.2185364	6.6190970	2.7036116
H	1.5550649	6.7465276	1.6568350
C	-0.2841067	6.3599582	2.7725472
O	1.3966488	7.8666172	3.4117928
C	0.3204936	8.7183587	2.9374630
C	-0.8869700	7.7857901	2.6989370
H	0.1461030	9.4839194	3.6990666
H	0.6452847	9.2124687	2.0055522
H	-0.5310166	5.8813271	3.7314909
H	-1.3428027	7.9849057	1.7191965
H	-1.6621728	7.9310042	3.4632365
H	-0.6322807	5.7037508	1.9634849

TS_a

B	1.7266171	2.6764039	0.2691737
H	1.7631104	1.8119355	-0.5767010
Mg	0.0860464	0.4526955	-0.0178287
C	0.2137103	1.7141073	1.7957473
O	1.1305387	3.9038676	-0.0704275
O	2.8444188	2.8567987	1.1072881
C	1.7471216	4.9353498	0.7594759
C	1.8425015	6.2114876	-0.0711101
H	2.3471607	6.0322476	-1.0287569
H	2.3909394	6.9925698	0.4762543
H	0.8316631	6.5893247	-0.2817459
C	0.8551900	5.1801573	1.9805938
H	0.7964379	4.2930869	2.6227586
H	-0.1609076	5.4157369	1.6333071
H	1.2221992	6.0281243	2.5772773
H	2.9799718	4.3583594	3.2960419
H	4.6320988	4.1449543	2.6722895
C	3.6742354	4.6569829	2.5011954
H	3.8482324	5.7411781	2.5718964
C	3.1369000	4.2837219	1.1248971
H	3.8363587	4.2625954	-0.9438530
C	4.2093695	4.5302389	0.0551003
H	5.0781222	3.8936732	0.2747219
H	4.5407692	5.5784644	0.0398681
H	-0.5070335	2.5451059	1.8015468
H	-0.2986648	0.8722298	2.3087541
H	1.0599101	1.9604886	2.4493617
C	0.3016230	-2.5947184	-0.6761069
C	-0.4183716	-3.7251749	-1.1874277
H	-0.2369042	-5.7308062	-2.0034986
C	1.6934487	-4.8741649	-1.5505226
C	0.2938808	-4.8574760	-1.6121782
H	1.8151910	-6.8515362	-2.4265489
C	2.4771694	-6.0852706	-1.9990547
H	3.2259407	-5.8236730	-2.7635176
H	3.0221871	-6.5477308	-1.1599521
C	2.3819025	-3.7397827	-1.0527832
H	3.4751138	-3.7683249	-1.0279387
C	1.7115662	-2.5977226	-0.6049736
C	-1.8080980	-3.3335625	-1.1479296
C	-3.0278130	-3.9231490	-1.5161110
H	-3.0516145	-4.9388504	-1.9220575
C	-4.2257158	-3.2103317	-1.3755698
C	-5.5484936	-3.8278349	-1.7652986
H	-6.2233888	-3.9193231	-0.8986826
H	-6.0738673	-3.2194260	-2.5188997
H	-5.4097661	-4.8340705	-2.1853174
C	-4.1944815	-1.8920182	-0.8555998
H	-5.1399743	-1.3490060	-0.7636887
C	-3.0032536	-1.2719174	-0.4678546
C	-1.8040118	-2.0008502	-0.6169180
N	-0.5332814	-1.5566755	-0.3241748
O	-0.1062051	0.9580964	-2.0913726
C	-0.3596787	0.6214843	-4.4466026
H	0.0597510	-0.0147342	-5.2370161
H	-1.3832708	0.9007080	-4.7391829
H	-0.9268997	2.7652396	-2.7595073
C	0.4761767	1.8817829	-4.1777115
H	0.2787222	2.6906938	-4.8935498
H	0.7668390	2.8371080	-2.1931883
C	0.0458866	2.2435242	-2.7655255
H	1.5525224	1.6504262	-4.1998453
C	-0.3637061	-0.0892484	-3.0929912
H	0.4408515	-0.8323529	-2.9992258
P	-2.7661682	0.4099199	0.2427270
H	-1.3202399	-0.5697459	-2.8499526
C	-4.0731109	1.4777269	-0.5745104
H	-5.0690251	1.0420224	-0.3789695
C	-3.8472932	1.5166357	-2.0950091
C	-4.0195651	2.8943076	0.0247300
H	-4.2266966	2.8638574	1.1063994
H	-2.9922012	3.2887351	-0.0853480
H	-2.8159758	1.8577061	-2.2906944
C	-5.0065319	3.8407171	-0.6727403
H	-6.0384072	3.5016836	-0.4702719
H	-4.9181333	4.8528420	-0.2459645
H	-3.9269708	0.5020054	-2.5150608
C	-4.8348228	2.4649279	-2.7875914
H	-5.8593021	2.0655971	-2.6772753
H	-4.6256969	2.4967849	-3.8691997
C	-4.7740825	3.8748198	-2.1877745
H	-3.7792457	4.3125628	-2.3903740
H	-5.5124325	4.5317457	-2.6746733
H	-5.4254174	0.8341832	1.7972012
H	-5.1696589	-0.9172518	1.7046529
C	-4.8555872	-0.0006661	2.2343004
C	-5.2009972	-0.1317887	3.7270488
H	-4.9742114	0.8242544	4.2327417
H	-6.2836076	-0.3017712	3.8460071
H	-4.6365726	-1.3024543	5.4735221
H	-4.7151128	-2.2263849	3.9655702
C	-4.4046401	-1.2578514	4.3972961
C	-2.8975110	-1.0743052	4.1802382
H	-2.3398280	-1.9178875	4.6185639
H	-2.5579721	-0.1631491	4.7050895
H	-2.8223344	-1.8940313	2.1751132
C	-2.5636378	-0.9520647	2.6881255
H	-1.4799480	-0.8173410	2.5475086
C	-3.3473747	0.1997659	2.0316763
H	-3.0412547	1.1433539	2.5208688
H	1.0496539	-0.9713846	2.6184860
C	1.7702749	-1.8026473	2.6604114
H	1.2582511	-2.6860716	2.2401973
C	2.1684674	-2.0833559	4.1152349
H	2.5712038	-1.1577538	4.5644327
H	1.2741641	-2.3544663	4.7001173
H	2.7836614	-4.1414007	3.8548670
H	3.5256569	-3.3499476	5.2537845
C	3.2248718	-3.1910761	4.2056835
H	5.1827887	-3.6801581	3.3847087
C	4.4486182	-2.8589239	3.3441927
H	4.9515265	-1.9646319	3.7549296
H	3.6311961	-3.5095908	1.4464389
C	4.0500912	-2.5878338	1.8851869
H	4.9428691	-2.3300030	1.2928768
H	3.4350959	-0.5289656	2.1676970
C	2.9991780	-1.4743763	1.7950666
P	2.4234343	-1.0368660	0.0575538
C	3.9818468	-0.7433393	-0.9436317
H	4.5537146	-1.6867854	-1.0019310
H	5.2168315	-0.0165032	0.6982203
C	4.8560056	0.3355493	-0.2808480
H	4.2466859	1.2324409	-0.0789570
C	6.0528350	0.7153910	-1.1639093
H	6.7343630	-0.1500659	-1.2538505
H	6.6282111	1.5202332	-0.6776681
C	5.6067427	1.1489298	-2.5651329
H	6.4813291	1.3982674	-3.1875282
H	4.4215836	0.3832293	-4.2272027
H	5.0018207	2.0702907	-2.4829690
C	4.7674284	0.0541499	-3.2335706
H	5.3978063	-0.8381723	-3.3992733
C	3.5620285	-0.3271470	-2.3658953
H	2.9880398	-1.1399421	-2.8394599
H	2.8827268	0.5408835	-2.2883809

Int_b

P	4.6722345	9.5406167	3.0005520
P	1.1831435	9.3168414	7.1692084
Mg	3.1458539	8.7225658	5.2307075
N	2.2419486	10.5087763	4.5718902
C	3.5448387	10.9035499	2.4832783
C	3.5936220	11.6584714	1.3066094
H	4.3863073	11.4700230	0.5771900
C	2.6407099	12.6646672	1.0119321
C	1.6026273	12.9153363	1.9191636
H	0.8607204	13.6857263	1.6887063
C	1.5101447	12.1730241	3.1064862
C	2.4911371	11.1638894	3.3858716
C	1.0870976	11.0763471	5.0671350
C	0.5858837	12.1151456	4.2146552
C	-0.5991463	12.7795469	4.5634215
H	-0.9974623	13.5728247	3.9234530
C	-1.2883360	12.4245647	5.7296891
C	-0.7771379	11.3893987	6.5500468
H	-1.3403038	11.1175425	7.4476775
C	0.4052664	10.7071375	6.2460731
C	2.7646488	13.4587323	-0.2675768
H	3.6414790	14.1267205	-0.2458611
H	1.8766368	14.0842304	-0.4358498
H	2.8842178	12.8006369	-1.1426864
C	-2.5562439	13.1403698	6.1317194
H	-2.9348743	13.7696877	5.3138294
H	-2.3923233	13.7951259	7.0036221
H	-3.3515078	12.4303848	6.4071239
C	5.1564497	8.7075876	1.3898808
H	5.4966967	9.4817419	0.6797417
C	6.3027746	7.7063611	1.6134261
H	7.1992526	8.2235313	1.9899064
H	6.0039824	6.9844877	2.3947977
C	6.6435473	6.9493022	0.3211591
H	7.0443588	7.6643692	-0.4197747
H	7.4433382	6.2177984	0.5179824
C	5.4114814	6.2514705	-0.2678438
H	5.0735159	5.4639546	0.4300543
H	5.6722102	5.7460402	-1.2115407
C	4.2673436	7.2477560	-0.4926873
H	3.3720742	6.7288569	-0.8726092
H	4.5635131	7.9741434	-1.2699886
C	3.9229478	8.0035194	0.7971935
H	3.1233837	8.7374447	0.6111857
H	3.5336111	7.2893546	1.5457792
C	6.2249419	10.4322422	3.5936510
H	6.9182198	9.6123443	3.8577787
C	5.8846963	11.1941030	4.8880468

H	5.1013158	11.9411303	4.6732526
H	5.4642294	10.4963354	5.6317667
C	7.1178610	11.8979187	5.4697233
H	6.8299069	12.4688509	6.3677320
H	7.8471830	11.1365751	5.7993568
C	7.7788160	12.8176156	4.4366348
H	7.0826680	13.6371926	4.1825609
H	8.6800793	13.2872903	4.8624571
C	8.1317086	12.0467056	3.1588706
H	8.9006179	11.2885737	3.3921673
H	8.5731170	12.7242034	2.4097517
C	6.8969340	11.3499623	2.5659216
H	6.1704074	12.1150865	2.2429873
H	7.1830015	10.7814772	1.6659481
C	-0.2646108	8.3576230	7.8808443
H	-0.9232187	9.0575035	8.4253231
C	-1.0660004	7.7222055	6.7307909
H	-0.3822449	7.0937779	6.1323110
H	-1.4452840	8.5069071	6.0578528
C	-2.2200599	6.8571487	7.2539704
H	-2.9526591	7.5038301	7.7690265
H	-2.7515207	6.3914213	6.4081494
C	-1.7171680	5.7849805	8.2282031
H	-2.5609716	5.1959749	8.6214161
H	-1.0650118	5.0780566	7.6833283
C	-0.9234138	6.4144313	9.3797364
H	-0.5311970	5.6326090	10.0499260
H	-1.6006616	7.0410296	9.9870389
C	0.2331802	7.2818604	8.8618852
H	0.9713882	6.6399368	8.3472937
H	0.7597433	7.7466483	9.7101588
C	2.0061562	10.1449182	8.6496426
H	2.4354717	9.3001856	9.2195221
C	1.0759733	10.9496198	9.5658067
H	0.5858472	11.7393170	8.9710412
H	0.2746827	10.3076373	9.9659936
C	1.8525051	11.5983187	10.7222048
H	2.2622787	10.8059605	11.3749871
H	1.1657701	12.1950061	11.3443367
C	3.0026585	12.4704833	10.2043980
H	2.5843918	13.3177487	9.6316451
H	3.5636332	12.9044588	11.0476513
C	3.9397172	11.6637686	9.2975433
H	4.7393144	12.3082649	8.8969139
H	4.4365383	10.8777423	9.8939563
C	3.1755778	11.0080508	8.1399833
H	3.8620454	10.3880803	7.5395335
H	2.7827716	11.7904514	7.4669723
H	2.0391990	5.6752542	5.3078066
C	1.9628431	5.9415741	4.2444337
H	2.8625449	5.5808761	3.7192488
C	0.6772687	5.4743187	3.5696790
O	1.9334076	7.3971237	4.1512499
C	0.8823217	7.8271172	3.2260525
C	0.4541020	6.5570745	2.5019892
H	0.0669928	8.2688475	3.8194312
H	1.3080598	8.6008195	2.5743275
H	-0.1556064	5.4669530	4.2898167
H	1.0984169	6.3755021	1.6282112
H	-0.5868615	6.6122402	2.1577254
H	0.7758970	4.4655225	3.1482069
H	4.3800438	7.9412494	6.2285373

Int_c

C	4.5141330	9.4964100	2.8880900
C	3.6621125	9.5327235	4.1663666
C	3.9014623	8.1493212	4.7625323
O	5.2509277	7.7766964	4.3405135
C	5.7465907	8.7254837	3.3393344
Mg	6.4463031	6.2129292	5.0698834
N	8.2056572	6.7158096	4.0469931
C	8.5161840	6.4419448	2.7340707
C	9.6408925	7.2040873	2.2737195
C	10.0357723	8.0132004	3.4034592
C	9.1159517	7.6693977	4.4482172
C	7.8269121	5.5607867	1.8734073
C	8.2836916	5.4557987	0.5554023
C	9.3990550	6.1876918	0.0791973
C	10.0706715	7.0594608	0.9461118
C	11.0147492	8.9899719	3.6434185
C	11.0823172	9.6270851	4.8891964
C	10.1562399	9.2748781	5.9027053
C	9.1734472	8.2987451	5.7104243
P	6.3696478	4.7310077	2.6388265
C	6.9618756	2.9735348	2.9813325
C	8.0123282	3.0205759	4.1059734
C	8.4906145	1.6145920	4.4905408
C	9.0096376	0.8437582	3.2706563
C	7.9509318	0.7871517	2.1624232
C	7.4776818	2.1941964	1.7652939
C	9.8537409	6.0108176	-1.3505502
C	12.1354046	10.6736756	5.1708851
P	7.8719878	7.7452753	6.8917547
C	8.7813048	6.6350485	8.1117950
C	9.9430576	7.2899167	8.8685142
C	10.6203615	6.2942078	9.8226936
C	11.0881684	5.0368367	9.0795266
C	9.9264194	4.3764658	8.3278113
C	9.2385902	5.3625779	7.3743061
C	5.1358512	4.5701522	1.2328146
C	3.9620218	3.6627237	1.6348600
C	2.8979394	3.5984174	0.5295654
C	2.4020495	4.9965044	0.1420091
C	3.5695286	5.9047392	-0.2606394
C	4.6327715	5.9710537	0.8432143
C	7.4084545	9.2857860	7.8547715
C	6.7085254	10.2731360	6.9048038
C	6.2235159	11.5264683	7.6444407
C	5.3130708	11.1597030	8.8222832
C	6.0123163	10.1838965	9.7758043
C	6.4986629	8.9254708	9.0416929
O	3.7872999	6.5476333	7.8933564
C	3.4670926	5.6181526	7.2207116
N	2.8876103	4.7392846	6.6206929
C	3.2191260	3.6467527	5.7439974
H	7.7649252	4.7938758	-0.1441312
H	10.9258223	7.6328333	0.5755660
H	11.7250979	9.2665621	2.8585192
H	10.2180849	9.7957097	6.8624836
H	10.2613793	5.0011738	-1.5235970
H	10.6398181	6.7336355	-1.6101261
H	9.0226963	6.1480306	-2.0605163
H	12.6886229	10.9372108	4.2583696
H	12.8693832	10.3196737	5.9133618
H	11.6908633	11.5972556	5.5737923
H	5.6474679	4.1222389	0.3623941
H	4.3188521	2.6477269	1.8696884
H	3.5045205	4.0576213	2.5601966
H	3.3316080	3.1064162	-0.3594869
H	2.0562578	2.9680950	0.8590693
H	1.8751649	5.4451506	1.0040141
H	1.6669623	4.9286898	-0.6758550
H	3.2069480	6.9195495	-0.4915782
H	4.0315783	5.5175342	-1.1862727
H	5.4784311	6.6012710	0.5259962
H	4.1981868	6.4492512	1.7401017
H	6.0647084	2.4645315	3.3819626
H	8.8733890	3.6262497	3.7725231
H	7.5880681	3.5290825	4.9880422
H	9.2724293	1.6875771	5.2642016
H	7.6503192	1.0574919	4.9425621
H	9.9132090	1.3467989	2.8818974
H	9.3145203	-0.1745018	3.5611251
H	7.0851113	0.1983213	2.5164148
H	8.3473656	0.2637461	1.2772014
H	8.3209164	2.7491121	1.3194242
H	6.6977999	2.1218983	0.9895702
H	8.3311010	9.7561347	8.2384590
H	5.8417768	9.7625690	6.4491929
H	7.3858121	10.5481130	6.0807268
H	7.0976240	12.0892613	8.0186461
H	5.6977551	12.1943162	6.9424412
H	4.9999622	12.0671190	9.3633779
H	4.3919023	10.6882457	8.4346708
H	5.3348174	9.8955610	10.5953569
H	6.8769104	10.6900071	10.2417696
H	5.6292812	8.3537167	8.6712493
H	7.0296603	8.2667638	9.7468150
H	7.9966564	6.3422662	8.8336641
H	10.6852677	7.6529233	8.1368932
H	9.5929441	8.1703053	9.4313090
H	9.9048996	6.0042578	10.6132846
H	11.4696979	6.7819378	10.3281277
H	11.8757654	5.3160941	8.3568621
H	11.5445327	4.3230561	9.7843222
H	10.2808084	3.4987266	7.7628715
H	9.1860473	4.0035927	9.0582623
H	8.3723063	4.8793116	6.8931548
H	9.9359186	5.6429393	6.5658713
H	3.8716582	8.1224456	5.8601828
H	3.2008477	7.3978549	4.3628545
H	6.4937494	9.3737716	3.8227932
H	6.2371489	8.1461283	2.5469671
H	4.0278229	10.3146003	4.8493019
H	3.9896863	8.9504785	2.0890392
H	4.7703603	10.4961266	2.5136538
H	2.5976043	9.7171718	3.9713262
H	5.6844126	5.0209203	6.1348661
H	4.2684456	3.7406095	5.4162252
H	3.0794165	2.6896039	6.2679234
H	2.5480585	3.6599788	4.8734524

TS_b

P	2.6516654	-0.0550048	0.6003591
P	-2.6795116	0.1521976	-0.0551743
Mg	0.0480262	0.8254799	0.0086052
O	0.3000104	0.9086630	-2.1326579
N	-0.0201227	-1.2941684	-0.0827014
C	-1.7255937	-4.2567719	-1.3223553
H	-1.4648521	-5.2754180	-1.6256376
C	0.7011912	-3.4272178	-0.7018077
C	-3.0587275	-3.8334570	-1.4088984
C	-1.1038067	-2.0449746	-0.4749881
C	4.2029858	0.5511869	-0.2595295
H	5.0339656	-0.1411028	-0.0372932
C	2.3042344	-1.1322618	4.6492244
H	1.5173798	-1.7278496	5.1397932
H	2.2513471	-0.1184164	5.0859356
C	3.1287995	-0.2561896	2.4163474
H	3.1190474	0.7787259	2.8072441
C	1.7058109	-4.3809433	-0.9275487
H	1.4483623	-5.3814810	-1.2884478
C	2.0253913	-1.0476191	3.1426341
H	1.0441738	-0.5868549	2.9596336
H	1.9838595	-2.0660233	2.7195549
C	-0.7331438	-3.3759159	-0.8648807
C	2.4169956	-1.7824791	0.0073708
C	1.0682218	-2.1234762	-0.2281749
C	3.3861215	-2.7583100	-0.2425811
H	4.4429404	-2.5213655	-0.0886423
C	-4.1418604	-4.7729338	-1.8853537
H	-4.8077983	-5.0751039	-1.0600779
H	-3.7134220	-5.6891672	-2.3157569
H	-4.7759396	-4.3037461	-2.6540604
C	4.5639017	1.9557333	0.2567176
H	3.6860104	2.6158213	0.1331523
H	4.7829207	1.9251368	1.3361552
C	-2.4410140	-1.6025246	-0.5613834
C	3.0499726	-4.0563317	-0.7024934
C	-3.9123217	0.8450271	-1.2855734
H	-4.8258712	0.2256974	-1.2658254
C	4.5062546	-0.8749799	2.6864367
H	4.5336051	-1.8898839	2.2530561
H	5.3029071	-0.2944797	2.1951410
C	-3.6121114	0.0389655	1.5828629
H	-3.6170622	1.0807880	1.9543692
C	4.7867047	-0.9616983	4.1955079
H	5.7686413	-1.4325337	4.3662125
H	4.8509469	0.0612972	4.6089237
C	3.6854453	-1.7350120	4.9306577
H	3.8870345	-1.7508545	6.0139650
H	3.6953974	-2.7866582	4.5913888
C	-3.3952299	-2.5085965	-1.0340382
H	-4.4376505	-2.1924018	-1.1326548
C	4.1445043	-5.0711854	-0.9379376
H	4.9065192	-4.6914282	-1.6373597
H	3.7394024	-6.0026140	-1.3577559
H	4.6671151	-5.3280473	-0.0018513
C	0.3467190	-0.2221478	-3.0614494
H	-0.5001696	-0.8803151	-2.8328809

H	1.2832125	-0.7722720	-2.8819291
C	3.9683606	0.5689485	-1.7792481
H	3.7522909	-0.4495062	-2.1380992
H	3.0691650	1.1742968	-1.9871961
C	-5.0594531	-0.4655263	1.5036956
H	-5.0598826	-1.4874848	1.0859988
H	-5.6588636	0.1597144	0.8232457
C	-2.7928633	-0.8128000	2.5700790
H	-2.7292660	-1.8430367	2.1796040
H	-1.7635112	-0.4326191	2.6360200
C	-3.4451726	-0.8337561	3.9592940
H	-3.4218557	0.1852431	4.3869186
H	-2.8561866	-1.4726536	4.6369856
C	-3.3130307	0.7925820	-2.7013741
H	-2.3463419	1.3252913	-2.6934508
H	-3.0961458	-0.2505363	-2.9793678
C	5.7600444	2.5471407	-0.5029607
H	5.9687292	3.5648379	-0.1354821
H	6.6597260	1.9427066	-0.2887328
C	-5.7138008	-0.4881951	2.8950936
H	-5.7962668	0.5478964	3.2704917
H	-6.7417884	-0.8781434	2.8176079
C	-4.8969947	-1.3219907	3.8896776
H	-4.9060286	-2.3787621	3.5674553
H	-5.3634641	-1.2916547	4.8877387
C	-4.2744697	2.2893062	-0.8969011
H	-4.7480973	2.3137205	0.0978112
H	-3.3436654	2.8795036	-0.8166257
C	5.1653766	1.1623413	-2.5331524
H	6.0402042	0.4998063	-2.4069862
H	4.9482481	1.1928794	-3.6137474
C	-5.2031264	2.9363098	-1.9343694
H	-5.4145165	3.9787613	-1.6465247
H	-6.1721476	2.4055677	-1.9343017
C	0.5064644	2.1587641	-2.8573876
H	-0.4573873	2.6920886	-2.9113104
H	1.2064195	2.7706554	-2.2738221
C	5.5124944	2.5638473	-2.0161521
H	6.3931828	2.9623564	-2.5447496
H	4.6737396	3.2491702	-2.2373353
C	-4.5983443	2.8806933	-3.3426639
H	-3.6822183	3.4979487	-3.3665481
H	-5.2942600	3.3187161	-4.0761246
C	-4.2436635	1.4411305	-3.7339786
H	-5.1707870	0.8455656	-3.8118450
H	-3.7703949	1.4178405	-4.7294788
C	0.2980226	0.4007144	-4.4521638
H	0.7885086	-0.2322112	-5.2034584
H	-0.7449512	0.5632842	-4.7652465
C	1.0088656	1.7454578	-4.2362617
H	2.1006581	1.6046785	-4.2234621
H	0.7662237	2.4919397	-5.0041098
H	0.1122577	2.6384033	0.1771229
C	-0.1432585	2.5876020	2.2518970
O	-0.2078480	1.3802354	2.3075084
N	-0.1148873	3.7755788	2.4794751
C	-0.2224103	4.5786210	3.6819574
H	-1.0611248	5.2810241	3.5768084
H	0.6954299	5.1699561	3.8087184
H	-0.3799956	3.9648181	4.5820972

Int_d

C	2.6093560	0.7674684	1.3195338
C	1.1048150	0.5980557	1.1392055
O	0.7026438	1.6972305	0.2641060
C	1.7909801	2.6701463	0.1307801
C	2.7861303	2.2914969	1.2202303
Mg	-1.0788579	1.8547718	-0.7761473
O	-2.3099186	0.4188978	-0.3853781
C	-2.5390975	-0.7948557	-0.8359908
N	-3.6797894	-1.3474242	-1.0858672
C	-4.8595051	-0.5146120	-0.8579613
N	-0.8016758	3.5516310	-1.9243881
C	-0.9949091	4.8485349	-1.5103331
C	-0.4623153	5.7983280	-2.4429939
C	0.1014598	5.0008834	-3.5107480
C	-0.1394374	3.6408512	-3.1266090
C	0.2831887	2.5584144	-3.9253033
C	0.9640321	2.8588390	-5.1085286
C	1.2174564	4.1933610	-5.5147510
C	0.7804542	5.2563405	-4.7125358
C	-0.5654564	7.1669091	-2.1502934
C	-1.1763967	7.5897033	-0.9614851
C	-1.6943133	6.6273137	-0.0587356
C	-1.6228281	5.2544112	-0.3145598
C	-1.3021916	9.0596456	-0.6354859
P	-0.1320597	0.9036668	-3.2248932
C	-1.5727264	0.2830342	-4.2654165
C	-2.8067014	1.1574244	-3.9789940
C	-4.0422628	0.6308702	-4.7204185
C	-3.7834193	0.5121907	-6.2271750
C	-2.5507458	-0.3558960	-6.5107495
C	-1.3096749	0.1703637	-5.7715987
P	-2.2190154	3.8561980	0.7290417
C	-4.0890886	3.8552051	0.5247035
C	-4.8005774	5.1647680	0.8854026
C	-6.3173058	5.0527831	0.6634020
C	-6.6428463	4.6246872	-0.7729169
C	-5.9356472	3.3120962	-1.1306810
C	-4.4208979	3.4094610	-0.9109869
C	1.9488264	4.4494073	-6.8116634
C	1.3242397	-0.1849165	-3.6809443
C	1.0192376	-1.6601024	-3.3705075
C	2.2354222	-2.5541460	-3.6518423
C	3.4771731	-2.0760826	-2.8896014
C	3.7852989	-0.6065197	-3.2007796
C	2.5726228	0.2889902	-2.9168595
C	-1.8873817	4.4009999	2.4912663
C	-0.3677303	4.4996617	2.7115247
C	-0.0283714	4.8763170	4.1595332
C	-0.6626158	3.8961522	5.1533158
C	-2.1779581	3.7982366	4.9410926
C	-2.5252428	3.4234866	3.4925486
H	-0.1661269	7.9137750	-2.8428180
H	1.5115040	-0.0813528	-4.7643679
H	-4.9018042	1.2931038	-4.5270118
H	-4.3071038	-0.3600081	-4.3112689
H	-1.7774452	-0.7225896	-3.8542253
H	0.9768557	6.2846011	-5.0307758
H	-3.0050116	1.1826302	-2.8960177
H	-2.5980158	2.1955425	-4.2907807
H	1.3183738	2.0469912	-5.7498569
H	-2.3558252	9.3834917	-0.6276516
H	-0.7710751	9.6774488	-1.3730694
H	-0.8874778	9.2917472	0.3583172
H	0.7337264	-1.7534605	-2.3065069
H	0.1546552	-2.0093536	-3.9565874
H	-2.3323713	5.4019853	2.6360015
H	-1.0465467	1.1676071	-6.1643535
H	-0.4490168	-0.4889258	-5.9695201
H	-4.4266381	3.0549561	1.2096358
H	-2.3497601	-0.3973799	-7.5936446
H	-2.7531892	-1.3919096	-6.1852467
H	-4.6676412	0.0969452	-6.7367388
H	-3.6191976	1.5208181	-6.6480100
H	-2.1589665	6.9828229	0.8653445
H	2.9451229	3.9789772	-6.8144409
H	2.0866597	5.5258729	-6.9851246
H	1.3980785	4.0403483	-7.6741254
H	1.3558512	3.6719262	0.2392457
H	2.2140162	2.5697186	-0.8804228
H	2.7966869	1.3366270	-3.1727242
H	2.3498339	0.2648725	-1.8348979
H	-4.4001739	5.9745089	0.2510700
H	-4.5929248	5.4456461	1.9307347
H	-3.9895770	4.1326408	-1.6253246
H	-3.9509828	2.4332386	-1.1115986
H	-6.3382706	2.4964481	-0.5034123
H	-6.1414411	3.0329499	-2.1766336
H	0.0840003	3.5185396	2.4765291
H	0.0690620	5.2278647	2.0103177
H	1.9988678	-3.5972262	-3.3882494
H	2.4479664	-2.5426121	-4.7358703
H	-6.7334921	4.3099298	1.3675467
H	-6.8000880	6.0154757	0.8977788
H	-6.3133788	5.4165931	-1.4695548
H	-7.7320442	4.5213489	-0.9033435
H	-3.6186464	3.3990497	3.3657919
H	-2.1617843	2.4013498	3.2792647
H	4.0674439	-0.5091665	-4.2641654
H	4.6511086	-0.2602834	-2.6128686
H	-2.6167949	3.0599496	5.6310153
H	-2.6417231	4.7713811	5.1828920
H	0.5560247	0.6990273	2.0891145
H	0.8096859	-0.3425309	0.6532950
H	4.3440655	-2.7106963	-3.1328775
H	3.3001086	-2.1865683	-1.8038867
H	-0.2120792	2.8960921	5.0139165
H	-0.4394756	4.1998538	6.1883623
H	-0.3982762	5.8965669	4.3659298
H	1.0655651	4.9067119	4.2904805
H	3.8106079	2.5883329	0.9610607
H	2.5169926	2.7738584	2.1726018
H	3.1546018	0.2626587	0.5076073
H	2.9575847	0.3557055	2.2756359
H	-1.6485068	-1.4313126	-1.0132308
H	-5.0335495	0.1733441	-1.7058309
H	-4.7817208	0.1141839	0.0480113
H	-5.7473664	-1.1577311	-0.7722925

TS_c

Mg	-0.2109247	0.9391765	0.0705426
O	1.9070303	1.3384924	-0.1713699
C	2.4616074	2.4290285	-0.4033097
N	2.0943884	3.6294782	0.0794856
B	1.1147691	3.8805255	1.2004734
C	-1.0582924	2.9569724	0.2657357
C	2.7921722	4.8143540	-0.4474948
H	3.5671235	4.4970530	-1.1582236
H	2.0848278	5.4771130	-0.9625913
H	3.2619189	5.3799000	0.3680932
O	0.7613304	5.2230217	1.3352491
H	3.3399794	2.4632568	-1.0805161
O	1.1389912	3.2033470	2.4209658
C	1.1180492	4.2475551	3.4540352
C	0.3873441	3.7359000	4.6870522
H	-0.6077617	3.3518942	4.4347170
H	0.9632063	2.9284562	5.1604860
H	0.2739553	4.5448780	5.4240109
H	3.0677816	3.6188151	4.1185119
C	2.5807181	4.5504232	3.8000623
H	3.1259601	4.9393023	2.9277542
H	2.6607046	5.2825639	4.6159504
H	-1.4469253	5.6932942	3.8695727
C	0.9081133	6.8284029	3.1256474
H	1.9756635	6.9424514	2.8998761
H	0.3553637	7.5960238	2.5658581
H	0.7516377	7.0098227	4.1990120
C	0.3947637	5.4470063	2.7311856
C	-1.1296745	5.4053210	2.8573902
H	-1.5291676	4.4110208	2.6273315
H	-1.5644425	6.1177131	2.1427469
H	-1.7592697	2.6582653	-0.5411564
H	-1.6536316	2.9988030	1.1926399
H	-0.8104417	3.9963830	0.0083184
O	-0.0082233	0.7920743	-2.0731400
H	1.4982173	-0.6474849	-2.1900057
C	0.5640921	-0.3840449	-2.7156880
H	-0.1622971	-1.1993956	-2.6049188
C	0.8238372	0.0416381	-4.1558197
H	1.6256370	-0.5447868	-4.6237590
H	-0.0894645	-0.0734248	-4.7580498
C	1.1804783	1.5283074	-3.9949632
H	1.0383305	2.1102677	-4.9155940
H	2.2298700	1.6356682	-3.6786799
C	0.2379521	1.9754511	-2.8801543
H	-0.7351377	2.3259725	-3.2585930
H	0.6513663	2.7590348	-2.2293248
C	3.1134482	0.6466368	3.2887025
H	2.5933201	0.9891035	4.1980799
H	2.9810283	1.4493709	2.5464328
C	4.6062401	0.4486124	3.5832506
H	4.7258336	-0.2665400	4.4171749
H	5.0475695	1.4014453	3.9196013
H	5.3102164	0.6699000	1.5484306
C	5.3534927	-0.0851812	2.3552338
H	6.4194858	-0.2378383	2.5890910
H	5.2432235	-1.7554129	0.9587797
C	4.7186093	-1.3888316	1.8561531
H	4.8373541	-2.1687195	2.6304786
H	2.7795730	-2.1554413	1.2291270

C	3.2283441	-1.2005517	1.5426726
H	3.1158097	-0.5008795	0.6983381
C	2.4620659	-0.6403260	2.7561355
H	2.4761197	-1.4020101	3.5579991
N	-1.3582106	-0.9356008	0.0070299
C	-0.8661019	-2.0081229	0.7387452
C	0.0410154	-1.9849592	1.8242103
C	0.3998672	-3.1989996	2.4197894
H	1.1099281	-3.1950657	3.2522098
C	-0.1109091	-4.4436552	1.9857044
H	-0.0822293	-6.6019378	2.1593770
C	0.3063903	-5.7167016	2.6826359
H	-0.0675962	-5.7532826	3.7192347
H	1.4028427	-5.8107517	2.7334837
H	-1.4285620	-5.4142544	0.5748431
C	-1.0168390	-4.4608034	0.9203978
C	-1.4003220	-3.2626846	0.3017588
C	-2.3008072	-2.9367098	-0.7661744
C	-2.2619520	-1.5012469	-0.8922944
H	-3.1174441	-4.8181158	-1.4681510
C	-3.1179420	-3.7297214	-1.5825821
H	-4.8474637	-4.9955395	-3.1436628
C	-4.8276486	-3.9384507	-3.4451335
H	-5.8645632	-3.5666416	-3.4385112
H	-4.4786970	-3.8977269	-4.4902965
C	-3.9424493	-3.1259769	-2.5308184
C	-3.9494235	-1.7156631	-2.6074425
H	-4.6430405	-1.2597521	-3.3178193
C	-3.1525731	-0.8811836	-1.8118884
P	-3.3206669	0.9656498	-1.8492681
C	-4.0763696	1.2938227	-3.5510739
H	-4.9915943	0.6905081	-3.6830551
C	-3.0860939	0.9175363	-4.6661217
H	-2.8283809	-0.1506400	-4.6007126
H	-2.1464008	1.4769716	-4.5117381
H	-3.5816480	3.4022343	-3.4469566
C	-4.4696026	2.7781139	-3.6586198
H	-5.2194324	3.0336774	-2.8935003
H	-4.5280046	0.6314143	-6.2563073
C	-3.6376029	1.2550410	-6.0571250
H	-2.8939096	0.9969770	-6.8289465
C	-4.0237204	2.7354901	-6.1577828
H	-4.4487155	2.9579014	-7.1498803
H	-3.1122500	3.3529922	-6.0587564
C	-5.0142148	3.1221962	-5.0527716
H	-5.2515661	4.1972032	-5.1069939
H	-5.9642310	2.5808024	-5.2127022
C	-4.8169901	1.2088027	-0.6947875
H	-4.9884567	2.3018694	-0.7260488
C	-6.1171935	0.4952414	-1.0854448
H	-5.9284724	-0.5913146	-1.1279469
H	-6.4411891	0.8003224	-2.0935181
C	-7.2437320	0.7757158	-0.0780271
H	-8.1526417	0.2235044	-0.3697372
H	-7.5030213	1.8497504	-0.1115341
H	-5.7188824	2.2118766	1.7917067
C	-5.5306877	1.1235155	1.7460765
H	-5.2147532	0.8159696	2.7566346
H	-6.6635105	-0.6877513	1.4045702
C	-6.8254347	0.4040038	1.3493068
H	-7.6332784	0.6410098	2.0608936
C	-4.4035286	0.8457589	0.7423915
H	-4.1351467	-0.2237696	0.7810389
H	-3.4955757	1.4020052	1.0222976
C	-0.2130749	0.0948748	3.8923323
H	0.1689478	1.1018968	4.1250833
H	-2.1016704	-0.7602591	3.2593448
C	-1.7209818	0.2152121	3.6074826
H	-1.8918099	0.9251230	2.7823812
C	-2.4991646	0.6521069	4.8557573
H	-3.5781070	0.6751719	4.6320073
H	-2.2119472	1.6850458	5.1226589
H	-2.7538522	0.0854556	6.9427068
C	-2.2183204	-0.2707076	6.0478807
H	-2.6088151	-1.2798808	5.8245295
C	-0.7139652	-0.3680691	6.3284176
H	-0.3373233	0.6232962	6.6398288
H	-0.5215367	-1.0562102	7.1675146
C	0.0584246	-0.8314768	5.0831450
H	-0.2539548	-1.8575055	4.8227140
H	1.1367425	-0.8708764	5.3054036
P	0.6690113	-0.3294631	2.2884845

Pdt

C	16.8821630	10.6402055	16.8816217
N	17.8869309	9.6987669	16.8049738
O	16.0880949	10.8750013	15.9757568
C	17.9968636	8.9320942	15.5567553
H	18.1687258	9.6093156	14.7088958
H	17.0681574	8.3765288	15.3673166
H	18.8331578	8.2314121	15.6441466
H	21.6787942	6.8559265	18.9216081
H	20.1736857	6.7198801	19.8616295
C	21.0319798	7.3682036	19.6474670
H	21.6059068	7.5114067	20.5746920
H	22.2946729	8.9459817	17.7851077
O	19.7333924	8.4667474	17.9105814
C	20.5931068	8.7116387	19.0833264
C	21.7991621	9.5109917	18.5863247
H	22.5265173	9.6784734	19.3928372
H	19.2825003	8.1618152	21.6765350
B	18.7923798	9.4769752	17.9152665
C	18.7232280	8.6710365	20.8795753
C	19.6445682	9.5459159	20.0265879
H	21.0700955	10.0946813	21.5621245
H	21.4933490	10.4862046	18.1818437
H	18.2122530	7.9130148	20.2692316
C	20.3510460	10.5823569	20.8878168
O	18.7852815	10.2519578	19.0591412
H	17.9599633	9.3088414	21.3456854
H	20.8856051	11.3188978	20.2761577
H	19.6137581	11.1158495	21.5039076
H	16.8598108	11.1713589	17.8547663

Int_b´

P	4.8189181	9.3403257	2.8648959
P	1.3254788	9.0874062	7.3358589
Mg	3.2692411	8.4851445	5.2443659
N	2.4746370	10.3516941	4.7032446
C	3.7089418	10.7829695	2.5527656
C	3.7211807	11.5946316	1.4113320
H	4.4473890	11.3895492	0.6203801
C	2.8163932	12.6651703	1.2196171
C	1.8497837	12.9206726	2.1994296
H	1.1345538	13.7357531	2.0537425
C	1.7871834	12.1220535	3.3495054
C	2.7230791	11.0476949	3.5364716
C	1.3671873	10.9517427	5.2719536
C	0.9016340	12.0593713	4.4850554
C	-0.2354727	12.7750688	4.8815513
H	-0.5934292	13.6182011	4.2824563
C	-0.9312035	12.4040280	6.0375235
C	-0.4693457	11.2992787	6.7894964
H	-1.0478768	11.0023646	7.6683109
C	0.6733993	10.5664317	6.4454577
C	2.9118389	13.5171484	-0.0240727
H	3.7807413	14.1948987	0.0164447
H	2.0145517	14.1393856	-0.1518135
H	3.0269008	12.9004224	-0.9289781
C	-2.1501504	13.1696111	6.4945812
H	-2.5468277	13.8055644	5.6902715
H	-1.9183652	13.8266563	7.3493661
H	-2.9550058	12.4918452	6.8183047
C	4.7865391	8.3681705	1.2509283
H	5.1905350	9.0153908	0.4525524
C	5.6866951	7.1272692	1.3936810
H	6.7227726	7.4234039	1.6247678
H	5.3338159	6.5307490	2.2548575
C	5.6625483	6.2616297	0.1262301
H	6.1167131	6.8270039	-0.7078819
H	6.2854067	5.3647315	0.2743055
C	4.2315278	5.8649782	-0.2545180
H	3.8145894	5.2136573	0.5359207
H	4.2303066	5.2729166	-1.1835647
C	3.3405905	7.1032132	-0.4063326
H	2.3046926	6.8064206	-0.6408496
H	3.6941212	7.7057522	-1.2626386
C	3.3605313	7.9661987	0.8614102
H	2.7414477	8.8658791	0.7239435
H	2.9183176	7.3995721	1.6959502
C	6.5850073	10.0411888	2.8572215
H	7.1871467	9.1862200	3.2196560
C	6.6910123	11.1629010	3.8957049
H	6.0534752	12.0064677	3.5806423
H	6.2830924	10.8118077	4.8521920
C	8.1345009	11.6440376	4.0783866
H	8.1640237	12.4650229	4.8128161
H	8.7409272	10.8227859	4.5029508
C	8.7430668	12.0855832	2.7426376
H	8.2062527	12.9805761	2.3799101
H	9.7959787	12.3812680	2.8761561
C	8.6297405	10.9733984	1.6932463
H	9.2507345	10.1140284	2.0056749
H	9.0299168	11.3153663	0.7250676
C	7.1765878	10.5011320	1.5161586
H	6.5743624	11.3350384	1.1178149
H	7.1442338	9.6939861	0.7685655
C	-0.1851972	7.9876409	7.5842954
H	-0.9079985	8.5313911	8.2165842
C	-0.8684278	7.6659376	6.2515101
H	-0.1217668	7.2159346	5.5792900
H	-1.2094137	8.5963333	5.7724672
C	-2.0430314	6.6967743	6.4333119
H	-2.8337329	7.1886421	7.0277530
H	-2.4896071	6.4629851	5.4524576
C	-1.6024744	5.4113271	7.1429398
H	-2.4620398	4.7385253	7.2931035
H	-0.8855019	4.8691696	6.4992447
C	-0.9301950	5.7281520	8.4837113
H	-0.5801767	4.8028285	8.9686934
H	-1.6741599	6.1799794	9.1648461
C	0.2460050	6.6986874	8.3061118
H	1.0406911	6.2103947	7.7133104
H	0.6896043	6.9331498	9.2874250
C	1.6806594	9.6633324	9.1152492
H	2.2386956	8.8083353	9.5434484
C	0.4669797	9.9421256	10.0151942
H	-0.1332560	10.7562334	9.5747743
H	-0.1874409	9.0601919	10.0828532
C	0.9006724	10.3608506	11.4287604
H	1.4241094	9.5158610	11.9124431
H	0.0096117	10.5711950	12.0425425
C	1.8308205	11.5775933	11.3936955
H	1.2770459	12.4471093	10.9953807
H	2.1521327	11.8467121	12.4126267
C	3.0453489	11.3003370	10.5035678
H	3.6982853	12.1863888	10.4458136
H	3.6474640	10.4957423	10.9642201
C	2.6240316	10.8730630	9.0917432
H	3.5055370	10.6322933	8.4837841
H	2.1167455	11.7141596	8.5886034
H	4.7917587	8.0755563	9.0163313
H	5.5426493	10.0026819	9.8690671
O	5.0810347	9.6380310	6.8660123
H	4.8149779	7.0532665	7.5537541
C	5.4361531	7.6536334	8.2348075
B	5.5165770	10.9562644	7.0177283
C	6.6160558	9.8027338	9.7563572
H	6.8550937	8.8682429	10.2824696
C	6.1287963	8.7430926	7.4262829
H	6.1833307	6.9996073	8.7084634
H	7.1662770	10.6240954	10.2354766
C	7.0174150	9.7340556	8.2813439
O	6.7094807	11.0457398	7.7073205
H	6.1274988	7.5971485	5.6143145
C	6.8630897	8.1283869	6.2362072
H	7.3576665	8.8959202	5.6261240
C	8.5189515	9.5001306	8.1596357
H	7.6212750	7.4083324	6.5737103
H	8.7879008	8.5000558	8.5292635
H	9.0543075	10.2446912	8.7652022
H	8.8591791	9.5940164	7.1210900
H	1.6776216	5.6889562	4.7572613
C	1.5826169	6.1401952	3.7608583
H	2.4212834	5.7813514	3.1406790
C	0.2332992	5.9141415	3.0847743
O	1.7083688	7.5846838	3.9179747
C	0.6991826	8.2673146	3.1064951
C	0.0629642	7.1854998	2.2371972
H	-0.0251994	8.7361705	3.7879646

H	1.2025230	9.0564978	2.5355791
H	-0.5689650	5.8386694	3.8338689
H	0.6036558	7.0869868	1.2844215
H	-0.9877106	7.4102937	2.0102143
H	0.2249112	4.9945965	2.4844706
H	3.9300017	6.8848822	5.6160317
C	4.7480147	12.2274007	6.5262756
H	3.9660753	11.9878634	5.7966609
H	5.4444224	12.9571804	6.0877241
H	4.2704694	12.7264375	7.3848292

Int_c´

P	4.9080915	9.3122626	2.9460253
P	1.3625042	9.1279830	7.4134537
Mg	3.3148691	8.5140240	5.3971799
N	2.5153487	10.3343295	4.7514790
C	3.7697249	10.7292977	2.6041000
C	3.7787795	11.5123609	1.4422412
H	4.5157737	11.3008731	0.6636445
C	2.8577223	12.5608250	1.2120869
C	1.8720325	12.8205731	2.1713020
H	1.1422005	13.6166068	1.9956903
C	1.8097974	12.0490253	3.3393726
C	2.7662086	11.0004786	3.5683395
C	1.3859315	10.9245370	5.2875334
C	0.9077388	11.9975134	4.4625622
C	-0.2525507	12.6964176	4.8203584
H	-0.6200846	13.5136872	4.1920458
C	-0.9586090	12.3405434	5.9747053
C	-0.4825916	11.2694026	6.7656898
H	-1.0676697	10.9837153	7.6438506
C	0.6836632	10.5563466	6.4617217
C	2.9563113	13.3858364	-0.0494400
H	3.8054973	14.0881763	-0.0070424
H	2.0455843	13.9803430	-0.2098138
H	3.1072464	12.7519197	-0.9369382
C	-2.2045587	13.0861316	6.3897133
H	-2.5868994	13.7115766	5.5705337
H	-2.0112211	13.7500696	7.2486168
H	-3.0071458	12.3953413	6.6907959
C	4.8979461	8.3422436	1.3278285
H	5.2022852	9.0295670	0.5192517
C	5.9093738	7.1851464	1.4024209
H	6.9274580	7.5675582	1.5770010
H	5.6601435	6.5523311	2.2715135
C	5.8874354	6.3274955	0.1297027
H	6.2405975	6.9353302	-0.7229989
H	6.5948139	5.4887436	0.2326982
C	4.4775156	5.8077973	-0.1726194
H	4.1636686	5.1204316	0.6346658
H	4.4757153	5.2207388	-1.1047912
C	3.4760917	6.9647349	-0.2638535
H	2.4581184	6.5806241	-0.4432180
H	3.7288337	7.5985125	-1.1326434
C	3.4929113	7.8199828	1.0087404
H	2.7947676	8.6656146	0.9111445
H	3.1430971	7.2146702	1.8613991
C	6.6602637	10.0457664	2.9303587
H	7.2821438	9.1879918	3.2522323
C	6.7728372	11.1322023	4.0040587
H	6.1229550	11.9795777	3.7273806
H	6.3849791	10.7449618	4.9549531
C	8.2155825	11.6181265	4.1805161
H	8.2513188	12.4130111	4.9429689
H	8.8334277	10.7862022	4.5664567
C	8.8004425	12.1103439	2.8516601
H	8.2547430	13.0161186	2.5311555
H	9.8543130	12.4052369	2.9788381
C	8.6732955	11.0377253	1.7630252
H	9.3047834	10.1706578	2.0299738
H	9.0524791	11.4190259	0.8011504
C	7.2191758	10.5649331	1.5970311
H	6.6042186	11.4129886	1.2518175
H	7.1714387	9.7929595	0.8140938
C	-0.1121285	7.9912426	7.6979902
H	-0.8561099	8.5400062	8.3006131
C	-0.7755032	7.5927825	6.3757265
H	-0.0098819	7.1434153	5.7256919
H	-1.1478385	8.4901050	5.8579677
C	-1.9143022	6.5880672	6.5917022
H	-2.7253470	7.0725550	7.1645335
H	-2.3476455	6.3003725	5.6192361
C	-1.4280065	5.3487723	7.3520013
H	-2.2610988	4.6476935	7.5208784
H	-0.6829701	4.8132160	6.7356681
C	-0.7816251	5.7438175	8.6846676
H	-0.3975358	4.8526242	9.2059545
H	-1.5502241	6.1899962	9.3420562
C	0.3590572	6.7506560	8.4780507
H	1.1802602	6.2649833	7.9230097
H	0.7768088	7.0444165	9.4548614
C	1.6903805	9.7823995	9.1708037
H	2.2626050	8.9580147	9.6379021
C	0.4580232	10.0657311	10.0435011
H	-0.1588903	10.8424229	9.5608968
H	-0.1716760	9.1690229	10.1415533
C	0.8602979	10.5575016	11.4425922
H	1.4005948	9.7500412	11.9694875
H	-0.0454337	10.7681250	12.0342728
C	1.7556564	11.7979634	11.3660298
H	1.1839095	12.6323987	10.9208147
H	2.0538159	12.1216457	12.3761270
C	2.9908413	11.5153165	10.5068620
H	3.6203019	12.4155735	10.4175693
H	3.6074266	10.7501190	11.0129680
C	2.6034854	11.0134414	9.1097226
H	3.5017858	10.7682220	8.5285860
H	2.0858424	11.8182140	8.5598522
H	4.7173640	8.1629823	9.1341214
H	5.4554289	10.1007543	9.9462655
O	5.0647360	9.6507212	6.9315310
H	4.7638608	7.0914207	7.7116203
C	5.3756460	7.7124040	8.3810187
B	5.4995194	10.9749260	7.0581211
C	6.5308644	9.8983791	9.8620263
H	6.7589655	8.9804027	10.4207892
C	6.0942272	8.7697191	7.5536495
H	6.1070580	7.0695811	8.8929658
H	7.0708769	10.7341262	10.3275972
C	6.9635153	9.7861912	8.3988122
O	6.6705488	11.0801492	7.7800650
H	6.1347845	7.5645395	5.7845098
C	6.8577335	8.1123833	6.4054863
H	7.3722767	8.8542913	5.7802069
C	8.4673553	9.5490339	8.3171013
H	7.6019432	7.4002630	6.7882074
H	8.7275201	8.5599202	8.7208900
H	8.9886845	10.3105613	8.9137150
H	8.8315030	9.6145139	7.2844472
H	1.7220918	5.6758381	4.9779016
C	1.6695752	6.0849691	3.9602647
H	2.5284279	5.6992135	3.3860525
C	0.3447507	5.8265803	3.2477508
O	1.7948413	7.5350619	4.0572928
C	0.7871401	8.1801477	3.2146441
C	0.1933072	7.0684944	2.3552787
H	0.0375912	8.6451129	3.8717511
H	1.2853421	8.9695610	2.6397827
H	-0.4804617	5.7692604	3.9730777
H	0.7704456	6.9476190	1.4267889
H	-0.8504590	7.2750457	2.0838247
H	0.3624144	4.8876193	2.6786103
H	3.9856586	6.9111138	5.7555330
C	4.7573719	12.2378996	6.5091788
H	4.0153696	11.9912561	5.7418099
H	5.4788618	12.9614493	6.1024167
H	4.2328706	12.7468538	7.3337832
N	4.6280059	4.2271184	5.5842869
H	5.0457105	5.9030030	4.4207868
C	5.3028188	4.8297236	4.4654243
H	6.3909528	4.7102261	4.5747278
H	4.9988977	4.3293718	3.5335417
C	3.8806046	4.6060666	6.4646143
O	3.1517183	4.6896596	7.4020903

TS_b´

P	4.7176628	9.2495653	2.8122564
P	1.2713002	8.9540070	7.2480689
Mg	3.2742087	8.4448518	5.2288512
N	2.2077691	10.0745867	4.4873535
C	3.4538044	10.5175062	2.3511476
C	3.3979754	11.2404281	1.1530621
H	4.1838248	11.0958437	0.4071485
C	2.3494505	12.1401986	0.8470986
C	1.3055573	12.3090416	1.7652973
H	0.4829519	12.9901719	1.5269064
C	1.3082343	11.5966911	2.9724327
C	2.3909581	10.7002290	3.2742918
C	1.0096598	10.5403068	4.9820431
C	0.4004525	11.4870466	4.0885825
C	-0.8485756	12.0395860	4.4026863
H	-1.3206071	12.7588316	3.7262866
C	-1.5089046	11.6621484	5.5780419
C	-0.8953108	10.7249548	6.4427546
H	-1.4380755	10.4291094	7.3445061
C	0.3598945	10.1601763	6.1851069
C	2.3741632	12.9068413	-0.4544702
H	3.1397215	13.7006043	-0.4424764
H	1.4055552	13.3873068	-0.6528311
H	2.6057396	12.2491321	-1.3066595
C	-2.8522567	12.2502086	5.9410710
H	-3.2812096	12.8133319	5.1000582
H	-2.7736877	12.9418674	6.7962734
H	-3.5732603	11.4680377	6.2253979
C	4.7649522	8.0627457	1.3466474
H	5.1563739	8.6086718	0.4706164
C	5.7189341	6.9035867	1.6902092
H	6.7351855	7.2835954	1.8842321
H	5.3809560	6.4298945	2.6299115
C	5.7653818	5.8536061	0.5711655
H	6.2179199	6.3027750	-0.3314757
H	6.4206640	5.0201711	0.8715630
C	4.3637404	5.3380313	0.2263295
H	3.9527775	4.7973653	1.0991609
H	4.4140180	4.6104156	-0.5997235
C	3.4273430	6.4967038	-0.1331875
H	2.4126751	6.1205378	-0.3458278
H	3.7826543	6.9786460	-1.0619547
C	3.3703217	7.5394529	0.9905249
H	2.7150667	8.3772412	0.7067669
H	2.9317271	7.0842990	1.8902922
C	6.4340856	10.0594902	2.6783680
H	7.0880098	9.2752461	3.1053321
C	6.5312811	11.2884672	3.5900043
H	5.8554232	12.0740624	3.2113848
H	6.1778169	11.0336880	4.5975095
C	7.9630339	11.8327098	3.6684133
H	7.9859538	12.7249413	4.3138421
H	8.6100338	11.0774098	4.1515400
C	8.5147666	12.1535416	2.2750192
H	7.9367441	12.9891961	1.8414916
H	9.5606983	12.4933997	2.3425806
C	8.4068009	10.9352351	1.3507958
H	9.0675610	10.1332514	1.7271639
H	8.7617034	11.1860798	0.3379877
C	6.9666429	10.3999224	1.2773074
H	6.3212638	11.1672410	0.8168825
H	6.9421001	9.5196086	0.6187776
C	0.0540393	7.5837733	7.6835335
H	-0.7390885	8.0008211	8.3264592
C	-0.6093823	6.9887615	6.4382994
H	0.1810616	6.6731984	5.7429482
H	-1.1990217	7.7623040	5.9222886
C	-1.4925544	5.7841116	6.7875942
H	-2.3371124	6.1190691	7.4167256
H	-1.9345993	5.3652464	5.8684015
C	-0.6976718	4.7095970	7.5390464
H	-1.3479760	3.8588796	7.7986366
H	0.0942881	4.3149406	6.8758413
C	-0.0489722	5.2939528	8.7991815
H	0.5535418	4.5276324	9.3138766
H	-0.8418421	5.5990276	9.5058847
C	0.8322695	6.5052408	8.4638788
H	1.6926153	6.1755058	7.8531404
H	1.2511854	6.9294635	9.3916828
C	1.4885679	9.8142184	8.9372994
H	2.2084620	9.1538364	9.4573125
C	0.2349906	9.9367777	9.8183737
H	-0.5264149	10.5327453	9.2880982
H	-0.2068496	8.9482741	10.0122447

C	0.5500092	10.6179863	11.1591004
H	1.2406743	9.9772493	11.7369752
H	-0.3730187	10.7035557	11.7552244
C	1.1917550	11.9936131	10.9549539
H	0.4687771	12.6619091	10.4533727
H	1.4305699	12.4561631	11.9260747
C	2.4518850	11.8721883	10.0942260
H	2.8981789	12.8627579	9.9097072
H	3.2060928	11.2862244	10.6497536
C	2.1564434	11.1838502	8.7554283
H	3.0842649	11.0643847	8.1806782
H	1.4952611	11.8281717	8.1508084
H	4.5096759	8.5596483	8.9121980
H	5.0191274	10.5812193	9.5832071
O	4.7218288	9.8184233	6.5459310
H	4.7117247	7.3551086	7.6148592
C	5.2317562	8.1143043	8.2166753
B	4.9393819	11.2026041	6.5635667
C	6.1112761	10.5335641	9.4878075
H	6.4815159	9.7068566	10.1095092
C	5.8388877	9.1557111	7.2851479
H	6.0246261	7.6218340	8.7983508
H	6.5262659	11.4744094	9.8742430
C	6.5385689	10.3693515	8.0278190
O	6.0399456	11.5469430	7.3174283
H	6.1052704	7.7495023	5.6840708
C	6.7176353	8.4750363	6.2383752
H	7.1404394	9.1993188	5.5300458
C	8.0612549	10.3718953	7.9319637
H	7.5434699	7.9335431	6.7200968
H	8.4841183	9.4796263	8.4154578
H	8.4547892	11.2597749	8.4462131
H	8.4009859	10.4004302	6.8895541
H	2.0345316	5.3892641	5.0050904
C	1.8697852	5.7393837	3.9774566
H	2.7492731	5.4566604	3.3748666
C	0.5657801	5.2661969	3.3398927
O	1.7877026	7.1966215	4.0160843
C	0.6744140	7.6569100	3.1862496
C	0.1985118	6.4326486	2.4081685
H	-0.1045684	8.0574790	3.8512212
H	1.0413315	8.4708866	2.5488749
H	-0.2116571	5.1249159	4.1051928
H	0.7386278	6.3463529	1.4541713
H	-0.8763402	6.4819375	2.1872503
H	0.6928678	4.3149992	2.8052358
H	4.0688233	6.9089249	5.6442428
C	4.0627729	12.2916138	5.8596956
H	4.0151566	12.1444195	4.7733020
H	4.4660944	13.2931104	6.0634752
H	3.0209562	12.2558712	6.2069317
N	3.7070027	4.7333288	6.8315255
H	2.5820138	3.0079695	7.2357270
H	3.3901450	3.7259774	8.6423721
C	3.5099659	3.4927230	7.5744937
C	4.6541668	4.9959364	6.0968003
H	4.3430874	2.7815646	7.4578664
O	5.6462739	5.0204728	5.4365497

Int_d´

P	2.5521587	0.1429305	1.0425519
P	-2.7018248	-0.1184573	-0.3255291
Mg	-0.1387506	0.7300531	0.2771696
O	0.3528110	1.8032341	-1.4177914
N	0.1051430	-1.2923283	-0.0701756
C	-1.1724730	-4.4150909	-1.4191715
H	-0.7870331	-5.4092040	-1.6640723
C	1.0764257	-3.3619901	-0.5292472
C	-2.5231849	-4.1245757	-1.6511550
C	-0.8550638	-2.1411106	-0.5751671
C	4.2589977	0.7783234	0.5894365
H	5.0062097	0.0730642	0.9945662
C	1.2140231	-0.7771917	4.9174102
H	0.2783327	-1.2724573	5.2246359
H	1.1783877	0.2495136	5.3228090
C	2.5933769	-0.0490047	2.9197109
H	2.5952453	0.9920621	3.2912382
C	2.1702453	-4.2401105	-0.5747613
H	2.0456989	-5.2610263	-0.9475653
C	1.2806231	-0.7019622	3.3865428
H	0.4186484	-0.1323147	3.0059533
H	1.2077194	-1.7171831	2.9595150
C	-0.3230720	-3.4362443	-0.8816797
C	2.5295355	-1.5893157	0.4156345
C	1.2695104	-2.0288855	-0.0396338
C	3.5931598	-2.4942690	0.3469736
H	4.5880215	-2.1839847	0.6787780
C	-3.4532835	-5.1638095	-2.2316068
H	-4.2745328	-5.4047055	-1.5375229
H	-2.9181832	-6.0984250	-2.4510688
H	-3.9155079	-4.8148492	-3.1689368
C	4.5014315	2.1616366	1.2162349
H	3.7000454	2.8521055	0.8941265
H	4.4378455	2.1054583	2.3138918
C	-2.2154384	-1.8361170	-0.7861978
C	3.4332024	-3.8137993	-0.1442744
C	-3.9747089	0.3354699	-1.6254045
H	-4.6986612	-0.4980245	-1.6760350
C	3.8088290	-0.7895001	3.4907660
H	3.8360832	-1.8105000	3.0724673
H	4.7462564	-0.2949561	3.1900028
C	-3.6712141	-0.3051745	1.2801081
H	-3.9957062	0.7269740	1.5094899
C	3.7370430	-0.8694268	5.0245761
H	4.6038671	-1.4317430	5.4082324
H	3.8099196	0.1506096	5.4429367
C	2.4276887	-1.5141616	5.4947326
H	2.3818368	-1.5268365	6.5955618
H	2.4038372	-2.5682161	5.1634460
C	-3.0243939	-2.8386124	-1.3309186
H	-4.0817594	-2.6360912	-1.5235737
C	4.6235319	-4.7430042	-0.1861780
H	5.4396328	-4.3286154	-0.7996833
H	4.3504076	-5.7200843	-0.6089238
H	5.0353876	-4.9181733	0.8208342
C	0.7402888	1.1378695	-2.6551588
H	-0.0916532	0.4806132	-2.9380910
H	1.6391166	0.5249864	-2.4729366
C	4.4176896	0.8267791	-0.9388183
H	4.2780622	-0.1786738	-1.3657718
H	3.6176906	1.4619605	-1.3583430
C	-4.9023144	-1.2173397	1.2054531
H	-4.5798647	-2.2265328	0.8970496
H	-5.6084722	-0.8587887	0.4391568
C	-2.7071582	-0.7500988	2.3950094
H	-2.2718999	-1.7292555	2.1289546
H	-1.8755950	-0.0320783	2.4722960
C	-3.4232589	-0.8568652	3.7474872
H	-3.7406068	0.1517904	4.0669200
H	-2.7162923	-1.2190447	4.5115805
C	-3.2952918	0.4658093	-2.9985706
H	-2.5260301	1.2575943	-2.9402475
H	-2.7729279	-0.4700628	-3.2532538
C	5.8617008	2.7368459	0.7981631
H	5.9899251	3.7416883	1.2314059
H	6.6647572	2.1062004	1.2198097
C	-5.6109808	-1.3090686	2.5660826
H	-6.0171175	-0.3162814	2.8315858
H	-6.4724177	-1.9923722	2.4919848
C	-4.6497147	-1.7731062	3.6674598
H	-4.3189228	-2.8042036	3.4472528
H	-5.1679667	-1.8074188	4.6391609
C	-4.7350791	1.6196013	-1.2635929
H	-5.2516755	1.5046290	-0.2975505
H	-4.0254732	2.4541150	-1.1406812
C	5.7788712	1.4033829	-1.3485122
H	6.5781211	0.7162953	-1.0174802
H	5.8464131	1.4570045	-2.4471893
C	-5.7556628	1.9816461	-2.3529816
H	-6.2541019	2.9277813	-2.0887948
H	-6.5415311	1.2050184	-2.3862194
C	1.0505952	3.0925621	-1.3228070
H	0.3020773	3.8380254	-1.0279171
H	1.8097120	3.0134933	-0.5287557
C	6.0087927	2.7859911	-0.7269571
H	7.0024473	3.1717753	-1.0046515
H	5.2685906	3.4969272	-1.1391033
C	-5.0965755	2.0954645	-3.7330462
H	-4.4055022	2.9558944	-3.7300046
H	-5.8561454	2.3046980	-4.5028473
C	-4.3146184	0.8246763	-4.0891376
H	-5.0190369	-0.0172455	-4.2120152
H	-3.7997635	0.9473813	-5.0558078
C	1.0078487	2.2855512	-3.6160714
H	1.6534521	1.9834349	-4.4509040
H	0.0610304	2.6626256	-4.0274319
C	1.6691254	3.3396739	-2.7063028
H	2.7578019	3.1881299	-2.6750959
H	1.4840727	4.3640994	-3.0538462
H	1.1948247	3.0543202	2.1842670
C	0.2467844	2.6379726	2.5797066
O	-0.4911603	1.9574571	1.7306850
N	-0.0020451	2.8980388	3.8205478
C	-1.2442001	2.3515175	4.3629237
H	-1.0952023	1.3179760	4.7243396
H	-2.0673455	2.3151293	3.6279830
H	-1.5595420	2.9551666	5.2269861
H	-0.3384652	6.5636702	1.8571373
C	-1.2594080	5.9702382	1.9448679
H	-1.8011687	6.3170826	2.8374480
H	-0.9800495	4.9223493	2.0979216
H	-1.3324292	8.1143899	0.2376644
C	-2.1125651	6.1610161	0.7006868
C	-2.3137701	7.6502020	0.4077876
H	-2.7951262	8.1607158	1.2532388
O	-1.3930402	5.6057546	-0.4611422
H	-3.3171695	4.2082659	2.5454889
H	-2.4789421	3.4311517	1.1849979
C	-3.3630708	4.0229938	1.4634408
H	-2.9276407	7.8036133	-0.4915839
C	-3.4566501	5.3388243	0.6885133
H	-4.5788713	6.4701900	2.1579302
B	-2.3444264	5.0588859	-1.3029178
H	-1.8619031	3.4539358	-2.7264450
C	-4.6882932	6.1236575	1.1197756
C	-2.0220437	4.5441983	-2.7485993
H	-1.1163265	5.0071742	-3.1633181
H	-4.2613134	3.4257066	1.2556369
O	-3.6035937	4.9932932	-0.7369751
H	-4.8627683	6.9933464	0.4746471
H	-5.5735869	5.4741713	1.0689403
H	-2.8592913	4.7261943	-3.4373266