Supporting Information

to the manuscript

Hydroboration of Isocyanates: Cobalt-Catalyzed vs. Catalyst-Free Approaches

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1. Experimental details

All manipulations were carried out using conventional inert atmosphere glovebox and Schlenk techniques. Toluene and C_6D_6 were dried by distillation from sodium. EtOAc, hexanes, MeOH, $CDCl_3$, DMSO-d_6, MeOH-d_4, $Co(acac)_2$, dpephos, HBPin, HBCat, Et_3SiH, $PhSiH_3$, 4 M HCl in dioxane, 4 M HCl in diethyl ether, 1,3,5-trimethoxybenzene, all isocyanates and organic substrates for chemoselectivity tests were purchased from Sigma-Aldrich (Merk) and used without further purification. NMR spectra were obtained with JEOL ECA-500 MHz spectrometer (^{1}H: 500 MHz, ^{13}C: 126 MHz, ^{31}P: 202 MHz, ^{11}B: 160 MHz and ^{19}F: 471 MHz). All catalytic hydroboration reactions were performed under inert atmosphere using either NMR tubes equipped with Teflon valves (J. Young NMR tubes) or 10 and/or 20 mL pressure vials (Supelco headspace vials) equipped with magnetic screw caps having PTFE-faced butyl septa. For details of computational studies, see section 8 below.

General procedure for monohydroboration of isocyanates to formamides

Conditions A. HBPin (1.0 or 3.5 equiv.) was added to an isocyanate substrate (0.2 mmol) in a pressure vial, which was sealed with a magnetic screw cap having PTFE-faced butyl septum. The mixture was left with stirring at room temperature for 24 hours. Then a solution of 1,3,5-trimethoxybenzene (internal standard; 6.7 mg, 0.04 mmol, 0.2 equiv.) in 0.6 mL of benzene-d_6 was added, and the resulting mixture was transferred to an NMR tube for analysis.

Conditions B. A mixture of $Co(acac)_2$ (2 mol%), dpephos (2 mol%), isocyanate (0.2 or 1.0 mmol) and HBPin (1 equiv.; 0.2 or 1.0 mmol) in either benzene-d_6 (0.6 mL, 0.33 M; for NMR reactions with 0.2 mmol of the substrate) or toluene (1.4 mL; 0.7 M; for reactions in pressure vials with 1.0 mmol of the substrate) was left with stirring for 24 hours at 60 °C. For NMR scale reactions (with 0.2 mmol of the substrate), conversions of isocyanates to N-borylformamides were determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard (6.7 mg, 0.04 mmol, 0.2 equiv.). For reactions in pressure vials with 1.0 mmol of the substrate, isolated yields of formamides were determined. The solvent was removed under reduced pressure, and the residue was treated with 5 mL of methanol at room temperature overnight. All volatiles were pumped off, and the products were purified by column chromatography with silica gel using EtOAc/Haxanes (1/1) as an eluent. The yields and the spectroscopic data for isolated formamides can be found below (see section 2). NMR spectra of N-borylformamides (taken directly from the reaction mixtures) and isolated formamide products can be found in sections 4 and 5, respectively.

General procedure for deoxygenative hydroboration of isocyanates to N-methylamines

Conditions A. HBPin (101.6 µL, 0.7 mmol, 3.5 equiv.) was added to an isocyanate substrate (0.2 mmol) in a pressure vial. The mixture was left with stirring for 24 hours at either 25, 50 or 70 °C, depending on the substrates used. Then a solution of 1,3,5-trimethoxybenzene (internal standard; 6.7 mg, 0.04 mmol, 0.2 equiv.) in 0.6 mL of benzene-d_6 was added, and the resulting mixture was transferred to an NMR tube for analysis. NMR conversions of isocyanates to borylated N-methylamines were determined by integration of ^{1}H-NMR spectra against resonances of 1,3,5-trimethoxybenzene.

Conditions B. A mixture of $Co(acac)_2$ (4 mol%), dpephos (4 mol%), isocyanate (0.2 or 0.5 mmol) and HBPin (3.5-6 equiv., depending on the substrate used) in either benzene-d_6 (0.6 mL, 0.33 M for NMR scale reactions with 0.2 mmol of the substrate, or 0.7 mL, 0.7 M for reactions in pressure vials with 0.5 mmol of the substrate) was left with stirring for 24-48 h hours at 70-80 °C (depending on the substate used). For NMR scale reactions (with 0.2 mmol of the substrate), conversions of isocyanates to borylated N-methylamines were determined by ^{1}H-NMR using

1,3,5-trimethoxybenzene as internal standard (6.7 mg, 0.04 mmol, 0.2 equiv.). For reactions in pressure vials with 0.5 mmol of the substrate, N-methylamines were isolated as the corresponding hydrochloride salts. For this, the obtained mixture was treated with 2.5 equivalents of HCl (as 4 M solution of HCl in either dioxane or diethyl ether) for 1 hour at room temperature. All volatiles were pumped off, and the residue was washed with cold (-20 °C) Et_2O (5x4 mL) to give solid products, which were dried in vacuum. The yields and the spectroscopic data for isolated N-methylamine hydrochlorides can be found in section 3 below. NMR spectra of borylated N-methylamines (taken directly from the reaction mixtures) and isolated N-methylamine hydrochloride products can be found in sections 6 and 7, respectively.

Mercury drop test for monohydroboration of PhNCO

The reaction was performed according to the above procedure for catalytic hydroboration of isocyanates to N-borylformamides using 0.29 mmol (34.5 mg, 31.5 µL) of PhNCO, 0.29 mmol (37.7 mg, 42.7 µL) of HBPin and 2.0 mol% of $Co(acac)_2$/dpephos in 0.9 mL of C_6D_6. All components were mixed in a pressure vial and a drop of Hg (313 mg) was added to the reaction mixture. The reaction was left with intensive stirring for 24 h at 60 °C. Then, 1,3,5-trimethoxybenzene was added as internal standard (9.8 mg, 0.058 mmol, 0.2 equiv. to PhNCO) and the reaction mixture was analysed by ^{1}H-NMR showing 95% conversion of PhNCO to the corresponding N-borylformamide, PhN(BPin)COH.

General procedure for competitive $Co(acac)_2$/dpephos-catalyzed hydroboration of PhNCO.

Monohydroboration to N-borylformamides. Both catalyst-free and catalytic competitive monohydroboration reactions were performed according to above procedures for conversion of isocyanates to N-borylformamides using 0.2 mmol (23.8 mg, 21.7 µL) of PhNCO, 0.2 mmol of competing substrates, either 0.2 mmol (25.6 mg, 29.0 µL) or 0.7 mmol (89.6 mg, 101.6 µL) of HBPin (for catalytic and catalyst-free reactions, respectively), and 2 mol% (0.004 mmol) of $Co(acac)_2$/dpephos (for catalytic reactions) in 0.6 mL of C_6D_6 (for catalytic reactions). Catalyst-free transformations were performed under neat conditions. All components were mixed in either an NMR tube or in a pressure vial. The reactions were left at either room temperature or at 60 °C for 24 hours and then 1,3,5-trimethoxybenzene (6.7 mg, 0.04 mmol, 0.2 equiv. to PhNCO) was added as internal standard and the reaction mixtures were checked by ^{1}H-NMR to determine conversions of PhNCO and competing substrates. Note, for catalyst-free and solvent-free transformations, 0.6 mL of C_6D_6 were added for NMR analysis of the reaction mixtures. The results of these tests are summarized in the Table 2 in the main text of the manuscript.

Hydroboration to borylated N-methylamines. Both catalyst-free and catalytic competitive monohydroboration reactions were performed according to above procedures for conversion of isocyanates to borylated N-methylamines using 0.2 mmol (23.8 mg, 21.7 µL) of PhNCO, 0.2 mmol of competing substrates, 0.6 mmol (76.8 mg, 87.1 µL) of HBPin, and 4 mol% (0.008 mmol) of $Co(acac)_2$/dpephos (for catalytic reactions) in 0.6 mL of C_6D_6 (for catalytic reactions). Catalyst-free transformations were performed under neat conditions. All components were mixed in either an NMR tube or in a pressure vial. The reactions were left at 70 °C for 24 hours and then 1,3,5-trimethoxybenzene (6.7 mg, 0.04 mmol, 0.2 equiv. to PhNCO) was added as internal standard and the reaction mixtures were checked by ^{1}H-NMR to determine conversions of PhNCO and competing substrates. Note, for catalyst-free and solvent-free transformations, 0.6 mL of C_6D_6 were added for NMR analysis of the reaction mixtures. The results of these tests are summarized in the Table 3 in the main text of the manuscript.

Attempts for reduction of PhNCO with HBCat, $PhSiH_3$ and Et_3SiH.

The reactions of PhNCO with HBCat, $PhSiH_3$ and Et_3SiH were performed analogously to experiments with HBPin using both catalytic and catalyst-free conditions for monohydroboration and deoxygenative hydroboration of isocyanates to formamides and N-methylamines, respectively (see above). The results of these trials are summarized in the table below (where applicable, NMR conversions using 1,3,5-trimethoxybenzene as internal standard are shown).

Reducing agent (equivalents)	Conditions	Result
$PhSiH_3$ (1 equiv.)	2% $Co(acac)_2$/dpephos, 60 °C, 24 h, Solvent: toluene	No reaction was observed by ^{1}H-NMR
$PhSiH_3$ (1 equiv.)	Catalyst-free / solvent-free, room temperature, 24 h	No reaction was observed by ^{1}H-NMR
Et_3SiH (1 equiv.)	2% $Co(acac)_2$/dpephos, 60 °C, 24 h, Solvent: toluene	Formation of 4% of formamide product was observed by ^{1}H-NMR
Et_3SiH (3.5 equiv.)	4% $Co(acac)_2$/dpephos, 70 °C, 24 h, Solvent: toluene	Formation of 35% of $PhN(SiEt_3)Me$ and 9% of formamide product was observed by ^{1}H-NMR
HBCat (1 equiv.)	2% $Co(acac)_2$/dpephos, 60 °C, 24 h, Solvent: toluene	Formation of 17% of formamide product was observed by ^{1}H-NMR
HBCat (3.5 equiv.)	Catalyst-free / solvent-free, room temperature, 24 h	Formation of $PhN(BCat)CH_3$ (49%) was observed by ^{1}H-NMR. No other products were detected
HBCat (3.5 equiv.)	4% $Co(acac)_2$/dpephos, 70 °C, 24 h, Solvent: toluene	Formation of $PhN(BCat)CH_3$ (80%) was observed by ^{1}H-NMR. No other products were detected

Monohydroboration of PhNCO with HBPin using $Co(acac)_2/PPh_3$ (1/2 ratio) as pre-catalyst.

The reaction was done analogously to $Co(acac)_2$/dpephos-catalyzed experiment (see above) using 2 mol% of $Co(acac)_2$ and 4 mol% of PPh_3 as a pre-catalyst system. NMR analysis of the reaction mixture after 24 h at 60 °C showed formation of 69% of N-borylformamide product PhN(BPin)C(O)H and 4% of N,O-bis(boryl)hemiaminal $PhN(BPin)CH_2OBPin$ (determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard).

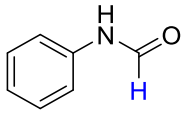
Deoxygenative hydroboration of PhNCO with 3.5 equiv. of HBPin using $Co(acac)_2/PPh_3$ (1/2 ratio) as pre-catalyst.

The reaction was done analogously to $Co(acac)_2$/dpephos-catalyzed experiment (see above) using 4 mol% of $Co(acac)_2$ and 8 mol% of PPh_3 as a pre-catalyst system. NMR analysis of the reaction mixture after 24 h at 70 °C showed formation of 74% of PhN(BPin)Me and 24% of N-borylformamide product PhN(BPin)C(O)H (determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard).

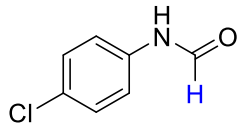
Monohydroboration of PhNCO with HBPin using $(dppe)CoCl_2$ as pre-catalyst.

The reaction was done analogously to $Co(acac)_2$/dpephos-catalyzed experiment (see above) using 2 mol% of $(dppe)CoCl_2$ as a pre-catalyst, which was activated with 4 mol% of $LiBHEt_3$ prior to addition of the substrate. NMR analysis of the reaction mixture after 24 h at 60 °C showed formation of 27% of N-borylformamide product PhN(BPin)C(O)H and 10% of N,O-bis(boryl)hemiaminal $PhN(BPin)CH_2OBPin$ (determined by ^{1}H-NMR using 1,3,5-trimethoxybenzene as internal standard).

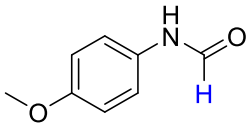
2. NMR data for isolated formamides



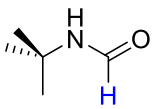
N-phenylformamide **(3'a):**[1] Yield 59%. A mixture of rotamers (approx. 1:1 ratio) was obtained. ^{1}H-NMR ($CDCl_3$, 500 MHz): δ = 8.70 (d, *J* = 11.4 Hz, 1H), 8.38 (d, *J* = 1.1 Hz, 1H), 8.29 (br s, 1H), 7.54 (d, *J* = 7.7 Hz, 2H), 7.43 (br s, 1H), 7.32-7.38 (m, 4H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.10 ppm (d, *J* = 7.7 Hz, 2H). ^{13}C{^{1}H}-NMR ($CDCl_3$, 126 MHz): δ = 162.9 (s), 159.4 (s), 136.9 (s), 136.8 (s), 129.9 (s), 129.2 (s), 125.5 (s), 125.0 (s), 120.2 (s), 119.0 ppm (s).



N-(4-chlorophenyl)formamide **(3'b):**[2,3] Yield 65%. A mixture of rotamers (approx. 1:1.5 ratio) was obtained. Major rotamer: ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 8.38 (s, 1H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 7.25 ppm (br s, 1H). ^{13}C{^{1}H}-NMR ($CDCl_3$, 126 MHz): δ = 158.9 (s), 135.5 (s), 129.3 (s), 121.3 ppm (s). Minor rotamer: ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 8.65 (d, *J* = 11.3 Hz, 1H), 7.95 (br s, 1H), 7.34 (d, *J* = 8.7 Hz, 2H), 7.03 ppm (d, *J* = 8.7 Hz, 2H). ^{13}C{^{1}H}-NMR ($CDCl_3$, 126 MHz): δ = 162.2 (s), 135.30 (s), 131.0 (s), 130.0 (s), 120.3 ppm (s).

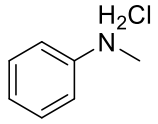


N-(4-methoxyphenyl)formamide **(3'f):**[4] Yield 69%. %. A mixture of rotamers (approx. 1:1.1 ratio) was obtained. Major rotamer: ^{1}H-NMR ($CDCl_3$, 500MHz): δ = 8.33 (s, 1H), 7.95 (br s, 1H), 7.45 (d, *J* = 9.0 Hz, 2H), 6.87 – 6.84 (m, 2H), 3.78 ppm (s, 3H). ^{13}C{^{1}H}-NMR ($CDCl_3$, 126 MHz): δ = 159.5 (s), 157.8 (s), 129.5 (s), 122.11 (s), 121.8 (s), 114.3 (s), 55.6 ppm (s). Minor rotamer: ^{1}H-NMR ($CDCl_3$, 500MHz): δ = 8.50 (d, *J* = 11.5 Hz, 1H), 8.30 (br s, 1H), 7.04 (d, *J* = 8.9 Hz, 2H), 6.90 – 6.87 (m, 2H), 3.80 ppm (s, 3H). ^{13}C{^{1}H}-NMR ($CDCl_3$, 126 MHz): δ = 163.3 (s), 157.0 (s), 129.8 (s), 122.1 (s), 115.0 (s), 55.7 ppm (s).

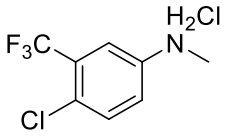


N-tert-butylformamide **(3'k):**[5] Yield 53%. A mixture of rotamers (1:1) was obtained. ^{1}H-NMR ($CDCl_3$, 500MHz):δ = 8.27 (d, *J* = 12.4 Hz, 1H), 8.03 (s, 1H), 5.94 (br s, 1H), 5.31 (br s, 1H), 1.37 (s, 12H), 1.33 ppm (s, 12H). ^{13}C{^{1}H}-NMR ($CDCl_3$, 126 MHz): δ = 163.0 (s), 160.6 (s), 51.5 (s), 50.5 (s), 31.1 (s), 29.1 ppm (s).

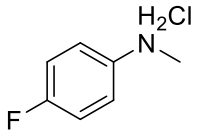
3. **NMR data for isolated N-methylamine hydrochlorides**



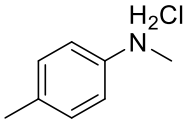
N-methylaniline hydrochloride **(5'a):**[6,7,8] Yield 78%. A mixture of rotamers (approx. 1:1 ratio) was obtained. ^{1}H-NMR (CD_3OD, 500 MHz): δ = 7.53-7.60 (m, 5H), 4.92 (br s, 2H), 3.08 ppm (s, 3H). $^{13}C\{^{1}H\}$-NMR (CD_3OD, 126 MHz): δ = 138.2 (s), 131.6 (s), 131.0 (s), 123.2 (s), 37.9 ppm (s).



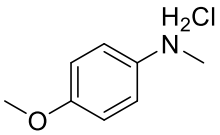
4-chloro-3-(trifluoromethyl)-N-methylaniline hydrochloride **(5'c):** Yield 68%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 7.24 (s, 1H), 6.91 (d, *J* = 2.8 Hz, 1H), 6.70 (dd, *J* = 8.7, 2.7 Hz, 1H), 4.94 (br s, 1H), 2.84 ppm (s, 3H). $^{13}C\{^{1}H\}$-NMR ($CDCl_3$, 126 MHz): δ = 146.96 (s), 132.17 (s), 128.87 (q, *J* = 30.8 Hz), 124.16 (s), 121.99 (s), 116.84 (s), 111.78 (d, *J* = 5.6 Hz), 31.22 ppm (s). ^{19}F-NMR ($CDCl_3$, 471 MHz): δ = -62.64 ppm (s).



4-fluoro-N-methylaniline hydrochloride **(5'd):**[7,9] Yield 72%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 11.6 (br s, 2H), 7.68 (br m, 2H), 7.15 (br m, 2H), 3.15 ppm (s, 3H). ^{1}H NMR (CD_3OD, 500 MHz): δ = 7.55-7.58 (m, 2H), 7.19-7.47 (m, 2H), 4.91 (br s, 2H), 3.07 ppm (s, 3H). $^{13}C\{^{1}H\}$-NMR ($CDCl_3$, 126 MHz): δ = 163.16 (d, *J* = 250.7 Hz), 133.15 (br s), 126.95 (d, *J* = 9.1 Hz), 117.62 (d, *J* = 23.3 Hz), 40.16 ppm (s). ^{19}F-NMR ($CDCl_3$, 471 MHz): δ = -110.03 ppm (s).



4-methyl-N-methylaniline hydrochloride **(5'e):**[6,7,10,11] Yield 88%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 11.42 (br s, 2H), 7.55 (br d, *J* = 6.4 Hz, 2H), 7.24 (br d, *J* = 6.3 Hz, 2H), 3.17 (br s, 3H), 2.36 ppm (s, 3H). $^{13}C\{^{1}H\}$-NMR ($CDCl_3$, 126 MHz): δ = 193.8 (s), 134.6 (s), 130.8 (s), 124.4 (s), 39.8 (s), 21.1 ppm (s). NMR data are consistent with those previously reported in the literature.[10]



4-methoxy-N-methylaniline hydrochloride **(5'f):**[6,7,12] Yield 90%. ^{1}H NMR ($CDCl_3$, 500 MHz): δ = 11.33 (br s, 2H), 7.57 (br d, *J* = 7.0 Hz, 2H), 6.92 (br d, *J* = 7.0 Hz, 2H), 3.80 (s, 3H), 3.09 ppm (br s, 3H). $^{13}C\{^{1}H\}$-NMR ($CDCl_3$, 126 MHz): δ = 160.2 (s), 129.8 (s), 125.3 (s), 115.4 (s), 55.7 (s), 39.5 ppm (s).

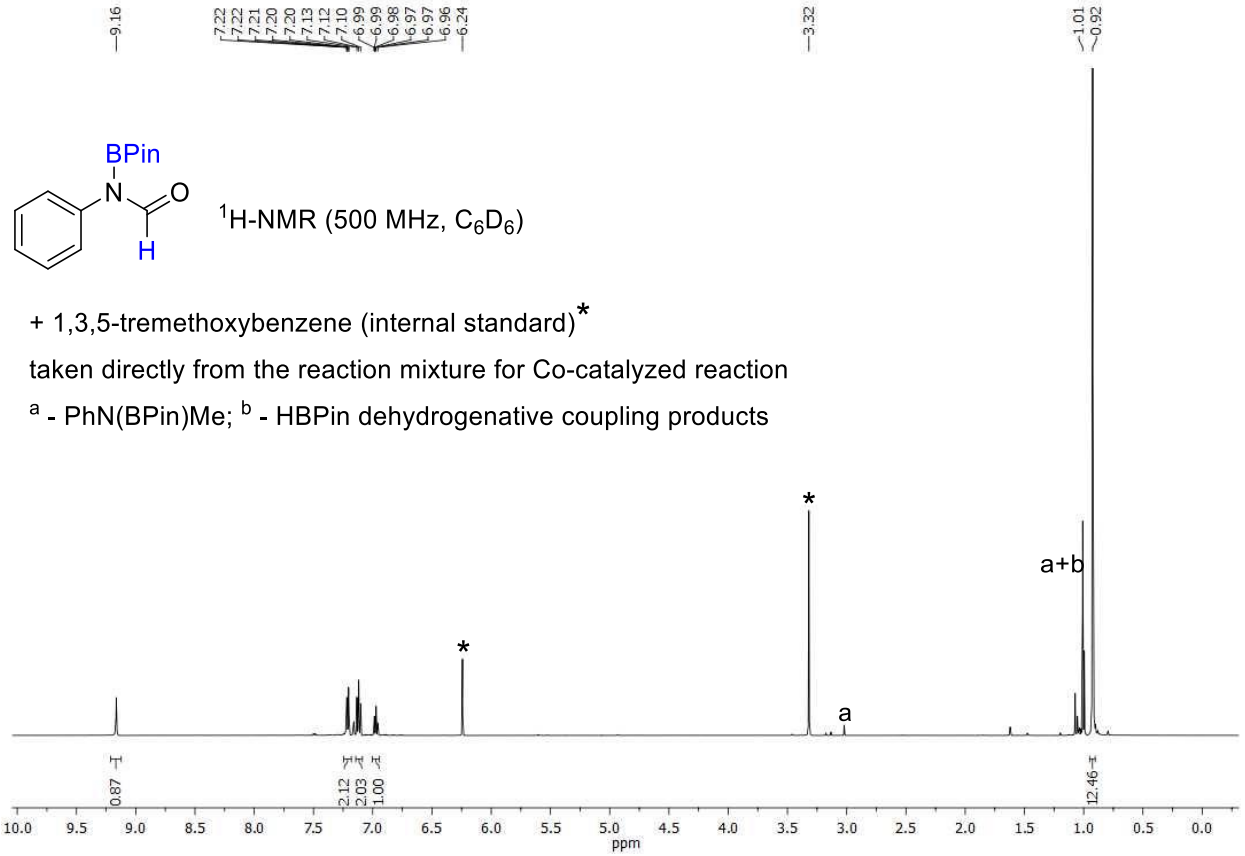
4. NMR spectra for N-borylformamides (taken directrly from reaction mixtures)

^{1}H-NMR (500 MHz, C_6D_6)

+ 1,3,5-tremethoxybenzene (internal standard)*

taken directly from the reaction mixture for Co-catalyzed reaction

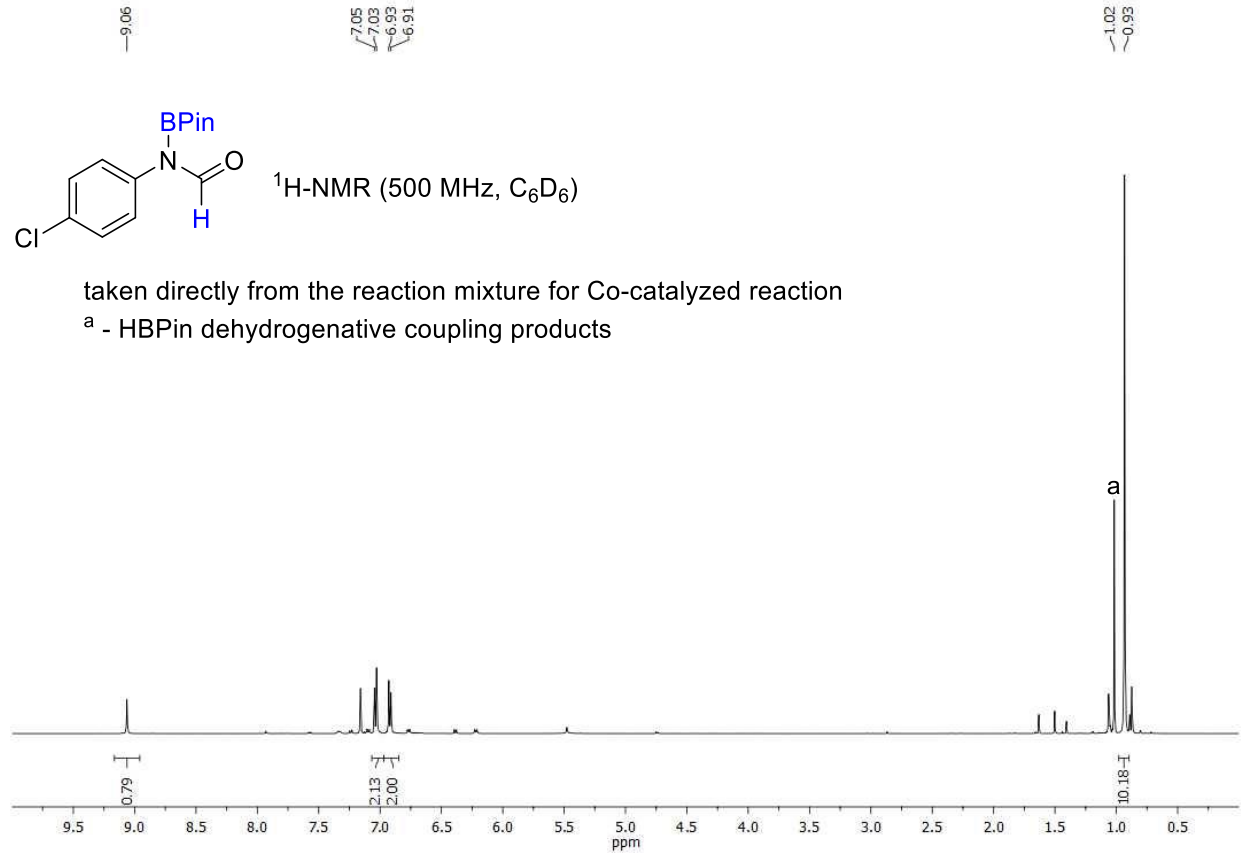
[a] - PhN(BPin)Me; [b] - HBPin dehydrogenative coupling products

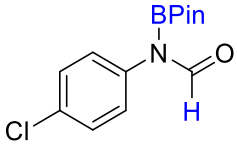


^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products

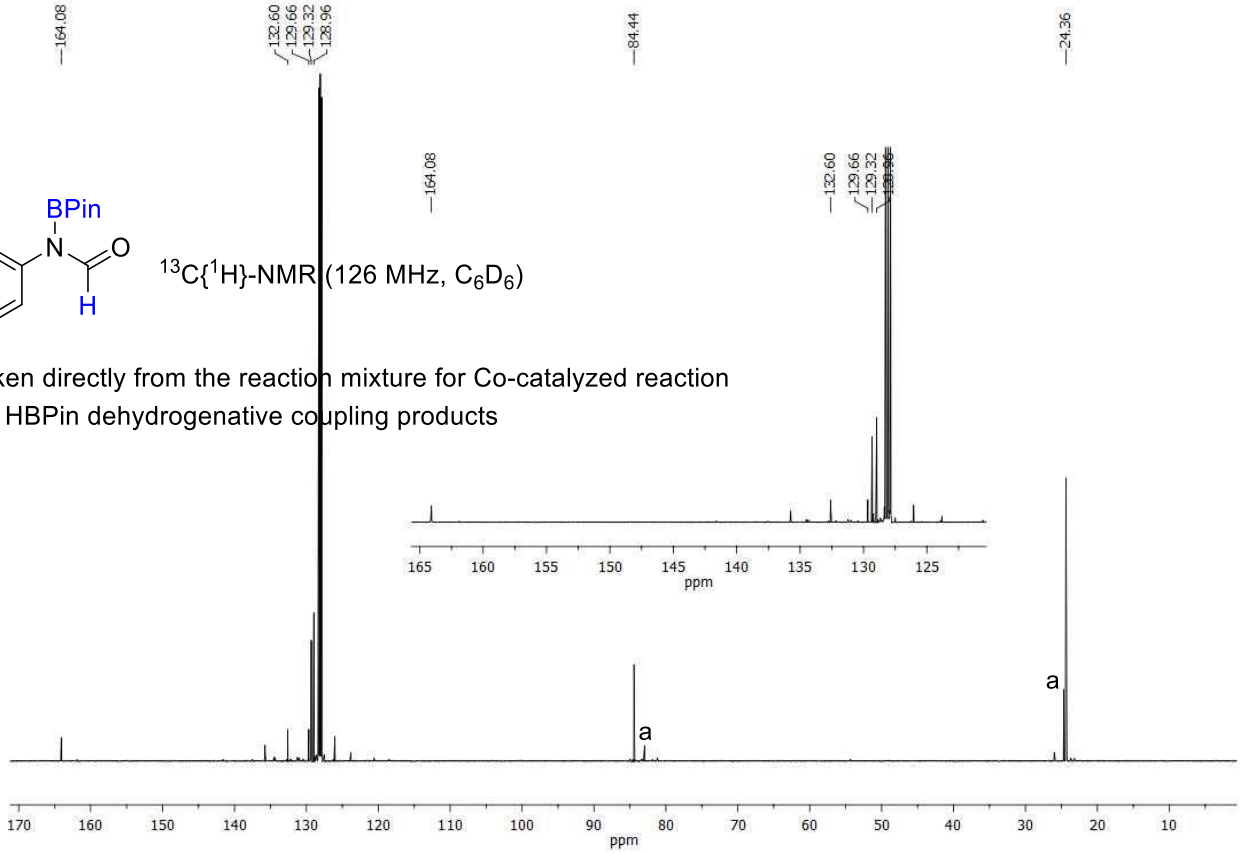


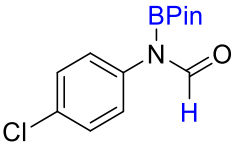


$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products

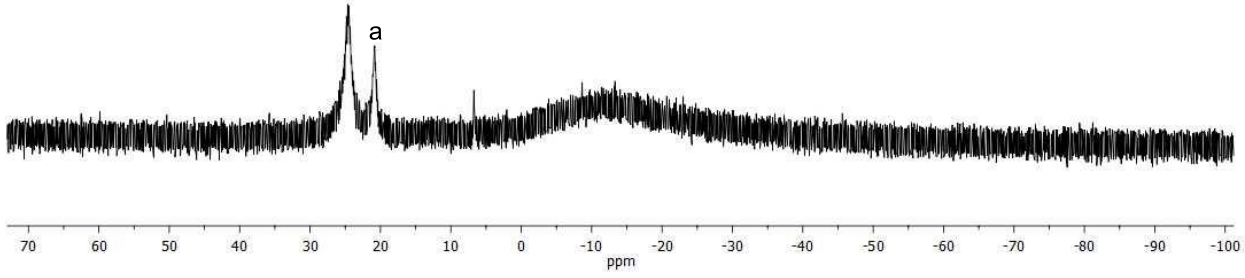


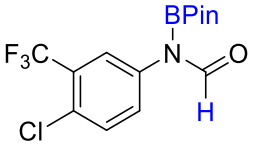


^{11}B-NMR (160 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products



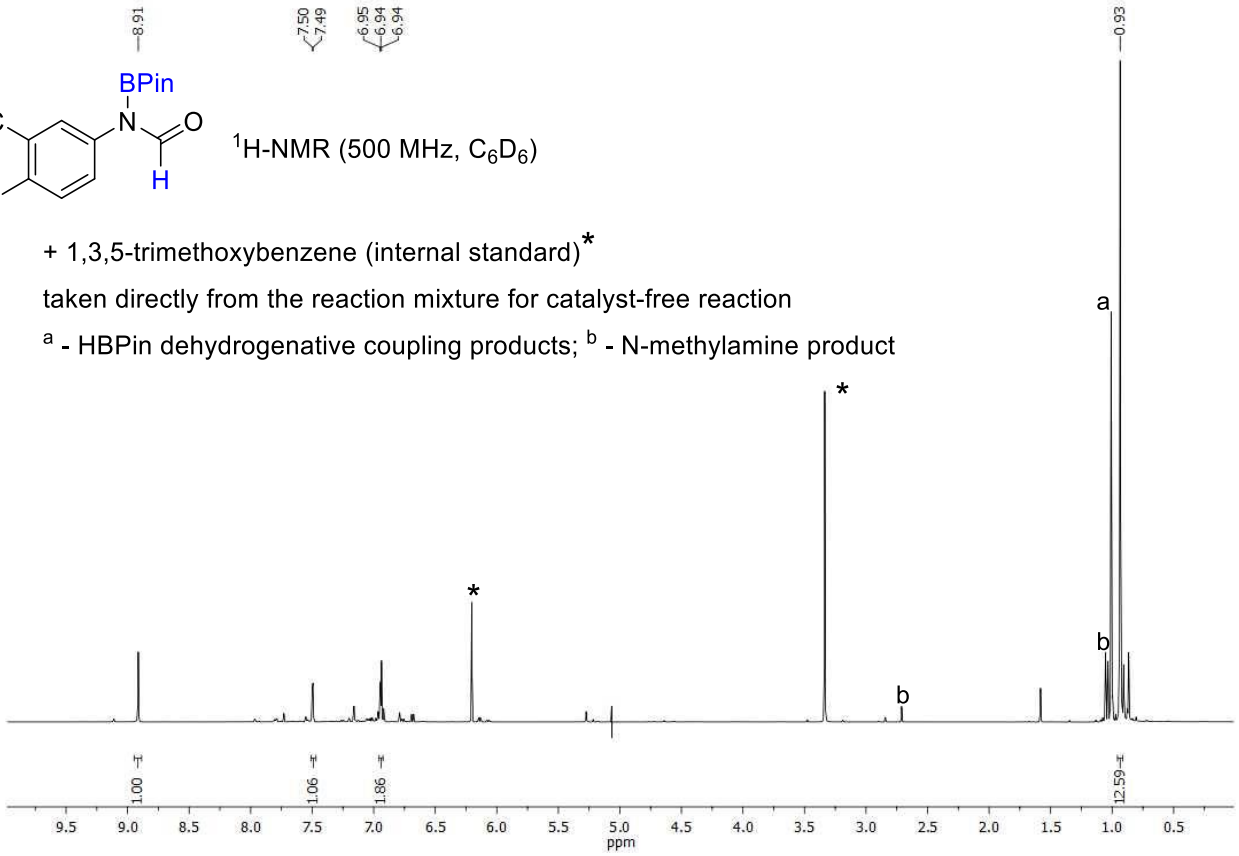


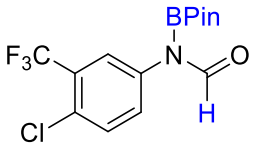
^{1}H-NMR (500 MHz, C_6D_6)

+ 1,3,5-trimethoxybenzene (internal standard)*

taken directly from the reaction mixture for catalyst-free reaction

[a] - HBPin dehydrogenative coupling products; [b] - N-methylamine product

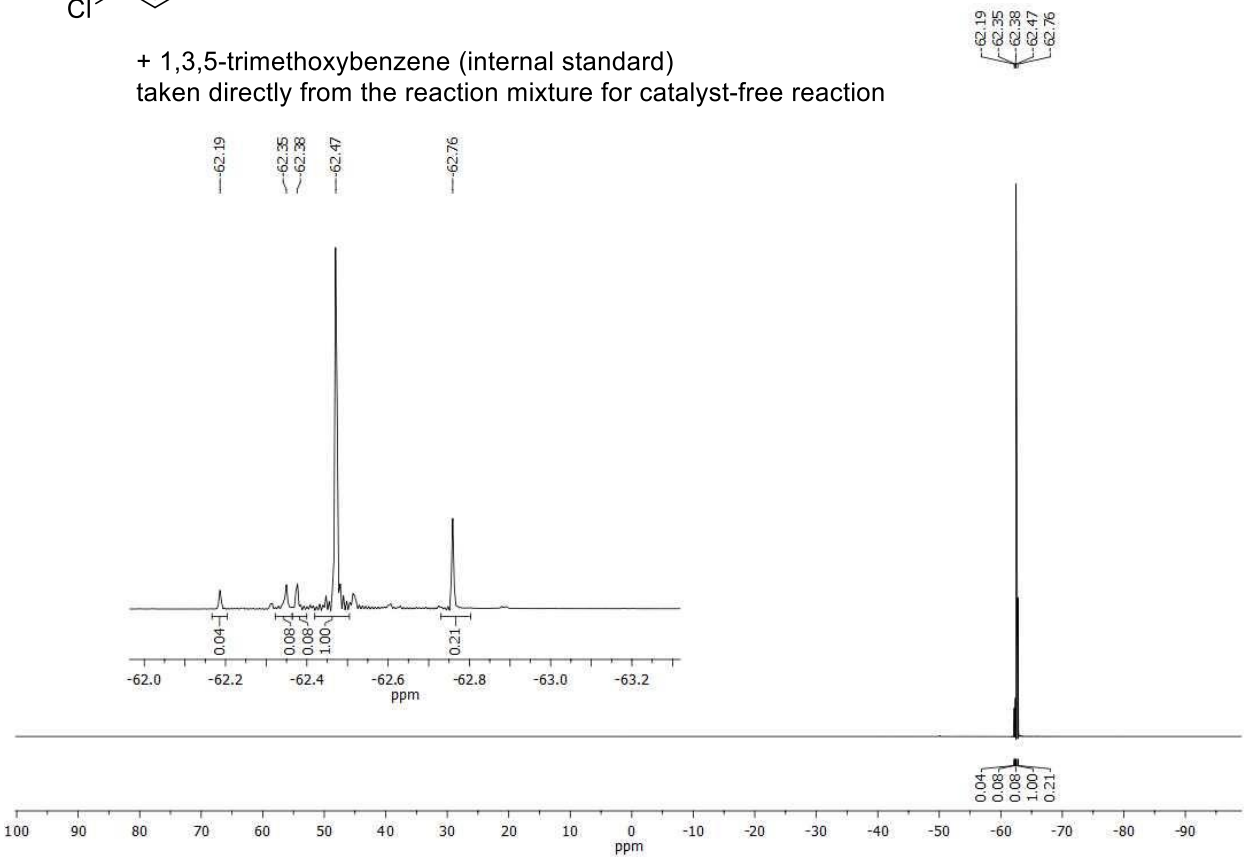


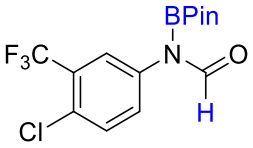


^{19}F-NMR (471 MHz, C_6D_6)

+ 1,3,5-trimethoxybenzene (internal standard)

taken directly from the reaction mixture for catalyst-free reaction

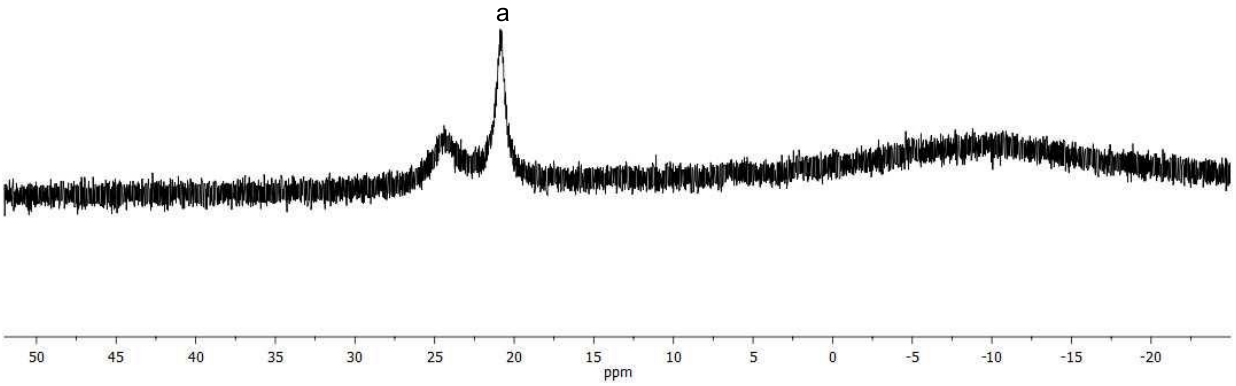




^{11}B-NMR (160 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

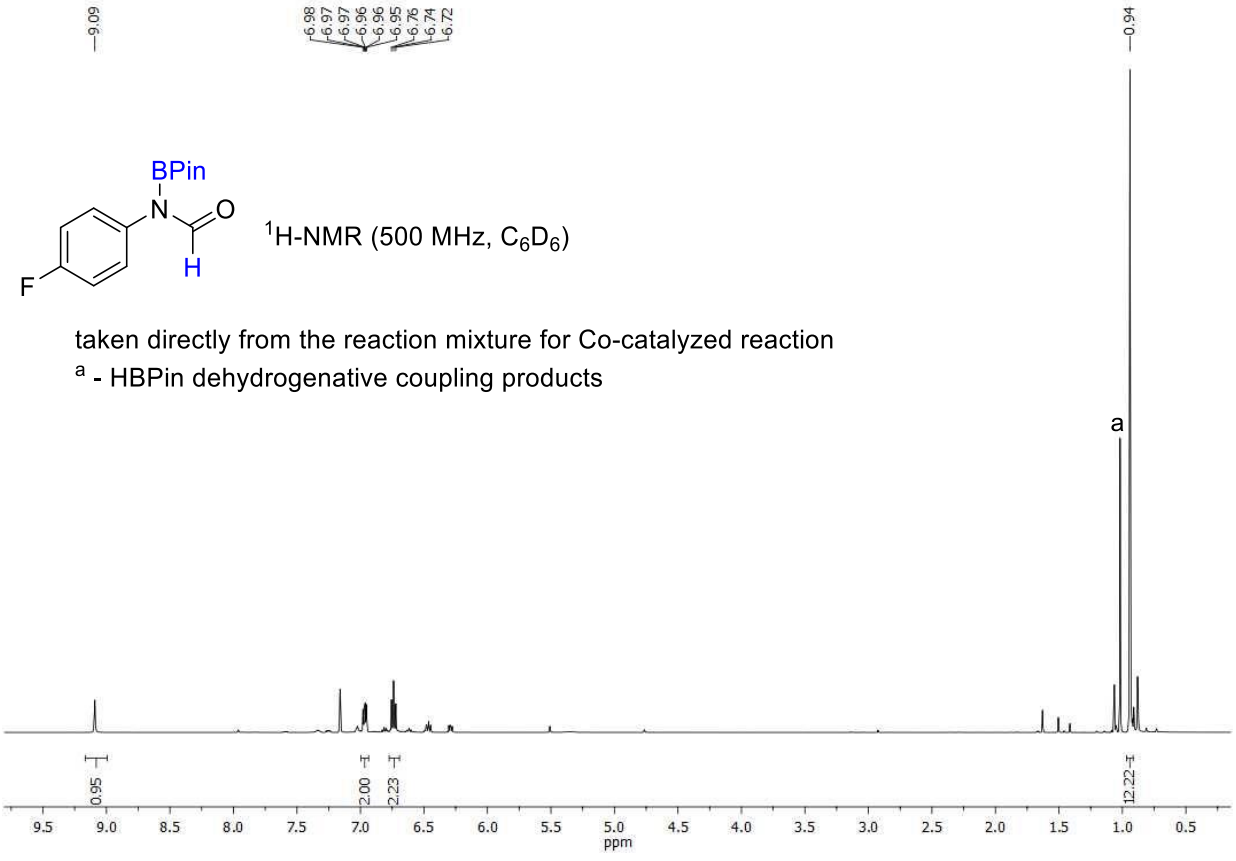
[a] - HBPin dehydrogenative coupling products

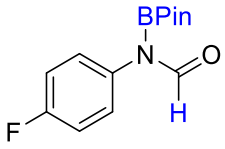


^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

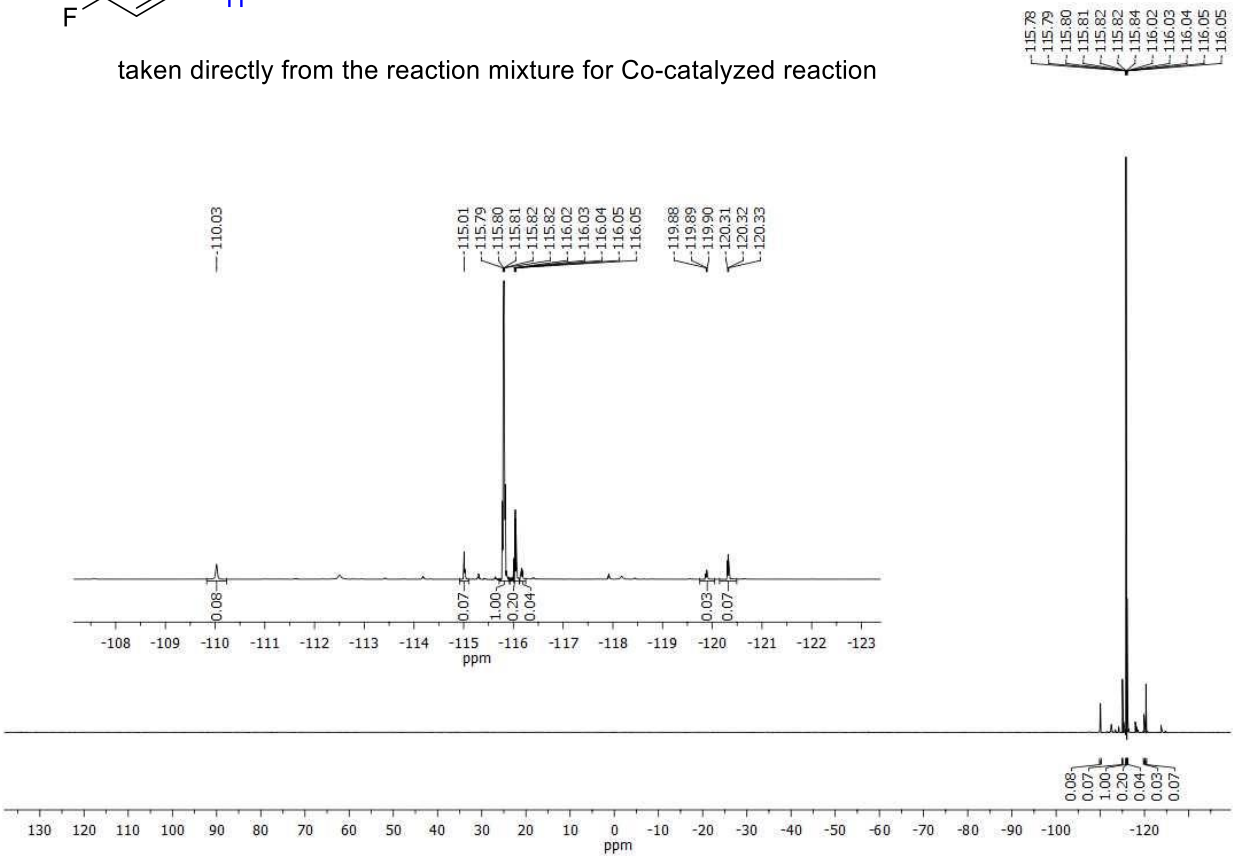
[a] - HBPin dehydrogenative coupling products

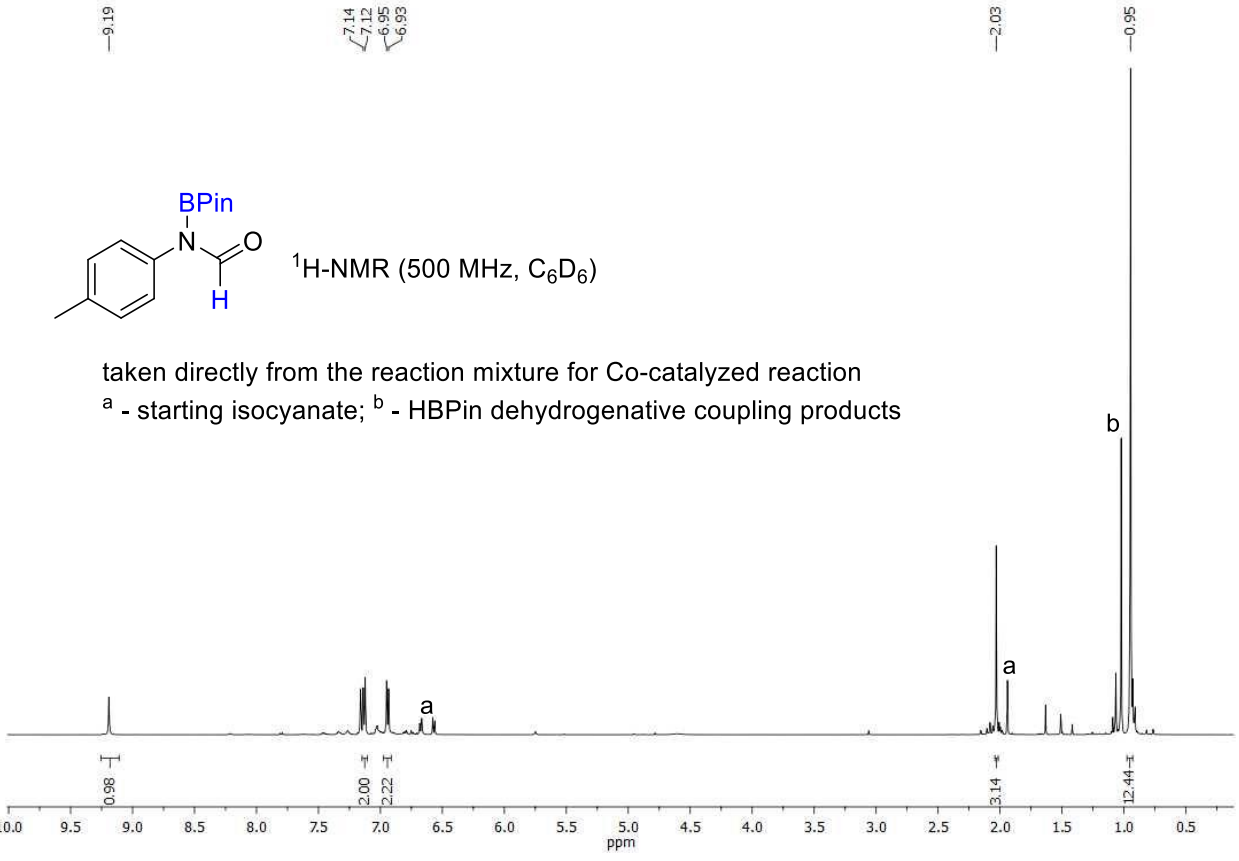




^{19}F-NMR (471 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

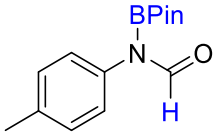




^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

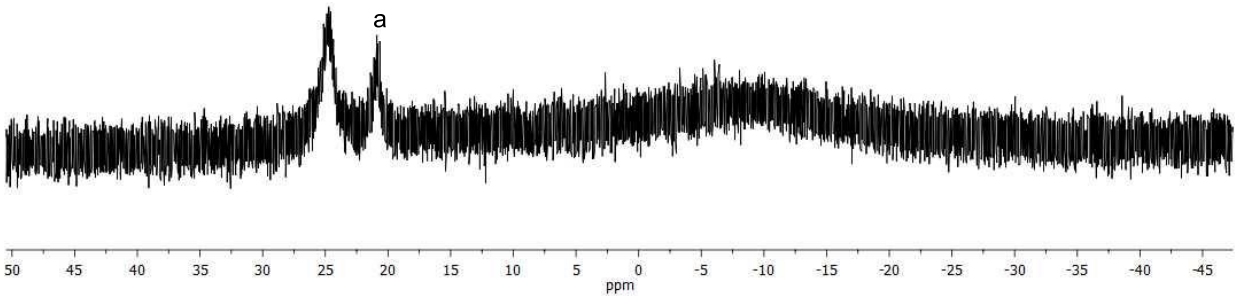
[a] - starting isocyanate; [b] - HBPin dehydrogenative coupling products



^{11}B-NMR (160 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

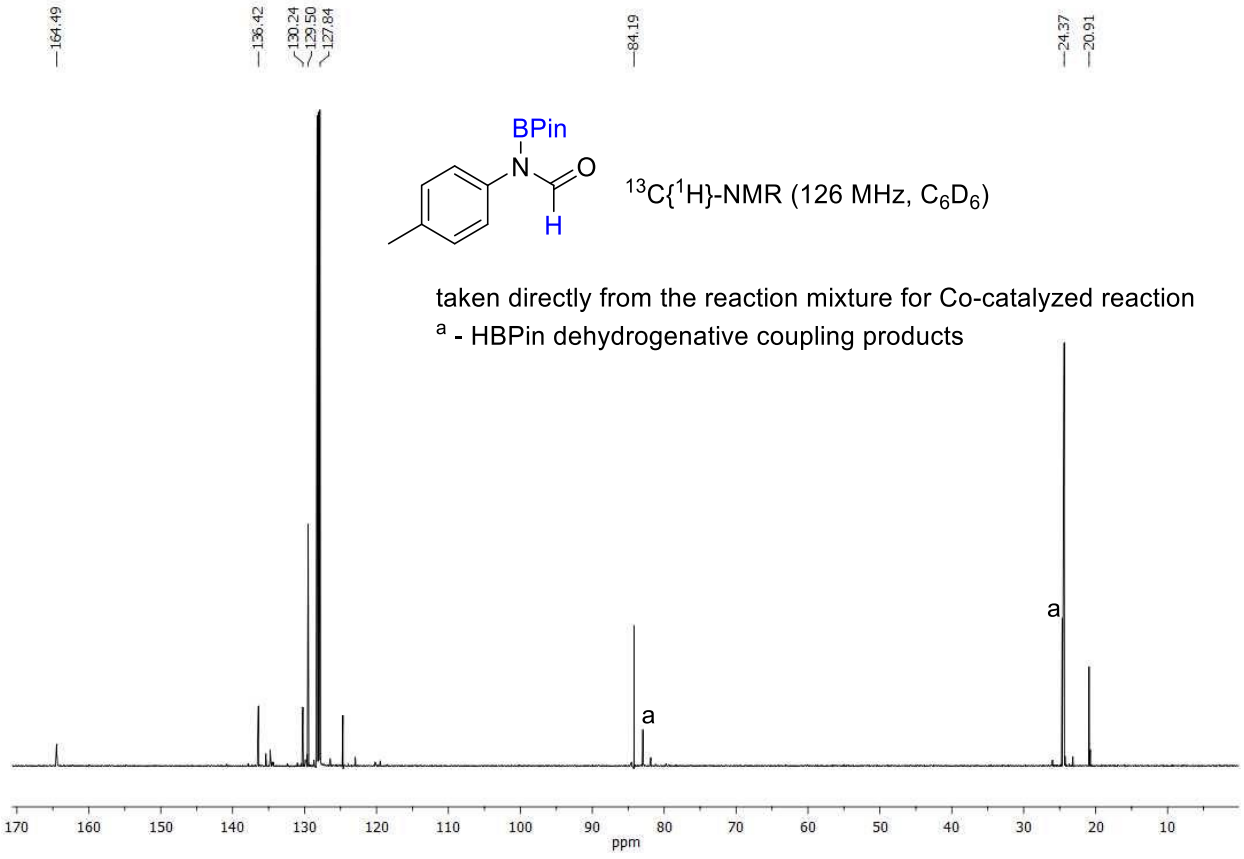
[a] - HBPin dehydrogenative coupling products

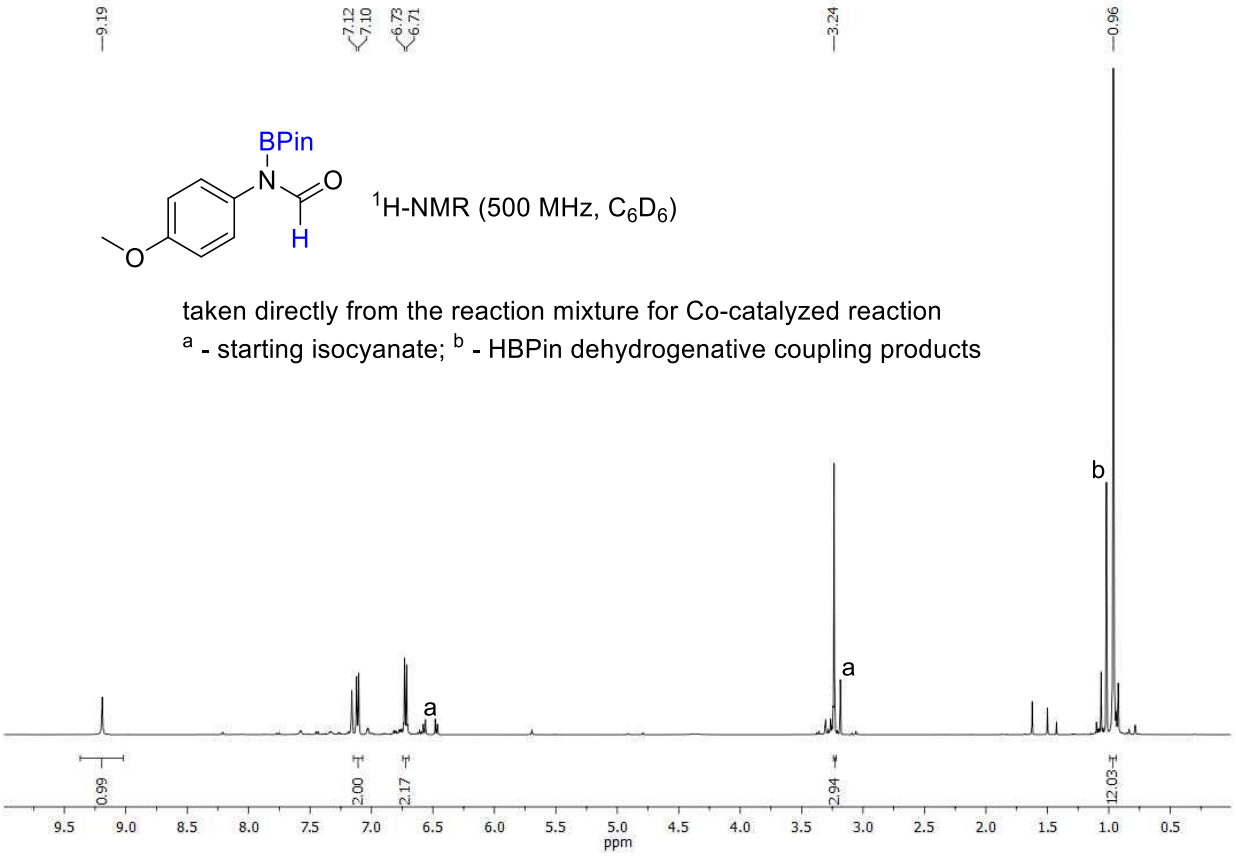


^{13}C{^{1}H}-NMR (126 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products

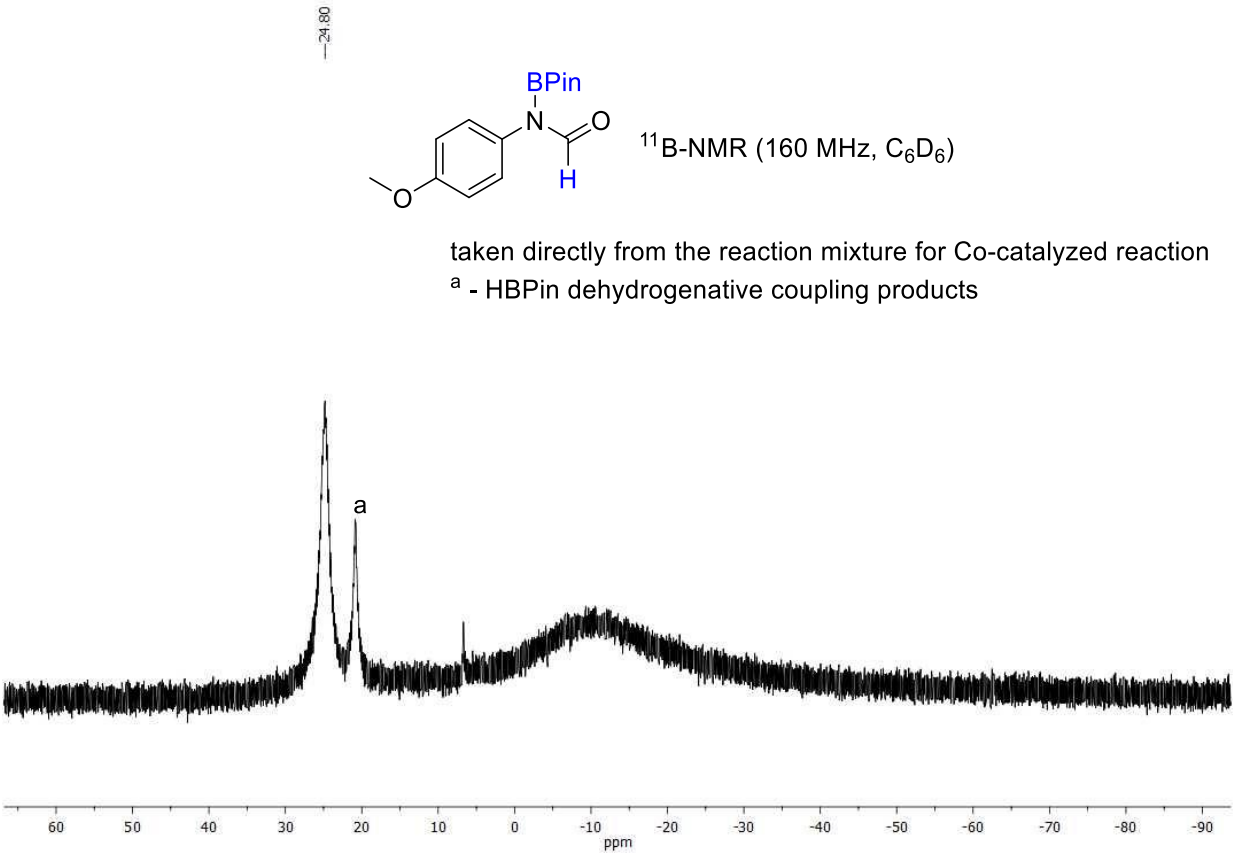




^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

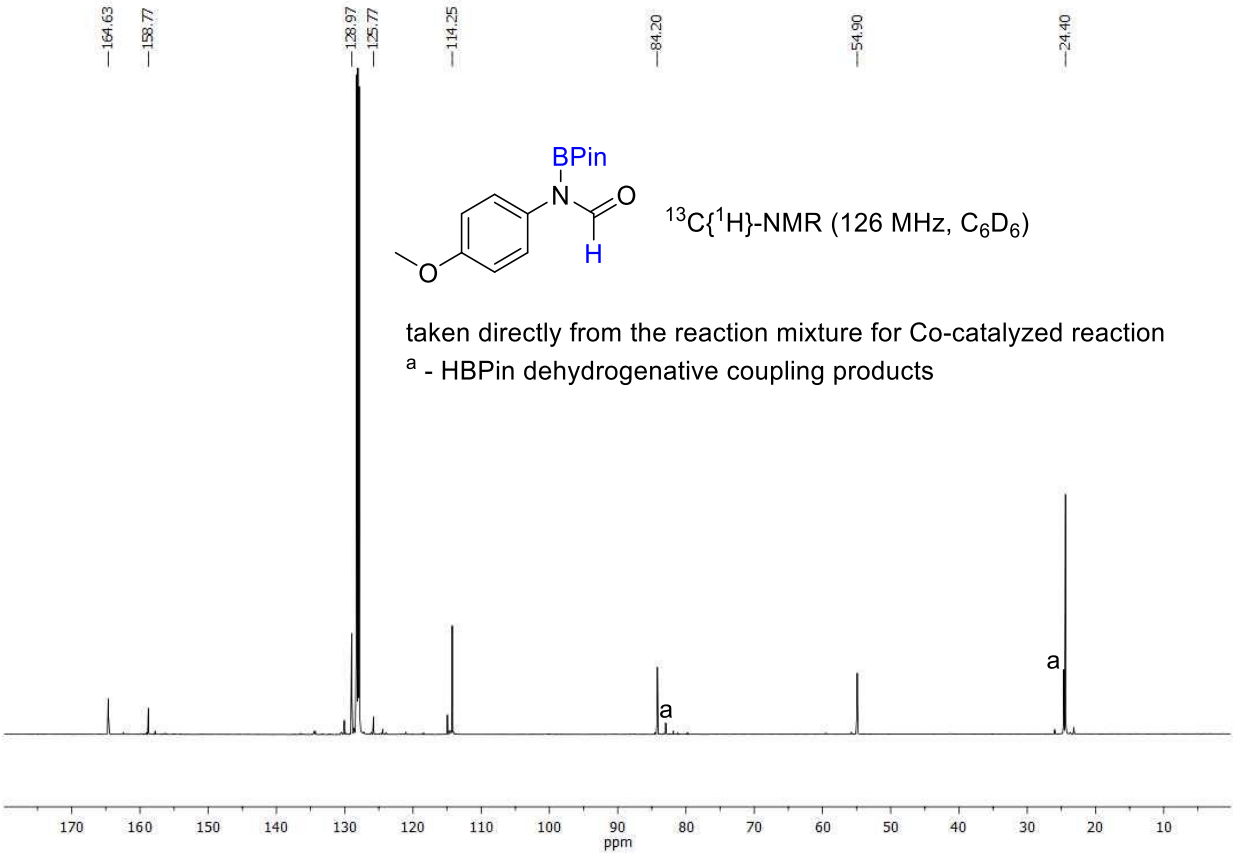
[a] - starting isocyanate; [b] - HBPin dehydrogenative coupling products



^{11}B-NMR (160 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

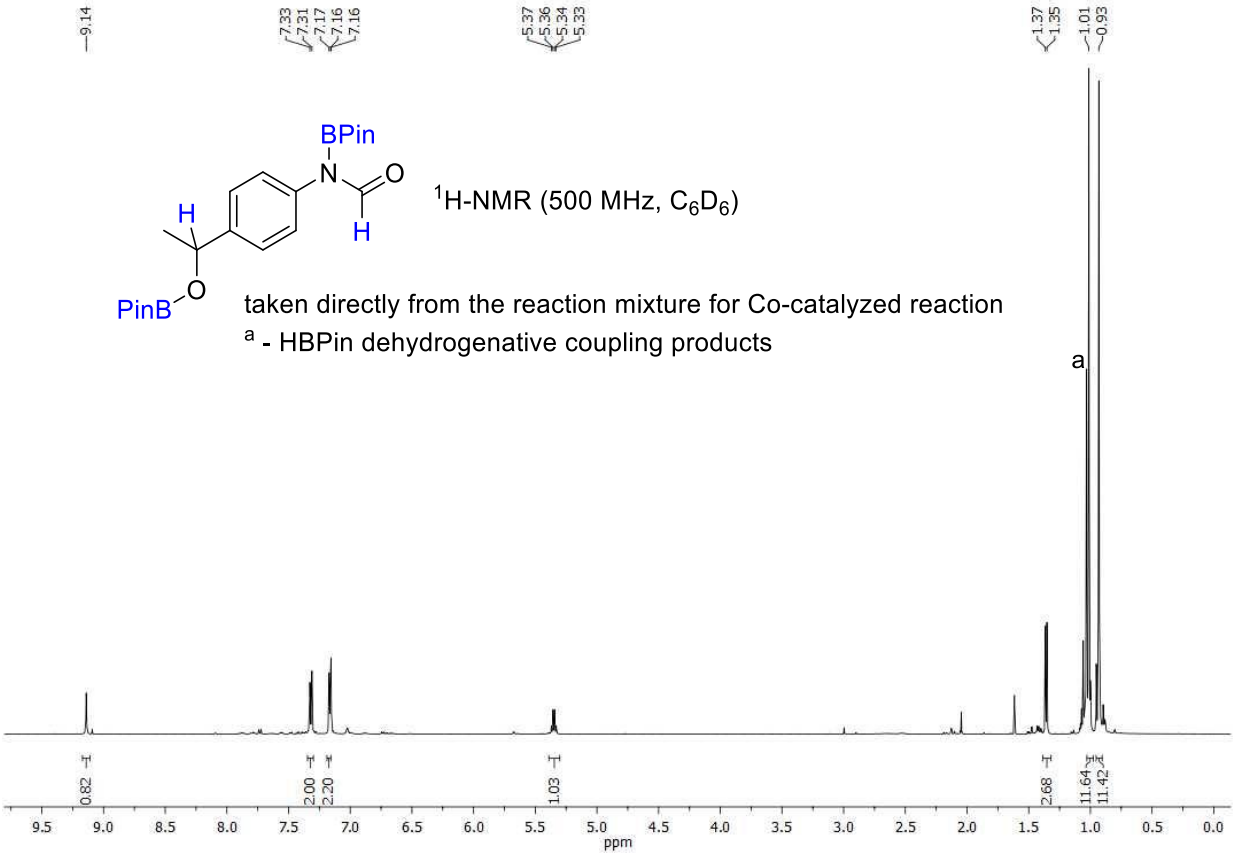
[a] - HBPin dehydrogenative coupling products



$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

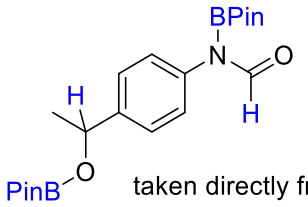
[a] - HBPin dehydrogenative coupling products



^{1}H-NMR (500 MHz, C_6D_6)

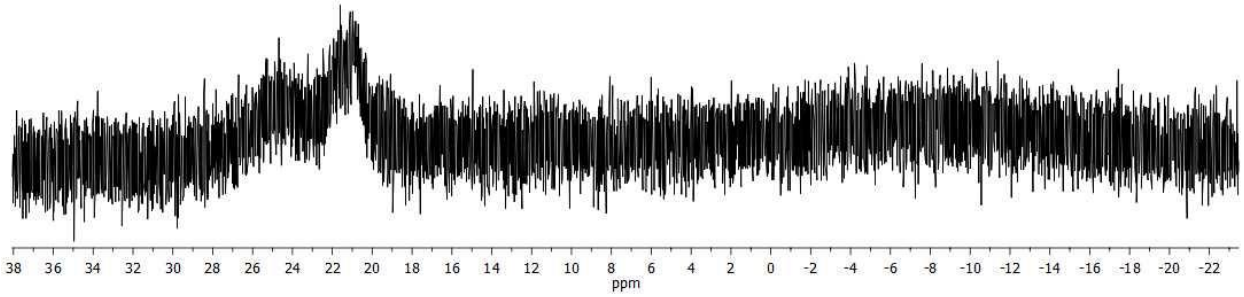
taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products



^{11}B-NMR (160 MHz, C_6D_6)

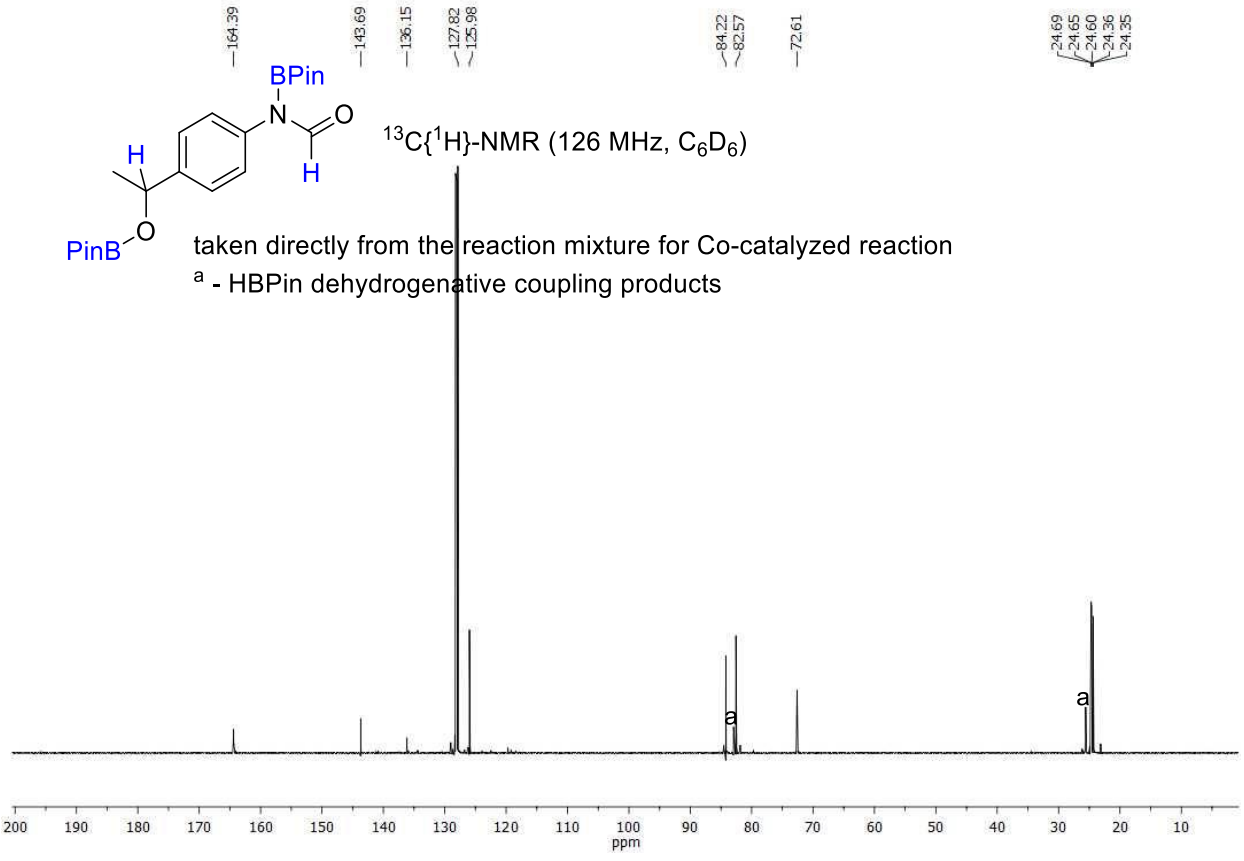
taken directly from the reaction mixture for Co-catalyzed reaction



^{13}C{^{1}H}-NMR (126 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

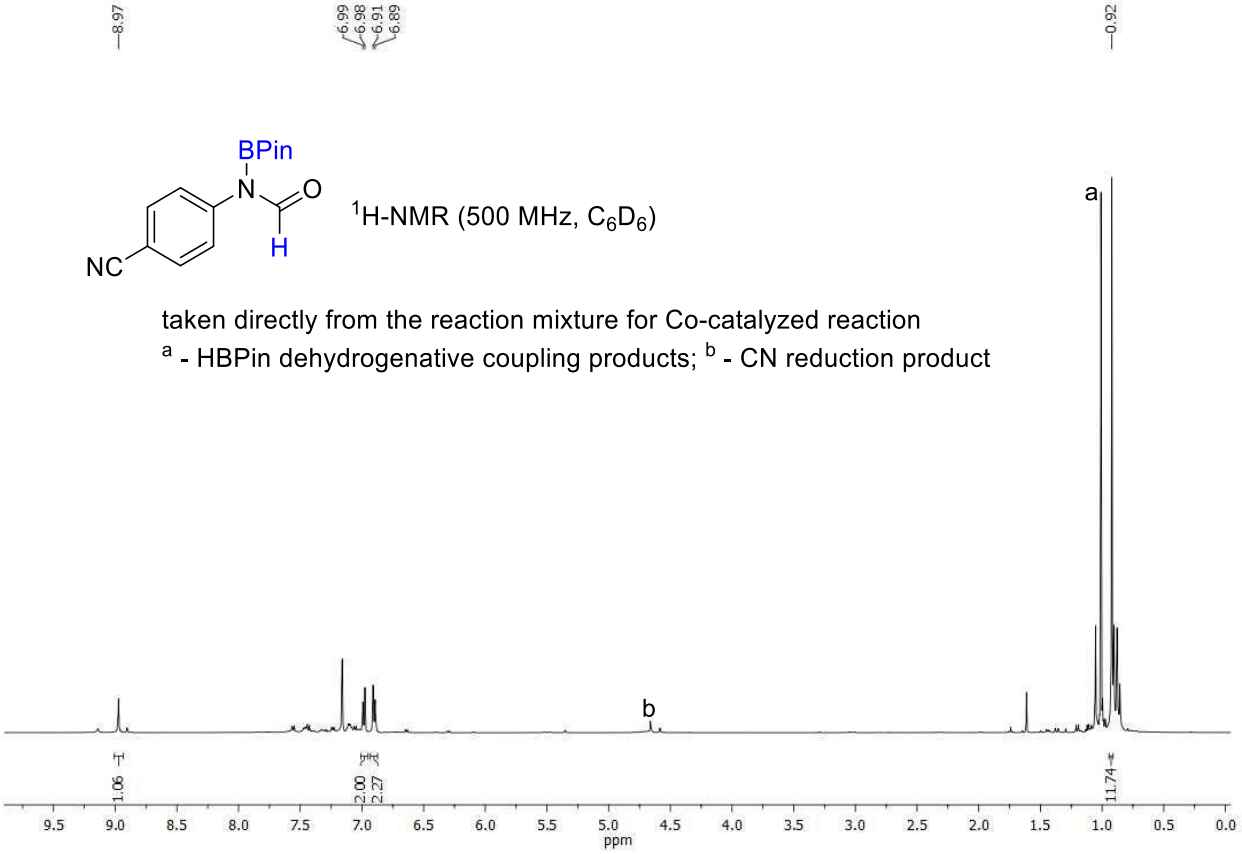
[a] - HBPin dehydrogenative coupling products



^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

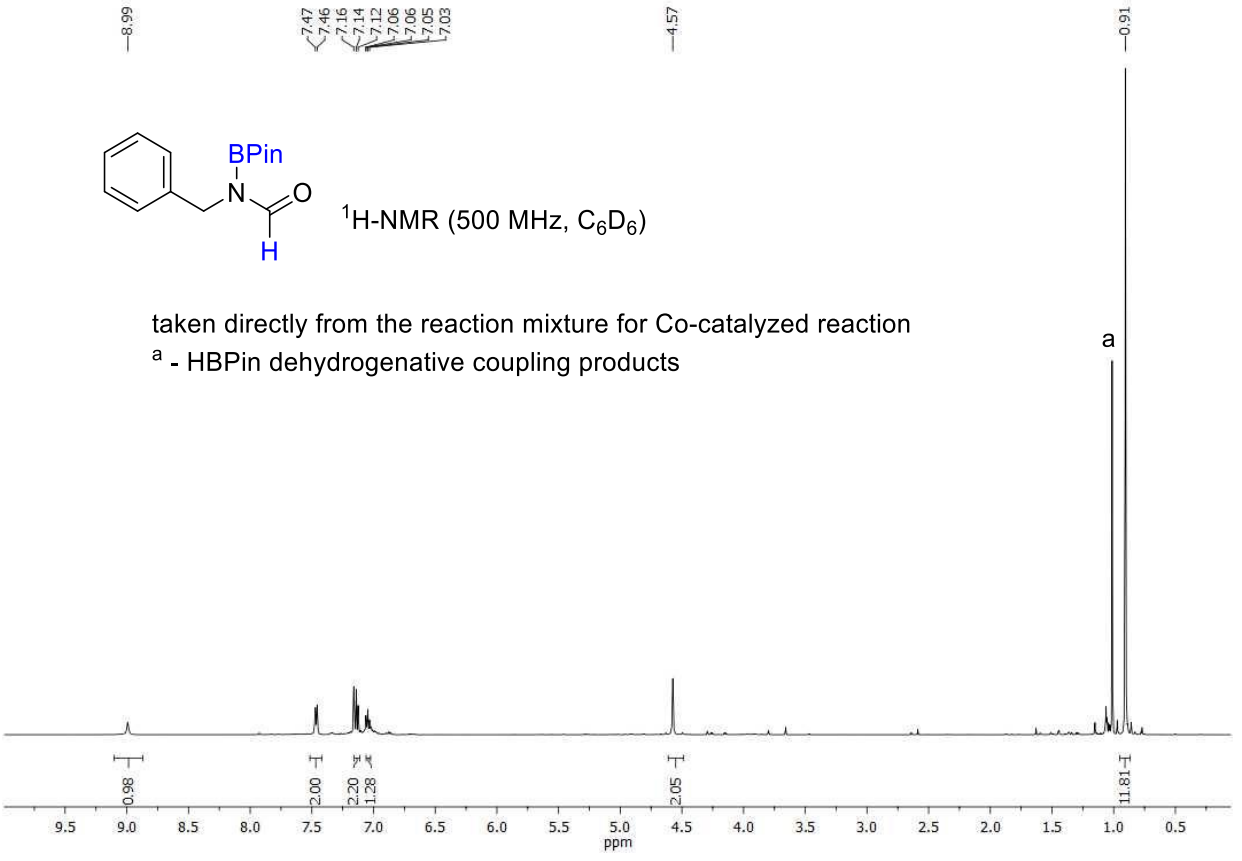
[a] - HBPin dehydrogenative coupling products; [b] - CN reduction product

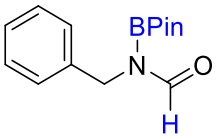


^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products

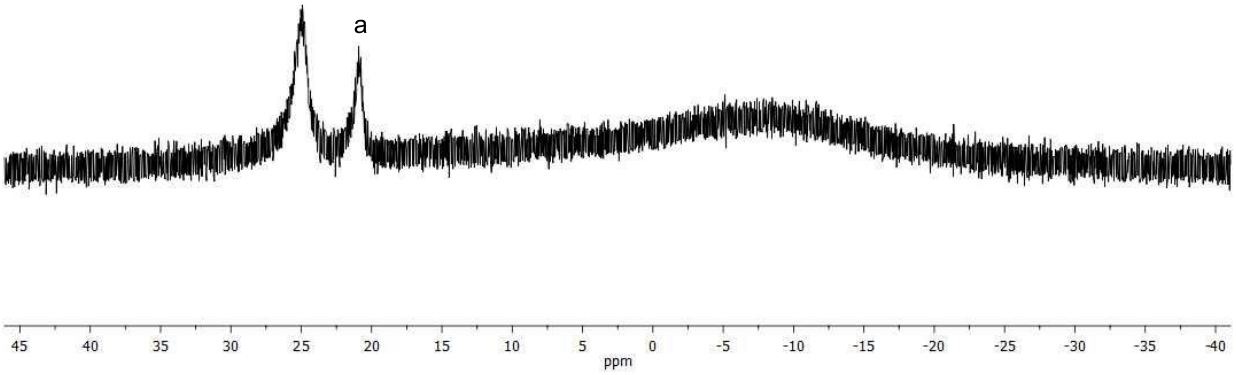




^{11}B-NMR (160 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

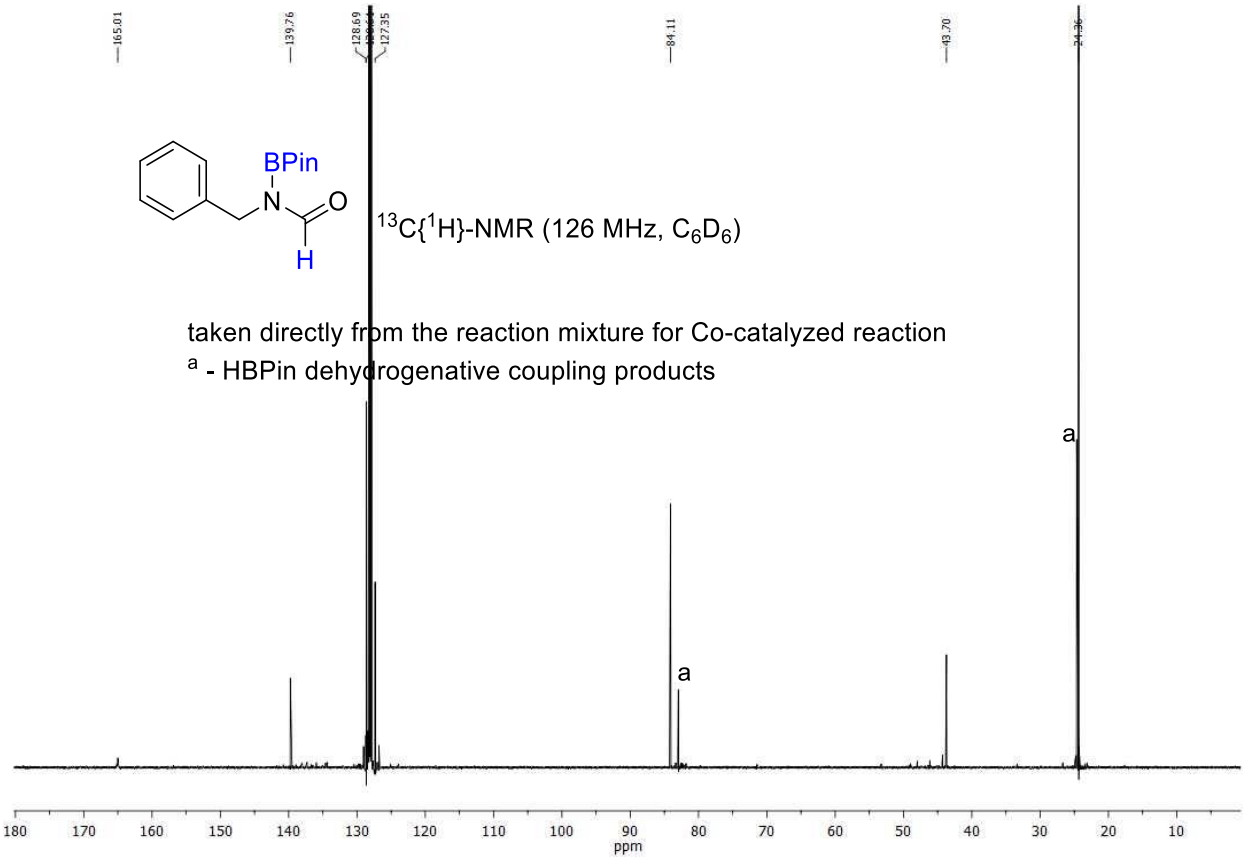
[a] - HBPin dehydrogenative coupling products

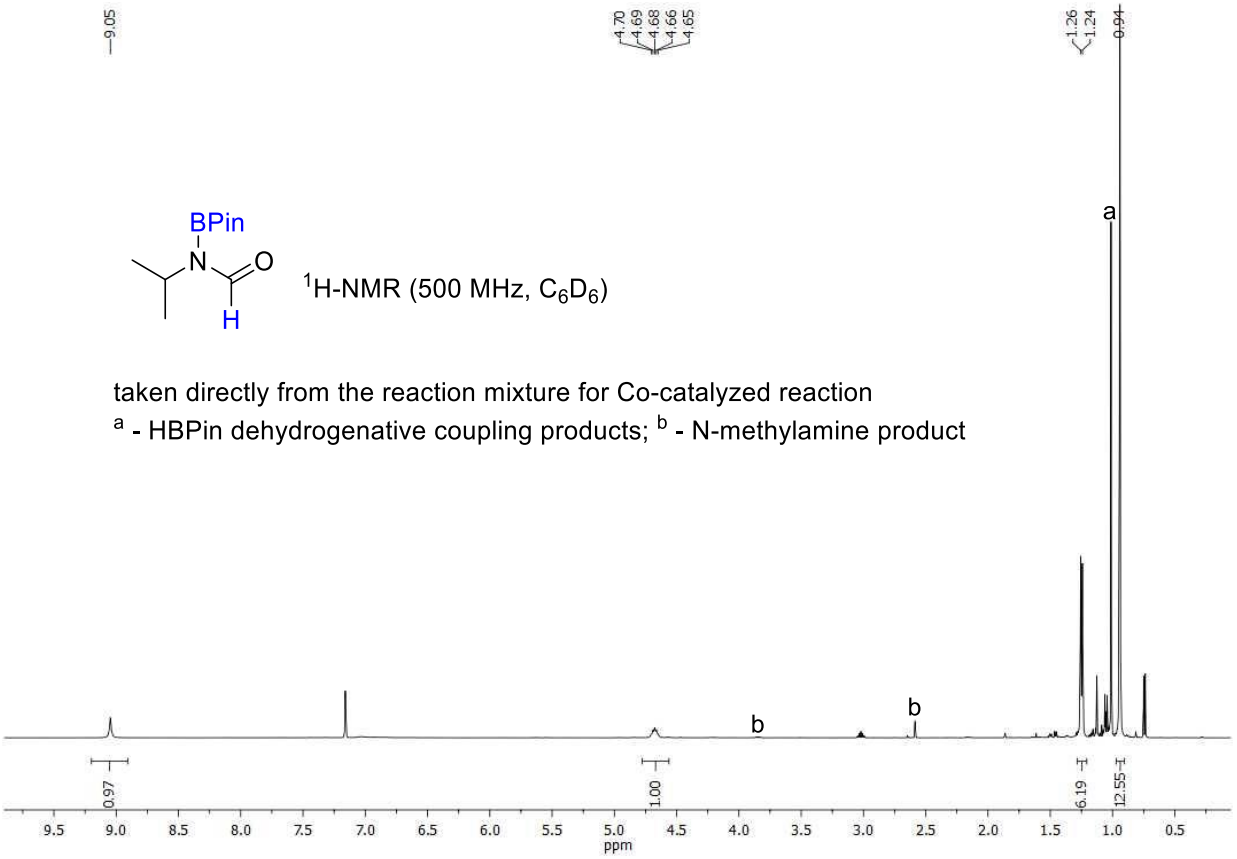


^{13}C{^{1}H}-NMR (126 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products

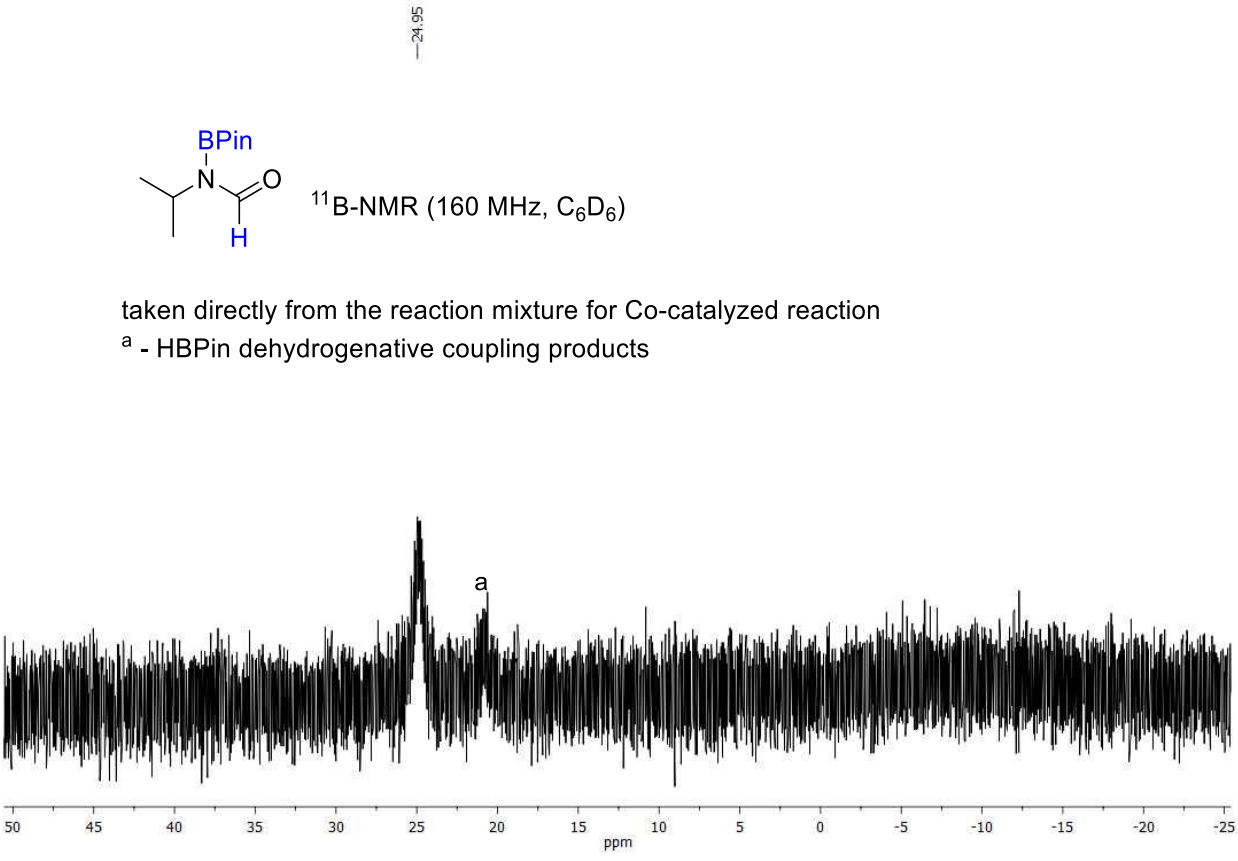




^{1}H-NMR (500 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

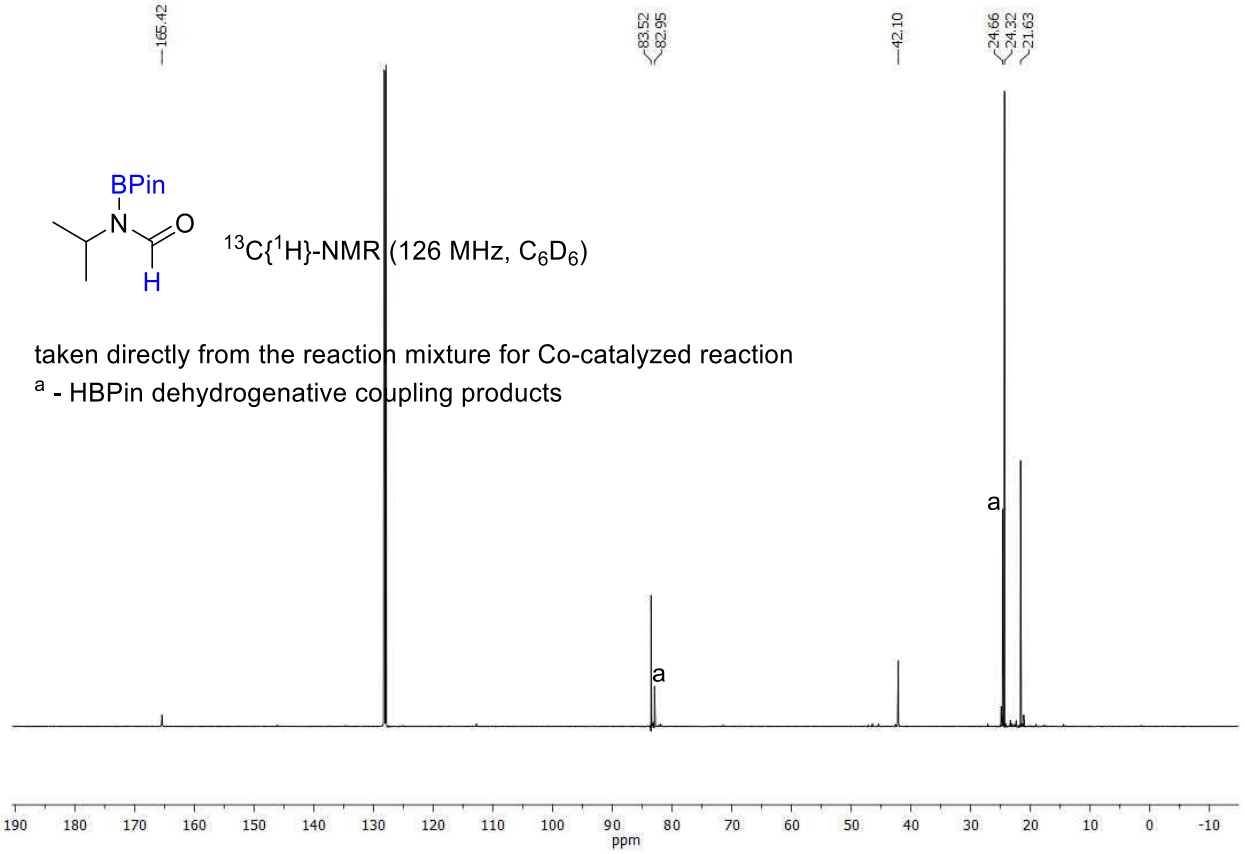
[a] - HBPin dehydrogenative coupling products; [b] - N-methylamine product



^{11}B-NMR (160 MHz, C_6D_6)

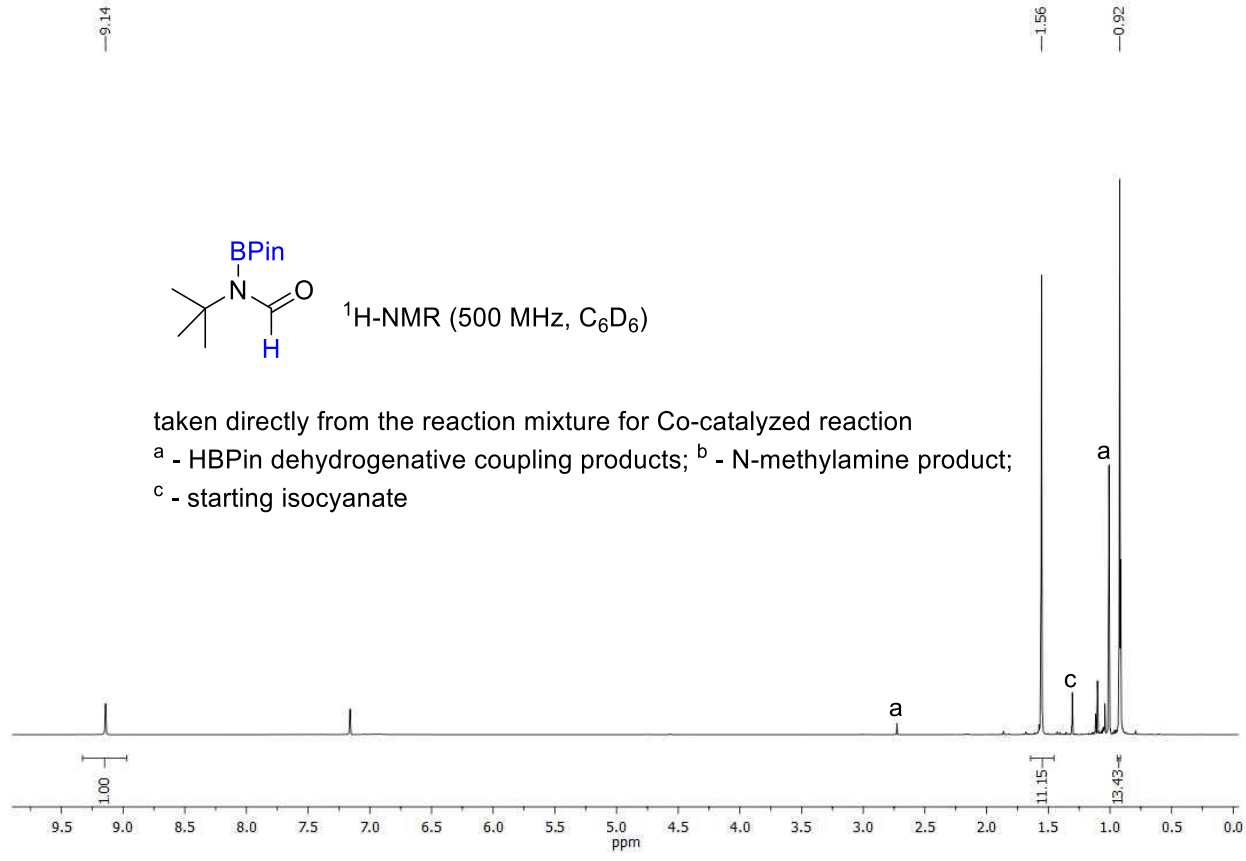
taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products



taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products



taken directly from the reaction mixture for Co-catalyzed reaction

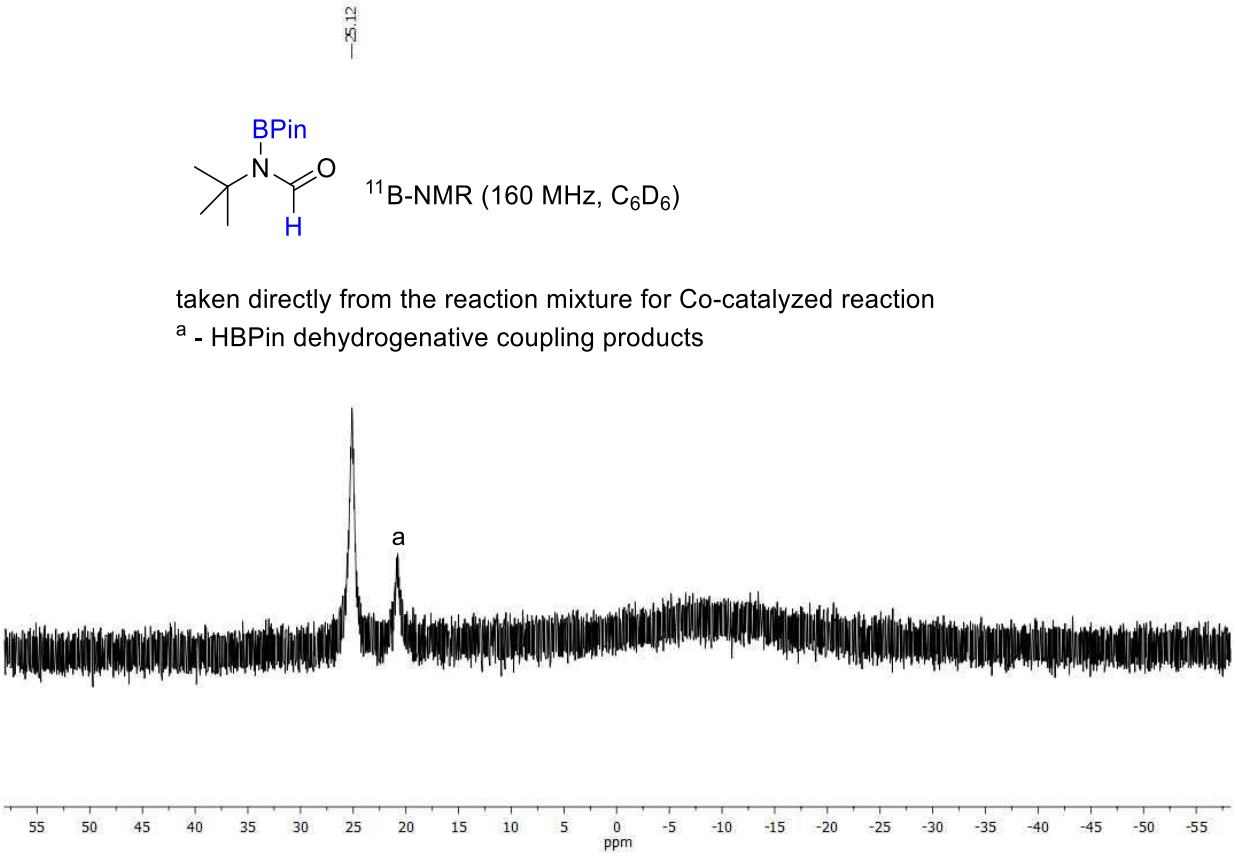
[a] - HBPin dehydrogenative coupling products; [b] - N-methylamine product;

[c] - starting isocyanate

^{11}B-NMR (160 MHz, C_6D_6)

taken directly from the reaction mixture for Co-catalyzed reaction

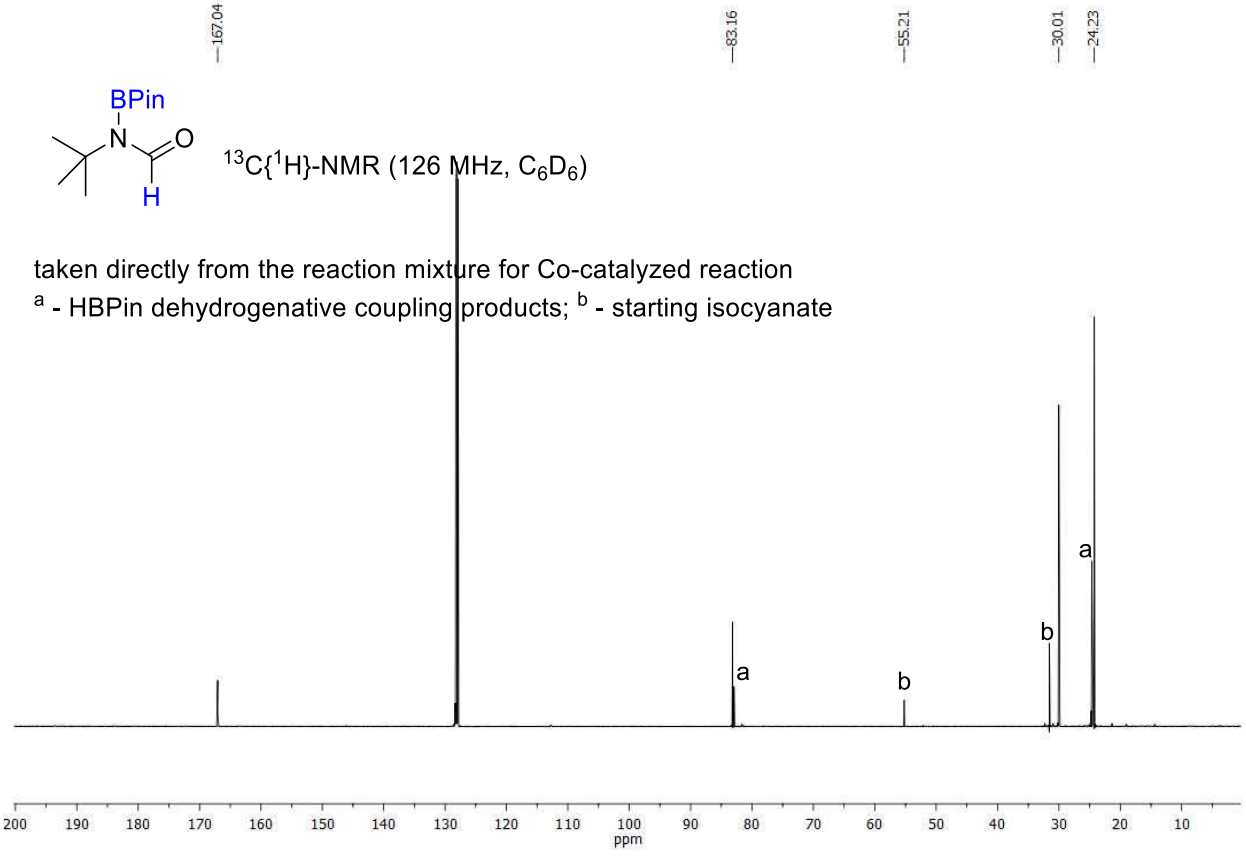
[a] - HBPin dehydrogenative coupling products



$^{13}C\{^1H\}$-NMR (126 MHz, C_6D_6)

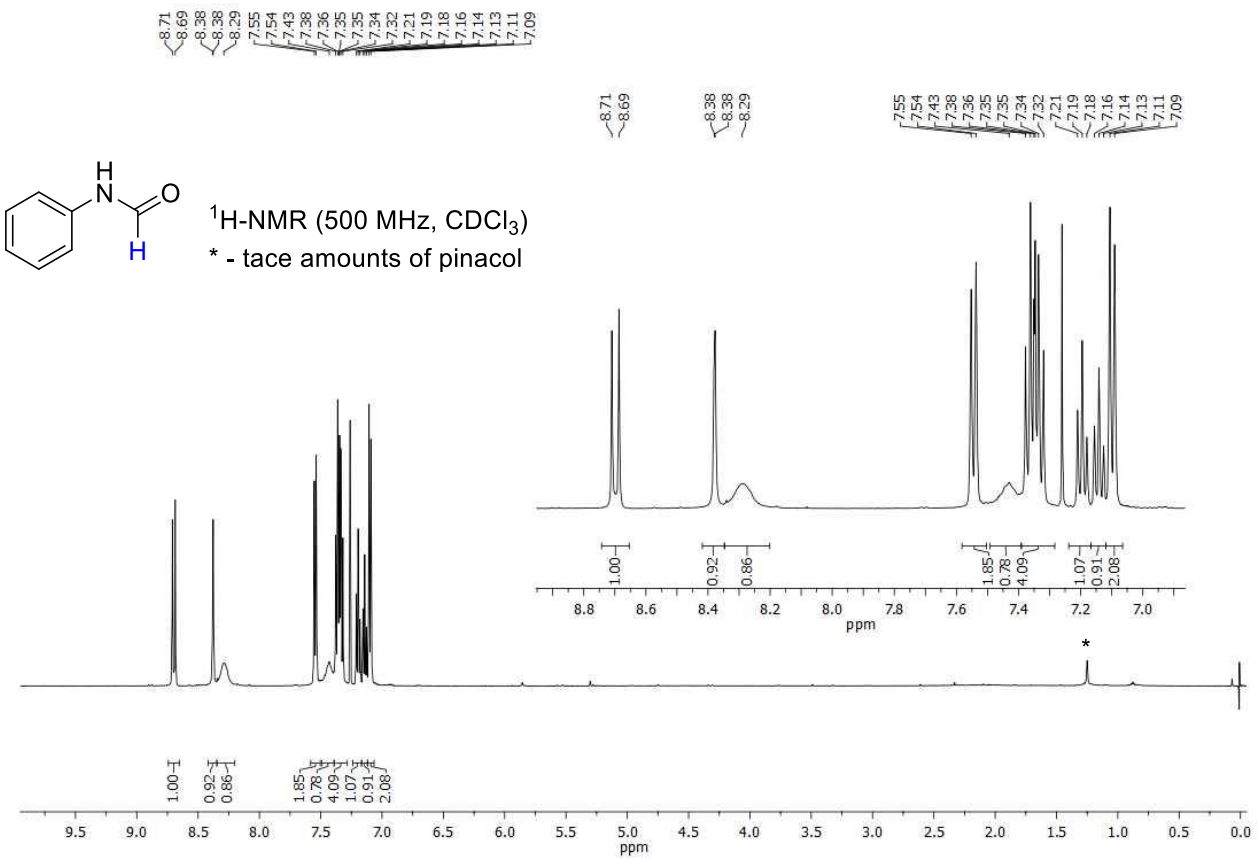
taken directly from the reaction mixture for Co-catalyzed reaction

[a] - HBPin dehydrogenative coupling products; [b] - starting isocyanate



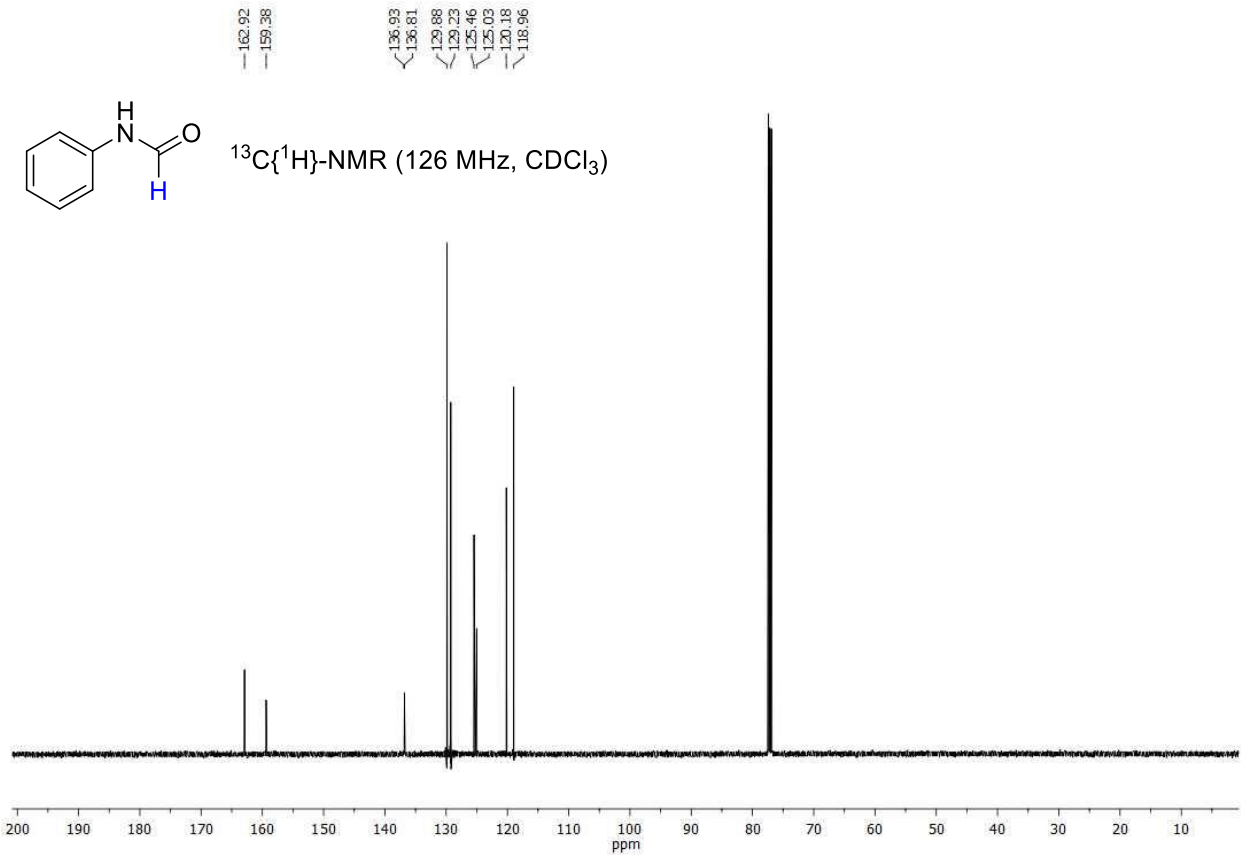
NMR spectra for borylated *N*-phenylformamide, *N*-(*p*-tolyl)formamide, *N*-(4-methoxyphenyl)formamide, *N*-(4-cyanophenyl)formamide, *N*-(4-fluorophenyl)formamide, and *N*-(4-chlorophenyl)formamide are consistent with those previously reported in the literature.[13]

5. NMR spectra for isolated formamides



^{1}H-NMR (500 MHz, $CDCl_3$)

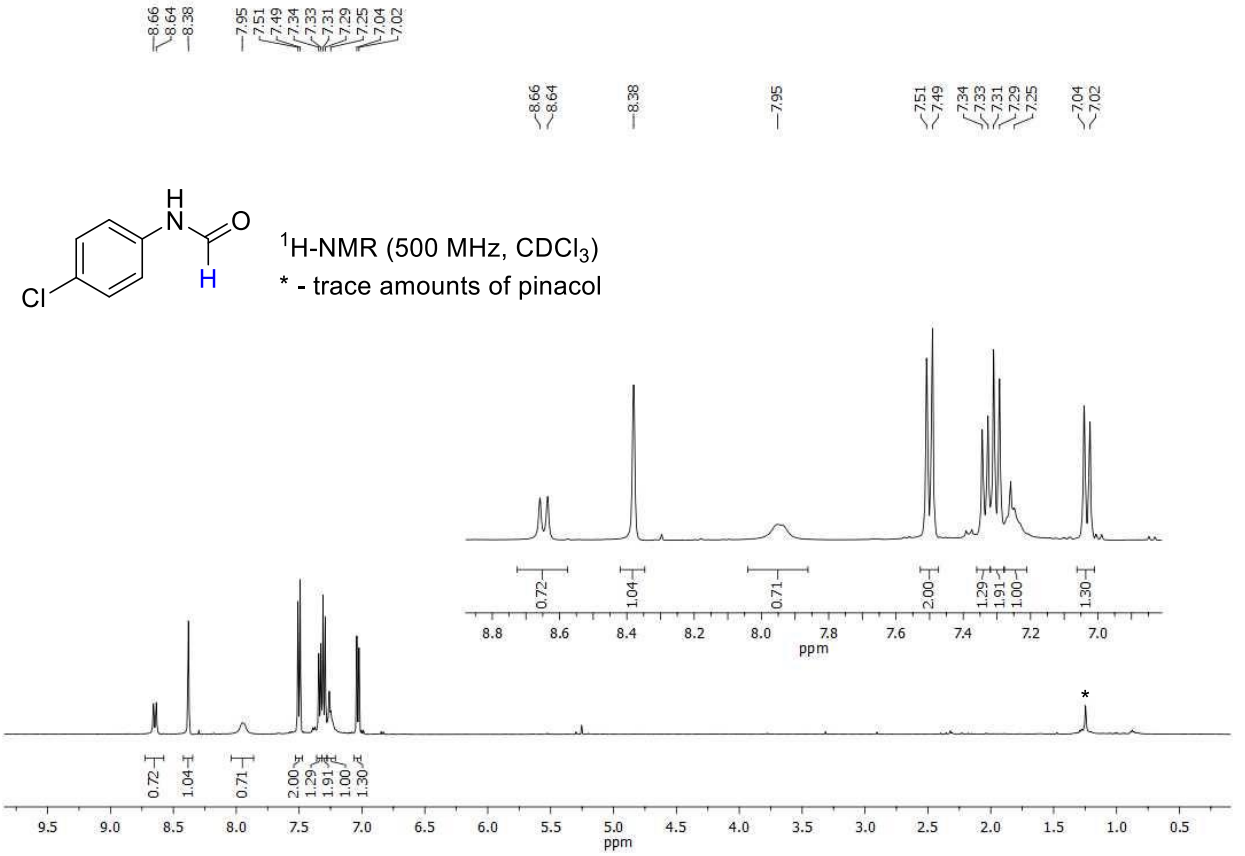
* - tace amounts of pinacol

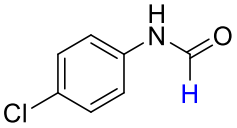


$^{13}C\{^{1}H\}$-NMR (126 MHz, $CDCl_3$)

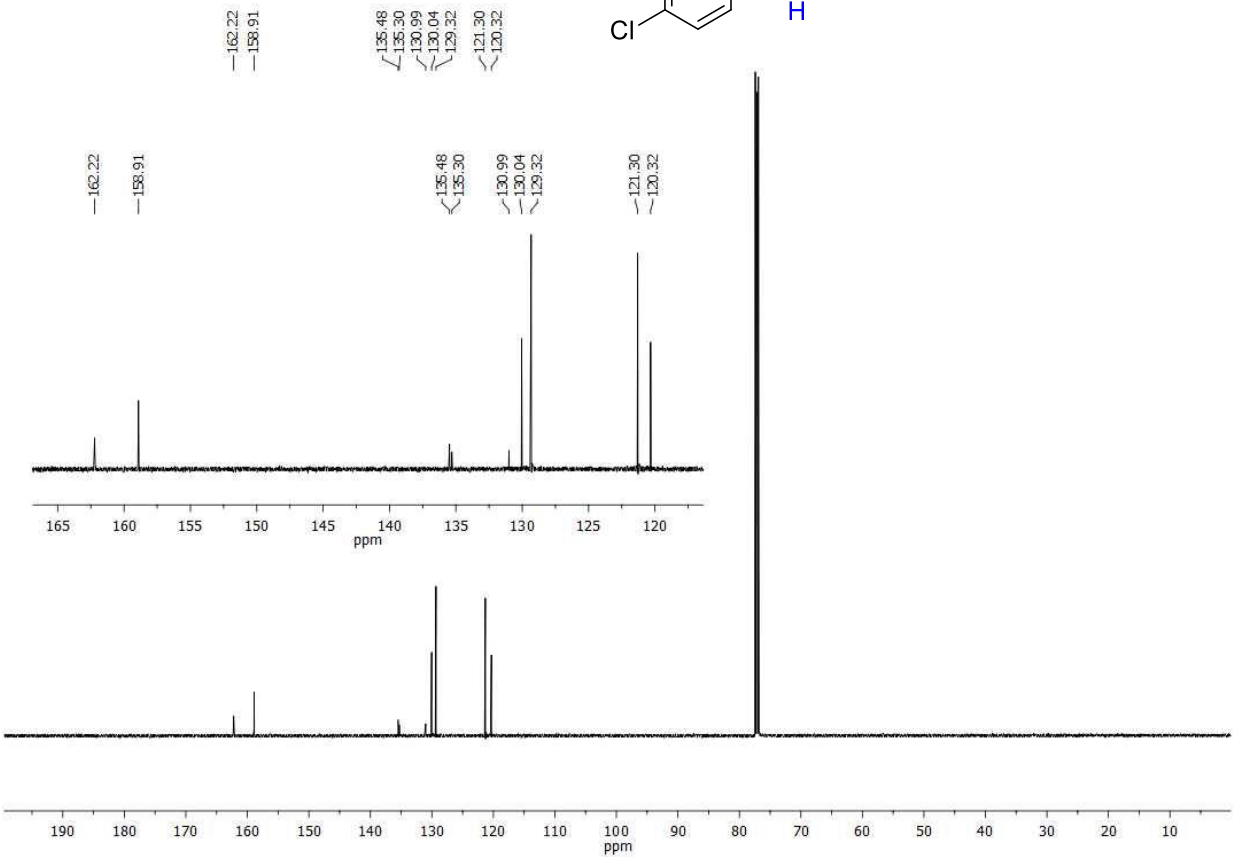
^{1}H-NMR (500 MHz, $CDCl_3$)

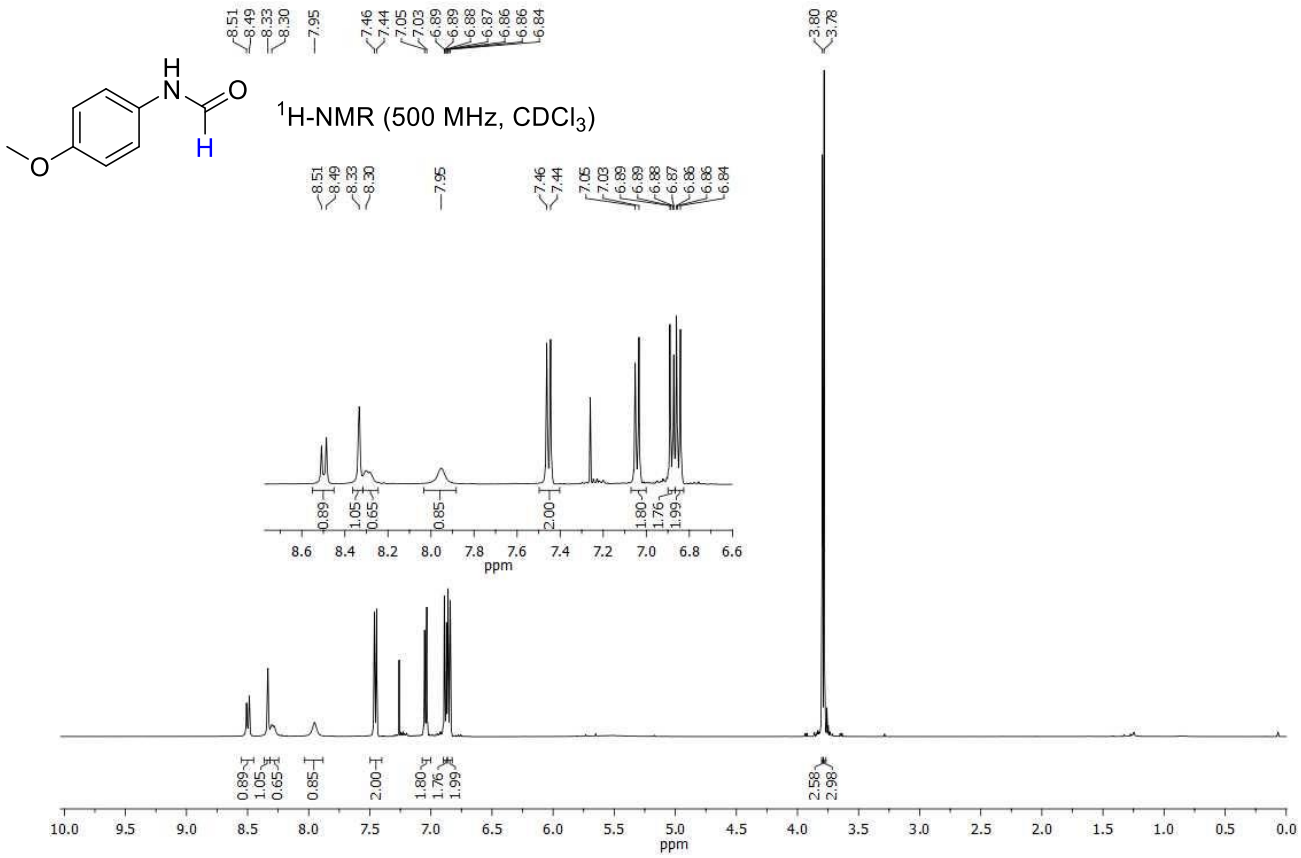
* - trace amounts of pinacol

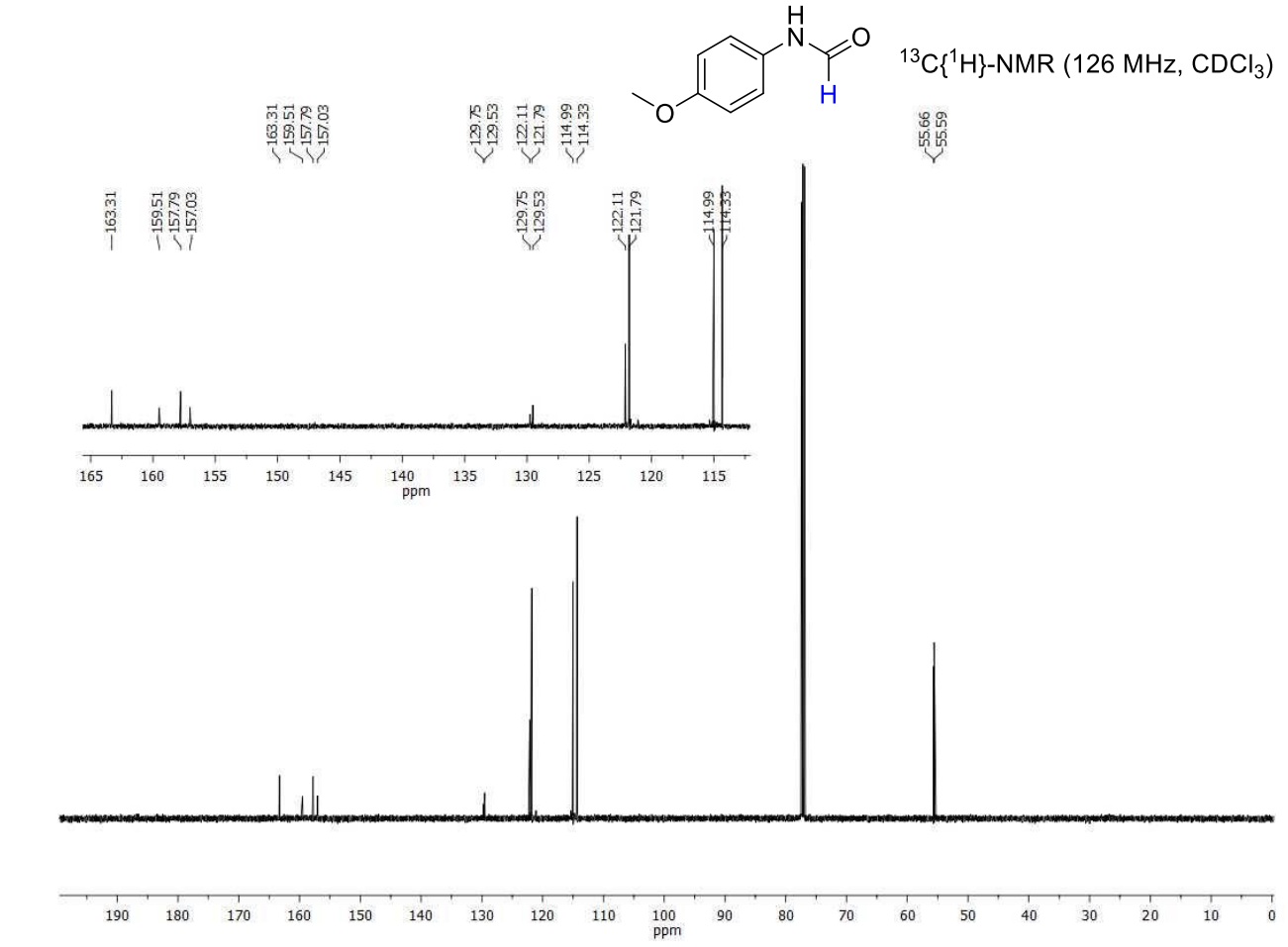


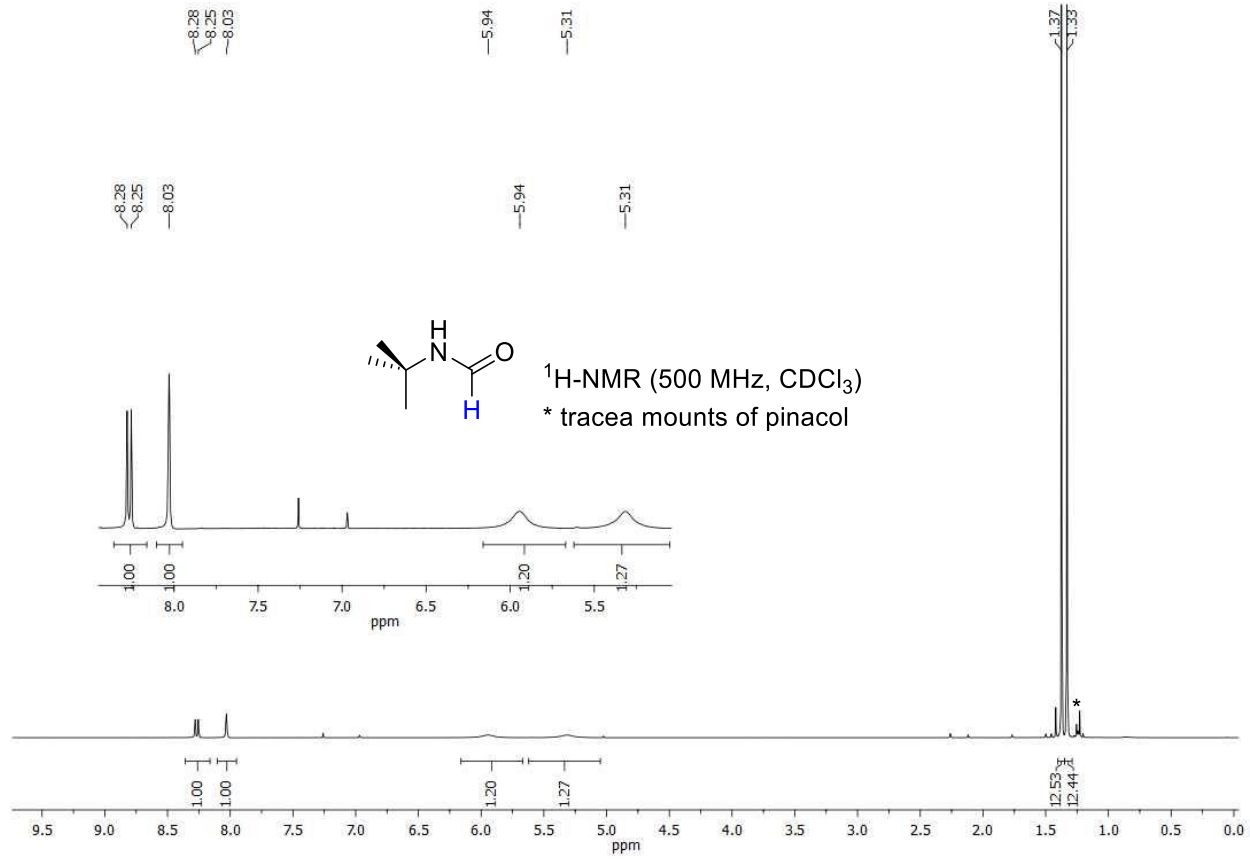


^{13}C{^{1}H}-NMR (126 MHz, $CDCl_3$)

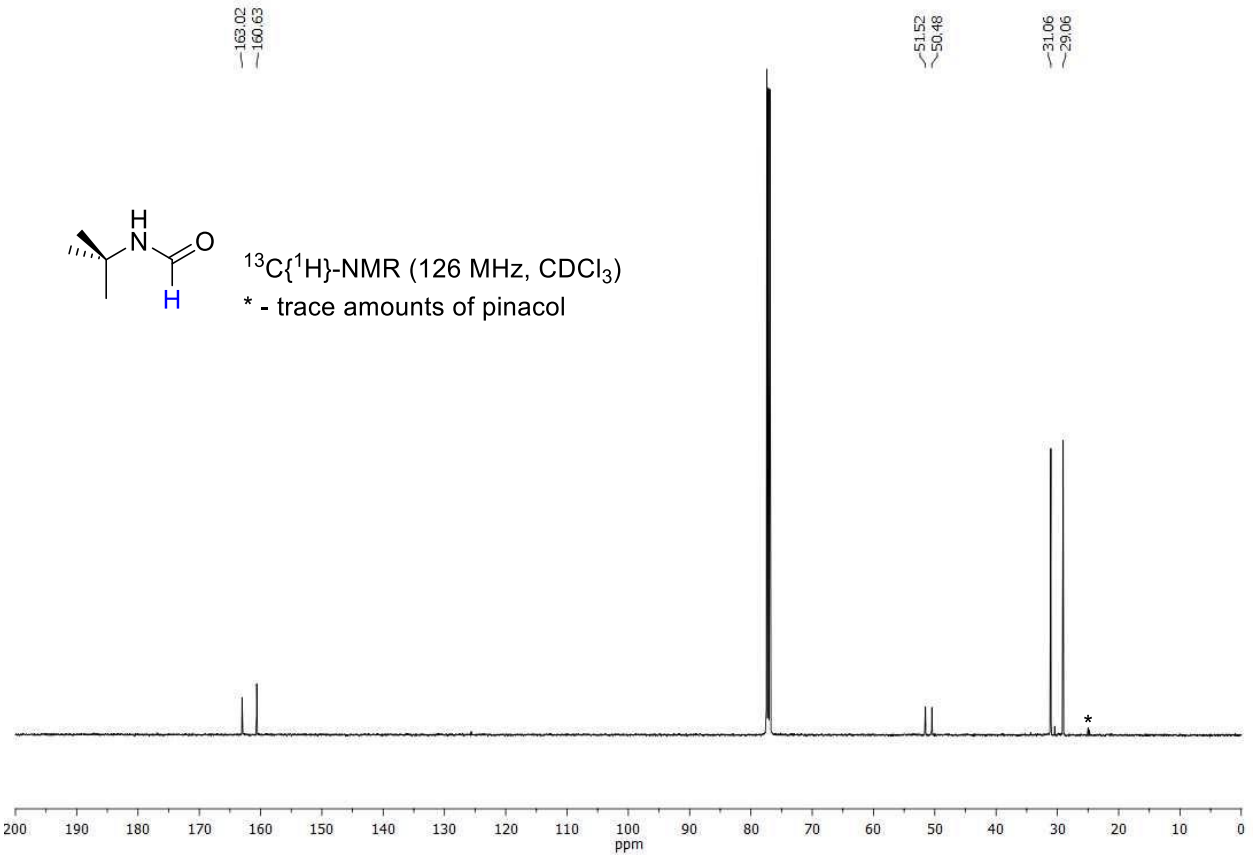



^{1}H-NMR (500 MHz, $CDCl_3$)
ppm


$^{13}C\{^1H\}$-NMR (126 MHz, $CDCl_3$)
ppm



^{1}H-NMR (500 MHz, $CDCl_3$)
* tracea mounts of pinacol

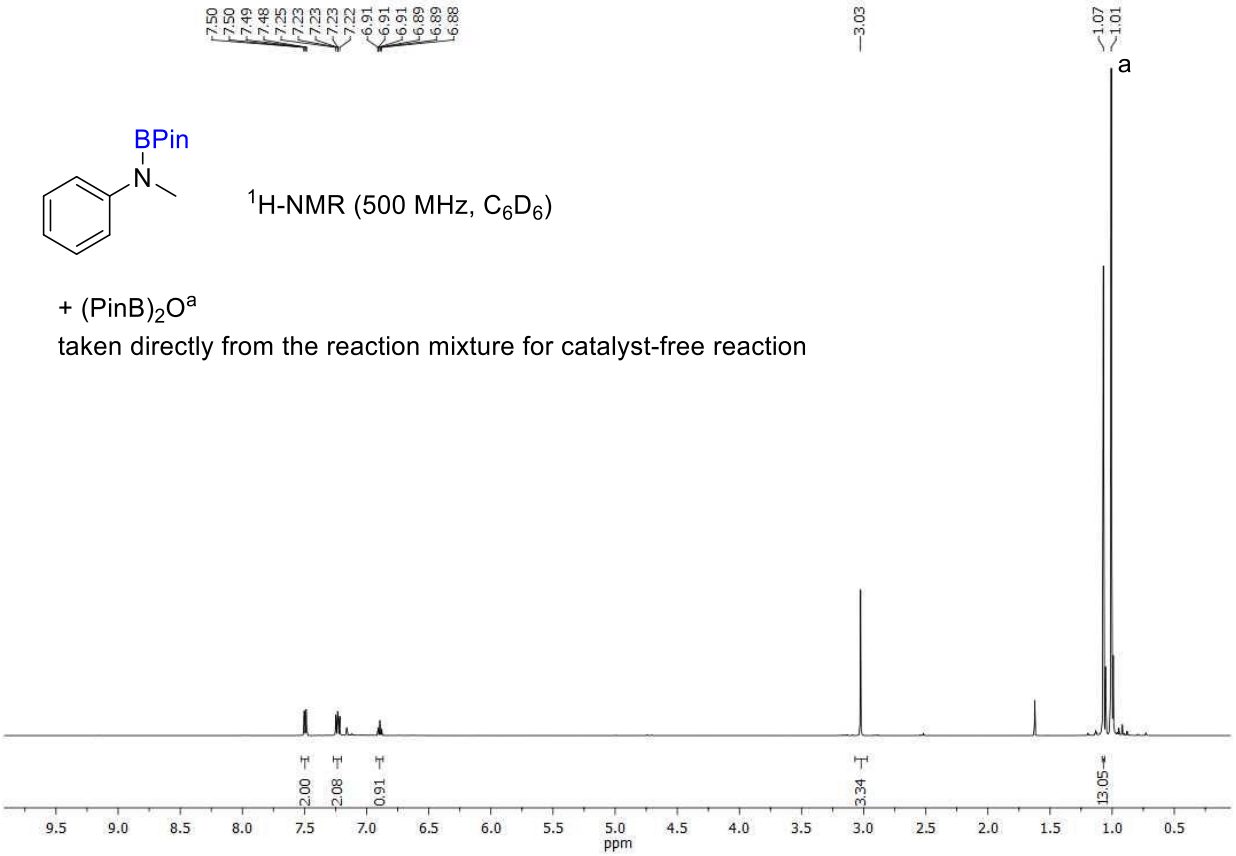


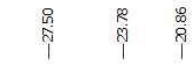
$^{13}C\{^{1}H\}$-NMR (126 MHz, $CDCl_3$)
* - trace amounts of pinacol

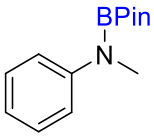
6. NMR spectra for borylated N-methylamines (taken directly from reaction mixtures)

^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a]
taken directly from the reaction mixture for catalyst-free reaction

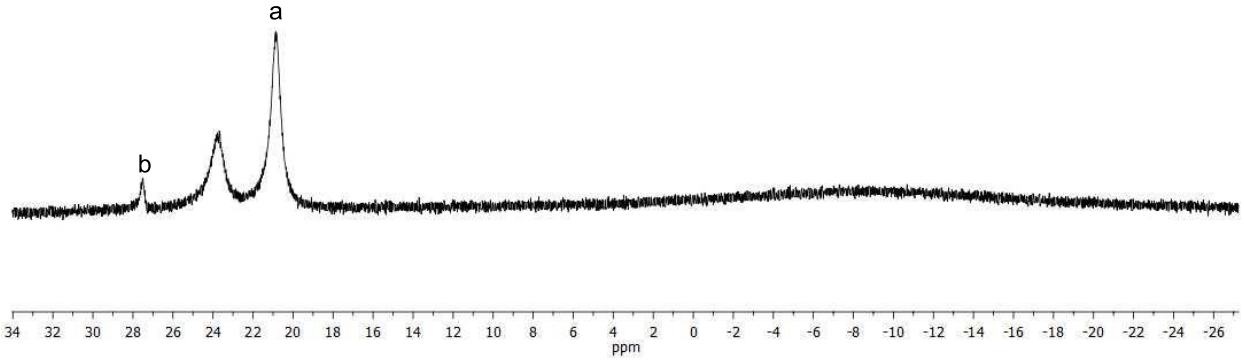






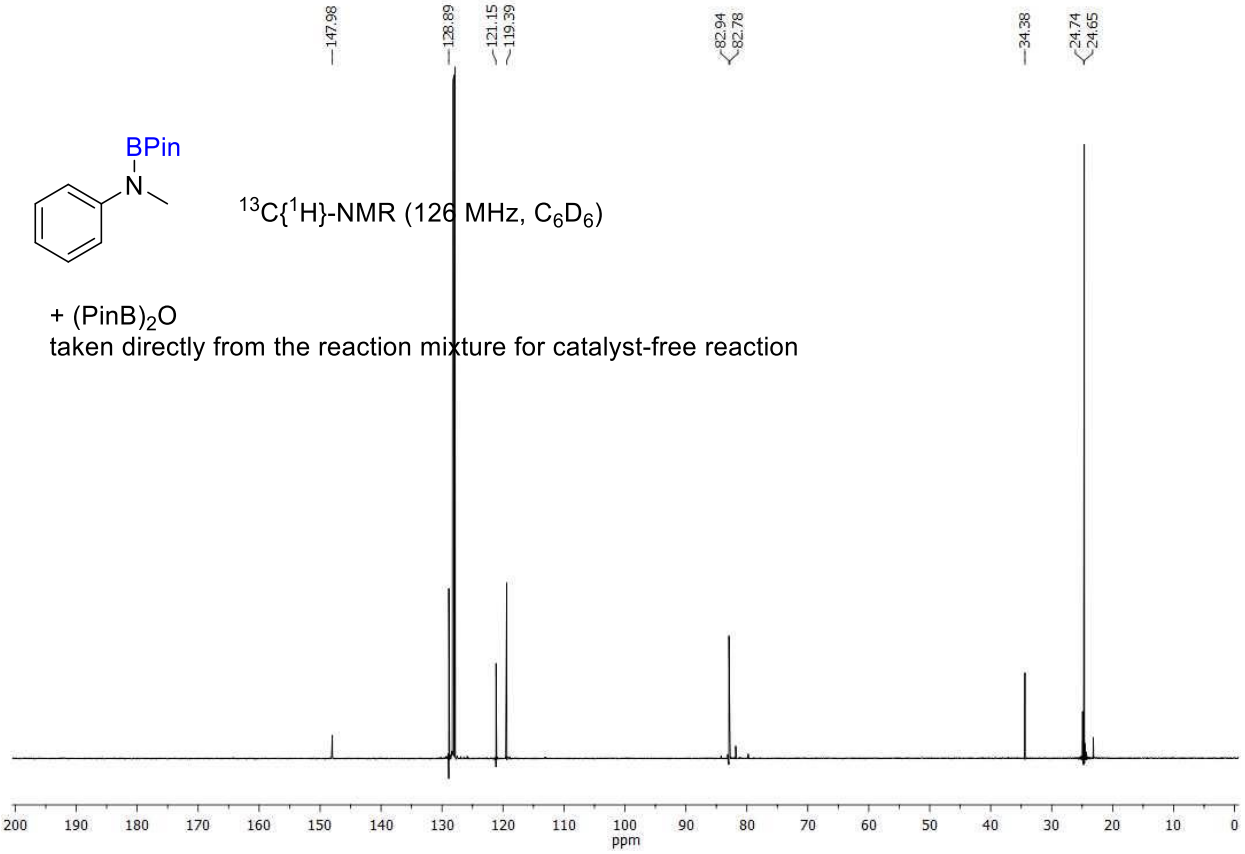
^{11}B-NMR (160 MHz, C_6D_6)

+ $(PinB)_2O$[a]
taken directly from the reaction mixture for catalyst-free reaction
[b] - excess HBPin



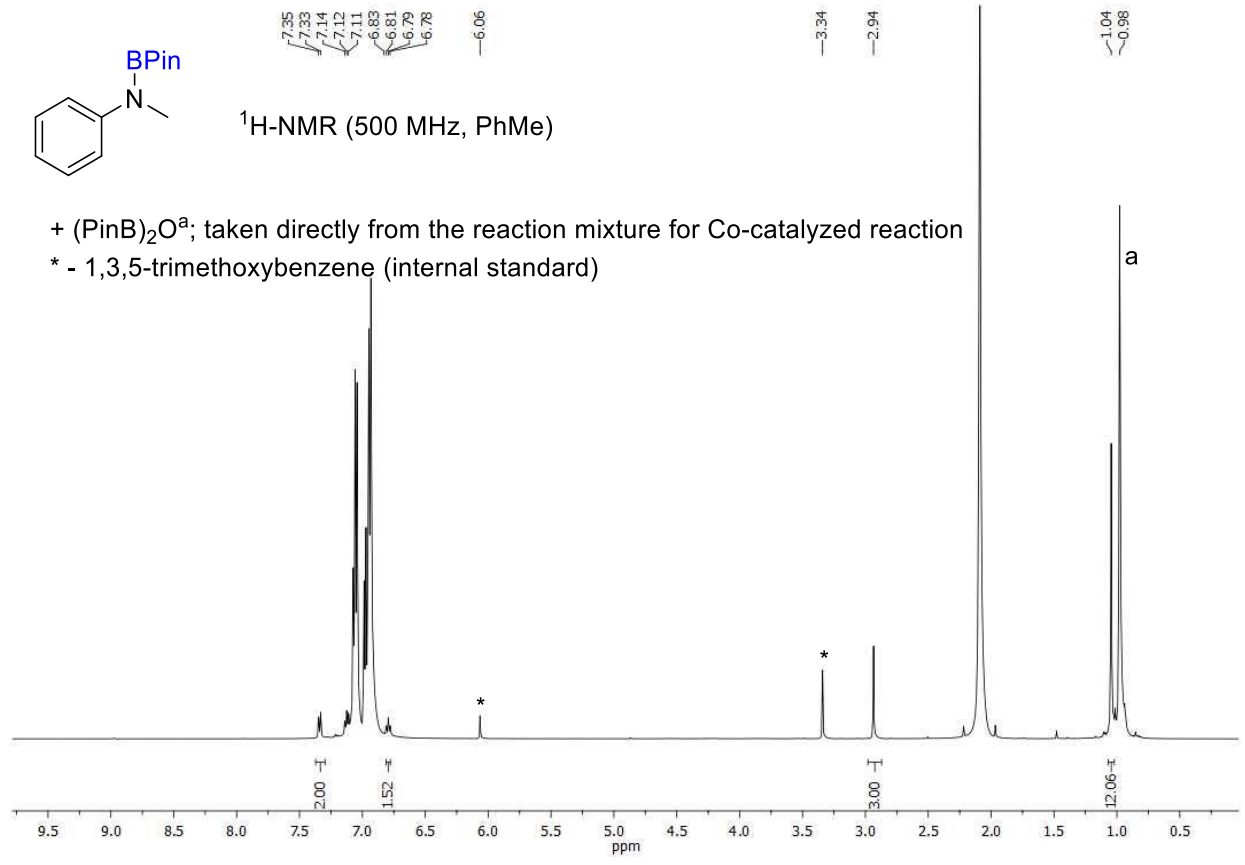
$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

+ $(PinB)_2O$
taken directly from the reaction mixture for catalyst-free reaction



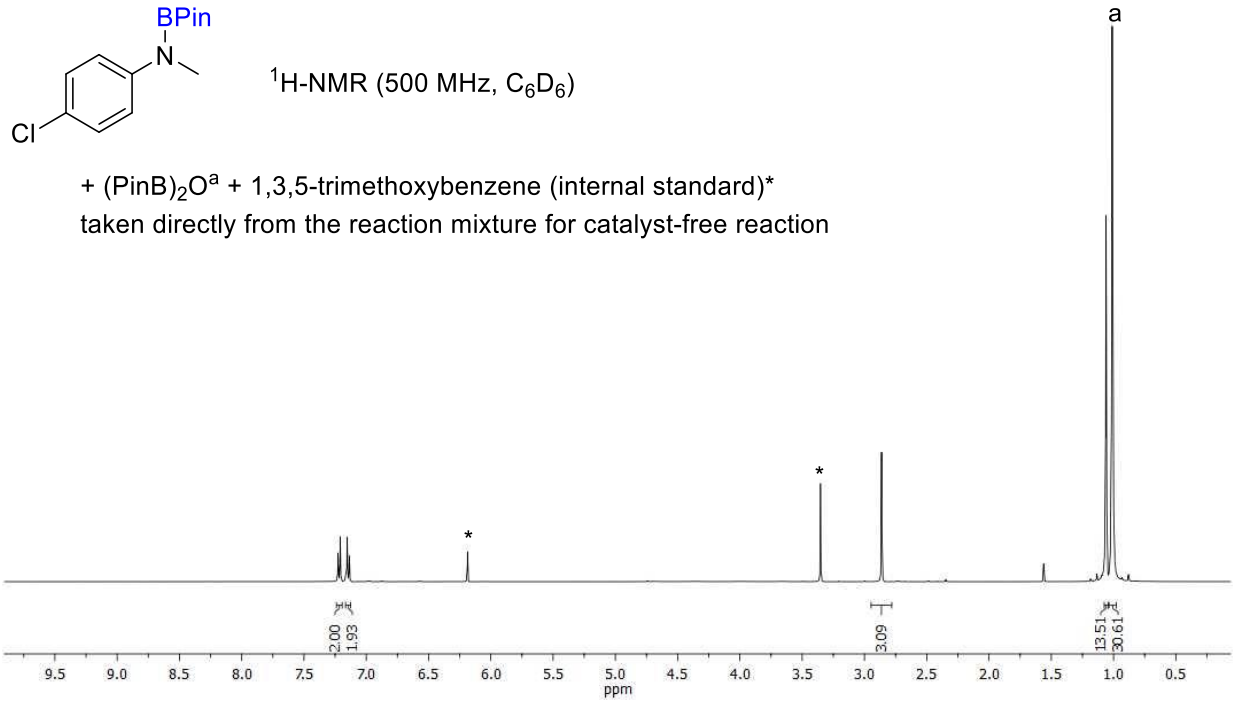
^{1}H-NMR (500 MHz, PhMe)

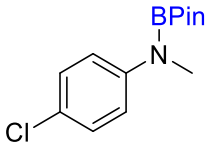
+ $(PinB)_2O^a$; taken directly from the reaction mixture for Co-catalyzed reaction
* - 1,3,5-trimethoxybenzene (internal standard)



^{1}H-NMR (500 MHz, C_6D_6)

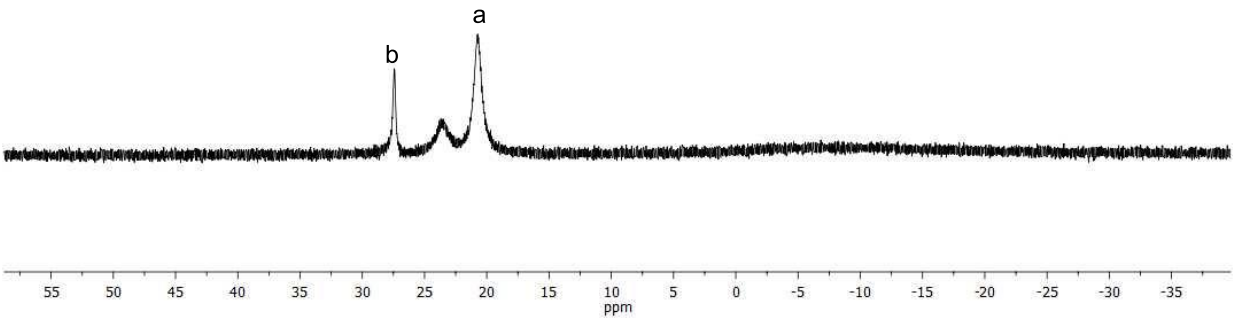
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction

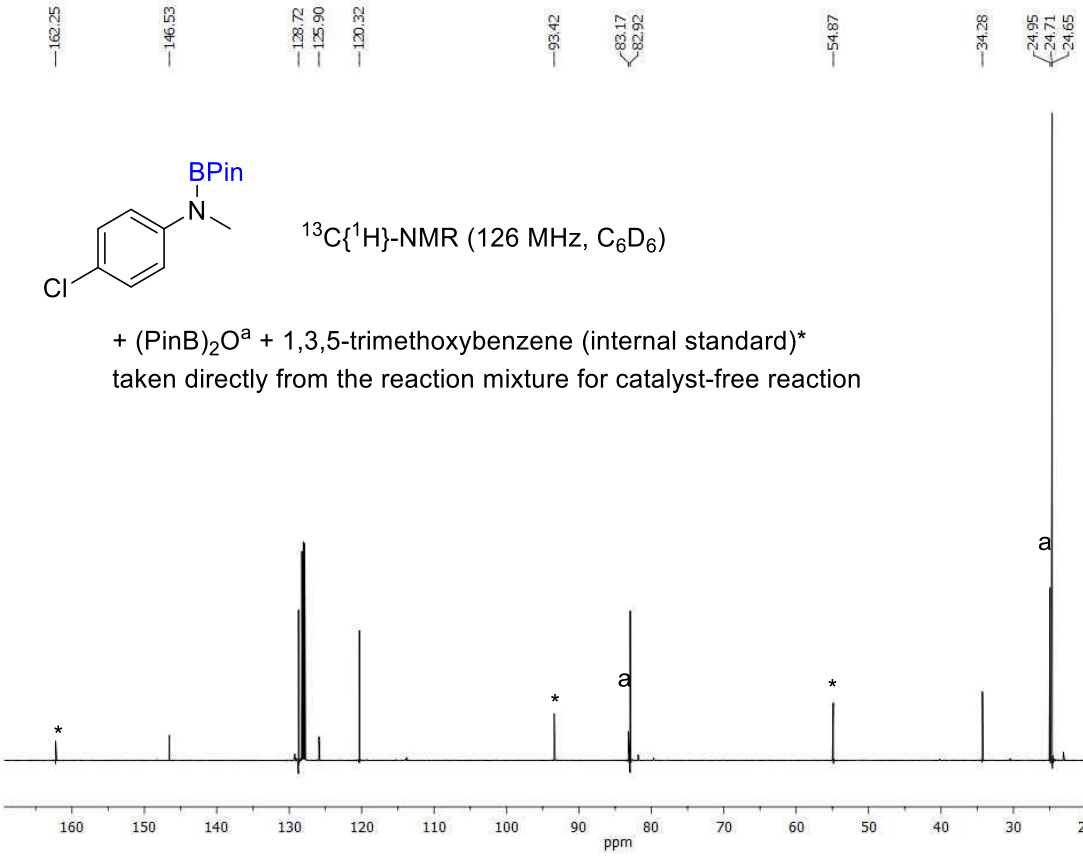




^{11}B-NMR (160 MHz, C_6D_6)

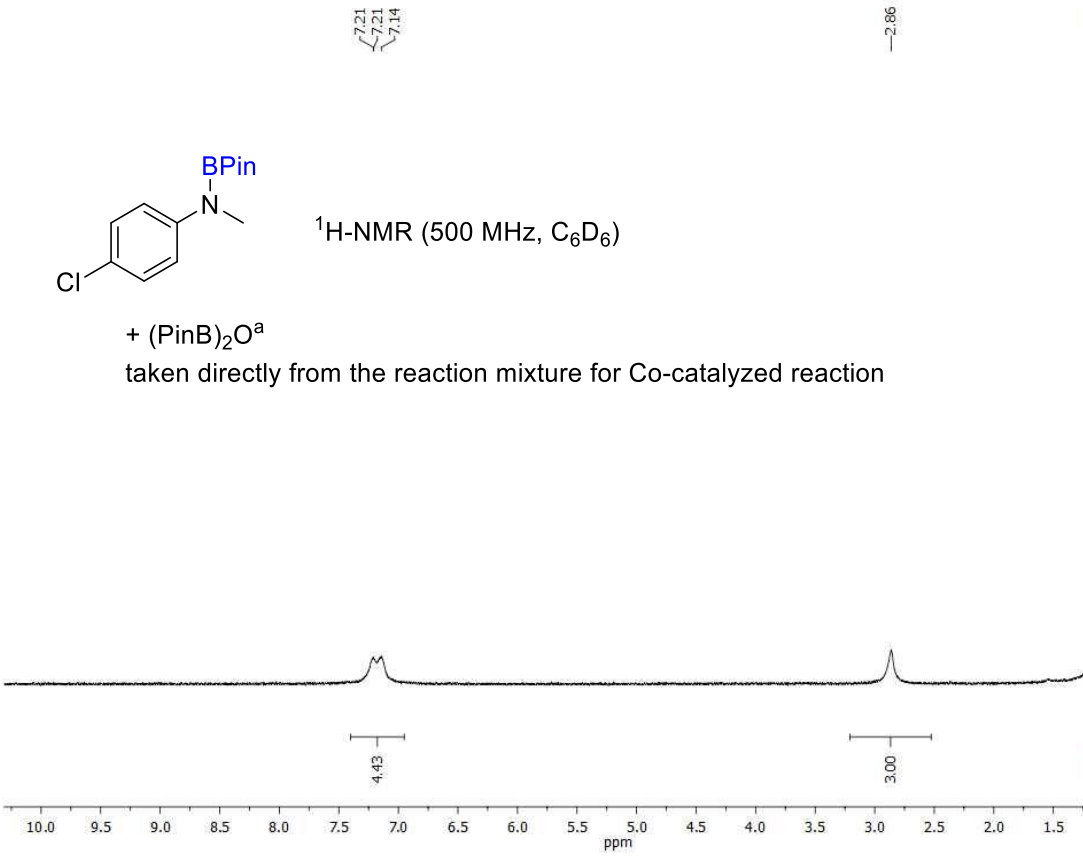
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction
[b] - excess HBPin





$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

+ $(PinB)_2O^a$ + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction

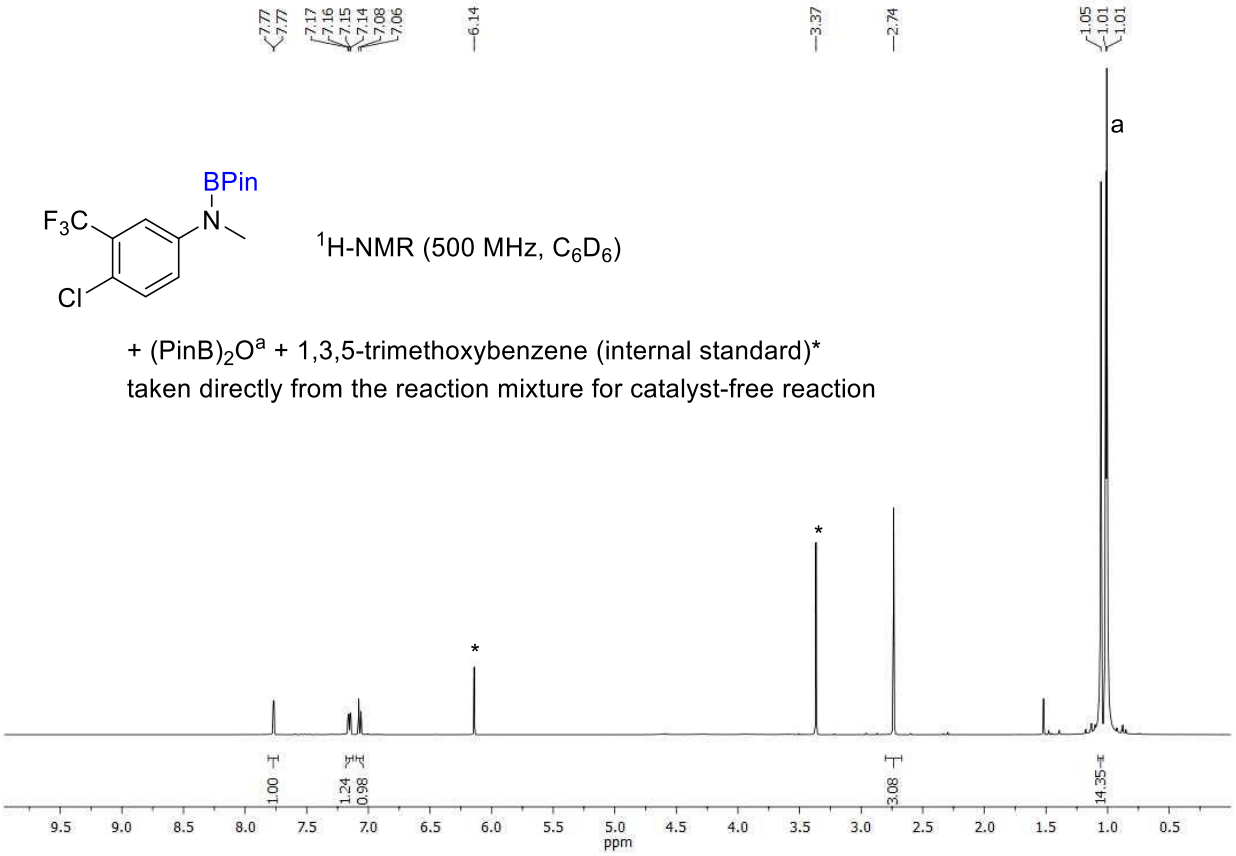


^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O^a$
taken directly from the reaction mixture for Co-catalyzed reaction

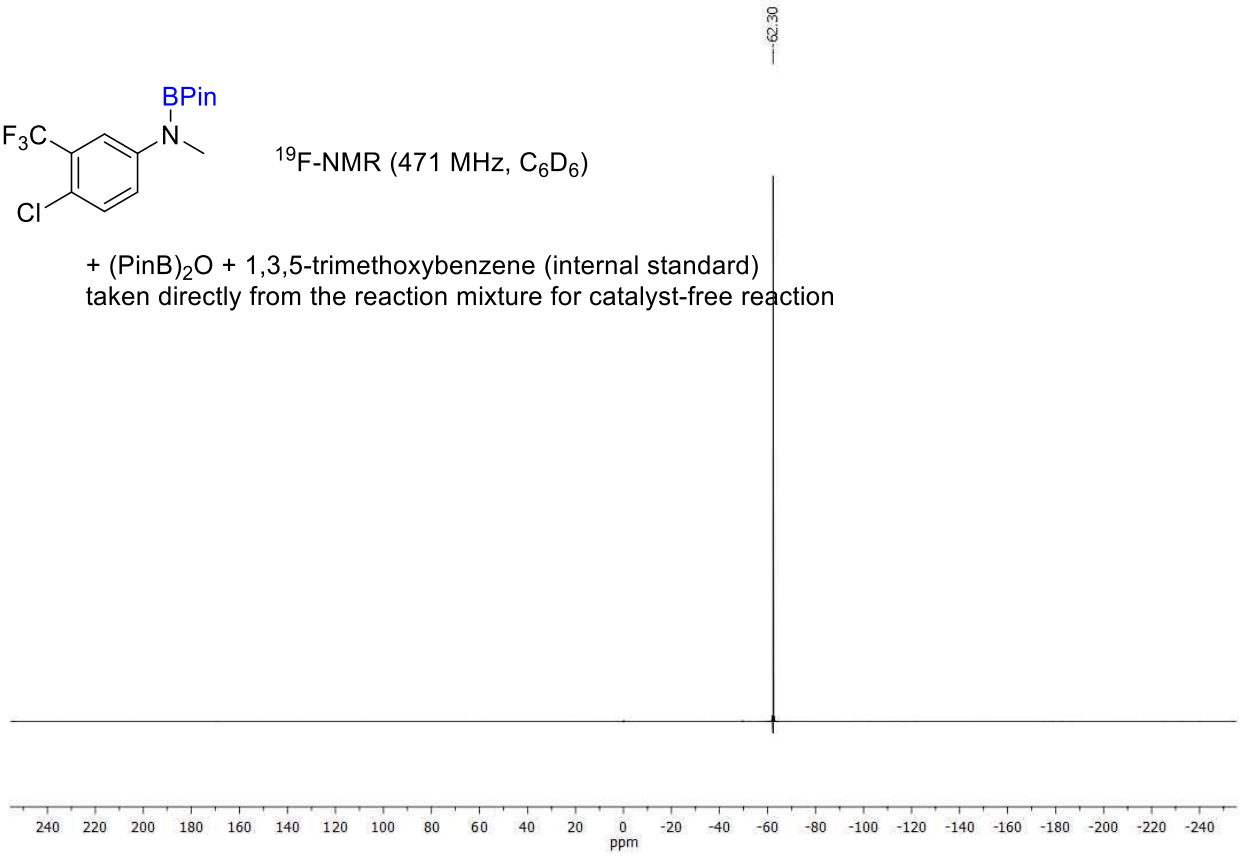
^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction



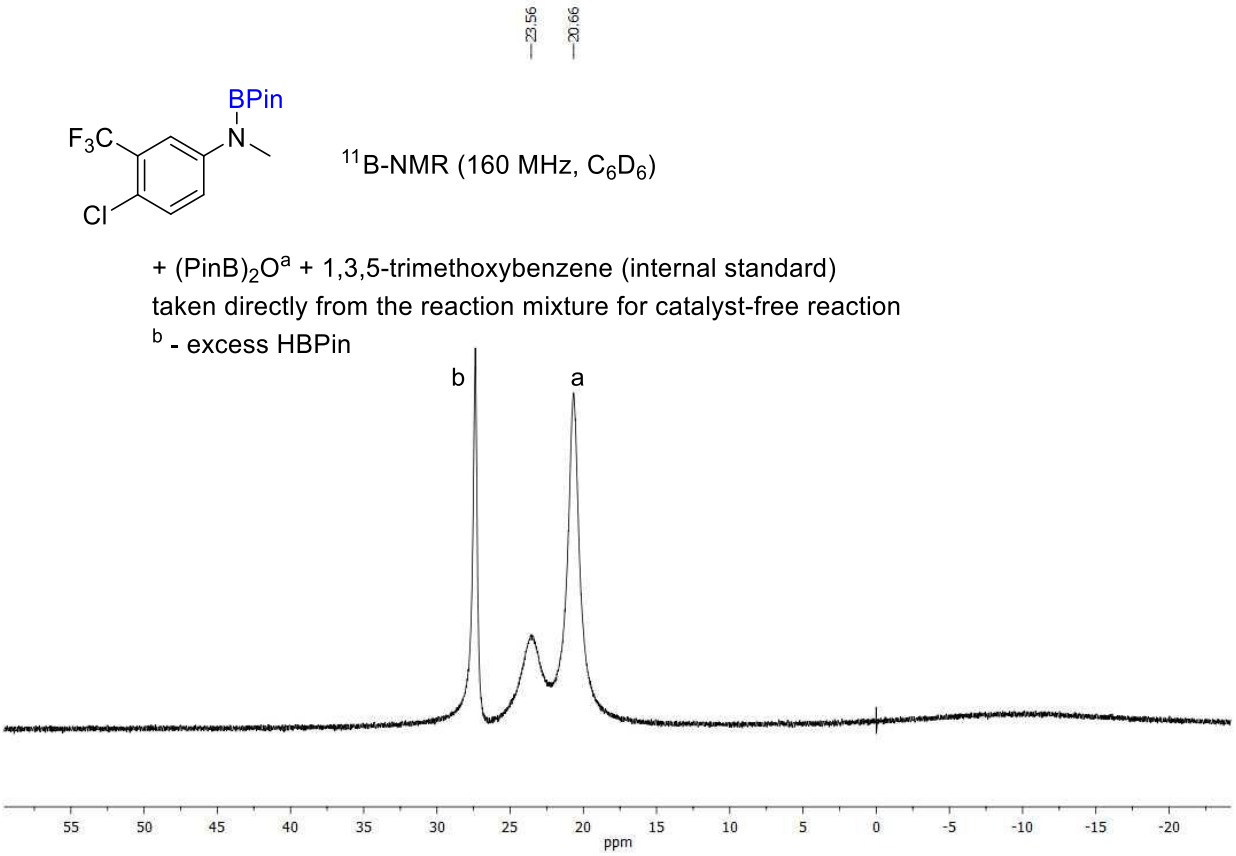
^{19}F-NMR (471 MHz, C_6D_6)

+ $(PinB)_2O$ + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction



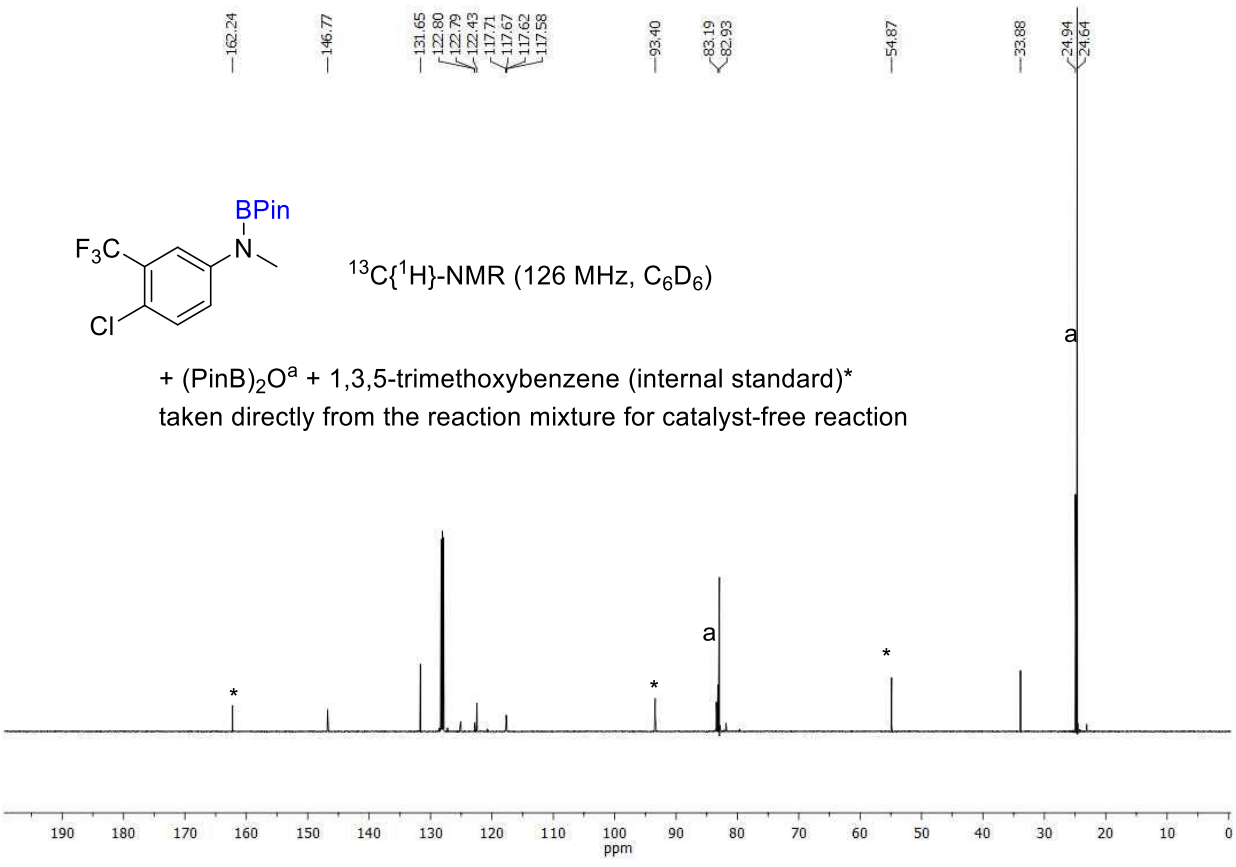
^{11}B-NMR (160 MHz, C_6D_6)

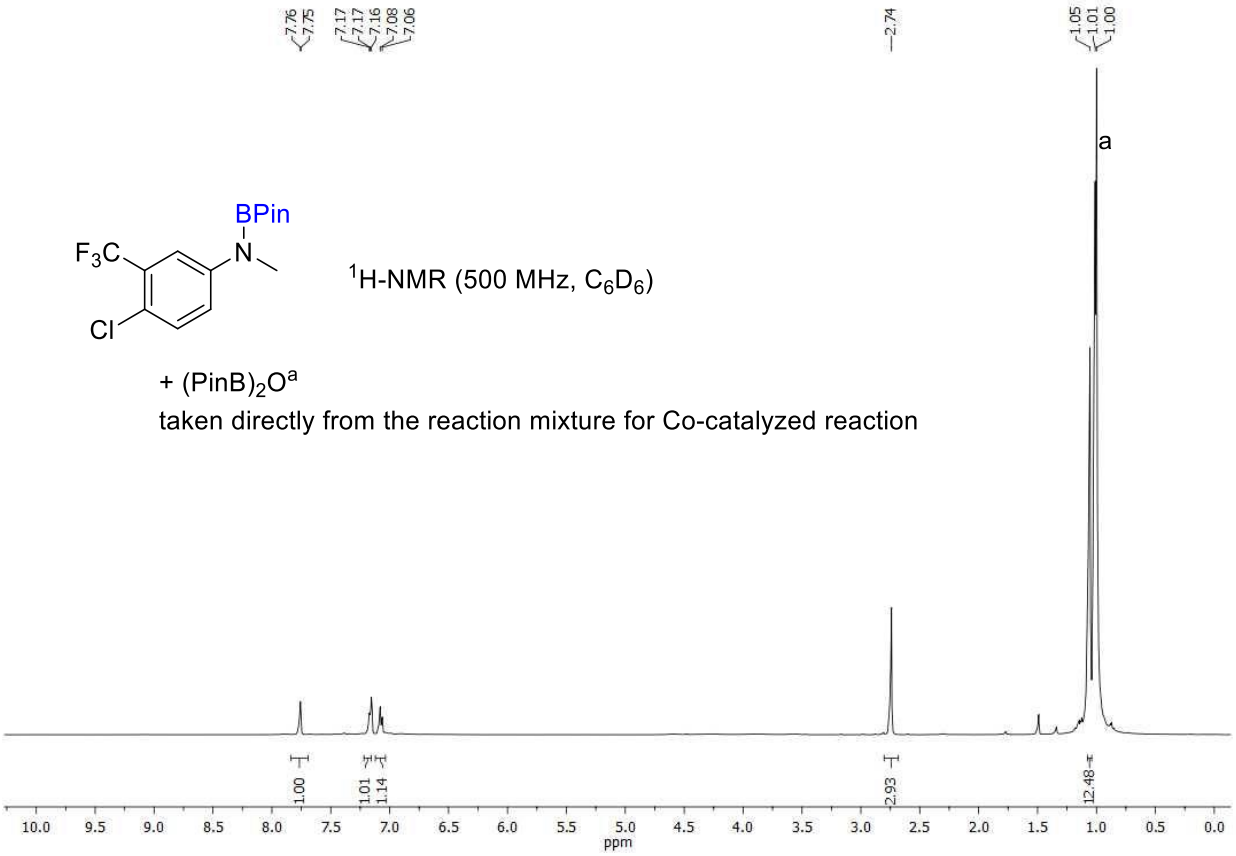
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction
[b] - excess HBPin



$^{13}C\{^1H\}$-NMR (126 MHz, C_6D_6)

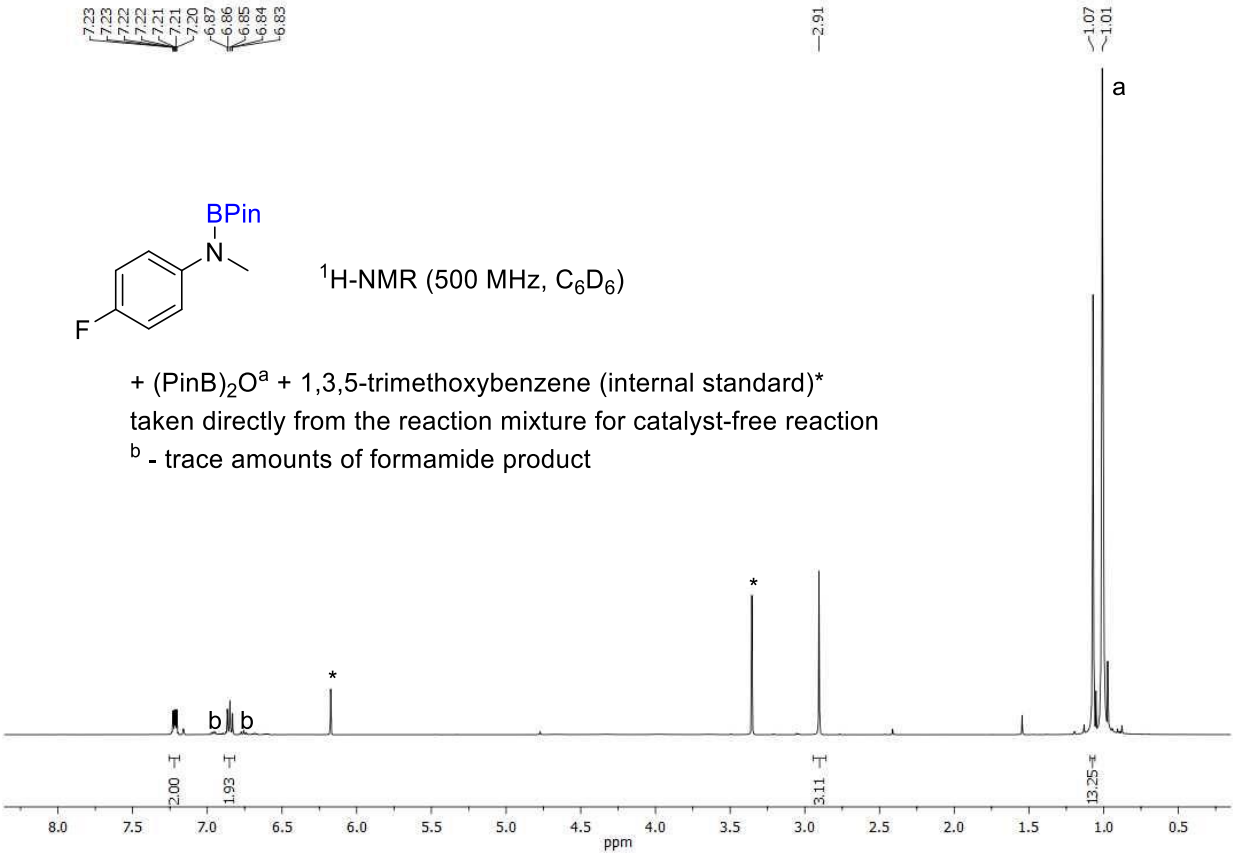
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction





^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a]
taken directly from the reaction mixture for Co-catalyzed reaction

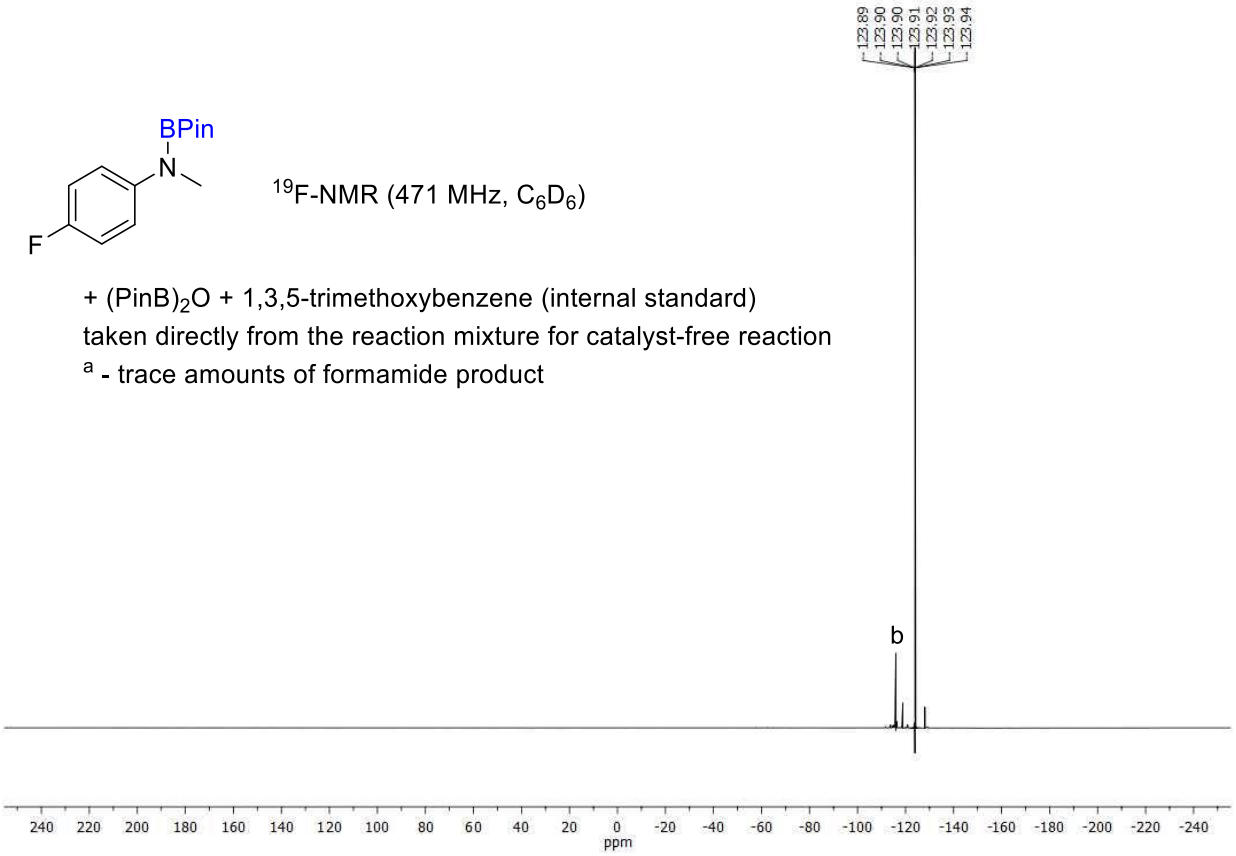


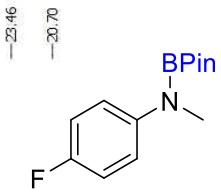
^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction
[b] - trace amounts of formamide product

^{19}F-NMR (471 MHz, C_6D_6)

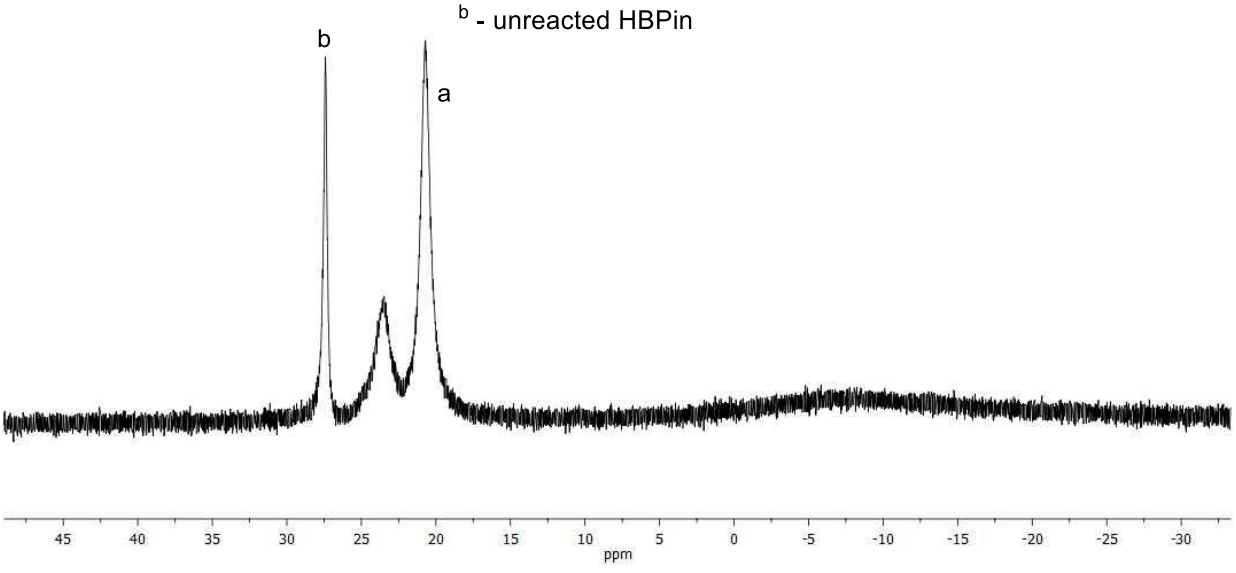
+ $(PinB)_2O$ + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction
[a] - trace amounts of formamide product

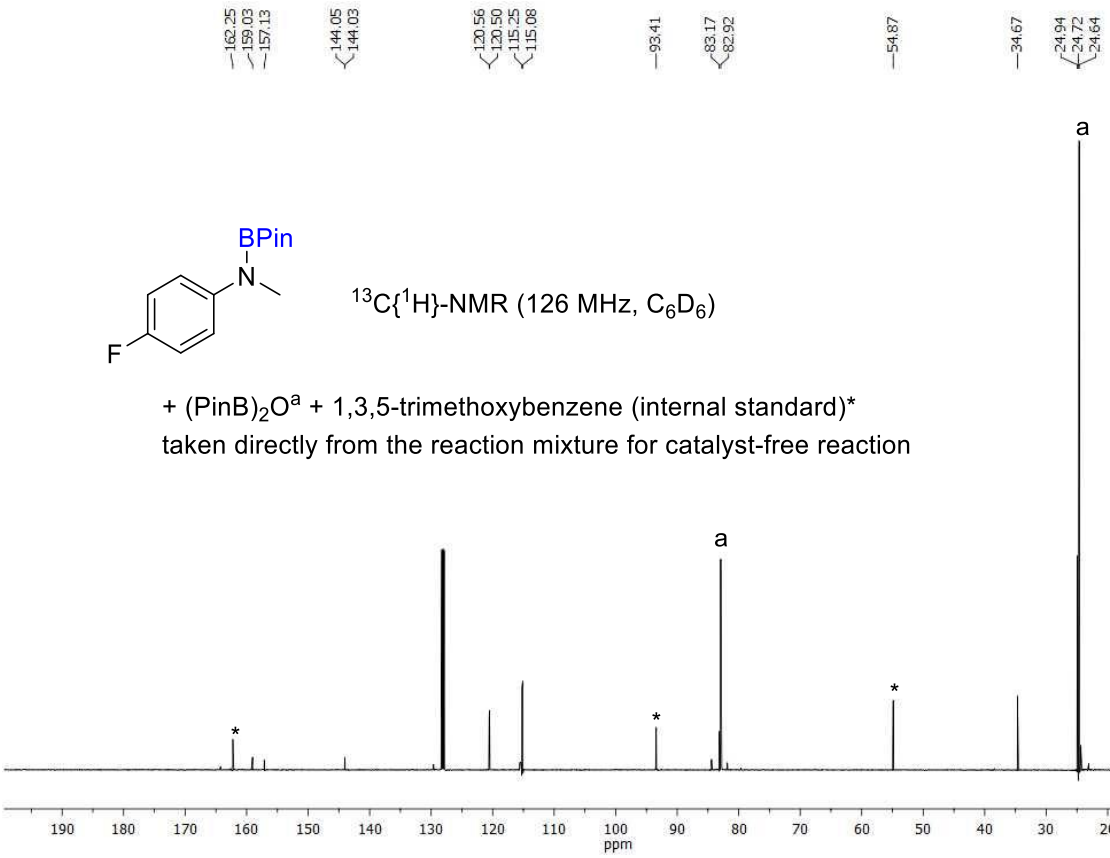




^{11}B-NMR (160 MHz, C_6D_6)

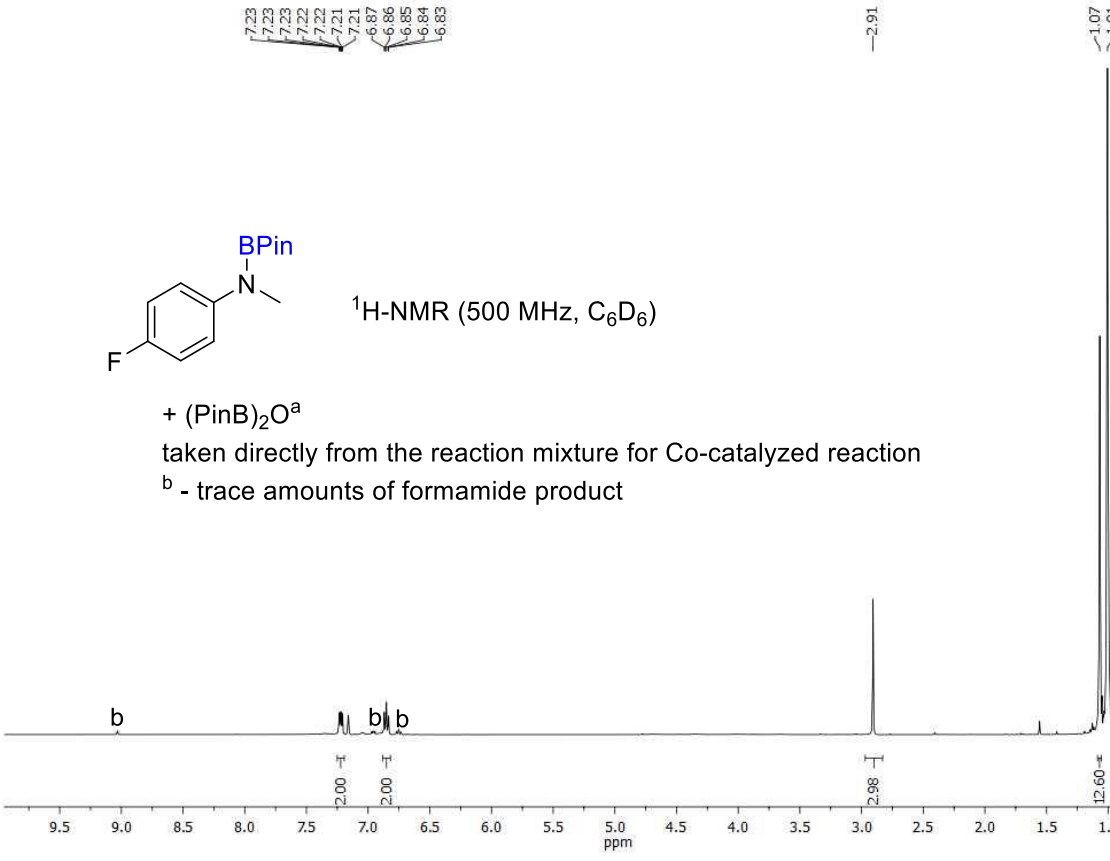
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction
[b] - unreacted HBPin





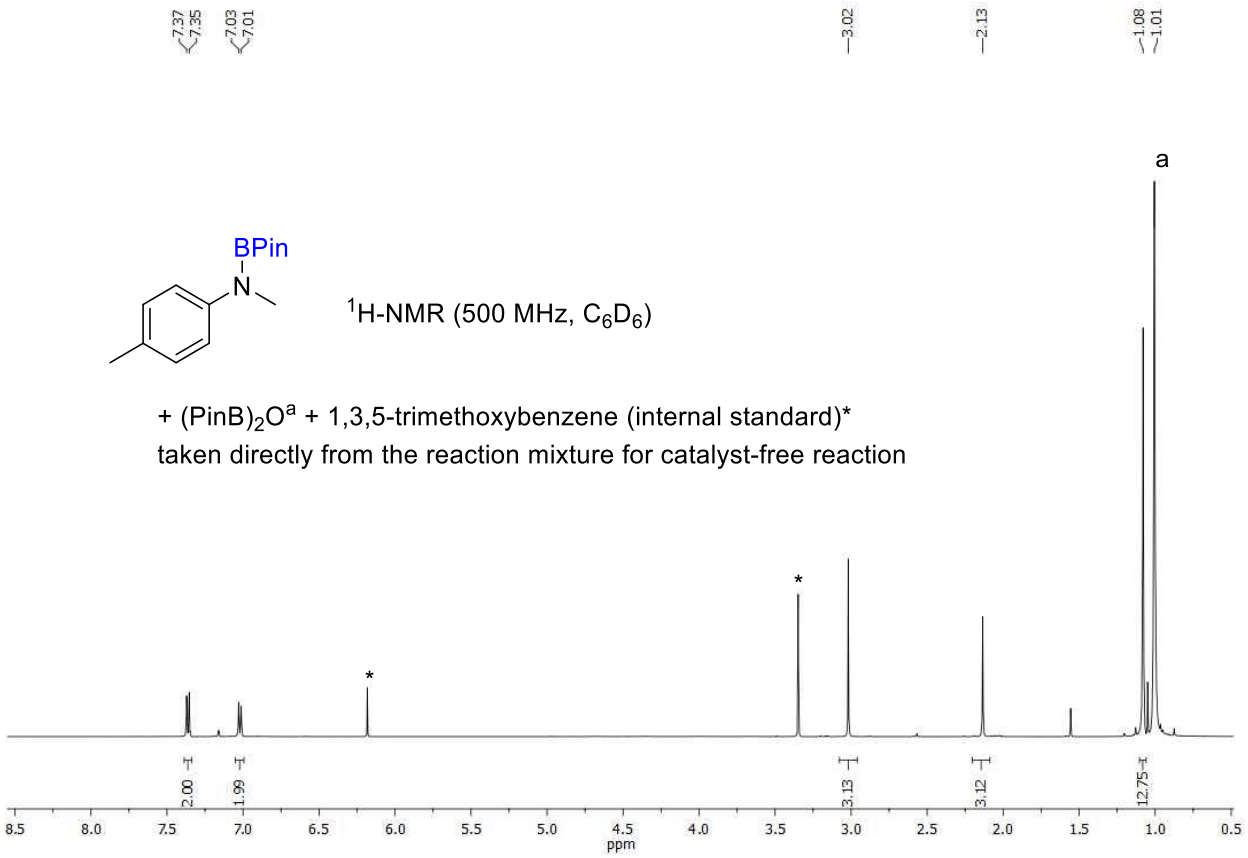
$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction



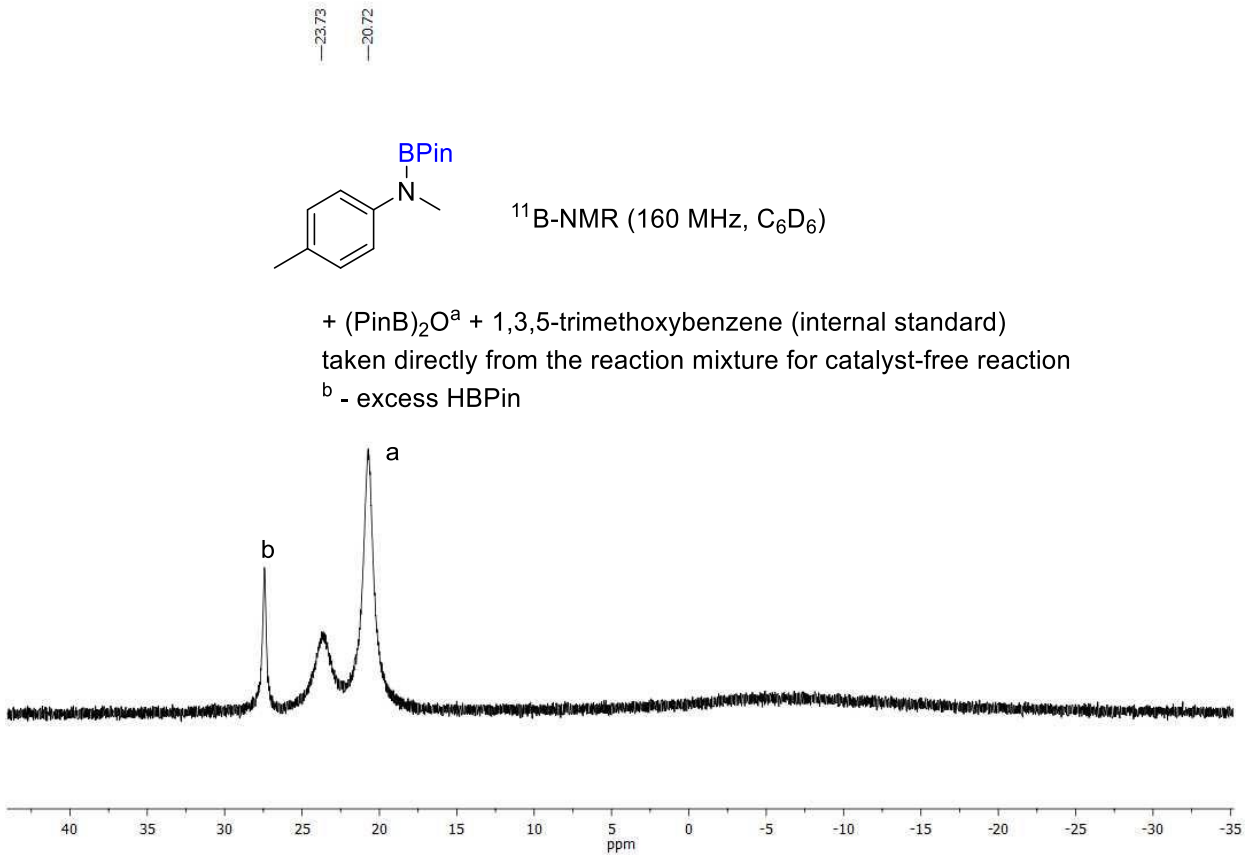
^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a]
taken directly from the reaction mixture for Co-catalyzed reaction
[b] - trace amounts of formamide product



^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O^a$ + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction

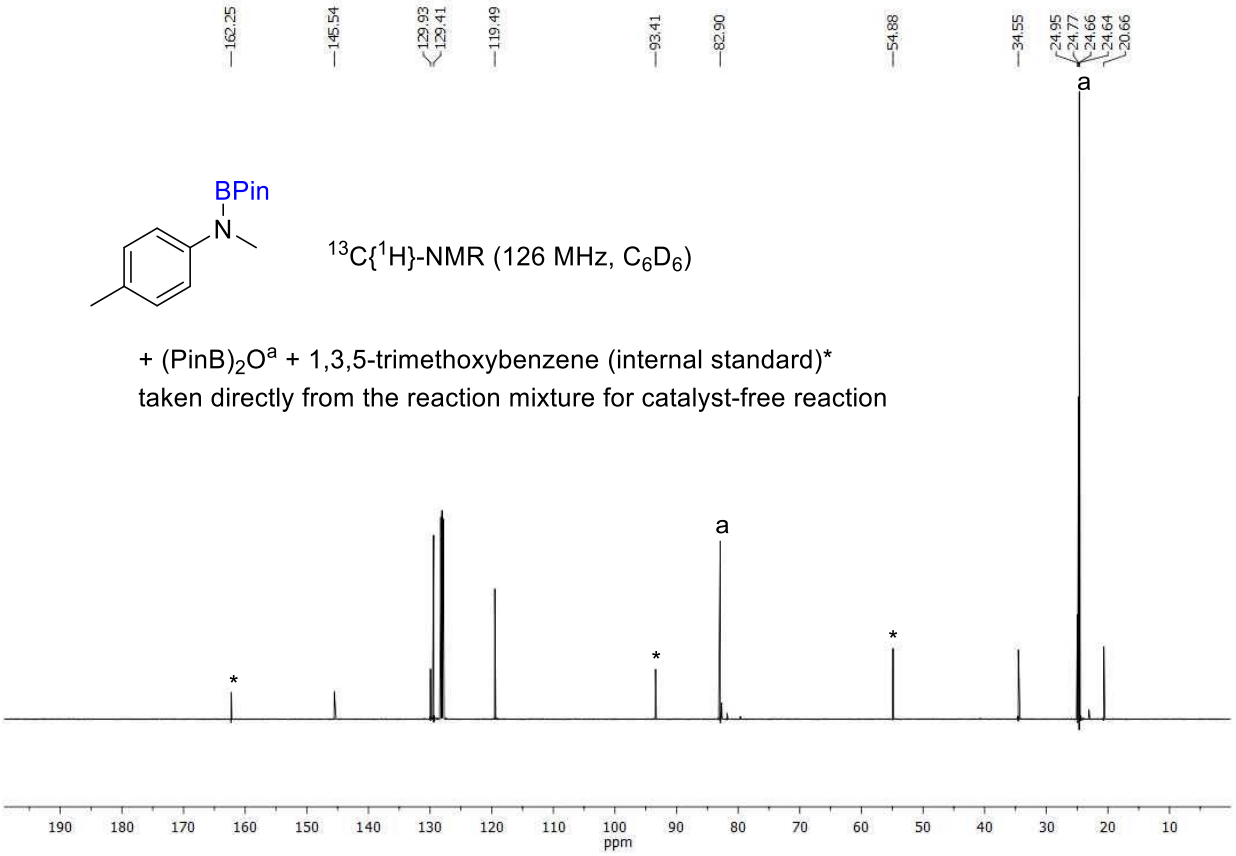


^{11}B-NMR (160 MHz, C_6D_6)

+ $(PinB)_2O^a$ + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction
[b] - excess HBPin

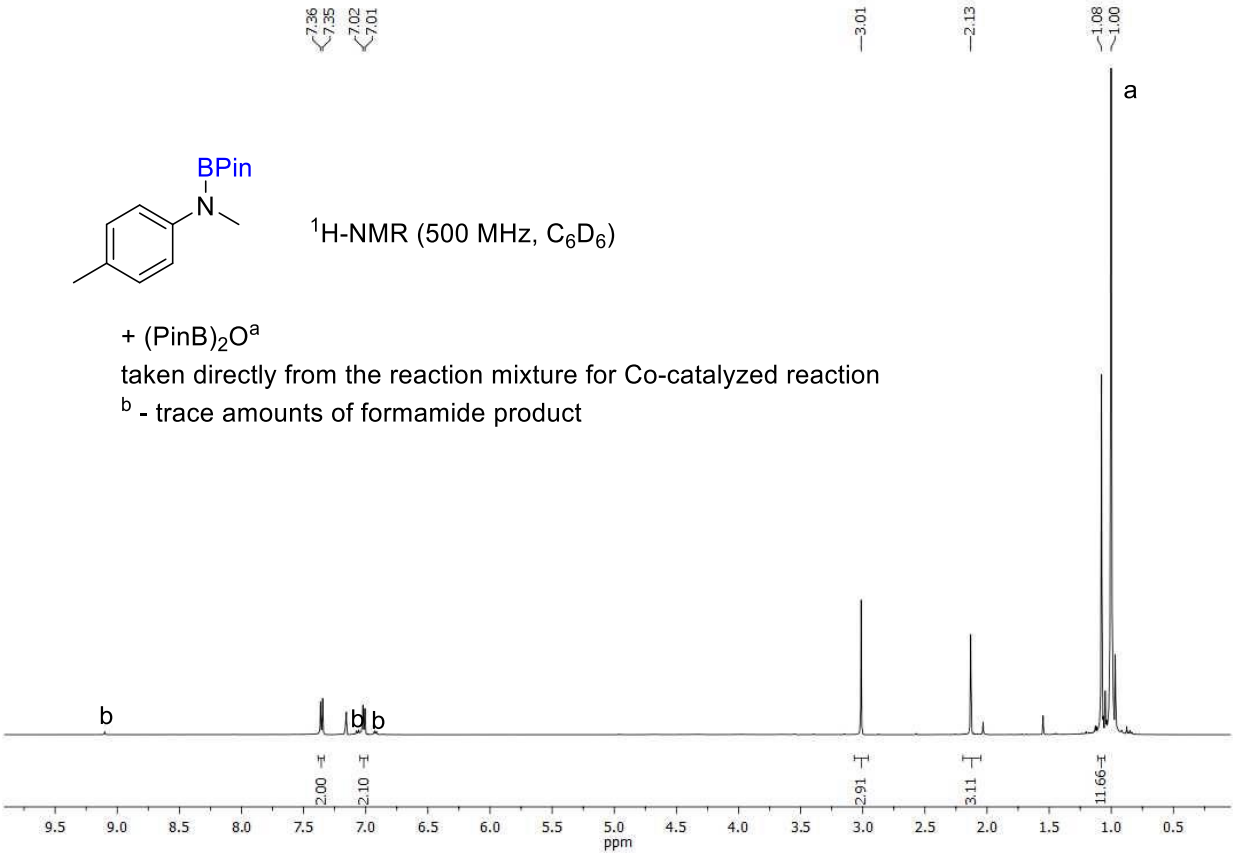
$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

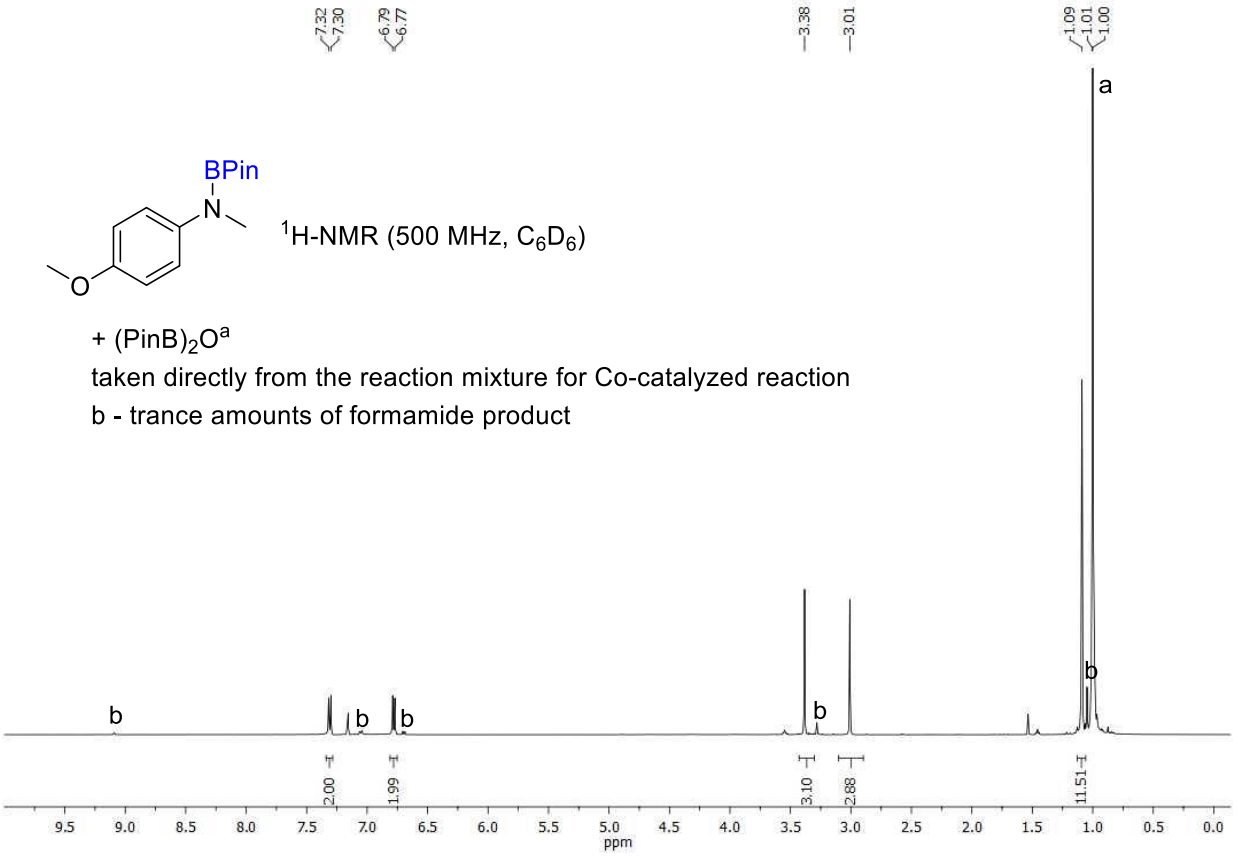
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction



^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a]
taken directly from the reaction mixture for Co-catalyzed reaction
[b] - trace amounts of formamide product



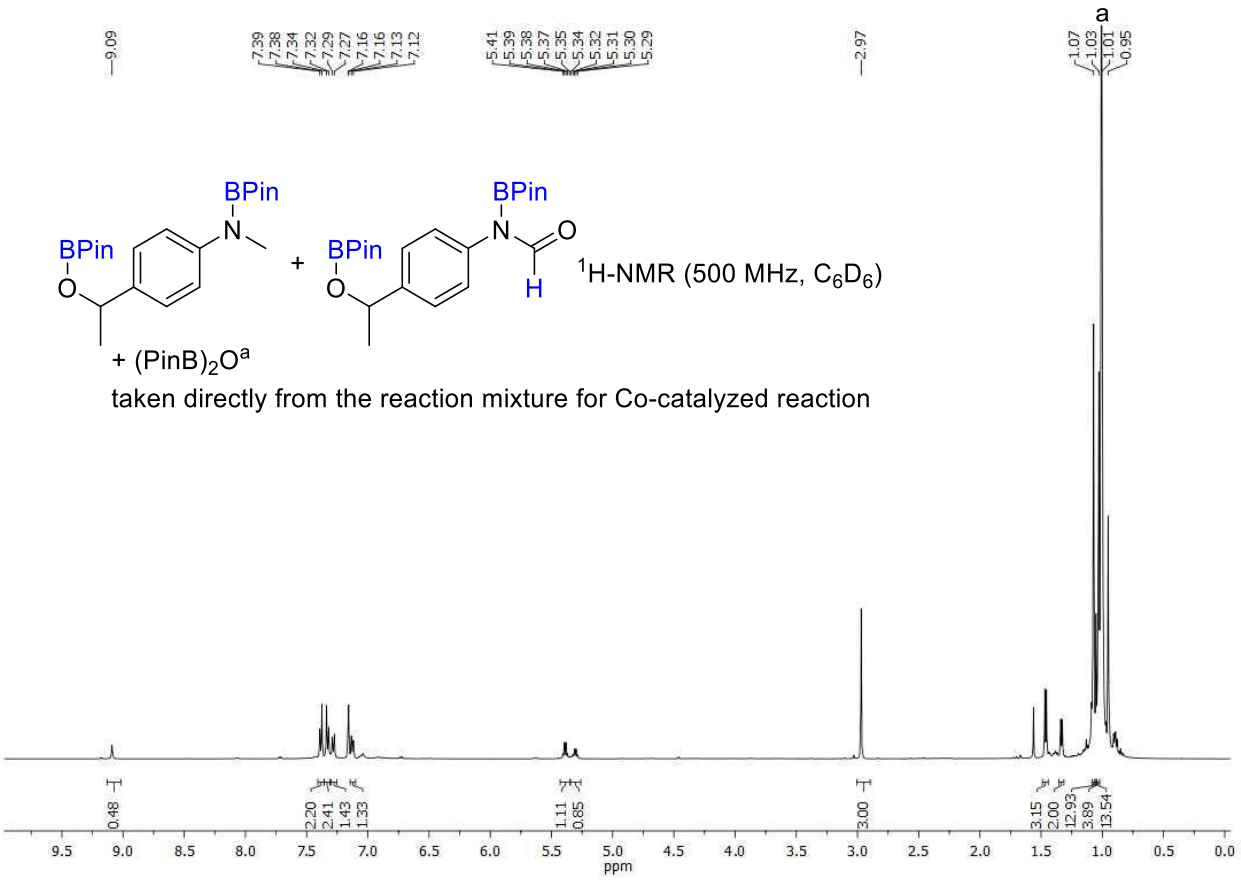


^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O^a$

taken directly from the reaction mixture for Co-catalyzed reaction

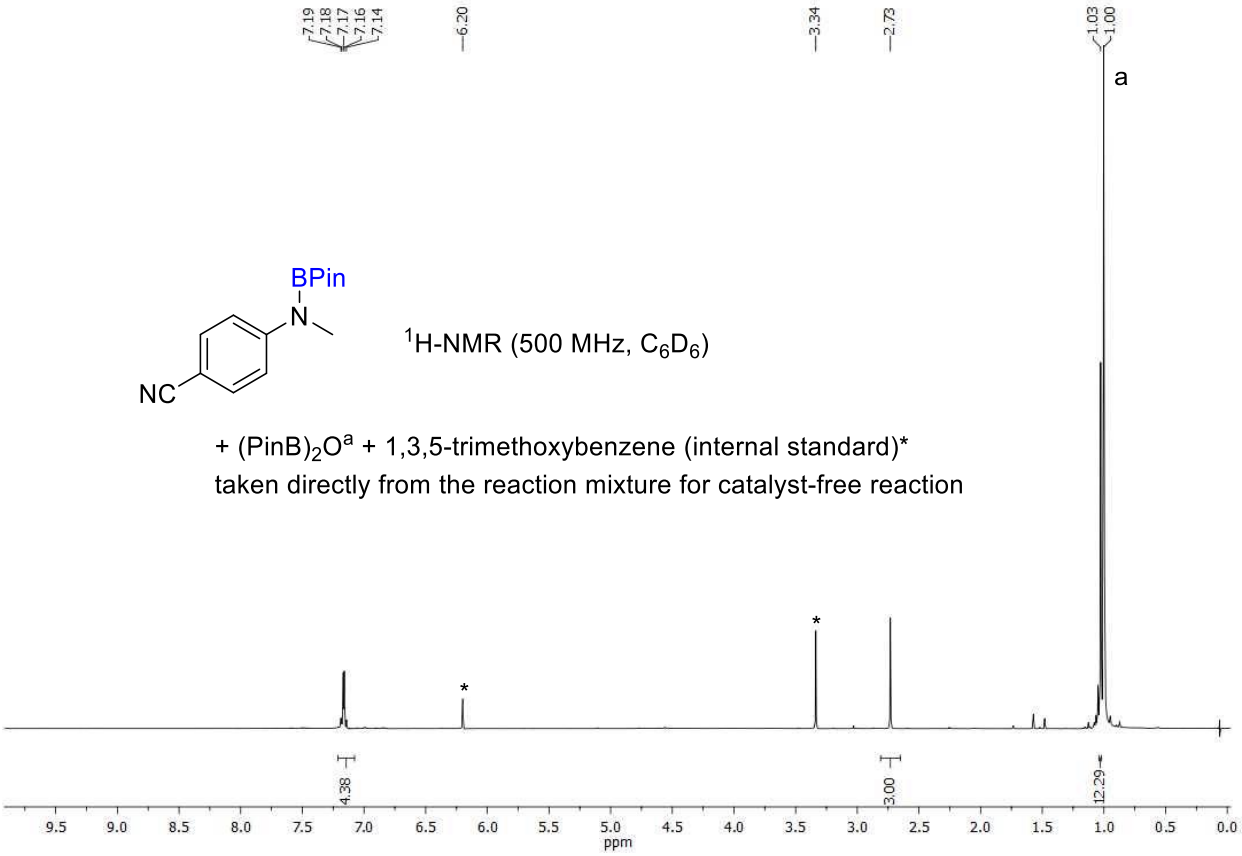
b - trance amounts of formamide product



^{1}H-NMR (500 MHz, C_6D_6)

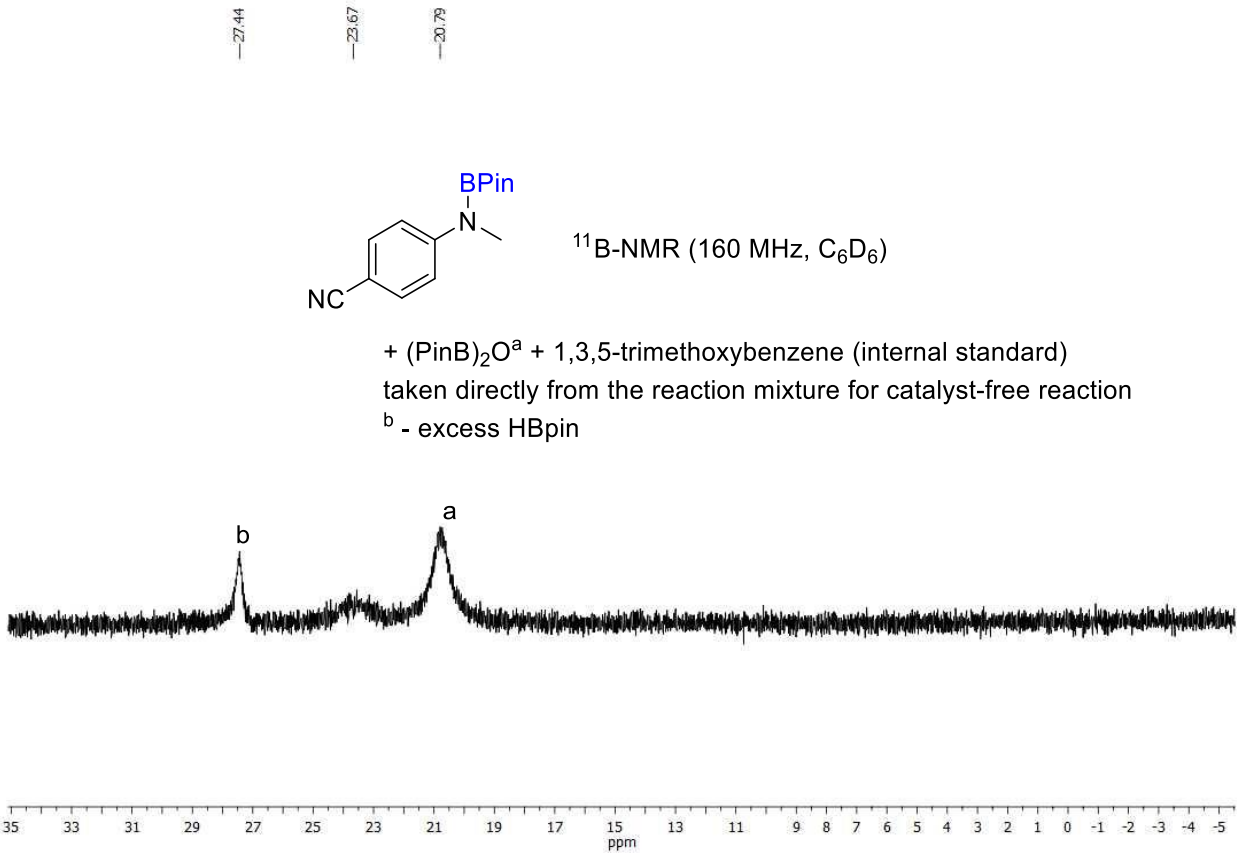
+ $(PinB)_2O^a$

taken directly from the reaction mixture for Co-catalyzed reaction



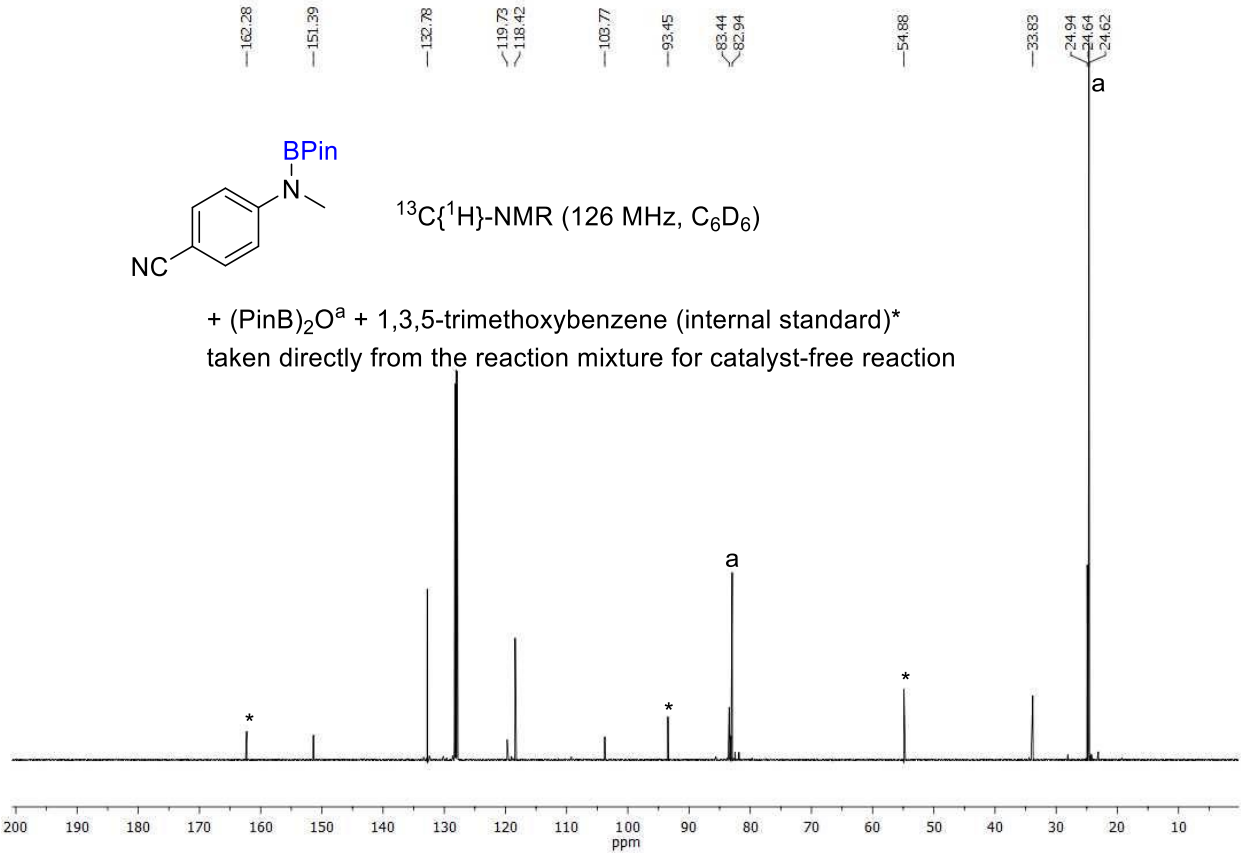
^{1}H-NMR (500 MHz, C_6D_6)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction



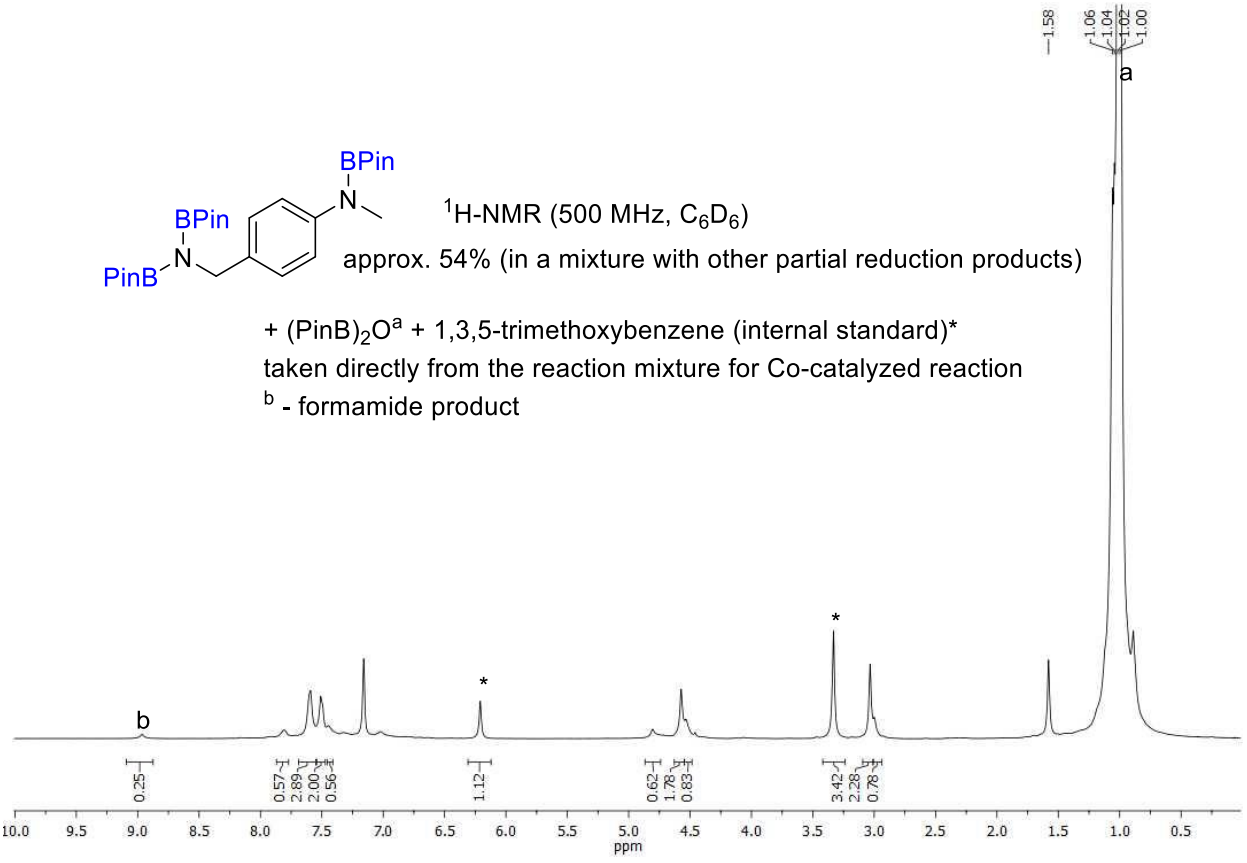
^{11}B-NMR (160 MHz, C_6D_6)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)
taken directly from the reaction mixture for catalyst-free reaction
[b] - excess HBpin



$^{13}C\{^{1}H\}$-NMR (126 MHz, C_6D_6)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction



^{1}H-NMR (500 MHz, C_6D_6)

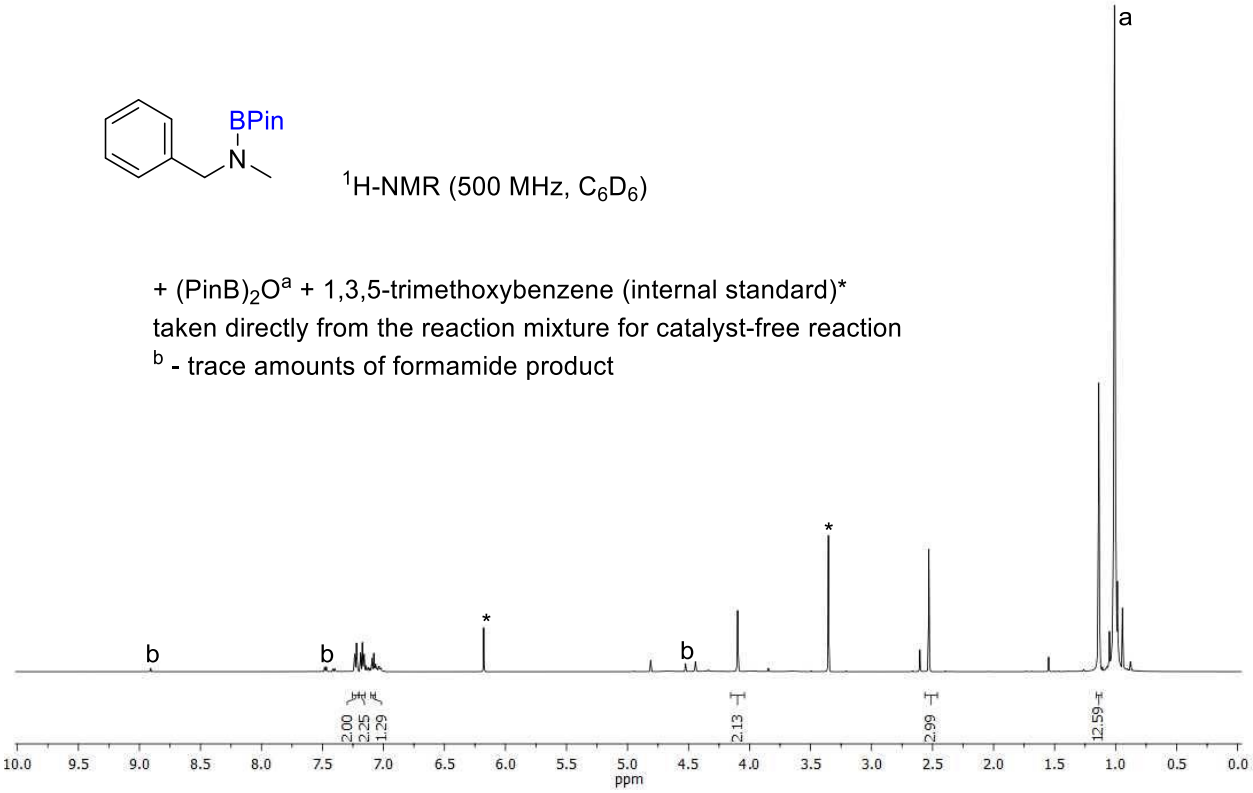
approx. 54% (in a mixture with other partial reduction products)

+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for Co-catalyzed reaction

[b] - formamide product

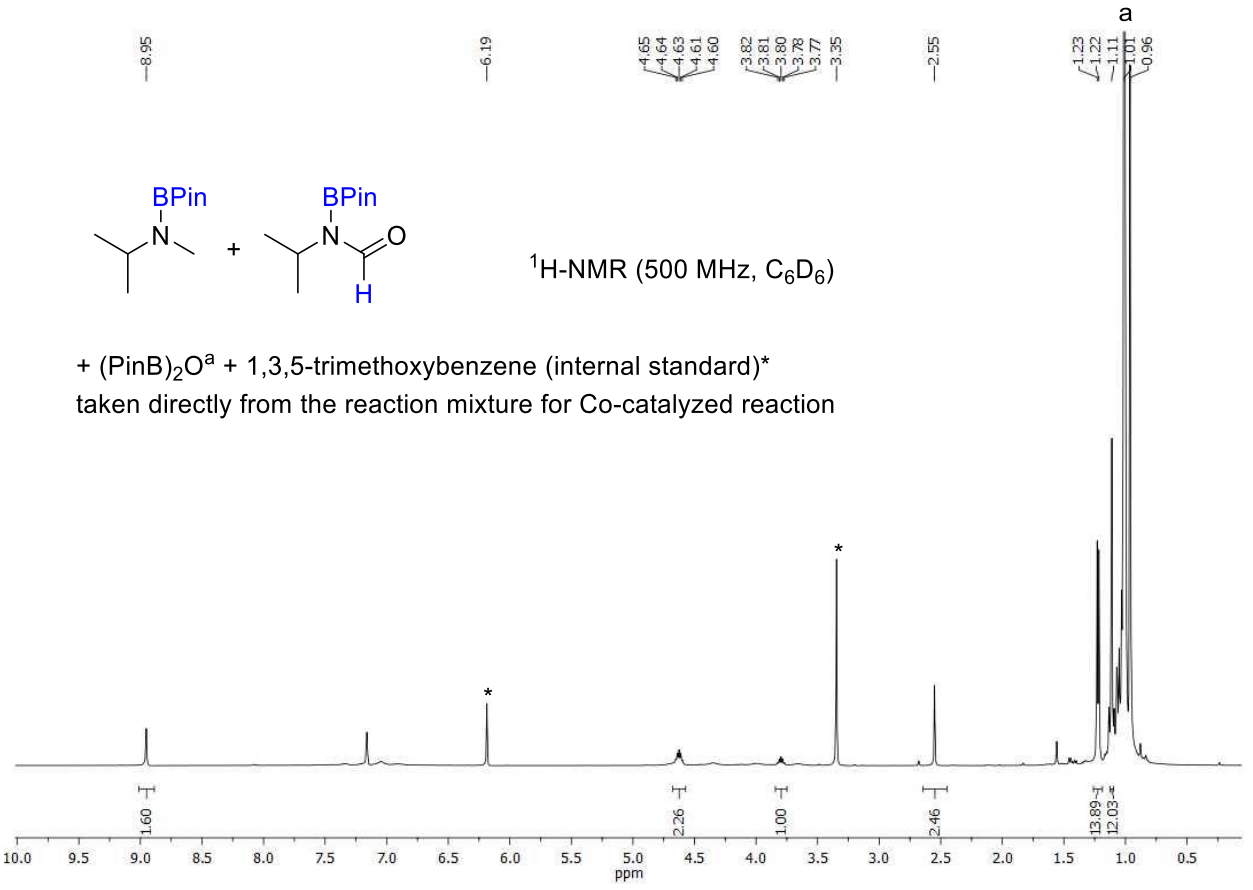
^{1}H-NMR (500 MHz, C_6D_6)

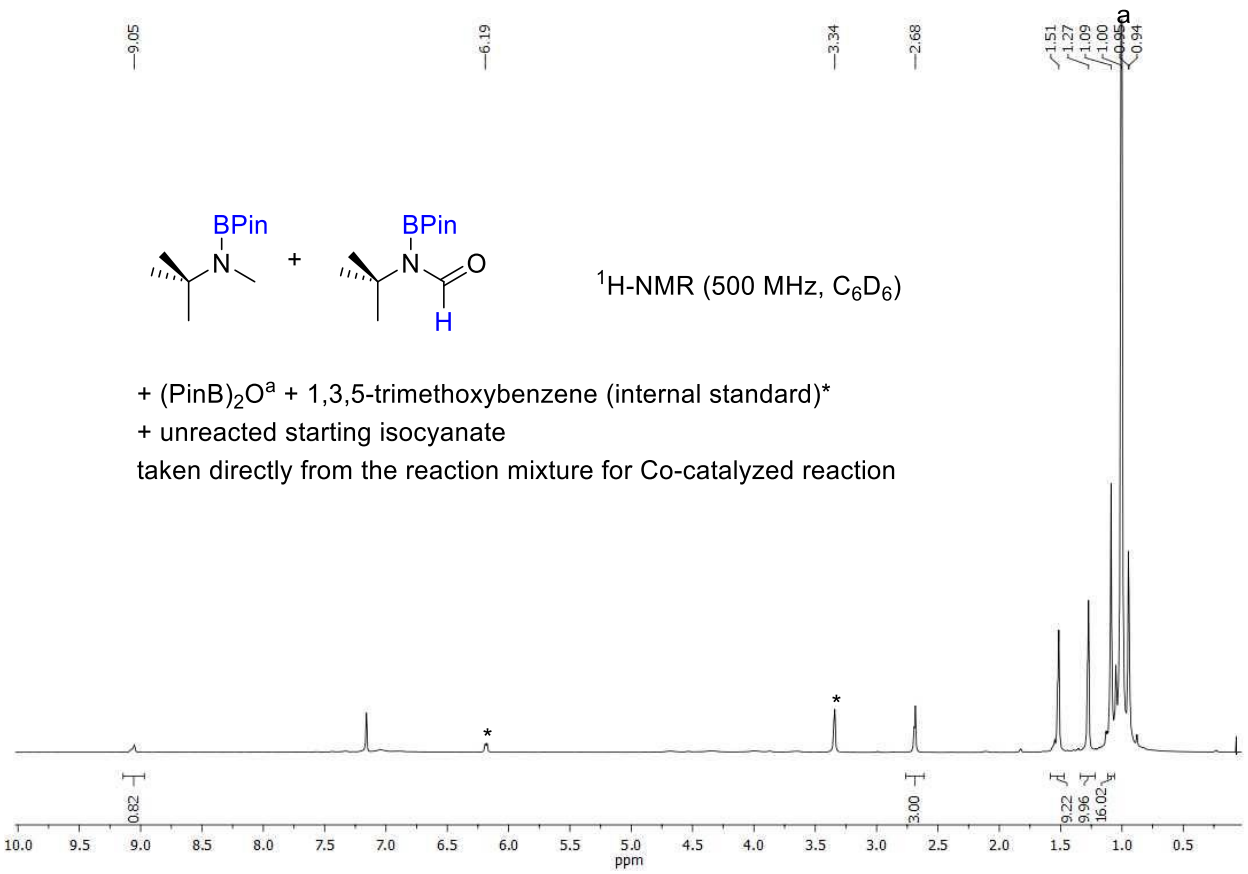
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for catalyst-free reaction
[b] - trace amounts of formamide product



^{1}H-NMR (500 MHz, C_6D_6)

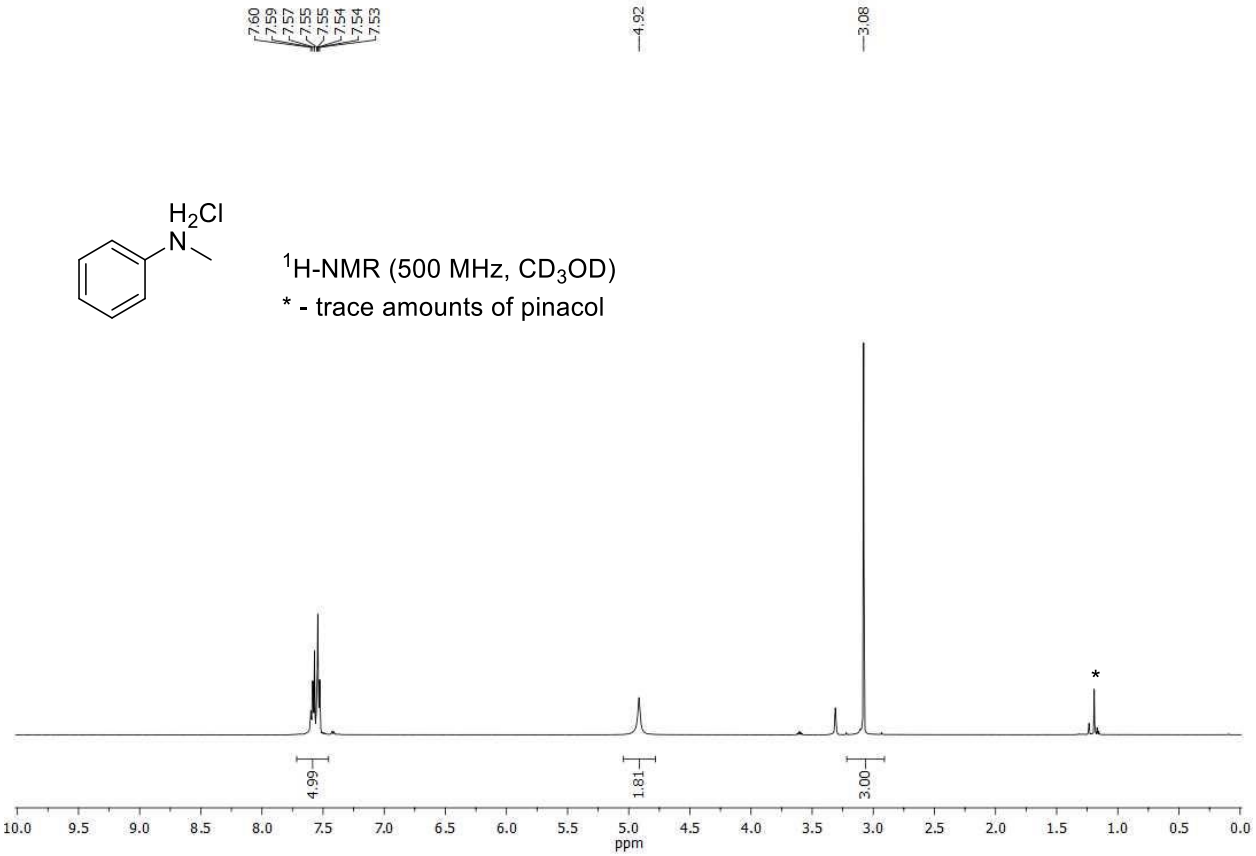
+ $(PinB)_2O$[a] + 1,3,5-trimethoxybenzene (internal standard)*
taken directly from the reaction mixture for Co-catalyzed reaction

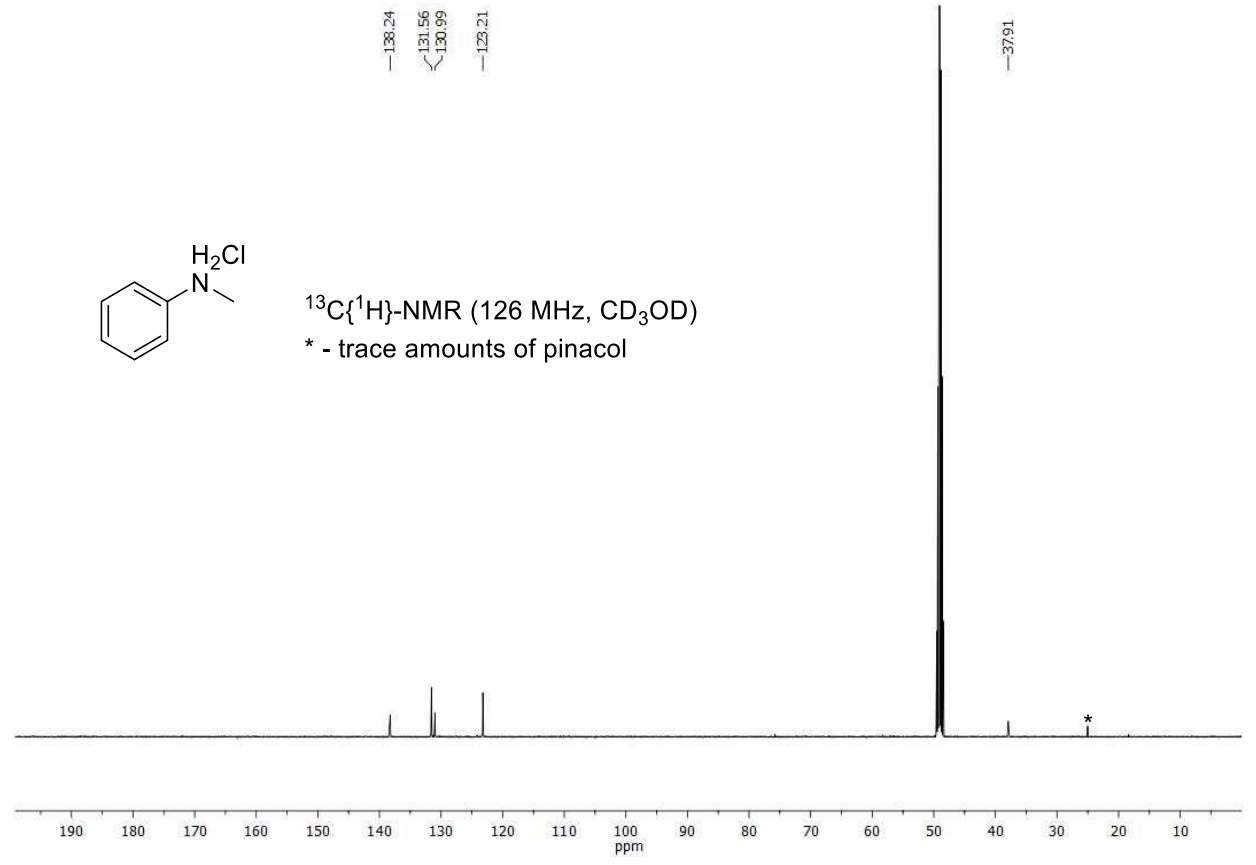


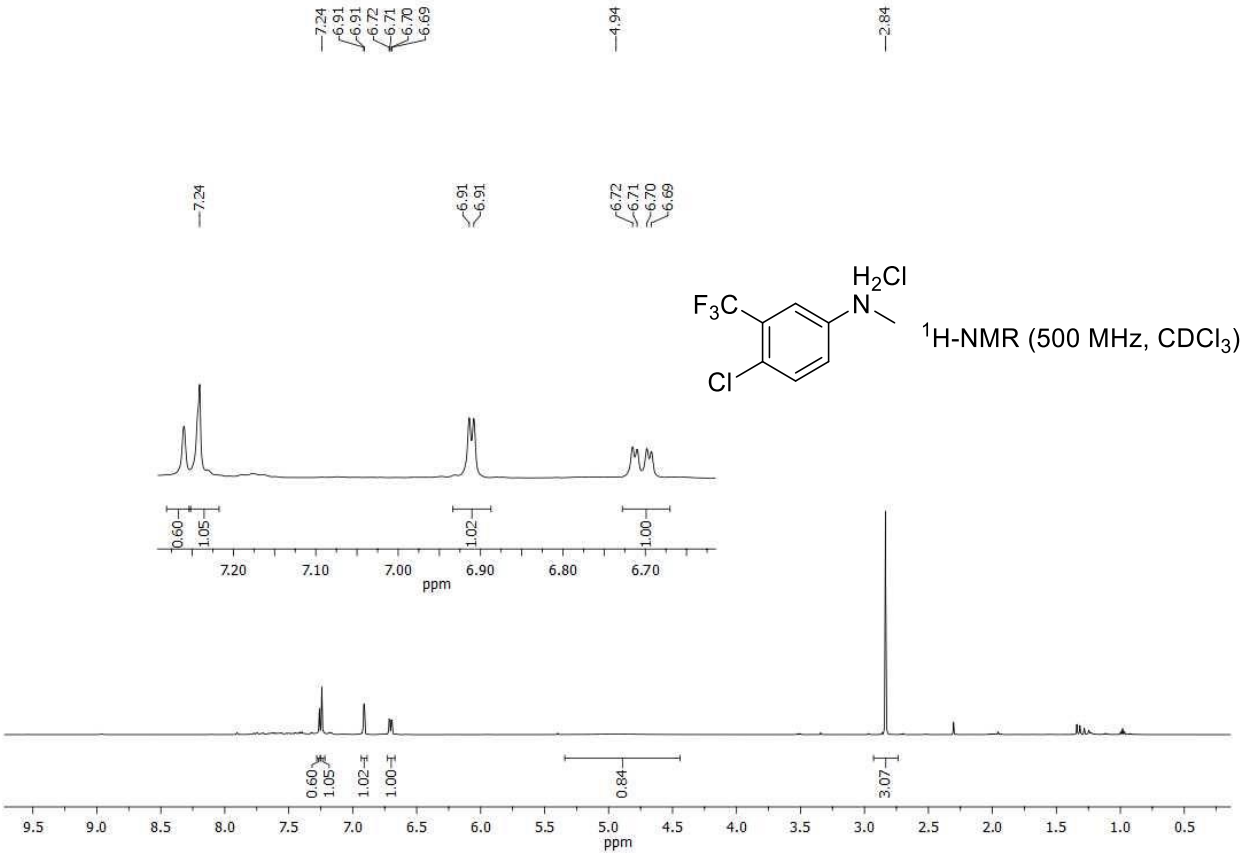


NMR spectra for borylated *N*-methylaniline,[14,15] 4-chloro-*N*-methylaniline,[13] 4-fluoro-*N*-methylaniline,[13] 4-methyl-*N*-methylaniline,[13] 4-methoxy-*N*-methylaniline,[13] 4-cyano-*N*-methylaniline,[13] *N*-methylbenzylamine,[16] *N*-methylisopropylamine,[15]and *N*-methyl-*tert*-butylamine[15] are consistent with those reported in the literature.

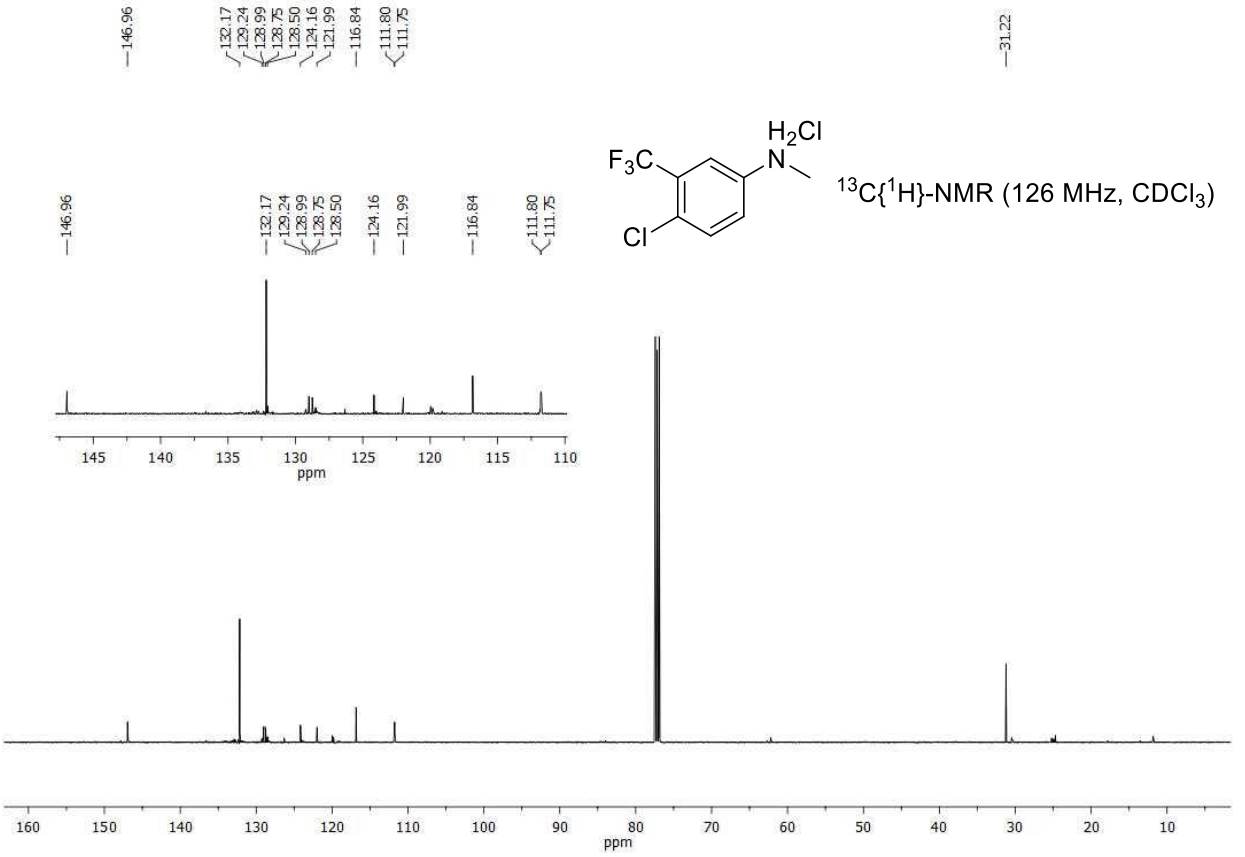
7. NMR spectra for isolated N-methylamine hydrochloride salts





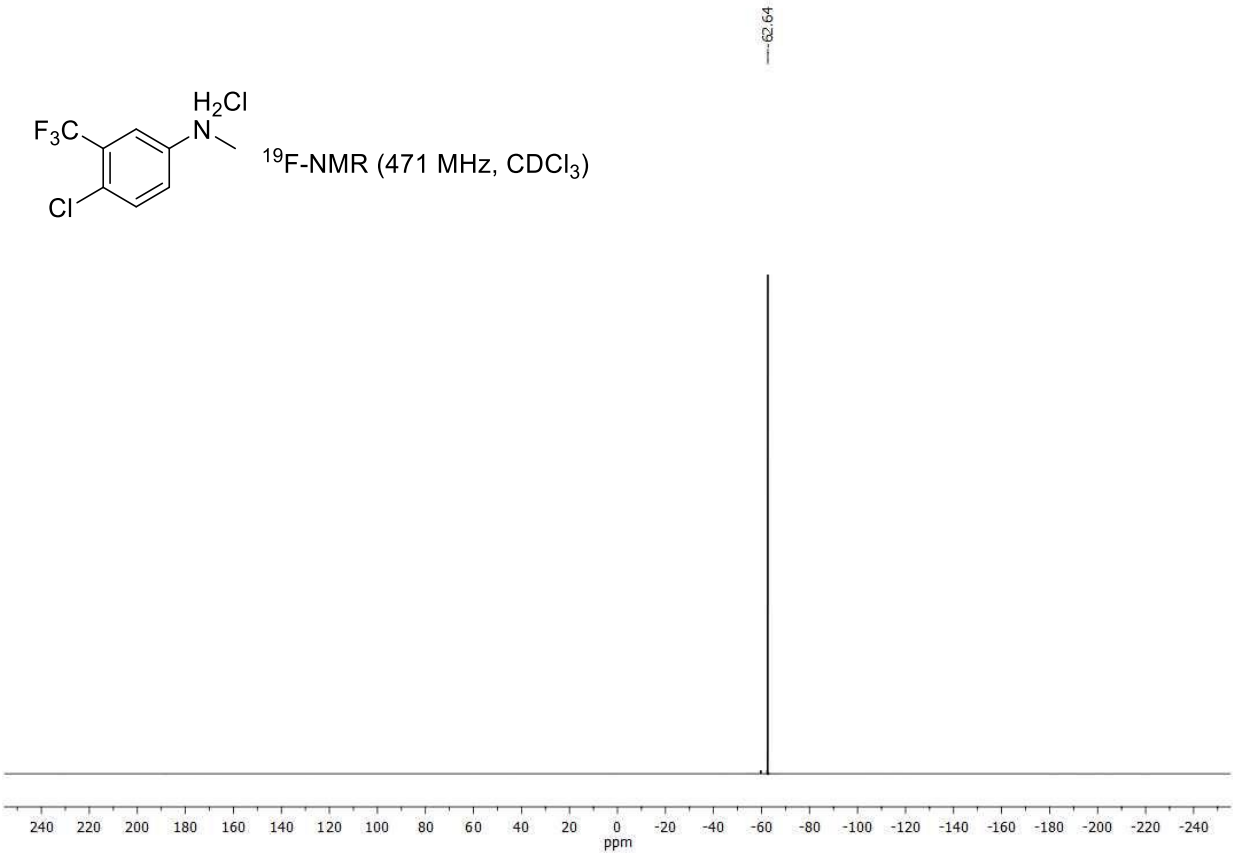


^{1}H-NMR (500 MHz, $CDCl_3$)



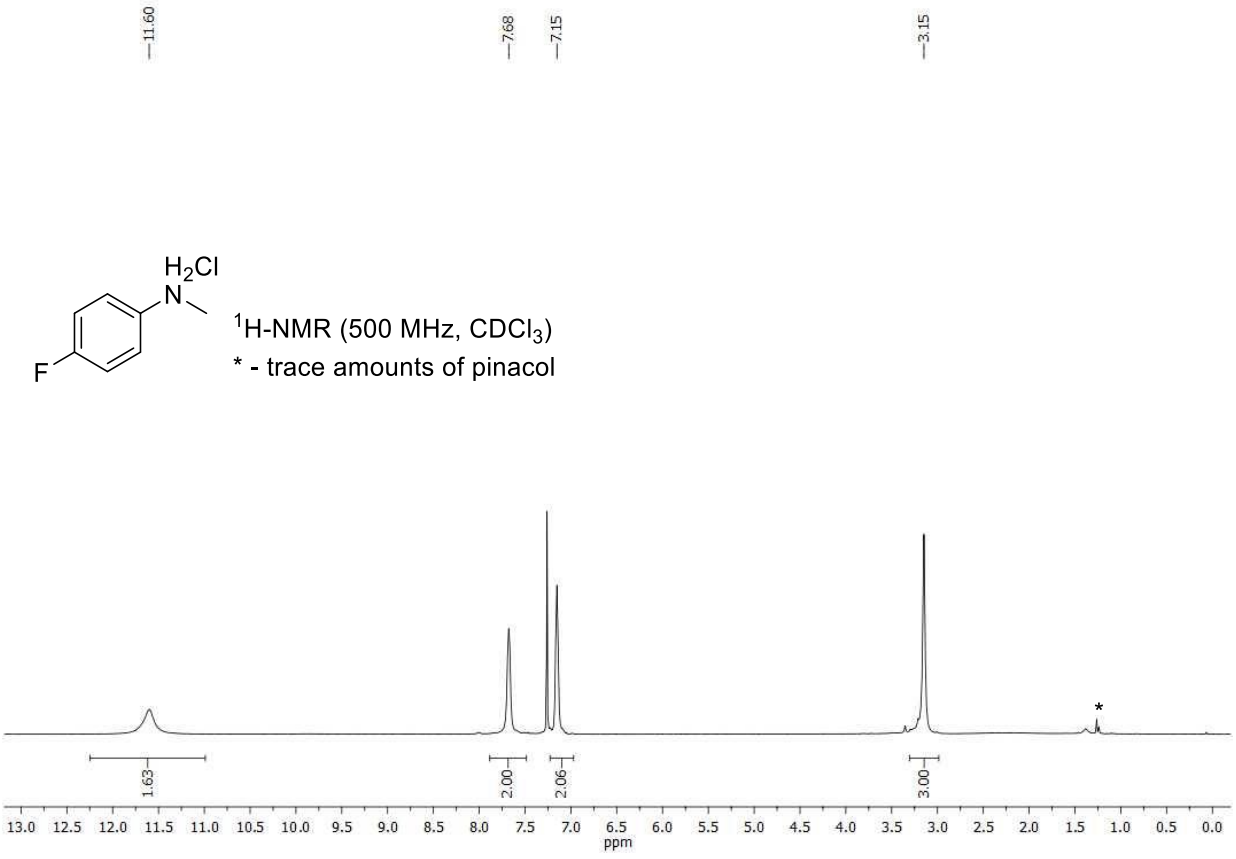
^{13}C{^{1}H}-NMR (126 MHz, $CDCl_3$)

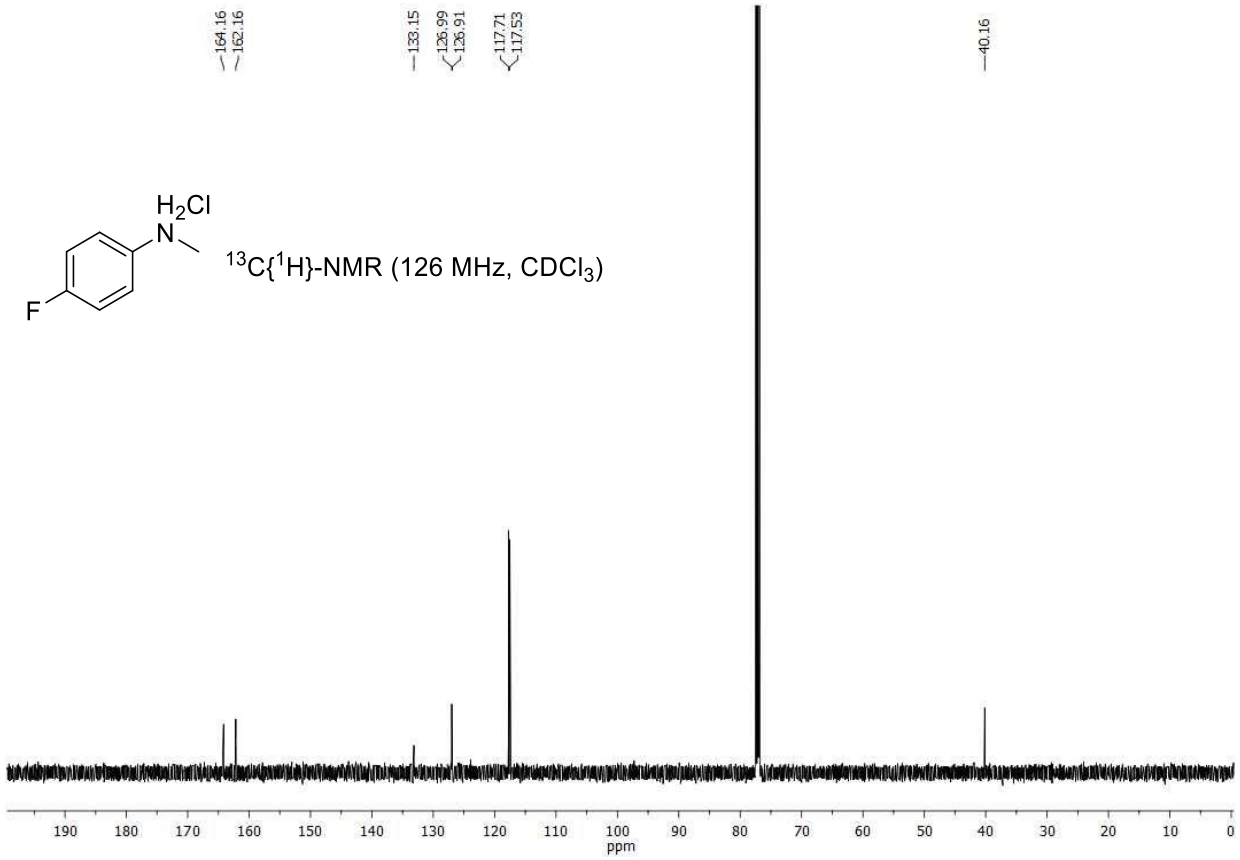
^{19}F-NMR (471 MHz, $CDCl_3$)



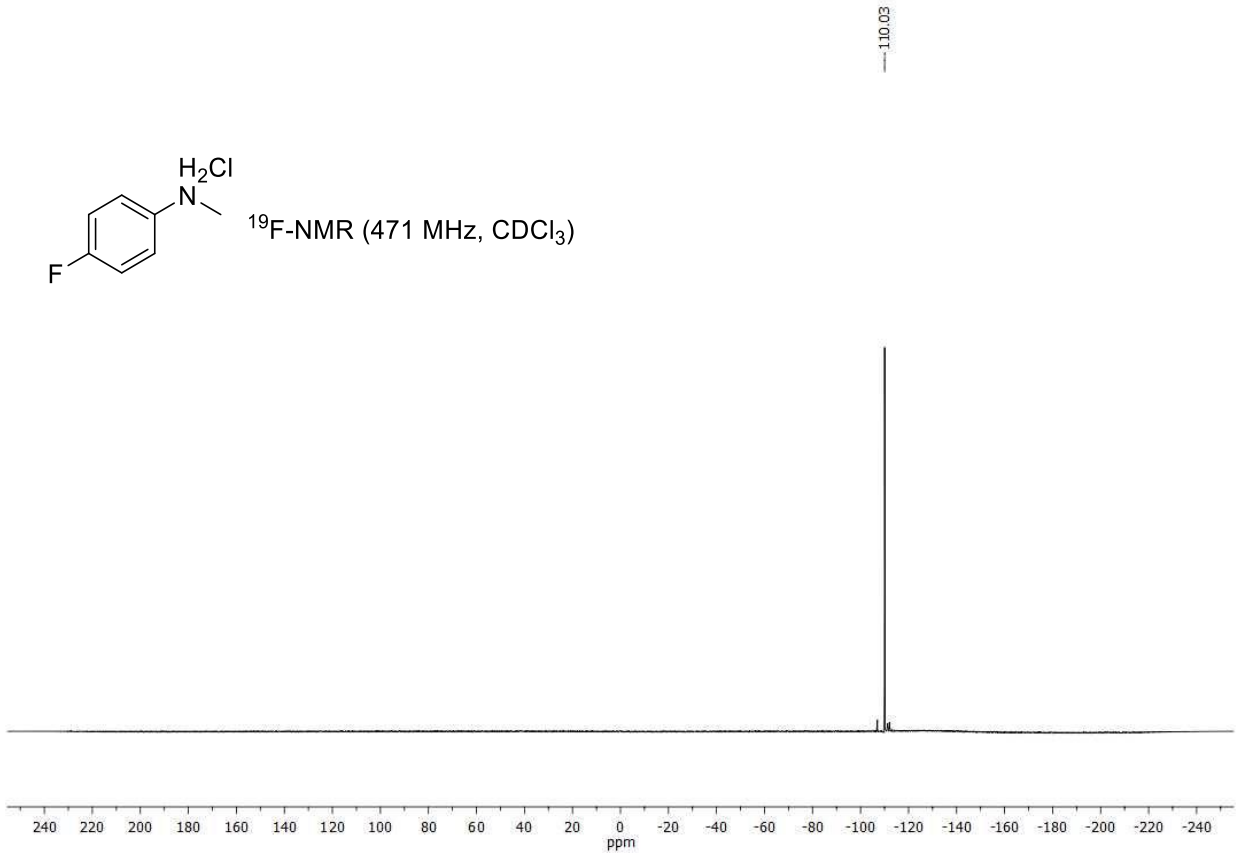
^{1}H-NMR (500 MHz, $CDCl_3$)

* - trace amounts of pinacol





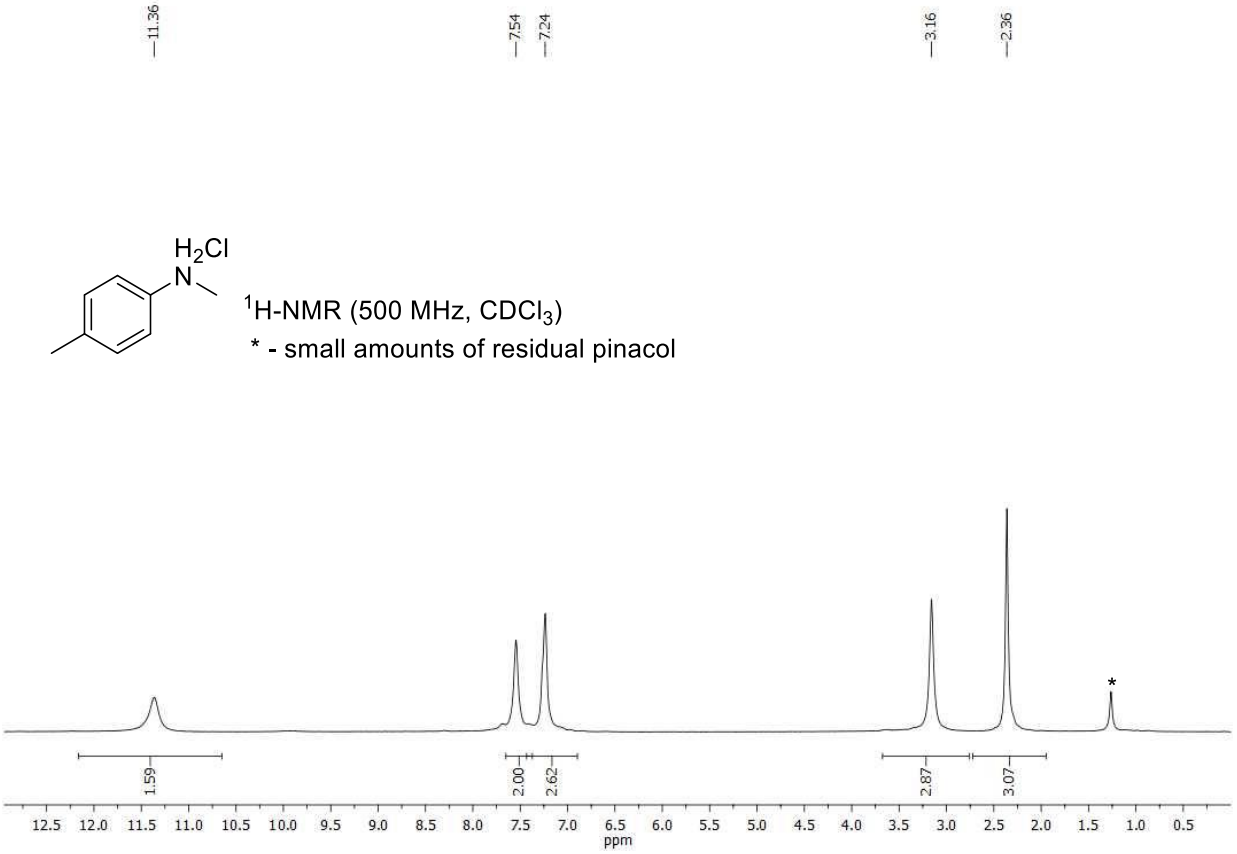
$^{13}C\{^{1}H\}$-NMR (126 MHz, $CDCl_3$)



^{19}F-NMR (471 MHz, $CDCl_3$)

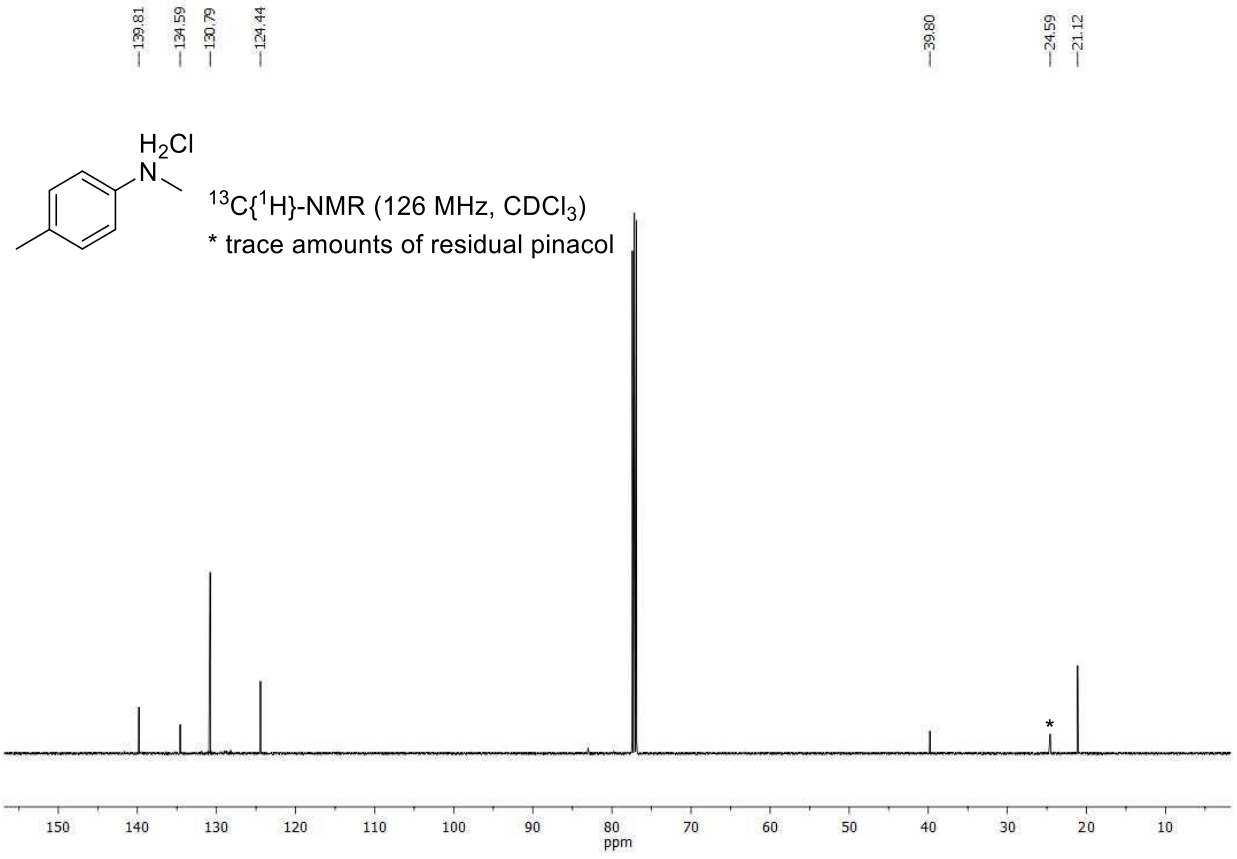
^{1}H-NMR (500 MHz, $CDCl_3$)

* - small amounts of residual pinacol



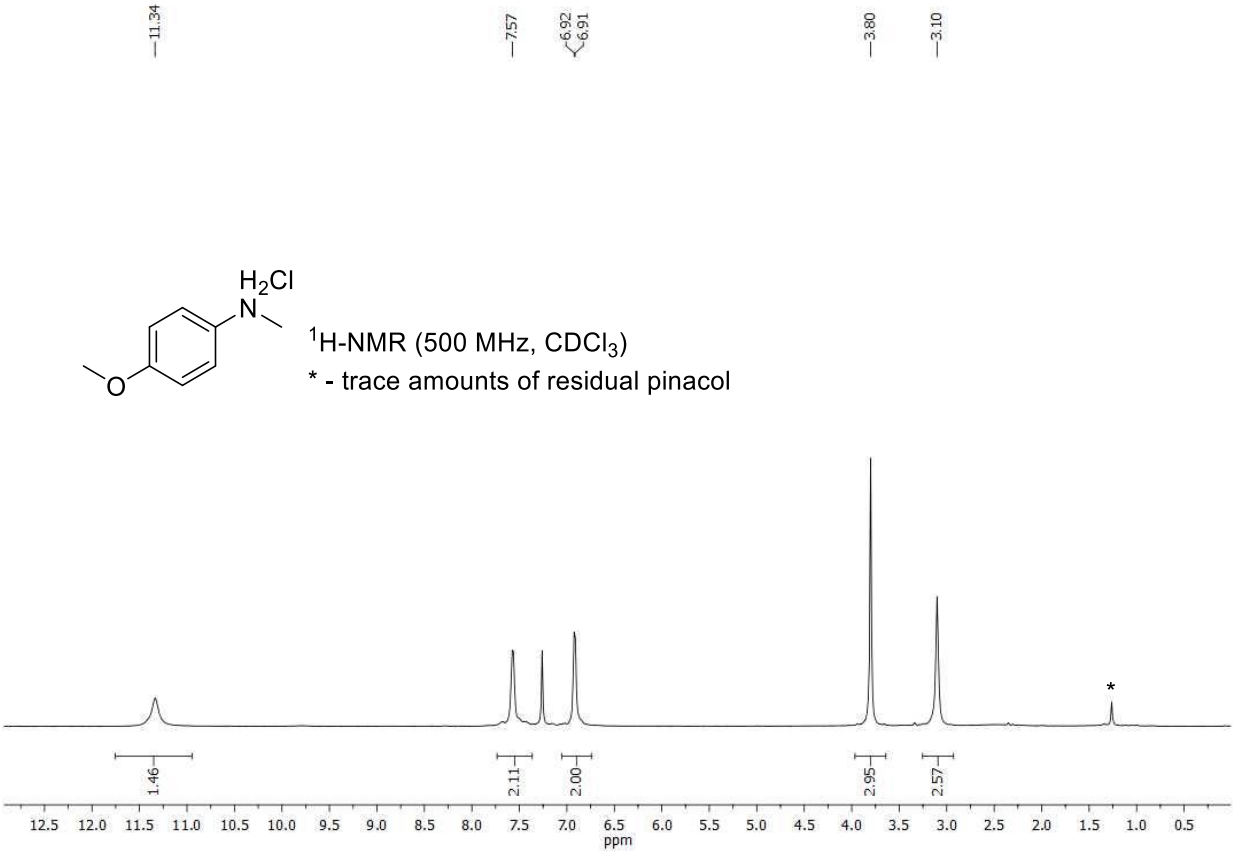
$^{13}C\{^1H\}$-NMR (126 MHz, $CDCl_3$)

* trace amounts of residual pinacol



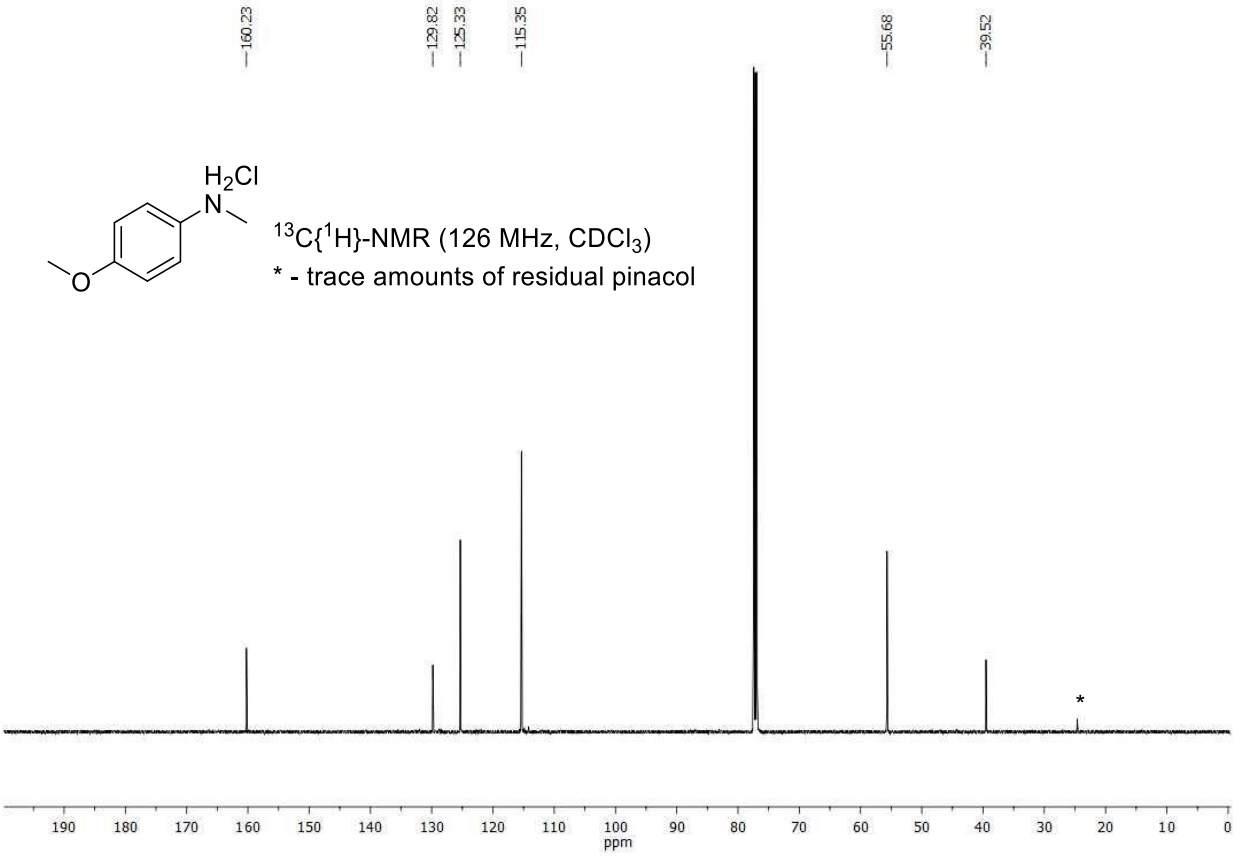
^{1}H-NMR (500 MHz, $CDCl_3$)

* - trace amounts of residual pinacol



$^{13}C\{^1H\}$-NMR (126 MHz, $CDCl_3$)

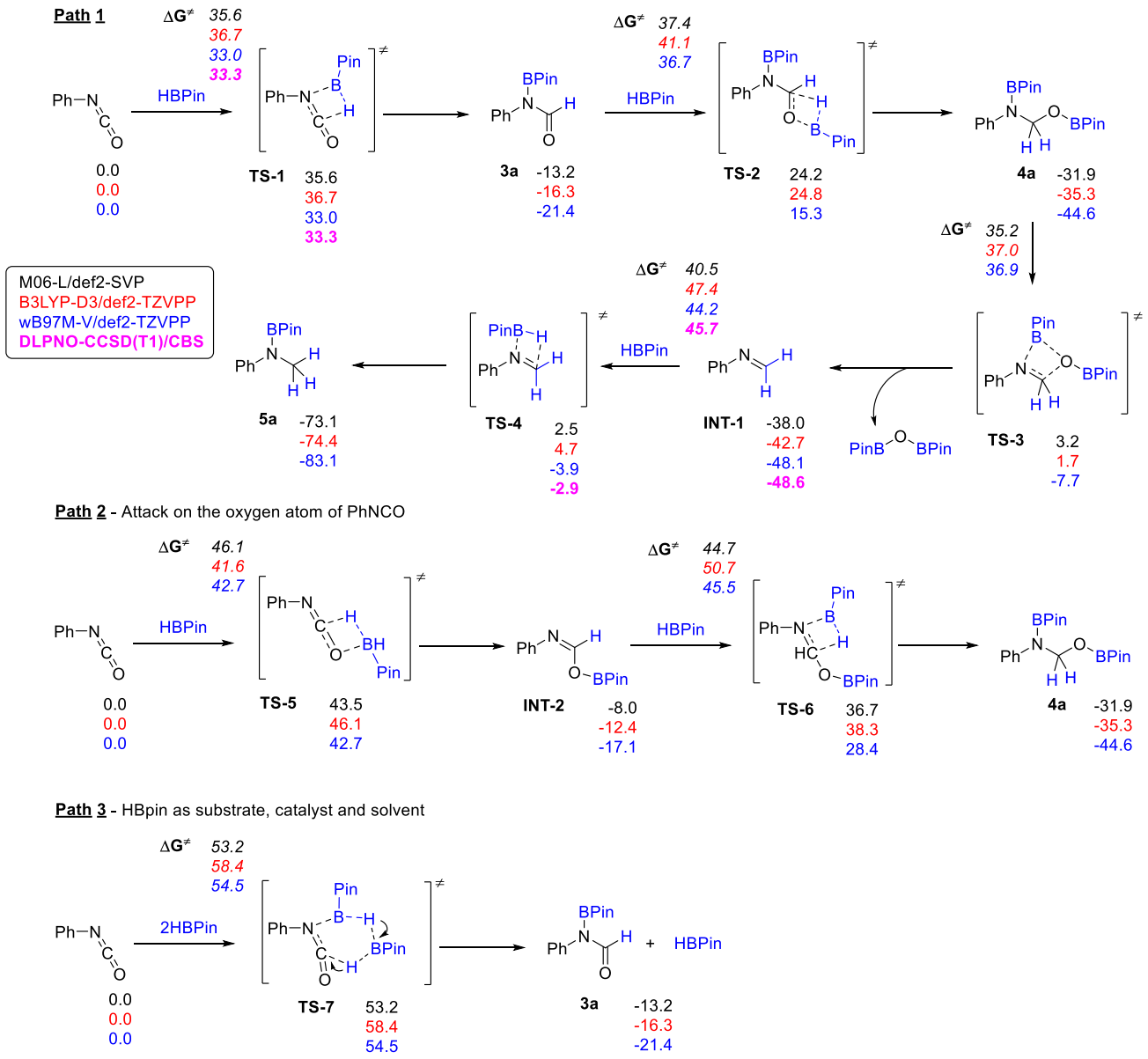
* - trace amounts of residual pinacol



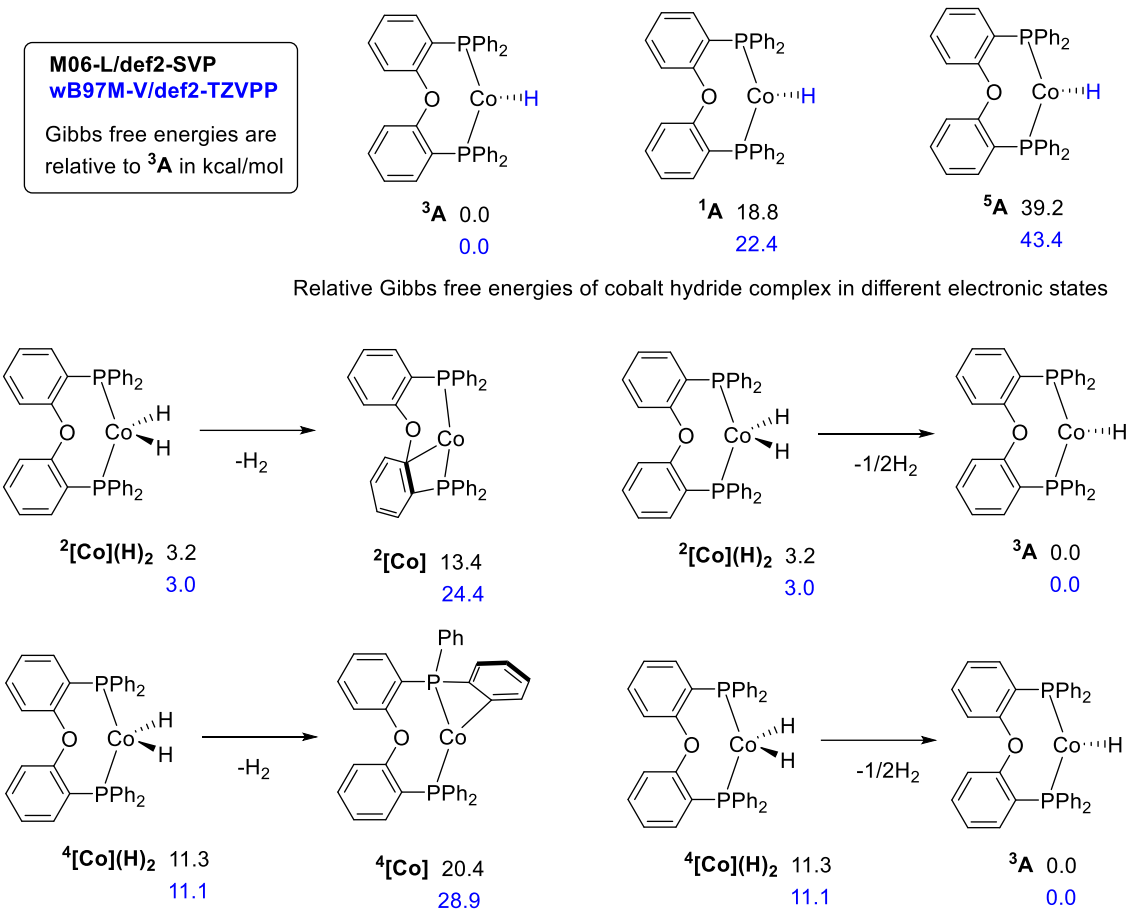
8. Computational details

All calculations were carried out with the Gaussian 09[17] and ORCA 4.2.1[18] suites of programs. Geometries were optimized using the meta-GGA functional M06-L[19] and the def2-SVP[20] basis set. Further single point calculations were performed on optimized geometries with a larger def2-TZVPP[20] basis set. For single point calculations the popular hybrid functional B3LYP[21-24] with D3BJ[25,26] correction (or B3LYP-D3) and the range-separated meta-GGA hybrid functional ωB97M-V[27] with nonlocal correlation were chosen. The ωB97M-V functional was applied to study both the catalyst-free and the catalyst-assisted reactions, while B3LYP-D3 was only used in the catalyst-free part. Recent systematic benchmark studies have shown that the ωB97M-V functional is highly robust in the calculations of main-group chemistry and also demonstrates a good accuracy towards transition metal complexes[28-30]. The default "Tight" convergence criterion and "UltraFine" grid were used in the Gaussian software. The ORCA "TightSCF" convergence criterion and “Grid5” numerical integration settings was employed throughout. To accelerate DFT calculations for the M06-L functional the resolution of the identity[31,32] approximation was used with automatically generated density fitting sets. For the exchange part in hybrid functionals the RIJCOSX method[33] was applied together with def2/J[34] auxiliary basis sets. The nature of the stationary points was confirmed by analytical calculation of vibrational frequencies in the harmonic approximation. Solvation effects were taken into account employing the polarized continuum solvation model (PCM)[35], the dielectric constants ε = 2.3741 for toluene and ε = 2.48 for HBpin[36] were used.

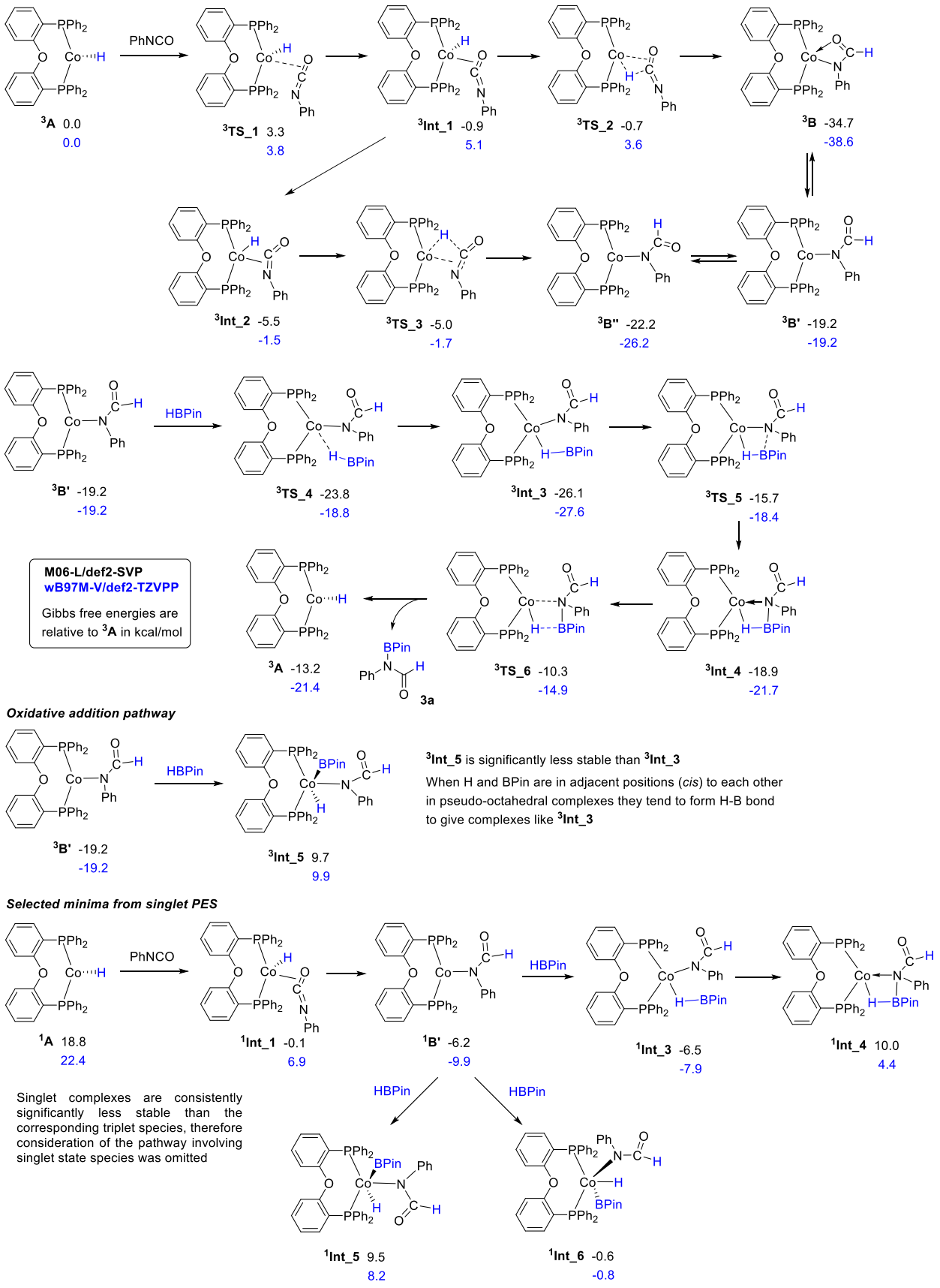
The domain based local pair natural orbital coupled-cluster DLPNO-CCSD(T1)[37,38] calculations were conducted to ensure the accuracy of DFT methods on selected structures in the catalyst-free part. DLPNO calculations were performed in combination with the def2-SVP and def2-TZVP[20] basis sets as implemented in ORCA 4.2.1 software. Auxiliary "/C" basis sets with maximum possible angular momentum ("autoauxlmax true") were generated using the automated auxiliary basis set construction module of ORCA (the so-called “autoaux”)[39]. The two-point extrapolation scheme for approaching the complete pair natural orbital space (CPS) limit was applied to reduce the local approximation error with the increasing system size[40]. Correlation energies obtained with two "TCutPNO" values (10^{-6} and 10^{-7}) for each basis set were extrapolated to the CPS limit, i.e. the CPS(6/7) scheme was used. A complete basis set (CBS) limit extrapolation was performed to minimize the basis set incompleteness and superposition errors, using the CBS(2/3) scheme described previously[41].



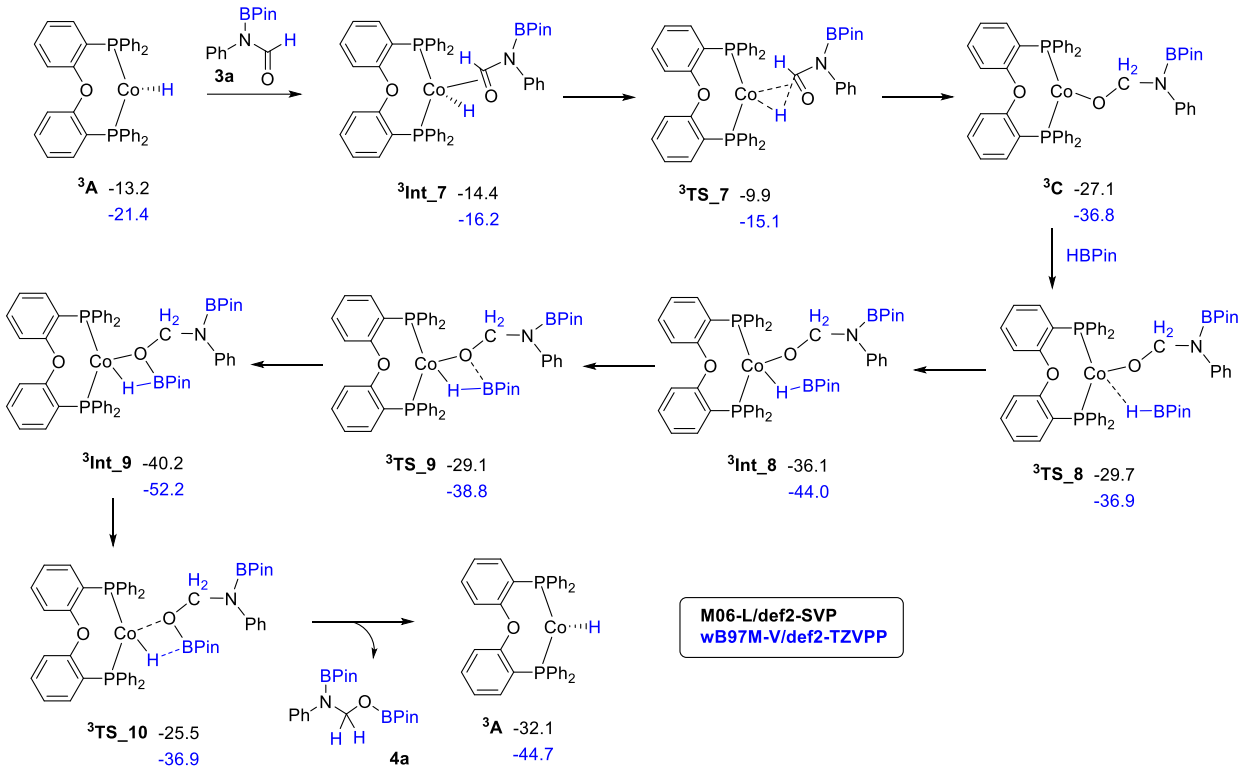
Scheme S1. DFT calculated pathways for catalyst-free hydroboration of PhNCO with HBPin to N-borylformamide **3a** and borylated *N*-methylaniline **5a** (Gibbs free energies are shown in kcal·mol^{-1}). Geometries were optimized using the M06L functional and the def2-SVP basis set. Additional single point calculations were performed on each optimized geometry with the aid of functionals B3LYP-D3 and *ω*B97M-V and the def2-TZVPP basis set, which all showed very similar results. Additional high-level *ab initio* DLPNO-CCSD(T1)/CBS calculations on selected structures demonstrate a high accuracy of the *ω*B97M-V/def2-TZVPP method. Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.48 for HBpin was used.



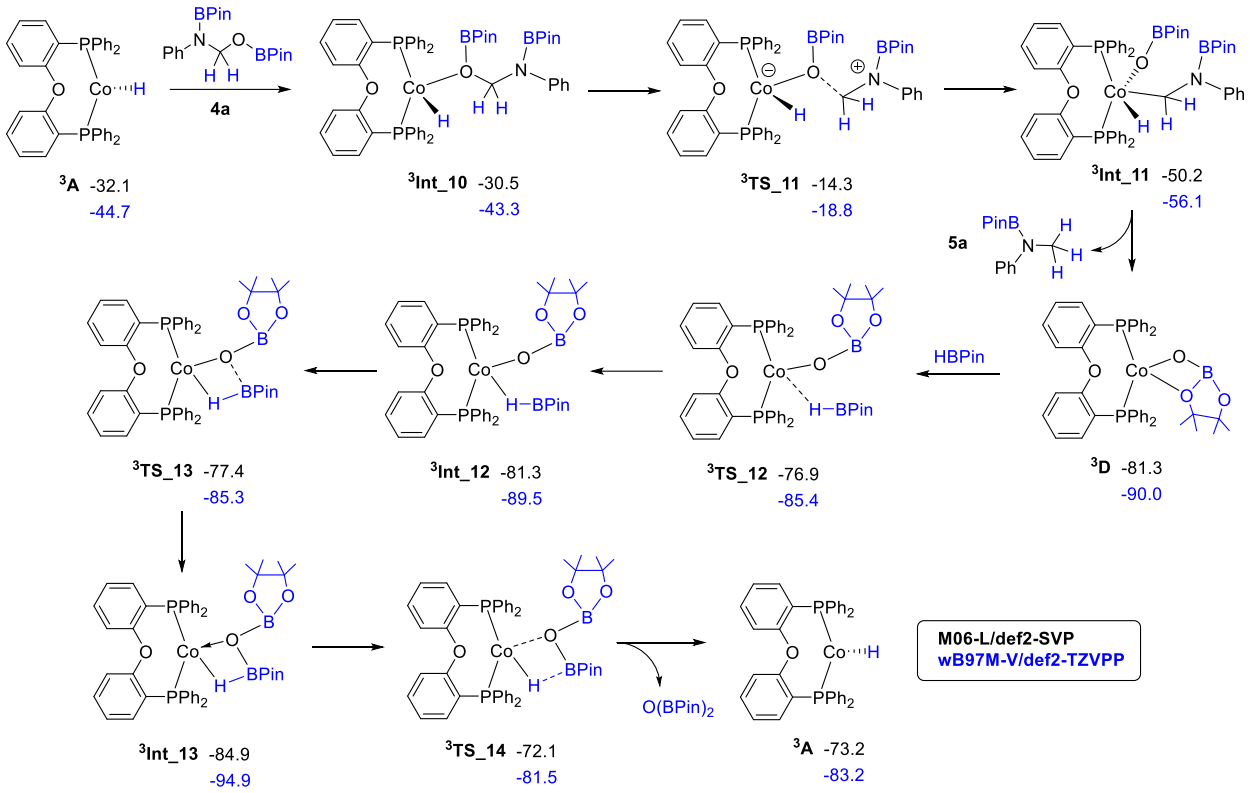
Scheme S2. DFT derived pathways for cobalt pre-catalyst activation (Gibbs free energies are shown in kcal·mol^{-1} relative to **A** in triplet state). Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used.



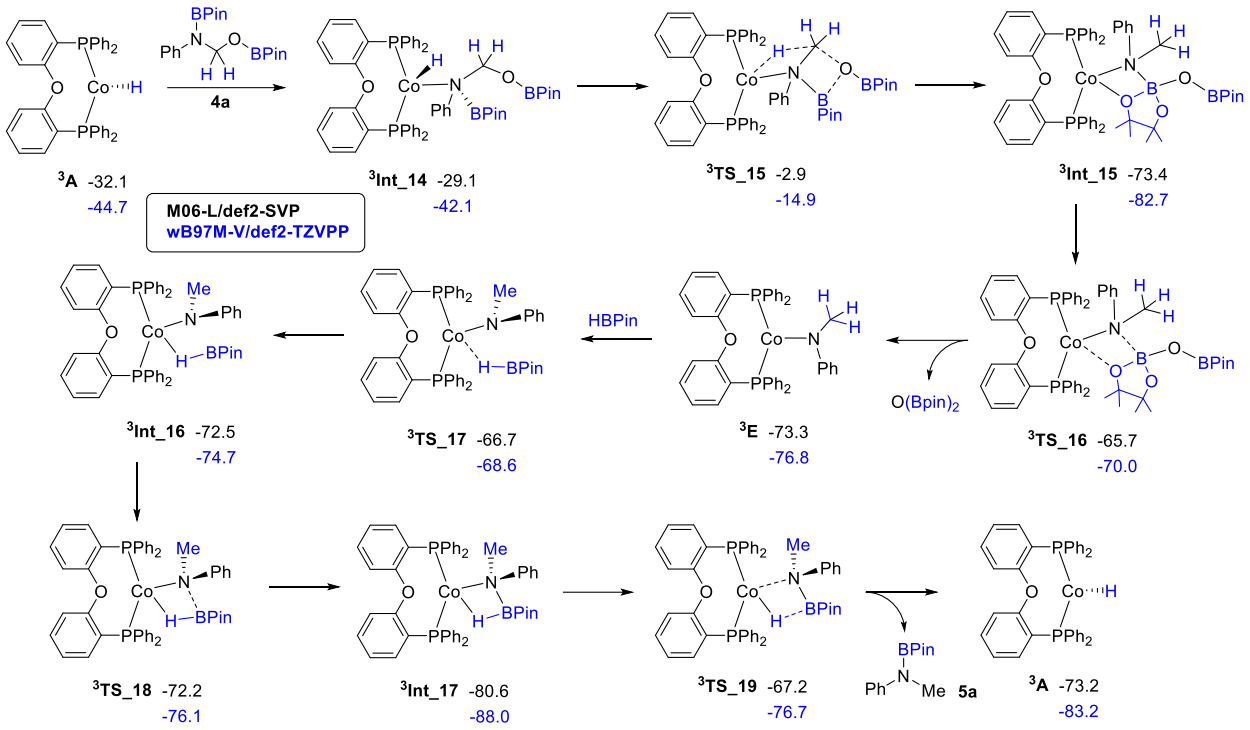
Scheme S3. DFT derived pathways for **A**-catalyzed monohydroboration of PhNCO with HBPin to N-borylformamide **3a** (cycle 1 in Scheme 6 in the manuscript). Gibbs free energies are shown in kcal·mol^{-1}. Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used.



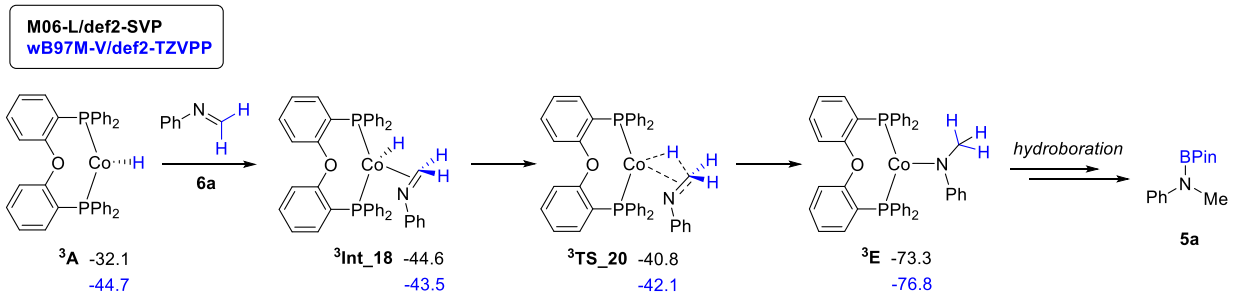
Scheme S4. DFT derived mechanism for **A**-catalyzed conversion of **3a** to **4a** (cycle 2 in Scheme 6 in the manuscript). Gibbs free energies are shown in kcal·mol^{-1}. Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used.



Scheme S5. DFT derived mechanism for **A**-catalyzed conversion of **4a** to **5a** via O-coordination of **4a** to **A** (cycle 3 in Scheme 6 in the manuscript). Gibbs free energies are shown in kcal·mol^{-1}. Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used. ^{3}**Int_11** was located separately, optimization from ^{3}**TS_11** leads directly to ^{3}**D**. No transition states for the reaction of **A** with **4a** to give Co-OBPin complex via either oxidative addition or metathesis routes could be localized.



Scheme S6. DFT derived mechanism for **A**-catalyzed conversion of **4a** to **5a** via N-coordination of **4a** to **A** (cycle 4 in Scheme 6 in the manuscript). Gibbs free energies are shown in kcal·mol^{-1}. Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used.



Scheme S7. DFT derived mechanism for **A**-catalyzed hydroboration of the imine **6a** to **5a**. Gibbs free energies are shown in kcal·mol^{-1}. Solvation effects were taken into account employing the PCM model, the dielectric constant ε = 2.3741 for toluene was used. Starting from intermediate **E** the following steps in Scheme S7 are identical to those in Scheme S6 and therefore were omitted.

Table S1. Electronic energies (E), thermal corrections to Gibbs free energy (G_{corr}), solvation energies (ΔG°_{solv}) and relative Gibbs free energies in solution ($\Delta\Delta_f G^{\circ}_s$) for the catalyst-free reaction calculated using different functionals: M06-L – (1), B3LYP-D3 – (2) and ωB97M-V – (3)

	E(1), a.u.	E(2), a.u.	E(3), a.u.	G_{corr}(1), a.u.	ΔG°_{solv}(1), kcal·mol^{-1}	$\Delta\Delta_f G^{\circ}_s$(1), kcal·mol^{-1}	$\Delta\Delta_f G^{\circ}_s$(2), kcal·mol^{-1}	$\Delta\Delta_f G^{\circ}_s$(3), kcal·mol^{-1}
HBpin	-411.51434	-412.07283	-411.85206	0.15740	-1.4	-	-	-
(Bpin)$_2$O	-897.11472	-898.31949	-897.88334	0.32022	-3.0	-	-	-
PhNCO	-399.40591	-399.91716	-399.74876	0.07176	-1.2	0.0	0.0	0.0
TS-1	-810.88456	-811.95251	-811.56925	0.24971	-2.3	35.6	36.7	33.0
3a	-810.96467	-812.03935	-811.65829	0.25364	-3.3	-13.2	-16.3	-21.4
TS-2	-1222.44318	-1224.07052	-1223.47575	0.43383	-4.0	24.2	24.8	15.3
4a	-1222.53914	-1224.17274	-1223.57765	0.43873	-3.0	-31.9	-35.3	-44.6
TS-3	-1222.48114	-1224.11186	-1223.51683	0.43642	-2.8	3.2	1.7	-7.7
INT-1	-325.40444	-325.83548	-325.67025	0.09079	-1.2	-38.0	-42.7	-48.1
TS-4	-736.87528	-737.85374	-737.47283	0.26897	-2.5	2.5	4.7	-3.9
5a	-737.00214	-737.98608	-737.60546	0.27393	-1.6	-73.1	-74.4	-83.1
TS-5	-810.87043	-811.93609	-811.55231	0.24798	-2.1	43.5	46.1	42.7
INT-2	-810.95616	-812.03287	-811.65120	0.25292	-3.0	-8.0	-12.4	-17.1
TS-6	-1222.42053	-1224.04630	-1223.45209	0.43114	-4.1	36.7	38.3	28.4
TS-7	-1222.39480	-1224.01487	-1223.41112	0.42983	-2.9	53.2	58.4	54.5

Table S2. Hartree-Fock energies (E_{HF}), CCSD(T1) correlation energies ($E_{C\text{-}CCSD(T1)}$) for different TCutPNO values and CPS(6/7) extrapolated correlation energies and total energies ($E_{CCSD(T1)}$) at the complete basis set limit for selected structures in the catalyst-free reaction

CBS(2/3)		TCutPNO=10^{-6}	TCutPNO=10^{-7}	CPS(6/7)	CPS(6/7)
	E_{HF}	$E_{C\text{-}CCSD(T1)}$	$E_{C\text{-}CCSD(T1)}$	$E_{C\text{-}CCSD(T1)}$	$E_{CCSD(T1)}$
HBpin	-409.59384	-1.86690	-1.86880	-1.86975	-411.46359
(Bpin)$_2$O	-893.07782	-3.96460	-3.96975	-3.97233	-897.05015
PhNCO	-397.59646	-1.73644	-1.73730	-1.73773	-399.33419
TS-1	-807.12758	-3.63208	-3.63619	-3.63825	-810.76583
INT-1	-323.80422	-1.50739	-1.50809	-1.50844	-325.31266
TS-4	-733.31011	-3.40838	-3.41237	-3.41436	-736.72447

Table S3. Electronic energies (E), thermal corrections to Gibbs free energy (G_{corr}), solvation energies (ΔG°_{solv}) and relative Gibbs free energies in solution ($\Delta\Delta_f G^{\circ}_{s}$) for the catalyst-assisted reaction calculated using two functionals: M06-L – (1) and ωB97M-V – (3)

	E(1), a.u.	E(3), a.u.	G_{corr}(1), a.u.	ΔG°_{solv}(1), kcal·mol^{-1}	$\Delta\Delta_f G^{\circ}_{s}$(1), kcal·mol^{-1}	$\Delta\Delta_f G^{\circ}_{s}$(3), kcal·mol^{-1}
^{3}A	-3528.35176	-3529.92385	0.46940	-4.6	0.0	0.0
^{1}A	-3528.32468	-3529.89116	0.47073	-3.6	18.8	22.4
^{5}A	-3528.28669	-3529.85216	0.46580	-4.0	39.2	43.4
^{2}[Co](H)$_2$	-3528.93819	-3530.50771	0.47511	-3.7	3.2	3.0
^{4}[Co](H)$_2$	-3528.92226	-3530.49172	0.47393	-4.9	11.3	11.1
^{2}[Co]	-3527.73943	-3529.29684	0.46070	-3.3	13.4	24.4
^{4}[Co]	-3527.72874	-3529.29021	0.46087	-3.2	20.4	28.9
H$_2$	-1.16721	-1.16137	-0.00148	-0.04	-	-
^{3}TS_1	-3927.77346	-3929.68765	0.56087	-5.0	3.3	3.8
^{3}Int_1	-3927.78044	-3929.68586	0.56207	-5.5	-0.9	5.1
^{3}TS_2	-3927.77993	-3929.68813	0.56210	-5.6	-0.7	3.6
^{3}Int_2	-3927.78997	-3929.69865	0.56307	-4.8	-5.5	-1.5
^{3}TS_3	-3927.78994	-3929.69958	0.56374	-4.7	-5.0	-1.7
^{3}B	-3927.84337	-3929.76444	0.56887	-4.1	-34.7	-38.6
^{3}B''	-3927.81660	-3929.73837	0.56638	-6.6	-22.0	-26.2
^{3}B'	-3927.82239	-3929.73736	0.56983	-2.4	-19.2	-19.2
^{3}TS_4	-4339.36635	-4341.61112	0.75048	-4.3	-23.8	-18.8
^{3}Int_3	-4339.36691	-4341.62197	0.74797	-4.7	-26.1	-27.6
^{3}TS_5	-4339.35741	-4341.61441	0.75410	-4.1	-15.7	-18.4
^{3}Int_4	-4339.35904	-4341.61621	0.75051	-4.0	-18.9	-21.7
^{3}TS_6	-4339.34401	-4341.60407	0.74956	-4.3	-10.3	-14.9
^{3}A	-3528.35176	-3529.92385	0.46940	-4.6	-13.2	-21.4
^{3}Int_5	-4339.31198	-4341.56422	0.74964	-4.4	9.7	9.9
^{1}Int_1	-3927.78980	-3929.69369	0.57300	-5.7	-0.1	6.9
^{1}B'	-3927.80135	-3929.72225	0.57235	-4.1	-6.2	-9.9
^{1}Int_4	-4339.31497	-4341.57667	0.75205	-3.7	10.0	4.4
^{1}Int_3	-4339.34567	-4341.60071	0.75706	-4.1	-6.5	-7.9
^{1}Int_5	-4339.31720	-4341.57200	0.75478	-4.5	9.5	8.2
^{1}Int_6	-4339.33251	-4341.58551	0.75589	-5.7	-0.6	-0.8
^{3}Int_7	-4339.35125	-4341.60685	0.75032	-4.3	-14.4	-16.2
^{3}TS_7	-4339.34254	-4341.60357	0.74917	-4.5	-9.9	-15.1
^{3}C	-4339.37030	-4341.63844	0.75086	-5.4	-27.1	-36.8
^{3}TS_8	-4750.91985	-4753.52175	0.93611	-4.7	-29.7	-36.9

^{3}Int_8	-4750.92447	-4753.52748	0.93082	-4.9	-36.1	-44.0
^{3}TS_9	-4750.91598	-4753.52181	0.93296	-4.6	-29.1	-38.8
^{3}Int_9	-4750.93723	-4753.54663	0.93687	-4.8	-40.2	-52.2
^{3}TS_10	-4750.90476	-4753.51332	0.92928	-5.6	-25.5	-36.9
^{3}A	-3528.35176	-3529.92385	0.46940	-4.6	-32.1	-44.7
^{3}Int_10	-4750.91957	-4753.53034	0.93598	-5.6	-30.5	-43.3
^{3}TS_11	-4750.88847	-4753.48603	0.93088	-5.7	-14.3	-18.8
^{3}Int_11	-4750.95315	-4753.55292	0.93589	-4.2	-50.2	-56.1
^{3}D	-4013.96929	-4015.97028	0.63492	-5.2	-81.3	-90.0
^{3}TS_12	-4425.50564	-4427.84393	0.81789	-4.4	-76.9	-85.4
^{3}Int_12	-4425.51212	-4427.85001	0.81687	-4.1	-81.3	-89.5
^{3}TS_13	-4425.50761	-4427.84496	0.81850	-4.0	-77.4	-85.3
^{3}Int_13	-4425.51638	-4427.85720	0.81647	-4.7	-84.9	-94.9
^{3}TS_14	-4425.49462	-4427.83436	0.81505	-4.7	-72.1	-81.5
^{3}A	-3528.35176	-3529.92385	0.46940	-4.6	-73.2	-83.2
^{3}Int_14	-4750.91519	-4753.52641	0.93338	-5.3	-29.1	-42.1
^{3}TS_15	-4750.87042	-4753.48011	0.92950	-4.7	-2.9	-14.9
^{3}Int_15	-4750.99121	-4753.59639	0.93978	-5.9	-73.4	-82.7
^{3}TS_16	-4750.97533	-4753.57257	0.93530	-5.4	-65.7	-70.0
^{3}E	-3853.84209	-3855.66949	0.58612	-3.5	-73.3	-76.8
^{3}TS_17	-4265.37429	-4267.53677	0.77041	-4.0	-66.7	-68.6
^{3}Int_16	-4265.38352	-4267.54662	0.77072	-4.1	-72.5	-74.7
^{3}TS_18	-4265.38074	-4267.54635	0.76849	-4.3	-72.2	-76.1
^{3}Int_17	-4265.39704	-4267.56836	0.77120	-4.1	-80.6	-88.0
^{3}TS_19	-4265.37577	-4267.55050	0.77057	-3.6	-67.2	-76.7
^{3}A	-3528.35176	-3529.92385	0.46940	-4.6	-73.2	-83.2
^{3}Int_18	-3853.79568	-3855.61574	0.58634	-4.1	-44.6	-43.5
^{3}TS_20	-3853.78837	-3855.61231	0.58437	-3.6	-40.8	-42.1

Table S4. Cartesian coordinates (in Å) and M06-L/def2-SVP electronic energies (in a.u.) of all optimized geometries

HBpin, -411.51434, NImag=0

C	-0.781325	-0.188248	0.051880
C	0.781343	-0.188202	-0.051901
C	-1.462165	-0.448038	-1.282173
O	-1.067188	1.189688	0.404522
C	-1.345169	-1.095616	1.123107
O	1.067132	1.189790	-0.404368
C	1.345272	-1.095411	-1.123224
C	1.462144	-0.448120	1.282136
H	0.987863	-0.822099	-2.122992
H	1.072479	-2.143685	-0.932714
H	2.441383	-1.032141	-1.133926
H	1.054445	0.195266	2.073963
H	2.534109	-0.228512	1.193337
H	1.354322	-1.494222	1.600493
H	-1.072329	-2.143850	0.932456
H	-2.441283	-1.032417	1.133860
H	-0.987735	-0.822391	2.122889
H	-1.054455	0.195399	-2.073954
H	-2.534121	-0.228396	-1.193330
H	-1.354396	-1.494113	-1.600632
B	-0.000060	1.934237	0.000072
H	-0.000129	3.125958	0.000018

PhNCO, -399.40591, NImag=0

C	0.000000	0.254311	0.000000
C	-1.247955	0.890660	0.000000
C	0.065987	-1.147455	0.000000
C	-2.413871	0.130888	0.000000
C	-1.107282	-1.894996	0.000000
C	-2.350910	-1.262410	0.000000
H	-1.283452	1.981188	0.000000
H	1.040805	-1.640245	0.000000
H	-3.382703	0.635256	0.000000
H	-1.047003	-2.985700	0.000000
H	-3.268066	-1.854668	0.000000
N	1.145665	1.034059	0.000000
C	2.350313	0.999540	0.000000
O	3.517885	1.100316	0.000000

TS-1, -810.88456, NImag=1

C	1.014679	-0.130118	0.216113
C	-0.243975	-0.401287	0.759380
C	1.751877	-1.129580	-0.423087
C	-0.765969	-1.687394	0.650147
C	1.218999	-2.412896	-0.517915
C	-0.039552	-2.694116	0.013523
H	-0.777781	0.402097	1.270816
H	2.732327	-0.900899	-0.847539
H	-1.748297	-1.905813	1.074555
H	1.792063	-3.197114	-1.017039
H	-0.453678	-3.701197	-0.066545
N	1.503080	1.198847	0.332531
C	2.707121	1.567312	0.468403
O	3.865383	1.595262	0.571109
C	-1.101771	3.776047	0.628488
C	-0.924024	3.479998	-0.902193
C	-0.713939	5.203871	0.989606
O	-0.145728	2.888622	1.225850
C	-2.475750	3.448551	1.175314
O	0.472149	3.170333	-0.993669
C	-1.221935	4.660761	-1.804960
C	-1.715954	2.263031	-1.360224
H	-0.552772	5.505515	-1.602581
H	-2.260897	5.001825	-1.682049
H	-1.086138	4.376973	-2.857467
H	-1.547177	1.399076	-0.702469
H	-1.388485	1.978033	-2.369352
H	-2.797533	2.458526	-1.397245
H	-3.252939	4.042507	0.671801
H	-2.522866	3.677202	2.248796
H	-2.721859	2.386370	1.050316
H	0.269193	5.466666	0.574399
H	-0.650540	5.296436	2.082154

(Bpin)$_2$O, -897.11472, NImag=0

C	-2.959415	0.665625	-0.558135
C	-3.423150	-0.415548	0.479393
C	-3.346480	0.310524	-1.985107
O	-1.520486	0.572671	-0.472879
C	-3.382619	2.080442	-0.228090
O	-2.338731	-1.367579	0.436019
C	-4.713188	-1.121010	0.122311
C	-3.484445	0.125859	1.899278
H	-4.636906	-1.654106	-0.832691
H	-5.546142	-0.405916	0.055614
H	-4.966790	-1.859141	0.894723
H	-2.562207	0.661574	2.164045
H	-3.598799	-0.710061	2.601838
H	-4.332243	0.809973	2.042915
H	-4.478609	2.162970	-0.187306
H	-3.023576	2.772969	-1.000979
H	-2.973332	2.415771	0.732063
H	-3.062625	-0.721722	-2.233086
H	-2.821562	0.977867	-2.681317
H	-4.426143	0.420028	-2.157722
B	-1.235951	-0.683867	-0.003282
O	-0.000013	-1.240596	-0.000473
C	3.422857	-0.414699	-0.480447
C	2.959704	0.664501	0.559378
C	3.483149	0.129349	-1.899371
O	2.338529	-1.366902	-0.438132
C	4.713161	-1.120693	-0.125478
O	1.520761	0.571727	0.474708
C	3.382808	2.079909	0.231705
C	3.347554	0.306696	1.985455
H	2.972868	2.416940	-0.727578
H	4.478780	2.162344	0.190243
H	3.024454	2.771094	1.006116
H	3.063852	-0.726025	2.231620
H	2.823030	0.972713	2.683230
H	4.427314	0.415891	2.157629
H	5.546053	-0.405602	-0.057933
H	4.966466	-1.857399	-0.899345
H	4.637422	-1.655436	0.828648
H	2.560667	0.665440	-2.162519
H	3.597139	-0.705250	-2.603557
H	4.330766	0.813836	-2.042297
B	1.235954	-0.683944	0.002950

3a, -810.96467, NImag=0

C	-2.653248	0.174390	-0.203186
C	-1.981376	-1.116937	0.373591
C	-2.962149	0.064351	-1.687468
O	-1.598974	1.158781	-0.064945
C	-3.867309	0.651863	0.561955
O	-0.581161	-0.889439	0.071549
C	-2.419963	-2.407777	-0.281141
C	-2.097418	-1.214280	1.885866
H	-2.198282	-2.420160	-1.354807
H	-3.500391	-2.564257	-0.149301
H	-1.900645	-3.260351	0.176103
H	-1.797816	-0.276101	2.373033
H	-1.434815	-2.009017	2.252683
H	-3.122353	-1.451974	2.202166
H	-4.659182	-0.111228	0.554572
H	-4.271675	1.560827	0.098060
H	-3.625687	0.891915	1.603813
H	-2.093636	-0.300030	-2.253813
H	-3.222475	1.056371	-2.078452
H	-3.806236	-0.611760	-1.881465
B	-0.428184	0.467362	-0.033837
N	0.895724	1.069380	-0.102447
C	1.083417	2.451368	-0.174131
O	0.221452	3.286478	-0.116095
H	2.167226	2.699909	-0.303955
C	2.063138	0.252028	-0.073855
C	3.110455	0.559686	0.802513
C	2.188621	-0.845756	-0.932570
C	4.271372	-0.211715	0.808793
C	3.343237	-1.622235	-0.909185
C	4.391670	-1.306604	-0.044357
H	3.003395	1.396761	1.496540
H	1.372923	-1.086337	-1.615733

H	-1.446247	5.939429	0.627488
B	0.896028	2.745552	0.281254
H	2.048106	3.232045	0.574235

TS-2, -1222.44318, NImag=1

C	0.689368	2.708401	-0.197603
C	2.199497	2.543221	0.181902
C	-0.216736	2.783829	1.018996
O	0.403619	1.448590	-0.862222
C	0.397091	3.836930	-1.160199
O	2.306087	1.103909	0.367122
C	2.609557	3.229323	1.464901
C	3.138066	2.911836	-0.954059
H	2.047210	2.853436	2.327524
H	2.447896	4.314564	1.393482
H	3.676904	3.062529	1.661367
H	2.838187	2.431801	-1.895793
H	4.155156	2.575535	-0.713824
H	3.168800	3.997611	-1.118516
H	0.684971	4.805190	-0.725587
H	-0.678066	3.873609	-1.379303
H	0.925392	3.712691	-2.112739
H	-0.021606	1.962248	1.721593
H	-1.261119	2.683424	0.700590
H	-0.101961	3.739026	1.549995
B	1.286102	0.556649	-0.355637
N	1.241038	-0.899111	-0.561005
C	0.141164	-1.547956	-1.027962
O	-0.846784	-0.923553	-1.572463
H	0.315732	-2.623259	-1.222765
C	2.344981	-1.716398	-0.145510
C	2.961393	-2.562142	-1.071096
C	2.783111	-1.691941	1.180256
C	4.010820	-3.386202	-0.669085
C	3.839404	-2.510228	1.572064
C	4.453568	-3.360245	0.652234
H	2.622845	-2.561248	-2.110265
H	2.293100	-1.029789	1.895053
H	4.489444	-4.044680	-1.397096
H	4.179956	-2.488506	2.609563
H	5.279113	-4.002568	0.965969
C	-3.945702	-1.211317	0.119948
C	-3.312440	0.197394	0.383520
C	-4.116546	-2.008796	1.406774
O	-2.943129	-1.842235	-0.681491
C	-5.243821	-1.183036	-0.661176
O	-1.927543	-0.127598	0.529228
C	-3.797007	0.877043	1.648021
C	-3.472614	1.121364	-0.819653
H	-3.537638	0.296227	2.541970
H	-4.888236	1.018857	1.630168
H	-3.337731	1.870329	1.753800
H	-3.173699	0.616686	-1.748631
H	-2.818375	1.996576	-0.699744
H	-4.505687	1.481846	-0.934926
H	-6.015534	-0.604366	-0.131180
H	-5.627038	-2.203720	-0.798115
H	-5.104484	-0.747487	-1.658106
H	-3.194800	-1.993008	2.005322
H	-4.338357	-3.055470	1.157574
H	-4.938828	-1.626692	2.029531
B	-1.712095	-1.246466	-0.327216
H	-0.855741	-2.027914	0.269346

TS-3, -1222.48114, NImag=1

C	-0.241761	2.210801	-0.958883
C	-0.695721	2.459469	0.524016
C	-1.370872	2.431747	-1.957843
O	0.075623	0.815141	-0.953218
C	0.991986	2.988410	-1.368509
O	-1.258299	1.187293	0.890970
C	-1.765265	3.523554	0.677172
C	0.466184	2.748320	1.461651
H	-2.679926	3.272538	0.125661
H	-1.404288	4.499204	0.318752
H	-2.035025	3.638328	1.736029
H	1.263009	2.000975	1.357895
H	0.107133	2.709553	2.498994
H	0.892000	3.747622	1.289129
H	0.826343	4.072759	-1.284379
H	1.250418	2.770573	-2.414445
H	1.854325	2.720785	-0.744189
H	-2.279040	1.885976	-1.663645
H	-1.062623	2.052376	-2.941488
H	5.080931	0.039987	1.497660
H	3.428081	-2.478544	-1.582242
H	5.298267	-1.915330	-0.033573

4a, -1222.53914, NImag=0

C	-0.835762	2.750675	-0.268378
C	-2.148575	2.588508	0.568894
C	-1.092758	3.297446	-1.663620
O	-0.402358	1.378970	-0.421218
C	0.248688	3.546461	0.424383
O	-2.630284	1.296834	0.131148
C	-3.209665	3.628736	0.285418
C	-1.882221	2.483228	2.062026
H	-3.532511	3.609455	-0.762276
H	-2.839176	4.638298	0.515741
H	-4.094559	3.447498	0.909732
H	-1.095498	1.747168	2.278166
H	-2.796572	2.152187	2.571320
H	-1.581364	3.447290	2.494959
H	-0.104361	4.562139	0.655767
H	1.130021	3.641145	-0.223541
H	0.569839	3.072862	1.359864
H	-1.899958	2.747914	-2.167717
H	-0.183756	3.187724	-2.270052
H	-1.362670	4.362474	-1.644885
B	-1.532712	0.598676	-0.304618
N	-1.501270	-0.796948	-0.615578
C	-0.243451	-1.327986	-1.059051
O	0.607068	-1.636430	0.032765
H	-0.425095	-2.251175	-1.631676
C	-2.533076	-1.707636	-0.295014
C	-2.229138	-3.023758	0.089213
C	-3.881160	-1.325045	-0.378813
C	-3.248730	-3.930200	0.370690
C	-4.890388	-2.236239	-0.082504
C	-4.585573	-3.545598	0.289543
H	-1.186828	-3.327408	0.200778
H	-4.131241	-0.309159	-0.683483
H	-2.988317	-4.947964	0.671870
H	-5.933295	-1.917884	-0.157401
H	-5.382115	-4.257684	0.515542
C	3.732961	-0.037254	-0.561558
C	4.018779	-0.912044	0.708387
C	3.436153	1.413235	-0.216694
O	2.503117	-0.612694	-1.052430
C	4.787482	-0.127060	-1.642483
O	2.688928	-1.268279	1.141635
C	4.721686	-0.179332	1.830442
C	4.747085	-2.204332	0.373934
H	4.131755	0.669331	2.196341
H	5.702401	0.194702	1.501737
H	4.888841	-0.856462	2.678604
H	4.262085	-2.733565	-0.458072
H	4.728883	-2.868472	1.247974
H	5.796990	-2.026782	0.102219
H	5.764355	0.210596	-1.266574
H	4.516232	0.514704	-2.491411
H	4.897589	-1.149841	-2.021947
H	2.689717	1.484600	0.586447
H	3.020094	1.915312	-1.100682
H	4.338258	1.957161	0.097007
B	1.883989	-1.182899	0.035513
H	0.246976	-0.594433	-1.713879

INT-1, -325.40444, NImag=0

N	-1.531165	-0.826220	-0.553325
C	-0.487625	-1.330280	-1.066218
H	-0.397345	-2.393926	-1.368678
C	-2.639614	-1.629454	-0.265577
C	-2.520630	-2.919738	0.277169
C	-3.919704	-1.097901	-0.487093
C	-3.659706	-3.664601	0.571156
C	-5.051895	-1.857623	-0.214265
C	-4.928127	-3.142606	0.318094
H	-1.527131	-3.319219	0.497283
H	-3.999130	-0.085017	-0.886962
H	-3.555348	-4.660997	1.007499
H	-6.042669	-1.438757	-0.405599
H	-5.819400	-3.729826	0.549404
H	0.390555	-0.693244	-1.240333

TS-4, -736.87528, NImag=1

C	2.011051	-0.502129	0.265497
C	1.913200	0.855656	0.607127

H	-1.629556	3.494543	-2.068416
B	-0.749951	0.214407	0.033040
N	-1.788737	-0.885125	-0.502472
C	-0.896760	-1.883435	-0.566687
O	0.139376	-0.987090	0.677060
H	-1.162588	-2.886220	-0.197898
C	-3.120058	-1.135589	-0.141865
C	-3.734675	-2.331763	-0.554990
C	-3.886604	-0.196572	0.569259
C	-5.060646	-2.601252	-0.229334
C	-5.216060	-0.472087	0.873744
C	-5.812898	-1.673158	0.488490
H	-3.175124	-3.041403	-1.170769
H	-3.417395	0.728982	0.898826
H	-5.514252	-3.538182	-0.561853
H	-5.794122	0.266932	1.434308
H	-6.856877	-1.878068	0.734293
C	3.474210	-1.378116	-0.519825
C	3.694073	-0.478331	0.745128
C	3.424031	-0.572188	-1.808030
O	2.135700	-1.889415	-0.299325
C	4.433826	-2.540368	-0.641810
O	2.346571	-0.047573	1.052208
C	4.552567	0.744570	0.506371
C	4.197796	-1.262745	1.945369
H	4.119551	1.407017	-0.252600
H	5.562293	0.456980	0.178737
H	4.654990	1.322166	1.434863
H	3.593603	-2.163729	2.119647
H	4.129744	-0.636543	2.844484
H	5.245669	-1.569880	1.823065
H	5.471044	-2.183408	-0.719891
H	4.212510	-3.121373	-1.546893
H	4.366154	-3.220301	0.215699
H	2.711499	0.260854	-1.725839
H	3.083810	-1.218478	-2.628155
H	4.410082	-0.171323	-2.080771
B	1.502152	-0.963140	0.490791
H	-0.095092	-1.854162	-1.313110

5a, -737.00214**,** NImag=0

C	2.132718	0.333622	-0.018835
C	2.175208	-1.056957	-0.244912
C	3.357757	1.000711	0.174073
C	3.387774	-1.736040	-0.265860
C	4.566010	0.306204	0.148498
C	4.596766	-1.067406	-0.069906
H	1.249553	-1.604402	-0.406192
H	3.380860	2.075060	0.353851
H	3.383436	-2.814408	-0.445214
H	5.496179	0.858603	0.304557
H	5.544728	-1.608844	-0.090154
N	0.919688	1.045578	0.002793
C	1.006230	2.491075	0.094007
H	1.623623	2.908130	-0.716914
H	1.445856	2.820212	1.049544
C	-2.126964	-0.967613	0.211879
C	-2.657142	0.450466	-0.180730
C	-2.251188	-1.247636	1.701193
O	-0.715977	-0.854145	-0.084896
C	-2.706916	-2.107219	-0.596525
O	-1.512666	1.285456	0.093705
C	-3.829497	0.935740	0.643634
C	-2.959239	0.570879	-1.666408
H	-3.577960	1.009229	1.708214
H	-4.690545	0.260096	0.536107
H	-4.143567	1.932615	0.306708
H	-2.124168	0.200221	-2.276995
H	-3.117899	1.626872	-1.921888
H	-3.863767	0.014366	-1.948493
H	-3.798528	-2.157931	-0.472975
H	-2.288536	-3.064511	-0.258346
H	-2.483874	-2.006274	-1.665220
H	-1.853927	-0.416542	2.300190
H	-1.673786	-2.146826	1.952809
H	-3.294468	-1.418840	2.000739
B	-0.395086	0.481376	-0.000015
H	0.004451	2.921798	0.019074

INT-2, -810.95616, NImag=0

N	-2.168839	-1.214010	-0.188433
C	-1.061058	-0.617001	-0.075458
O	0.089485	-1.297212	-0.224348
C	-3.353754	-0.483348	-0.109934
C	3.239356	-0.990250	-0.210789
C	3.003505	1.703169	0.447849
C	4.330100	-0.137827	-0.358991
C	4.217097	1.214493	-0.038389
H	0.963503	1.232157	0.986165
H	3.355178	-2.053774	-0.436344
H	2.906162	2.759010	0.711475
H	5.280993	-0.538281	-0.718810
H	5.074348	1.881202	-0.153337
N	0.904842	-1.338879	0.493393
C	0.714876	-2.386311	-0.286348
H	1.423579	-2.701285	-1.073921
H	0.034891	-3.171033	0.065392
C	-1.900290	0.785412	-0.596618
C	-2.390288	-0.166043	0.551257
C	-2.754782	0.664844	-1.850741
O	-0.591828	0.266358	-0.906876
C	-1.760931	2.237672	-0.191342
O	-1.788073	-1.417824	0.176459
C	-3.892411	-0.349591	0.610522
C	-1.851776	0.231943	1.917553
H	-4.285325	-0.791953	-0.312726
H	-4.400403	0.611373	0.779941
H	-4.160021	-1.018849	1.439288
H	-0.763037	0.372625	1.897560
H	-2.060185	-0.572844	2.635123
H	-2.319959	1.152801	2.293577
H	-2.731238	2.652429	0.119855
H	-1.397197	2.834385	-1.038771
H	-1.051785	2.369085	0.635028
H	-2.889873	-0.386521	-2.140781
H	-2.253516	1.179995	-2.680956
H	-3.749007	1.115597	-1.721131
B	-0.631449	-1.082026	-0.525555
H	-0.386799	-1.898334	-1.468786

TS-5, -810.87043, NImag=1

N	-2.048966	-1.380411	-0.534186
C	-0.830859	-1.296199	-0.526580
O	0.276154	-1.768217	-0.811377
C	-3.085112	-0.509307	-0.216367
C	-2.961189	0.873481	-0.421681
C	-4.277884	-1.034816	0.296851
C	-4.019326	1.716452	-0.093867
C	-5.327670	-0.180859	0.619081
C	-5.203101	1.195877	0.428458
H	-2.042043	1.276970	-0.852752
H	-4.360216	-2.113400	0.440199
H	-3.918020	2.791710	-0.257077
H	-6.253975	-0.596076	1.022189
H	-6.031084	1.861810	0.679720
C	2.768996	0.823470	-0.408443
C	2.978438	-0.277291	0.687378
C	2.506610	2.196087	0.192594
O	1.554752	0.382907	-1.053584
C	3.869414	0.895264	-1.444776
O	1.616631	-0.606724	1.043328
C	3.701195	0.197992	1.928410
C	3.632274	-1.532418	0.128743
H	3.153643	1.001444	2.435404
H	4.707885	0.565225	1.680009
H	3.813889	-0.628970	2.642219
H	3.139515	-1.864916	-0.795211
H	3.546645	-2.343718	0.863695
H	4.699502	-1.379055	-0.085344
H	4.837143	1.124036	-0.974429
H	3.655108	1.689652	-2.172242
H	3.966200	-0.045261	-1.999811
H	1.733970	2.149339	0.972868
H	2.151611	2.875695	-0.593628
H	3.413285	2.633138	0.634272
B	0.876134	-0.365381	-0.101658
H	-0.341969	0.022027	0.161763

TS-6, -1222.42053, NImag=1

N	1.114392	0.853338	-0.855914
C	-0.121377	0.927660	-0.386203
O	-1.111370	0.444040	-1.143770
C	2.077850	1.797799	-0.423169

C	-3.521677	0.760319	-0.743897
C	-4.438585	-1.034695	0.591824
C	-4.734191	1.439941	-0.655275
C	-5.641588	-0.343712	0.686775
C	-5.797377	0.896907	0.065033
H	-2.700408	1.175196	-1.334443
H	-4.308253	-2.010774	1.063456
H	-4.850908	2.401254	-1.161949
H	-6.472070	-0.782683	1.245164
H	-6.747916	1.430662	0.130298
C	2.866035	0.863681	0.425245
C	3.526841	-0.377371	-0.271408
C	3.005634	0.831524	1.937789
O	1.458466	0.664587	0.126514
C	3.298759	2.203063	-0.126664
O	2.472222	-1.369753	-0.200906
C	4.752549	-0.915908	0.431869
C	3.812703	-0.138781	-1.744867
H	4.527604	-1.248479	1.451862
H	5.541938	-0.152006	0.480955
H	5.154576	-1.777567	-0.116764
H	2.935815	0.271488	-2.264659
H	4.069212	-1.091994	-2.224854
H	4.652970	0.553534	-1.891528
H	4.382230	2.343668	-0.003098
H	2.793466	3.016231	0.410848
H	3.056172	2.305826	-1.190759
H	2.711904	-0.144200	2.349028
H	2.352124	1.593634	2.381998
H	4.035809	1.040530	2.256726
B	1.307604	-0.674842	-0.099059
H	-0.937534	0.459280	0.155767

TS-7, -1222.39480, NImag=1

N	0.886771	0.909515	0.849307
B	0.726481	-0.603600	0.192366
O	1.593742	-0.753068	-0.899970
C	2.049525	-2.115932	-0.856607
C	3.416149	-2.194112	-1.502814
C	0.173998	1.210068	1.862490
C	1.599761	1.980963	0.205148
C	0.952457	3.197348	-0.024647
C	1.640076	4.233496	-0.651407
C	2.961001	4.053859	-1.059151
C	3.592975	2.830861	-0.836538
C	2.919964	1.789172	-0.203266
O	0.915409	-1.640285	1.126859
C	2.030019	-2.420858	0.680357
C	3.278678	-1.921436	1.394499
C	1.782302	-3.875978	1.024213
C	1.044250	-2.967367	-1.621381
H	4.626511	2.681916	-1.156539
H	3.497598	4.866016	-1.553939
H	1.132558	5.183756	-0.830284
H	-0.092156	3.317577	0.272404
H	3.404583	0.829214	-0.033213
H	1.791924	-4.014829	2.113667
H	0.807177	-4.218037	0.658100
H	2.563473	-4.522677	0.597219
H	3.120498	-1.975978	2.479998
H	-0.509708	-0.541699	-0.160276
H	0.058261	-2.949445	-1.134652
C	2.082936	2.396777	0.844321
C	3.097540	2.116240	-1.328025
C	3.073418	3.314328	1.183099
C	4.089122	3.031441	-0.982972
C	4.079586	3.638078	0.272576
H	1.330810	2.117864	1.586453
H	3.083604	1.641445	-2.311516
H	3.068411	3.768674	2.176903
H	4.873529	3.274759	-1.703707
H	4.857344	4.355071	0.544534
C	-4.147215	0.614981	0.746387
C	-4.522553	-0.325335	-0.453575
C	-4.632727	2.040838	0.552342
O	-2.694013	0.649693	0.661803
C	-4.543172	0.090399	2.107571
O	-3.429761	-0.094195	-1.383682
C	-5.825668	0.018983	-1.138178
C	-4.477380	-1.797697	-0.082140
H	-5.815372	1.032137	-1.556547
H	-6.667325	-0.058315	-0.434934
H	-6.014164	-0.679780	-1.963427
H	-3.538747	-2.057360	0.426688
H	-4.539679	-2.405110	-0.994029
H	-5.313275	-2.078390	0.572915
H	-5.632832	-0.041376	2.171426
H	-4.246654	0.801828	2.889369
H	-4.064460	-0.869587	2.332402
H	-4.362568	2.428776	-0.439595
H	-4.170109	2.691527	1.305874
H	-5.722848	2.117055	0.663065
B	-2.389275	0.333609	-0.628172
H	-0.433727	1.665643	0.378205
C	2.223008	-2.363936	-0.528325
C	2.710018	-1.895641	0.886560
C	3.084494	-1.790758	-1.646330
O	0.917588	-1.771945	-0.605397
C	2.084010	-3.863848	-0.683056
O	2.131795	-0.585973	0.996362
C	4.213233	-1.766469	1.023826
C	2.141234	-2.758940	2.004046
H	4.616075	-1.014124	0.334131
H	4.714672	-2.726476	0.828963
H	4.475741	-1.452316	2.043354
H	1.056037	-2.890099	1.889129
H	2.320908	-2.267143	2.969666
H	2.606476	-3.754839	2.038551
H	3.045610	-4.370438	-0.511769
H	1.752930	-4.110076	-1.701210
H	1.344634	-4.276465	0.014211
H	3.250341	-0.713426	-1.510345
H	2.569939	-1.929561	-2.606634
H	4.064798	-2.285711	-1.705238
B	1.017077	-0.582259	0.130465
H	-0.081909	-0.326653	0.737977

^{3}**A**, -3528.35176, NImag=0

Co	0.027835	-0.833100	-1.529444
P	-1.801608	-0.052164	-0.529825
C	-1.713208	-0.650310	1.208579
C	-0.745961	-1.618173	1.526651
C	-2.514062	-0.157212	2.247760
C	-0.575446	-2.065033	2.838227
C	-2.351668	-0.591633	3.559892
C	-1.377256	-1.545517	3.851012
H	-3.261161	0.609324	2.023432
H	0.189909	-2.807070	3.068902
H	-2.981277	-0.184506	4.353457
H	-1.236849	-1.895259	4.876304
P	1.775985	0.049245	-0.433950
C	2.330175	-1.494238	0.416521
C	1.350978	-2.448478	0.728304
C	3.668273	-1.846788	0.626475
C	1.674712	-3.715410	1.199405
C	4.009641	-3.105320	1.121753
C	3.015938	-4.042261	1.399009
O	0.020827	-2.113582	0.485651
H	4.455733	-1.130257	0.376683
H	0.876908	-4.435265	1.391725
H	5.060428	-3.361053	1.273445
H	3.281781	-5.036668	1.763929
H	0.676425	-1.744954	-2.695806
C	1.714701	1.286426	0.917423
C	1.501526	0.920031	2.254656
C	1.705684	2.652730	0.588462

H	4.168158	-2.520113	1.150811
H	3.493636	-0.872348	1.147322
H	1.366267	-4.014899	-1.705833
H	0.926153	-2.564494	-2.636602
H	4.120216	-1.478750	-1.059249
H	3.842111	-3.203277	-1.401644
H	3.344322	-1.966797	-2.575081
B	-1.650614	-0.181288	0.693386
O	-2.130541	0.995423	0.114940
O	-2.560405	-1.218938	0.622270
C	-3.499919	0.738098	-0.261463
C	-3.526845	-0.823506	-0.376603
C	-3.801619	1.468351	-1.552759
H	-3.070891	1.232283	-2.335506
H	-4.804814	1.212212	-1.924596
H	-3.774660	2.554368	-1.390262
C	-4.384762	1.252211	0.864099
H	-4.166599	2.313467	1.043164
H	-5.453346	1.161661	0.622758
H	-4.195386	0.708811	1.800072
C	-3.020647	-1.315827	-1.725306
H	-2.862134	-2.401724	-1.679204
H	-3.737844	-1.112479	-2.532905
H	-2.062215	-0.848023	-1.993490
C	-4.859004	-1.458440	-0.043218
H	-5.163803	-1.246491	0.988379
H	-5.646902	-1.097155	-0.720533
H	-4.796873	-2.549282	-0.153325
H	-0.967199	-0.069879	1.742492
O	-0.147682	1.829254	2.797524

[1]A, -3528.32468, NImag=0

Co	-0.014351	0.378435	-1.282106
P	-1.886675	-0.035876	-0.460399
C	-2.376534	1.640496	0.131479
C	-1.317580	2.552764	0.241884
C	-3.676899	2.135609	0.283851
C	-1.519887	3.910954	0.446589
C	-3.901907	3.494304	0.515622
C	-2.829583	4.380074	0.588063
H	-4.524161	1.449913	0.194033
H	-0.669960	4.594612	0.470633
H	-4.923960	3.865149	0.619261
H	-3.004462	5.447306	0.738932
P	1.925938	0.018577	-0.608268
C	2.068530	1.233445	0.762729
C	0.963874	2.068815	0.992259
C	3.145172	1.300748	1.654265
C	0.891760	2.878954	2.123749
C	3.105813	2.130871	2.771757
C	1.967767	2.898854	3.012128
O	-0.034880	2.031082	0.014263
H	4.016378	0.663226	1.474137
H	0.009850	3.485327	2.327282
H	3.950082	2.164437	3.463186
H	1.908556	3.532517	3.899790
H	-0.014324	-0.777758	-2.232232
C	-3.395387	-0.654133	-1.300950
C	-3.399364	-0.616987	-2.700251
C	-4.521773	-1.145802	-0.626753
C	-4.516269	-1.043740	-3.416848
C	-5.638141	-1.573705	-1.342891
C	-5.637370	-1.520119	-2.737951
H	-2.497937	-0.264356	-3.212622
H	-4.520864	-1.199933	0.466915
H	-4.507951	-1.014825	-4.509091
H	-6.513379	-1.955192	-0.811074
H	-6.512014	-1.860961	-3.297374
C	-1.842902	-1.066178	1.054919
C	-1.755928	-0.509633	2.338182
C	-1.778316	-2.462662	0.917987
C	-1.630576	-1.330543	3.459335
C	-1.660032	-3.278722	2.037977
C	-1.589643	-2.716370	3.314272
C	1.271564	1.889037	3.231124
C	1.501685	3.619724	1.568192
C	1.274059	3.242298	2.893332
H	1.517673	-0.135589	2.540853
H	1.858416	2.961322	-0.450765
H	1.101469	1.581258	4.266160
H	1.506284	4.677413	1.292309
H	1.103184	4.001328	3.660516
C	3.269950	0.546694	-1.374132
C	3.343237	0.132777	-2.710913
C	4.327802	1.287055	-0.826730
C	4.458946	0.448319	-3.484211
C	5.439556	1.605099	-1.605099
C	5.507486	1.185257	-2.934194
H	2.506847	-0.443519	-3.123741
H	4.282639	1.618109	0.215287
H	4.506399	0.120413	-4.525458
H	6.259071	2.182789	-1.170353
H	6.379819	1.436621	-3.542511
C	-3.360821	-0.814086	-1.147919
C	-3.257950	-1.739397	-2.192843
C	-4.623560	-0.537814	-0.604281
C	-4.394186	-2.382502	-2.684704
C	-5.757758	-1.178513	-1.095819
C	-5.644177	-2.103779	-2.135928
H	-2.270835	-1.947285	-2.624503
H	-4.723830	0.193669	0.203480
H	-4.300357	-3.101161	-3.502190
H	-6.737597	-0.955483	-0.666567
H	-6.535791	-2.605092	-2.520252
C	-2.267420	1.706733	-0.332847
C	-1.687475	2.501121	0.667773
C	-3.106318	2.320356	-1.276073
C	-1.960727	3.865719	0.735874
C	-3.374102	3.685940	-1.207782
C	-2.805975	4.463271	-0.198851
H	-1.017581	2.050592	1.407125
H	-3.559634	1.722132	-2.071833
H	-1.504999	4.464033	1.529153
H	-4.034081	4.144430	-1.948156
H	-3.019853	5.533145	-0.142807

[5]A, -3528.28669, NImag=0

Co	0.061581	-0.324747	1.774953
P	1.873231	-0.002644	0.366027
C	2.140890	1.740929	-0.086274
C	1.050149	2.456561	-0.636008
C	3.259426	2.472853	0.348016
C	1.062184	3.846154	-0.701353
C	3.287119	3.862388	0.262464
C	2.186419	4.548787	-0.248314
H	4.110138	1.941920	0.780366
H	0.206463	4.395954	-1.088971
H	4.166853	4.410839	0.604780
H	2.192148	5.639549	-0.304126
P	-1.830448	0.003255	0.486013
C	-2.286983	1.413779	-0.598116
C	-1.265655	2.108215	-1.274100
C	-3.608768	1.849636	-0.780577
C	-1.563093	3.117379	-2.187210
C	-3.907892	2.901989	-1.641177
C	-2.887724	3.521227	-2.366066
O	0.019825	1.652566	-1.076150
H	-4.416344	1.343444	-0.245441
H	-0.761484	3.570250	-2.771964
H	-4.944549	3.220226	-1.767885
H	-3.118755	4.318398	-3.075533
H	0.214713	0.426841	3.174210
C	-1.788229	-1.393717	-0.704485
C	-1.726143	-2.685350	-0.156912
C	-1.762363	-1.236666	-2.092797
C	-1.679638	-3.801851	-0.989559
C	-1.682778	-2.358422	-2.924546
C	-1.653481	-3.637090	-2.375391
H	-1.716276	-2.803779	0.933964
H	-1.805164	-0.237227	-2.534407
H	-1.658526	-4.804210	-0.554491
H	-1.638686	-2.224795	-4.008289
H	-1.602430	-4.511521	-3.029577
C	-3.292782	-0.322319	1.509859
C	-4.426616	-0.999937	1.025698
C	-3.277225	0.120829	2.841739
C	-5.522555	-1.215335	1.862921
C	-4.373951	-0.094948	3.670075
C	-5.500636	-0.765343	3.180625

H	-1.797584	0.576946	2.466621
H	-1.817595	-2.911808	-0.079866
H	-1.573770	-0.881432	4.454245
H	-1.610472	-4.363478	1.913607
H	-1.494958	-3.358625	4.193303
C	1.989652	-1.610360	0.227687
C	1.790585	-1.775789	1.605449
C	2.129060	-2.756643	-0.573013
C	1.762479	-3.050660	2.169442
C	2.096888	-4.027844	-0.007631
C	1.919293	-4.180796	1.368936
H	1.651134	-0.902997	2.249903
H	2.263529	-2.647127	-1.653727
H	1.608469	-3.157949	3.246298
H	2.212309	-4.906931	-0.646821
H	1.896315	-5.178761	1.813526
C	3.606136	0.119876	-1.371775
C	4.705128	-0.648311	-0.963444
C	3.777592	1.037513	-2.416708
C	5.947032	-0.490132	-1.578204
C	5.018758	1.201843	-3.027155
C	6.107350	0.436189	-2.608440
H	4.589010	-1.381271	-0.158951
H	2.914526	1.621273	-2.754449
H	6.795924	-1.095641	-1.250449
H	5.135913	1.922299	-3.840491
H	7.080322	0.556041	-3.091058

^{2}[Co](H)$_2$, -3528.93819, NImag=0

Co	-0.004278	0.063734	-0.762911
P	-2.141893	0.003131	-0.436677
C	-2.230571	0.443572	1.357984
C	-1.086871	0.218460	2.146039
C	-3.340371	1.031501	1.971737
C	-1.038257	0.592052	3.487901
C	-3.318005	1.386998	3.320002
C	-2.164038	1.172087	4.070614
H	-4.232282	1.240732	1.373981
H	-0.121365	0.458919	4.063287
H	-4.195085	1.848374	3.777843
H	-2.126604	1.471405	5.120372
P	2.127961	0.091553	-0.409632
C	2.238573	-0.859759	1.172170
C	1.086676	-0.933777	1.976497
C	3.369924	-1.570704	1.585503
C	1.055689	-1.698884	3.141312
C	3.364172	-2.318343	2.762516
C	2.205059	-2.383167	3.533311
O	-0.015139	-0.298519	1.463876
H	4.265879	-1.558214	0.957685
H	0.133427	-1.784383	3.717331
H	4.258479	-2.866042	3.065967
H	2.181834	-2.988340	4.442279
H	0.227921	-1.453598	-1.099661
H	-0.234904	1.602479	-0.564111
C	3.035351	1.649080	-0.037175
C	2.501303	2.850926	-0.513843
C	4.235360	1.678470	0.687863
C	3.161332	4.058600	-0.286192
C	4.888444	2.885533	0.925204
C	4.353771	4.078310	0.434812
H	1.547633	2.820979	-1.050479
H	4.667911	0.749922	1.071731
H	2.735652	4.989999	-0.667398
H	5.819975	2.896334	1.496400
H	4.867377	5.024736	0.620933
C	3.321332	-0.814940	-1.468977
C	3.090269	-2.177946	-1.712044
C	4.410253	-0.192659	-2.091836
C	3.944070	-2.904399	-2.535676
C	5.257059	-0.920931	-2.929432
C	5.031005	-2.277462	-3.148749
H	2.222959	-2.661194	-1.251590
H	4.604150	0.870181	-1.926082
H	3.755944	-3.966923	-2.707833
H	6.100789	-0.420328	-3.410528
H	5.697244	-2.846978	-3.801088
C	-3.257182	1.239029	-1.201555
C	-3.057289	2.599342	-0.920117
C	-4.233154	0.881025	-2.140277
C	-3.835420	3.572269	-1.539785
C	-5.003332	1.859428	-2.770486
C	-4.811892	3.205502	-2.468031
H	-2.274473	2.890408	-0.213035
H	-4.396332	-0.171504	-2.386385
H	-4.448598	-1.358680	-0.007116
H	-2.385429	0.629682	3.223302
H	-6.398077	-1.744132	1.478821
H	-4.348235	0.255180	4.703831
H	-6.359747	-0.937721	3.832612
C	1.862837	-0.951612	-1.193315
C	1.666755	-2.335608	-1.108256
C	2.063827	-0.362721	-2.446801
C	1.698021	-3.123339	-2.254214
C	2.075994	-1.151054	-3.597024
C	1.901585	-2.531991	-3.502062
H	1.481401	-2.790690	-0.127126
H	2.216374	0.718071	-2.520074
H	1.551267	-4.203735	-2.176292
H	2.230854	-0.684778	-4.571673
H	1.919815	-3.148517	-4.403727
C	3.417253	-0.507335	1.183169
C	3.476654	-0.452864	2.583148
C	4.547795	-0.920980	0.461761
C	4.649122	-0.795460	3.251057
C	5.717564	-1.270123	1.135420
C	5.772258	-1.206582	2.528960
H	2.590463	-0.134191	3.144859
H	4.511979	-0.970125	-0.630569
H	4.685680	-0.747937	4.341504
H	6.594528	-1.591094	0.569212
H	6.690533	-1.479228	3.052532

^{4}[Co](H)$_2$, -3528.92226, NImag=0

Co	0.091384	-0.234946	1.829957
P	1.882102	-0.032976	0.360777
C	2.184762	1.704674	-0.108724
C	1.115412	2.423553	-0.681132
C	3.325792	2.412760	0.284224
C	1.166896	3.811408	-0.798626
C	3.401220	3.796564	0.135059
C	2.313755	4.490862	-0.386338
H	4.160171	1.871596	0.737484
H	0.318219	4.371016	-1.188940
H	4.300518	4.330789	0.446943
H	2.347502	5.578709	-0.478327
P	-1.792310	0.010107	0.498304
C	-2.232001	1.442437	-0.571012
C	-1.212625	2.096846	-1.286009
C	-3.550019	1.870912	-0.771503
C	-1.510223	3.076269	-2.235545
C	-3.850566	2.888576	-1.674528
C	-2.831602	3.475134	-2.422298
O	0.066331	1.638083	-1.091965
H	-4.358521	1.392529	-0.213188
H	-0.709094	3.502080	-2.840557
H	-4.886200	3.206640	-1.809782
H	-3.062236	4.244169	-3.162791
H	-0.054999	-1.762037	2.305257
H	0.254307	0.876161	2.974146
C	-1.862820	-1.381779	-0.690988
C	-1.879232	-2.681299	-0.157104
C	-1.833528	-1.218439	-2.081327
C	-1.902801	-3.788219	-1.000425
C	-1.841220	-2.331811	-2.921543
C	-1.886130	-3.616947	-2.385630
H	-1.866258	-2.816298	0.929039
H	-1.809096	-0.217260	-2.520179
H	-1.929118	-4.792955	-0.571328
H	-1.812808	-2.189261	-4.004628
H	-1.899354	-4.486951	-3.046952
C	-3.281519	-0.237793	1.527624
C	-4.449046	-0.862593	1.066266
C	-3.215976	0.199426	2.857634
C	-5.538839	-1.029015	1.918415
C	-4.310084	0.035898	3.705478
C	-5.471818	-0.576569	3.237064
H	-4.501751	-1.226354	0.035289
H	-2.288182	0.653910	3.224046
H	-6.444684	-1.518428	1.552542
H	-4.248764	0.377666	4.741173
H	-6.326480	-0.711632	3.904319
C	1.853682	-0.988915	-1.190925
C	1.534187	-2.351499	-1.089306
C	2.113355	-0.437647	-2.450581
C	1.502527	-3.151464	-2.227540
C	2.066344	-1.240213	-3.590673
C	1.768202	-2.597535	-3.480822
H	1.300844	-2.777758	-0.107125
H	2.359245	0.624595	-2.540512

H	-3.673584	4.626518	-1.302460
H	-5.758809	1.563116	-3.502126
H	-5.418379	3.970571	-2.958485
C	-3.140281	-1.545597	-0.503880
C	-4.471703	-1.603325	-0.063591
C	-2.531078	-2.711907	-0.975997
C	-5.176622	-2.803073	-0.098896
C	-3.239084	-3.914135	-1.014443
C	-4.560250	-3.962254	-0.575603
H	-4.968158	-0.699567	0.302727
H	-1.487072	-2.656375	-1.303640
H	-6.212711	-2.835617	0.246938
H	-2.752654	-4.818420	-1.388396
H	-5.114580	-4.903635	-0.603239

^{2}[Co], -3527.73943, NImag=0

Co	-0.153011	-0.427385	0.391411
P	-2.299248	-0.008719	0.533557
C	-1.650470	-0.714658	-1.024442
C	-0.435365	-0.144911	-1.569512
C	-2.040250	-1.979433	-1.551580
C	0.197777	-0.717757	-2.701304
C	-1.365968	-2.565384	-2.607511
C	-0.247254	-1.929621	-3.188515
H	-2.912967	-2.481953	-1.124631
H	1.069633	-0.220949	-3.135337
H	-1.718123	-3.518623	-3.008094
H	0.276004	-2.398866	-4.025057
P	1.958517	-0.062468	0.453636
C	2.131589	1.327587	-0.750472
C	1.003262	1.773884	-1.466499
C	3.353495	1.970950	-0.991621
C	1.100179	2.825698	-2.377487
C	3.457847	3.020543	-1.901228
C	2.325429	3.451346	-2.591901
O	-0.251075	1.239087	-1.270867
H	4.237821	1.657082	-0.429339
H	0.196484	3.141297	-2.902106
H	4.421825	3.507102	-2.064030
H	2.394473	4.277303	-3.303398
C	2.975783	-1.413824	-0.278954
C	2.289905	-2.531182	-0.772019
C	4.369596	-1.357861	-0.419380
C	2.977053	-3.569412	-1.398460
C	5.057395	-2.393941	-1.047746
C	4.362346	-3.499993	-1.540322
H	1.198687	-2.564293	-0.668428
H	4.926379	-0.504926	-0.019660
H	2.426103	-4.433617	-1.777798
H	6.143782	-2.339763	-1.152427
H	4.904730	-4.310892	-2.032553
C	3.010135	0.509202	1.849996
C	2.987215	1.852394	2.256102
C	3.724069	-0.412313	2.630997
C	3.677400	2.264802	3.393008
C	4.411049	0.000748	3.771084
C	4.394205	1.341121	4.154880
H	2.420684	2.585294	1.673688
H	3.746086	-1.467712	2.343380
H	3.653892	3.316957	3.687298
H	4.965426	-0.731909	4.362841
H	4.934879	1.665136	5.047073
C	-3.606868	-1.181364	1.023531
C	-3.208675	-2.342028	1.702853
C	-4.966464	-0.988787	0.744421
C	-4.145544	-3.298830	2.082328
C	-5.905529	-1.941404	1.138620
C	-5.498653	-3.097496	1.804049
H	-2.146232	-2.488493	1.928178
H	-5.292212	-0.090741	0.211921
H	-3.821020	-4.200979	2.606204
H	-6.963681	-1.781647	0.917633
H	-6.237314	-3.841996	2.110013
C	-3.196346	1.531831	0.148530
C	-3.317016	2.015261	-1.160096
C	-3.753737	2.270661	1.202984
C	-3.987540	3.212384	-1.408103
C	-4.433425	3.459296	0.951119
C	-4.548871	3.935155	-0.356183
H	-2.882447	1.445076	-1.985486
H	-3.656140	1.907199	2.230925
H	-4.076842	3.580072	-2.433370
H	-4.869841	4.021659	1.780104
H	-5.075714	4.871714	-0.553594
H	1.254187	-4.211639	-2.136941
H	2.271705	-0.801910	-4.570472
H	1.735683	-3.225020	-4.374959
C	3.444215	-0.543694	1.154688
C	3.505896	-0.491422	2.554062
C	4.562856	-0.976826	0.430560
C	4.677681	-0.850535	3.217611
C	5.730696	-1.340413	1.098306
C	5.790051	-1.274907	2.491101
H	2.622861	-0.166308	3.116569
H	4.518456	-1.030835	-0.661565
H	4.718219	-0.806895	4.308359
H	6.599483	-1.678565	0.528440
H	6.706359	-1.562545	3.012233

^{4}[Co], -3527.72874, NImag=0

Co	0.038151	-1.453652	-0.707973
P	-1.755546	-0.102101	-0.350553
C	-1.601137	1.545813	-1.129384
C	-0.524714	2.359347	-0.724551
C	-2.347842	1.952066	-2.242010
C	-0.193260	3.522865	-1.415803
C	-2.036920	3.124351	-2.930656
C	-0.956587	3.901301	-2.520485
H	-3.178556	1.330012	-2.584968
H	0.657885	4.126689	-1.097289
H	-2.634142	3.421901	-3.794730
H	-0.697713	4.814151	-3.061658
P	1.980971	-0.257365	-0.383551
C	2.458807	1.372073	0.318748
C	1.450401	2.301485	0.618268
C	3.784337	1.742565	0.584768
C	1.736847	3.533348	1.201723
C	4.084975	2.982169	1.146003
C	3.061876	3.875351	1.463471
O	0.143167	1.927715	0.392256
H	4.592705	1.043153	0.355959
H	0.914242	4.208702	1.446473
H	5.125077	3.246004	1.348936
H	3.293297	4.840684	1.918817
C	1.395070	-1.219197	1.029148
C	1.096754	-2.607388	0.703955
C	0.986693	-0.690426	2.272365
C	0.460306	-3.396920	1.716302
C	0.340003	-1.482922	3.205132
C	0.075545	-2.847785	2.916091
H	1.736186	-3.134524	-0.018874
H	1.184887	0.361556	2.501613
H	0.293336	-4.460396	1.523550
H	0.031128	-1.054400	4.161134
H	-0.423966	-3.470281	3.663758
C	3.592668	-0.969812	-0.867335
C	4.340879	-1.768152	0.010266
C	4.080296	-0.739820	-2.161915
C	5.557121	-2.314458	-0.399395
C	5.302233	-1.273812	-2.563797
C	6.041901	-2.065591	-1.682892
H	3.964917	-1.954583	1.021002
H	3.493928	-0.133941	-2.859904
H	6.131629	-2.936888	0.291106
H	5.676664	-1.078439	-3.571532
H	6.995530	-2.493667	-2.000847
C	-2.360688	0.206717	1.343074
C	-2.672342	-0.920046	2.118720
C	-2.482389	1.478916	1.916281
C	-3.115971	-0.777527	3.429882
C	-2.912159	1.617952	3.235126
C	-3.234936	0.492646	3.994541
H	-2.557848	-1.921261	1.689580
H	-2.250694	2.369771	1.327111
H	-3.356671	-1.666419	4.018697
H	-3.005826	2.616366	3.669532
H	-3.575370	0.606090	5.026420
C	-3.246523	-0.803484	-1.160348
C	-3.069435	-1.822587	-2.101929
C	-4.543146	-0.356255	-0.871145
C	-4.165945	-2.379838	-2.758449
C	-5.639275	-0.915209	-1.523799
C	-5.451832	-1.925574	-2.469694
H	-2.048115	-2.184611	-2.297227
H	-4.691532	0.434104	-0.128349
H	-4.015697	-3.176141	-3.491370
H	-6.647557	-0.563671	-1.291983
H	-6.314199	-2.364049	-2.977836

H_2, -1.16721, NImag=0

H	0.000000	0.000000	0.377177
H	0.000000	0.000000	-0.377177

^{3}TS_1, -3927.77346, NImag=1

Co	0.064054	-0.758182	-1.117735
P	1.143359	0.842339	-0.000058
C	1.589318	0.436352	1.742443
C	0.626059	-0.204583	2.549936
C	2.895560	0.511840	2.246640
C	0.950381	-0.740899	3.792643
C	3.226402	-0.011706	3.496129
C	2.255897	-0.644286	4.269421
H	3.681223	0.963505	1.636266
H	0.167265	-1.247057	4.360641
H	4.254476	0.063017	3.857816
H	2.513201	-1.069851	5.241743
P	-2.065214	-0.435600	-0.419033
C	-2.405392	0.720751	0.965709
C	-1.552404	0.627799	2.079565
C	-3.322252	1.778618	0.946034
C	-1.632059	1.515543	3.149339
C	-3.404749	2.685205	2.002978
C	-2.568348	2.546626	3.108663
O	-0.647725	-0.408818	2.067920
H	-3.972997	1.909055	0.077644
H	-0.952738	1.401670	3.997446
H	-4.124880	3.505020	1.957837
H	-2.634009	3.249994	3.942082
H	-0.032820	-1.909829	-2.250721
C	3.259189	-2.463396	-0.270374
C	4.479210	-1.932224	0.169467
C	3.091172	-2.809468	-1.620268
C	5.522482	-1.752238	-0.733796
C	4.145256	-2.627640	-2.510590
C	5.362690	-2.102785	-2.074456
H	4.590725	-1.675724	1.224762
H	2.125359	-3.191846	-1.958680
H	6.470255	-1.335075	-0.385404
H	4.008984	-2.899181	-3.560354
H	6.184901	-1.962759	-2.780010
N	2.247608	-2.656102	0.656982
C	1.081789	-2.965525	0.745564
O	-0.019234	-3.267905	1.010630
C	0.279789	2.462953	0.086383
C	-0.480547	2.811598	-1.037877
C	0.358236	3.357817	1.157962
C	-1.137020	4.036696	-1.101571
C	-0.306637	4.583255	1.098530
C	-1.049410	4.926925	-0.030133
H	-0.565044	2.095395	-1.862958
H	0.931505	3.090612	2.052165
H	-1.728417	4.291254	-1.984719
H	-0.248446	5.271980	1.945299
H	-1.569625	5.886858	-0.071019
C	2.725283	1.388816	-0.766484
C	3.154966	0.708781	-1.911059
C	3.455330	2.503208	-0.325142
C	4.303426	1.115491	-2.590087
C	4.608897	2.901577	-0.995223
C	5.035710	2.206717	-2.129349
H	2.572276	-0.146118	-2.273463
H	3.112350	3.071379	0.545317
H	4.623290	0.573578	-3.483327
H	5.171773	3.768174	-0.639863
H	5.935712	2.527693	-2.659461
C	-3.246809	0.076596	-1.723865
C	-2.726447	0.471468	-2.961730
C	-4.638122	0.032729	-1.554225
C	-3.574709	0.852958	-4.000905
C	-5.486705	0.412054	-2.591537
C	-4.955761	0.828874	-3.813923
H	-1.641394	0.443870	-3.114861
H	-5.057306	-0.307895	-0.602076
H	-3.155674	1.155920	-4.963296
H	-6.569543	0.375696	-2.449533
H	-5.623374	1.122207	-4.627689
C	-2.808084	-2.008581	0.159453
C	-3.355812	-2.194807	1.432811
C	-2.758649	-3.092556	-0.729447
C	-3.843583	-3.445446	1.812171
C	-3.258219	-4.334848	-0.352329
C	-3.797500	-4.516617	0.922201
H	-3.401790	-1.361416	2.139235
H	-2.294363	-2.956971	-1.711694

^{3}Int_1, -3927.78044, NImag=0

Co	0.425828	-0.897857	-0.008331
P	0.994205	1.327352	-0.050043
C	0.618047	2.373125	1.417615
C	-0.623133	2.236567	2.063003
C	1.546691	3.259603	1.981323
C	-0.919043	2.932225	3.232197
C	1.253993	3.972996	3.142072
C	0.023799	3.801397	3.774650
H	2.524904	3.382708	1.509002
H	-1.891144	2.772987	3.702319
H	1.996547	4.656433	3.558878
H	-0.204834	4.345676	4.693478
P	-1.873880	-0.955226	-0.053341
C	-2.698353	0.646948	-0.358736
C	-2.295318	1.715009	0.463165
C	-3.491440	0.941065	-1.474051
C	-2.631857	3.033850	0.167299
C	-3.851098	2.255475	-1.771874
C	-3.409815	3.298212	-0.959487
O	-1.561091	1.363794	1.565653
H	-3.808951	0.130671	-2.135860
H	-2.279332	3.843210	0.810890
H	-4.462999	2.465758	-2.651529
H	-3.671237	4.331317	-1.200012
H	0.554373	-2.441537	-0.288220
C	3.380358	-2.794360	0.582317
C	4.130927	-3.958476	0.822831
C	3.505408	-2.168645	-0.673079
C	4.963744	-4.483582	-0.159808
C	4.343139	-2.698013	-1.649684
C	5.076176	-3.859011	-1.403468
H	4.039966	-4.438493	1.799492
H	2.955677	-1.243197	-0.864794
H	5.534390	-5.392294	0.048782
H	4.430090	-2.187481	-2.612986
H	5.735700	-4.269849	-2.171229
N	2.601024	-2.288489	1.608236
C	1.519459	-1.647030	1.508413
O	0.701356	-1.011143	2.168449
C	-2.560990	-2.015856	-1.374873
C	-1.729203	-2.367724	-2.444404
C	-3.885763	-2.472899	-1.358418
C	-2.218959	-3.142039	-3.495445
C	-4.372203	-3.253470	-2.404717
C	-3.540834	-3.584490	-3.476302
H	-0.679888	-2.051948	-2.430848
H	-4.538533	-2.215459	-0.518150
H	-1.560745	-3.413527	-4.323879
H	-5.404983	-3.609332	-2.382957
H	-3.923479	-4.199493	-4.294296
C	-2.626796	-1.614347	1.469137
C	-3.747874	-1.039842	2.078954
C	-2.030831	-2.744727	2.045534
C	-4.276032	-1.598436	3.241923
C	-2.566089	-3.303194	3.202984
C	-3.688452	-2.731497	3.803302
H	-4.211449	-0.150221	1.641848
H	-1.138835	-3.177458	1.582066
H	-5.152059	-1.144943	3.711993
H	-2.095813	-4.184049	3.645723
H	-4.102743	-3.167431	4.715491
C	0.412990	2.338681	-1.458718
C	-0.245729	1.694175	-2.511593
C	0.605733	3.725970	-1.517963
C	-0.699369	2.420094	-3.612245
C	0.151901	4.450718	-2.616539
C	-0.500633	3.798278	-3.665020
H	-0.414091	0.611891	-2.456361
H	1.113709	4.240128	-0.695905
H	-1.218878	1.906436	-4.424585
H	0.306337	5.531597	-2.656355
H	-0.858928	4.369631	-4.524629
C	2.818076	1.416197	-0.148242
C	3.490874	1.756217	-1.328510
C	3.557197	0.931352	0.944646
C	4.877340	1.618896	-1.411436
C	4.938852	0.799392	0.857070
C	5.602893	1.139853	-0.322916
H	2.930799	2.124751	-2.192621
H	3.043053	0.642417	1.867191

H	-4.263969	-3.581214	2.811801
H	-3.213829	-5.171949	-1.053279
H	-4.179250	-5.495508	1.222294

^{3}TS_2, -3927.77993, NImag=1

Co	0.415222	-0.845021	0.079476
P	1.004032	1.349990	-0.047005
C	0.603091	2.418534	1.396291
C	-0.652460	2.301014	2.017312
C	1.529697	3.301661	1.968244
C	-0.965891	3.016181	3.169977
C	1.219871	4.033612	3.112841
C	-0.025791	3.883577	3.720170
H	2.519902	3.404977	1.516207
H	-1.948689	2.872284	3.622364
H	1.960905	4.713789	3.537549
H	-0.268388	4.442581	4.626481
P	-1.865114	-0.932657	-0.047463
C	-2.663478	0.666081	-0.428030
C	-2.278530	1.752423	0.378975
C	-3.412569	0.937154	-1.578876
C	-2.591468	3.065670	0.035750
C	-3.748396	2.246224	-1.924426
C	-3.326282	3.306503	-1.124668
O	-1.587626	1.426286	1.516710
H	-3.713251	0.112171	-2.230484
H	-2.253702	3.889049	0.669432
H	-4.325498	2.438199	-2.831379
H	-3.568505	4.335046	-1.402031
H	0.579077	-2.419094	0.088505
C	3.274926	-2.850814	0.644279
C	4.021763	-4.022129	0.866648
C	3.358948	-2.243535	-0.625356
C	4.804603	-4.571252	-0.143024
C	4.146445	-2.797461	-1.630470
C	4.872238	-3.965859	-1.399946
H	3.966072	-4.488444	1.852636
H	2.824622	-1.305022	-0.803490
H	5.371897	-5.484796	0.053811
H	4.202577	-2.298861	-2.602344
H	5.493800	-4.395781	-2.188628
N	2.542614	-2.319582	1.689546
C	1.437645	-1.706268	1.577399
O	0.656958	-1.037564	2.256759
C	0.480859	2.349065	-1.486541
C	-0.145801	1.695759	-2.553461
C	0.687847	3.733797	-1.557059
C	-0.553248	2.410573	-3.679202
C	0.279926	4.447321	-2.680753
C	-0.340381	3.786164	-3.743245
H	-0.325839	0.615944	-2.488950
H	1.170474	4.255023	-0.724233
H	-1.047604	1.890521	-4.503092
H	0.445528	5.526186	-2.729520
H	-0.662161	4.348705	-4.622877
C	2.830972	1.395999	-0.090164
C	3.516013	0.869726	1.018840
C	3.553815	1.742783	-1.238253
C	4.896013	0.703542	0.978161
C	4.938563	1.571102	-1.273484
C	5.610920	1.050688	-0.169804
H	2.960874	0.573505	1.915085
H	3.035156	2.142770	-2.114131
H	5.412195	0.279768	1.842407
H	5.492979	1.842801	-2.174917
H	6.692881	0.905703	-0.205525
C	-2.477256	-2.029511	-1.375714
C	-3.807419	-2.465957	-1.444068
C	-1.569418	-2.446682	-2.356523
C	-4.223216	-3.289639	-2.487587
C	-1.987139	-3.266435	-3.404222
C	-3.314575	-3.686897	-3.470493
H	-4.519352	-2.158853	-0.671166
H	-0.518371	-2.143931	-2.275913
H	-5.260959	-3.628391	-2.532876
H	-1.269732	-3.589564	-4.161862
H	-3.641871	-4.336615	-4.285654
C	-2.694592	-1.557775	1.449731
C	-3.830135	-0.959845	2.008277
C	-2.137761	-2.688018	2.064110
C	-4.409936	-1.495867	3.157587
C	-2.724352	-3.224150	3.206691
C	-3.860520	-2.629096	3.755998
H	-4.263998	-0.069807	1.542380
H	-1.234304	-3.139676	1.643466
H	5.391248	1.885971	-2.337911
H	5.497546	0.409253	1.710661
H	6.686368	1.022410	-0.394900

^{3}Int_2, -3927.78997, NImag=0

Co	0.190452	-0.651956	-1.011632
P	1.027464	1.260936	-0.079049
C	1.349935	1.369990	1.734147
C	0.380294	0.867872	2.619879
C	2.539122	1.859274	2.294484
C	0.586207	0.833406	3.996364
C	2.752528	1.841275	3.671706
C	1.779178	1.321870	4.524194
H	3.317771	2.252267	1.635134
H	-0.196438	0.417182	4.633678
H	3.688429	2.229417	4.079088
H	1.946785	1.296154	5.603106
P	-1.987430	-0.803245	-0.230482
C	-2.600535	0.667130	0.657140
C	-1.793354	1.162880	1.697256
C	-3.676773	1.451861	0.226995
C	-2.021861	2.415006	2.262585
C	-3.926962	2.698854	0.798357
C	-3.090775	3.182969	1.802612
O	-0.785598	0.332001	2.115359
H	-4.311673	1.091715	-0.587229
H	-1.358726	2.785977	3.047451
H	-4.765233	3.301573	0.443114
H	-3.267073	4.169729	2.236845
H	-0.099722	0.040679	-2.371208
C	2.667193	-2.616239	-0.644063
C	2.578084	-2.962326	0.713926
C	3.823321	-2.950426	-1.369220
C	3.628070	-3.630894	1.335592
C	4.865044	-3.621430	-0.735185
C	4.776980	-3.965263	0.615656
H	1.676574	-2.679548	1.266990
H	3.891080	-2.663558	-2.420923
H	3.550328	-3.890970	2.394324
H	5.762322	-3.877384	-1.304875
H	5.600101	-4.490608	1.104853
N	1.608307	-1.929267	-1.229008
C	1.607377	-1.201073	-2.309297
O	2.180331	-0.979544	-3.337465
C	-2.131248	-2.176445	0.972120
C	-1.352348	-3.317683	0.736248
C	-2.945346	-2.127855	2.110673
C	-1.401508	-4.399783	1.612441
C	-2.989730	-3.209818	2.988286
C	-2.221095	-4.347447	2.739795
H	-0.688176	-3.348178	-0.135077
H	-3.541532	-1.232923	2.315601
H	-0.786568	-5.281791	1.418489
H	-3.626291	-3.162729	3.875221
H	-2.255352	-5.192204	3.431739
C	-3.312250	-1.144970	-1.444960
C	-3.074865	-0.859121	-2.795024
C	-4.555455	-1.667798	-1.060723
C	-4.073066	-1.076481	-3.744720
C	-5.548339	-1.887285	-2.012167
C	-5.309166	-1.588966	-3.355011
H	-2.092341	-0.474498	-3.089602
H	-4.746921	-1.906270	-0.009913
H	-3.878571	-0.851927	-4.795971
H	-6.513798	-2.296518	-1.705329
H	-6.088740	-1.764563	-4.100193
C	2.686753	1.481328	-0.806983
C	2.914945	2.376279	-1.859505
C	3.703567	0.581881	-0.446355
C	4.138290	2.378376	-2.528542
C	4.924596	0.590474	-1.113485
C	5.144109	1.487644	-2.159561
H	2.127353	3.068769	-2.168969
H	3.537478	-0.140477	0.359989
H	4.301002	3.078010	-3.351608
H	5.701857	-0.119841	-0.821327
H	6.098146	1.486951	-2.691574
C	0.183735	2.858999	-0.406635
C	0.585405	4.050574	0.213882
C	-0.892523	2.882184	-1.299901
C	-0.077998	5.243894	-0.058866
C	-1.556823	4.078339	-1.571002
C	-1.151844	5.258930	-0.951573
H	1.424332	4.044001	0.916817
H	-1.200365	1.946596	-1.779297

H	-5.296605	-1.023819	3.587761
H	-2.283452	-4.104944	3.678721
H	-4.315633	-3.046336	4.657392

^{3}TS_3, -3927.78994, NImag=1

Co	0.204060	-0.672386	-0.959911
P	1.012211	1.268235	-0.072123
C	1.309644	1.413905	1.742631
C	0.335579	0.916292	2.626060
C	2.486563	1.927148	2.307431
C	0.526297	0.908421	4.005172
C	2.684226	1.936242	3.687082
C	1.707344	1.420232	4.537597
H	3.268149	2.317211	1.649789
H	-0.258862	0.494593	4.640928
H	3.610684	2.342827	4.098044
H	1.862845	1.415524	5.618616
P	-1.979595	-0.823863	-0.223805
C	-2.618241	0.655376	0.630955
C	-1.828480	1.175218	1.672793
C	-3.694905	1.424271	0.174145
C	-2.073782	2.434852	2.213686
C	-3.961979	2.678810	0.721035
C	-3.142493	3.186553	1.727366
O	-0.819442	0.360369	2.118586
H	-4.316593	1.045552	-0.641849
H	-1.423874	2.824300	3.000650
H	-4.800281	3.268652	0.344858
H	-3.332095	4.179032	2.142516
H	-0.036557	-0.080097	-2.376118
C	2.719128	-2.605824	-0.637724
C	2.658029	-2.954618	0.721416
C	3.865579	-2.929062	-1.383236
C	3.724538	-3.614457	1.323729
C	4.923997	-3.592062	-0.768562
C	4.863311	-3.938362	0.583063
H	1.764997	-2.678144	1.291334
H	3.913416	-2.639638	-2.435127
H	3.668101	-3.875843	2.383525
H	5.813220	-3.839384	-1.354510
H	5.699527	-4.457139	1.056843
N	1.642507	-1.927090	-1.199180
C	1.622398	-1.193971	-2.277825
O	2.201528	-0.960295	-3.300218
C	-2.128381	-2.177941	1.000128
C	-1.328237	-3.311196	0.799574
C	-2.965094	-2.121753	2.121777
C	-1.379150	-4.378859	1.693223
C	-3.011001	-3.189044	3.017184
C	-2.221442	-4.319361	2.803375
H	-0.647090	-3.346779	-0.058453
H	-3.577674	-1.232111	2.299719
H	-0.748101	-5.255041	1.526515
H	-3.665244	-3.136023	3.890821
H	-2.257116	-5.152560	3.509130
C	-3.285475	-1.197295	-1.450053
C	-3.031746	-0.935235	-2.801908
C	-4.530043	-1.722506	-1.073579
C	-4.014637	-1.178230	-3.761272
C	-5.507734	-1.967897	-2.034416
C	-5.252097	-1.693158	-3.379227
H	-2.048286	-0.549029	-3.091087
H	-4.734542	-1.942906	-0.021300
H	-3.806979	-0.972065	-4.813766
H	-6.474157	-2.379066	-1.733258
H	-6.019674	-1.889119	-4.131741
C	2.679377	1.495407	-0.780372
C	2.920046	2.386331	-1.833395
C	3.694628	0.602768	-0.398895
C	4.153884	2.390433	-2.483124
C	4.925911	0.613328	-1.046617
C	5.157620	1.506013	-2.093986
H	2.134723	3.074059	-2.158776
H	3.518887	-0.116308	0.408347
H	4.326496	3.086698	-3.307046
H	5.701522	-0.092069	-0.738562
H	6.119781	1.506820	-2.611167
C	0.154154	2.848225	-0.444846
C	0.526504	4.058149	0.157820
C	-0.902918	2.836742	-1.360971
C	-0.146934	5.235825	-0.155492
C	-1.577191	4.017191	-1.672974
C	-1.201203	5.216397	-1.071220
H	1.350368	4.078107	0.878188
H	-1.187989	1.885999	-1.824914
H	0.243647	6.168226	0.427209
H	-2.400053	4.083885	-2.266154
H	-1.673585	6.195601	-1.162823

^{3}B, -3927.84337, NImag=0

Co	0.308379	-0.863962	-0.517169
P	0.963415	1.241658	0.012198
C	1.002867	1.847879	1.750671
C	-0.067215	1.526797	2.606535
C	2.082543	2.551353	2.304529
C	-0.053486	1.869409	3.956418
C	2.100427	2.909847	3.651321
C	1.035361	2.561929	4.480976
H	2.931083	2.813198	1.666464
H	-0.903702	1.580939	4.577602
H	2.954610	3.457984	4.054415
H	1.049243	2.830697	5.539523
P	-1.857447	-0.937063	-0.070412
C	-2.664257	0.654594	0.332623
C	-2.079991	1.430526	1.349653
C	-3.660776	1.247336	-0.451640
C	-2.450497	2.755932	1.561057
C	-4.048612	2.570412	-0.242980
C	-3.436084	3.324733	0.755394
O	-1.134594	0.802375	2.124634
H	-4.119899	0.671311	-1.259793
H	-1.959501	3.337627	2.344768
H	-4.819537	3.016889	-0.874423
H	-3.722211	4.367309	0.912080
H	2.774234	-1.493501	-3.068156
C	3.055390	-2.506211	-0.562552
C	3.056308	-2.668706	0.836699
C	4.139357	-3.039369	-1.287936
C	4.103617	-3.309241	1.488712
C	5.184722	-3.678658	-0.627711
C	5.181951	-3.816936	0.761408
H	2.209680	-2.256820	1.398918
H	4.165180	-2.956460	-2.376309
H	4.077954	-3.413983	2.576569
H	6.015769	-4.082252	-1.212447
H	6.005746	-4.322492	1.269580
N	1.983621	-1.827386	-1.119301
C	1.929991	-1.344162	-2.356615
O	0.925295	-0.684182	-2.710035
C	0.102326	2.594326	-0.878916
C	0.237723	3.944045	-0.527636
C	-0.693181	2.245662	-1.976765
C	-0.412897	4.929376	-1.266326
C	-1.338996	3.234533	-2.718041
C	-1.201421	4.575421	-2.363009
H	0.856900	4.225799	0.330072
H	-0.792841	1.188071	-2.244090
H	-0.303839	5.980134	-0.986501
H	-1.957413	2.953000	-3.573850
H	-1.711205	5.349924	-2.941370
C	2.700167	1.422908	-0.534598
C	3.045500	2.085007	-1.719338
C	3.684262	0.678792	0.135890
C	4.348561	2.010277	-2.213553
C	4.982584	0.606081	-0.357079
C	5.318382	1.271707	-1.537890
H	2.289519	2.649519	-2.271668
H	3.425054	0.127325	1.045454
H	4.603125	2.529983	-3.140432
H	5.727309	0.006708	0.173025
H	6.334659	1.207976	-1.933793
C	-2.933696	-1.616102	-1.389889
C	-2.417928	-1.645541	-2.692717
C	-4.227912	-2.098377	-1.151280
C	-3.196537	-2.131344	-3.743710
C	-4.999842	-2.588099	-2.202226
C	-4.485960	-2.601616	-3.500381
H	-1.395867	-1.293790	-2.877577
H	-4.634419	-2.091850	-0.135069
H	-2.787491	-2.149911	-4.756557
H	-6.007235	-2.964210	-2.008009
H	-5.092514	-2.987797	-4.323164
C	-2.221416	-2.001179	1.377811
C	-1.367427	-3.089075	1.604331
C	-3.276279	-1.766876	2.268142
C	-1.578611	-3.942742	2.685146
C	-3.483739	-2.617496	3.352678
C	-2.638803	-3.708055	3.560693
H	-0.524467	-3.258581	0.922801
H	-3.934947	-0.905831	2.115728

H	0.151402	6.175060	0.316688
H	-2.405069	3.996024	-2.386038
H	-1.730595	6.140969	-1.314247

^{3}B'', -3927.81660, NImag=0

Co	-0.127463	-0.474832	-0.780875
P	1.730328	0.818687	-0.346298
C	2.042588	0.725377	1.464382
C	0.931261	0.524855	2.300174
C	3.305715	0.781708	2.066642
C	1.059680	0.374443	3.676260
C	3.447707	0.643571	3.446490
C	2.327822	0.438328	4.252055
H	4.191505	0.925862	1.442038
H	0.164335	0.200666	4.276692
H	4.442624	0.689482	3.894169
H	2.439248	0.319551	5.331802
P	-2.292308	-0.337925	-0.233077
C	-2.284670	1.223226	0.736662
C	-1.188075	1.433351	1.597245
C	-3.196088	2.271005	0.569161
C	-0.996935	2.646684	2.251303
C	-3.021851	3.489271	1.226578
C	-1.920334	3.674605	2.058713
O	-0.316378	0.373261	1.712909
H	-4.050219	2.132438	-0.100092
H	-0.122905	2.791492	2.889890
H	-3.743274	4.295606	1.079964
H	-1.766249	4.630936	2.563696
H	-0.895514	-2.173517	-2.911579
C	1.509605	-2.872248	-0.694404
C	1.610990	-2.544557	0.677082
C	2.514243	-3.700083	-1.243651
C	2.675362	-2.978966	1.460299
C	3.577991	-4.126563	-0.452197
C	3.679274	-3.768276	0.895731
H	0.800694	-1.954617	1.123487
H	2.442708	-3.989774	-2.290409
H	2.717118	-2.698695	2.517218
H	4.352088	-4.755372	-0.902192
H	4.520801	-4.113814	1.500800
N	0.448424	-2.299782	-1.385376
C	-0.007668	-2.783111	-2.568258
O	0.388971	-3.726199	-3.235526
C	-2.787473	-1.600442	0.991557
C	-2.291464	-2.899547	0.815882
C	-3.595515	-1.312803	2.100483
C	-2.621287	-3.902552	1.725910
C	-3.918328	-2.318137	3.009883
C	-3.434116	-3.613652	2.821521
H	-1.627000	-3.111033	-0.028655
H	-3.969841	-0.295502	2.254361
H	-2.228702	-4.911653	1.582845
H	-4.548511	-2.088730	3.872635
H	-3.685270	-4.399077	3.538347
C	-3.726389	-0.128732	-1.342863
C	-3.488616	0.442652	-2.601177
C	-5.030374	-0.512153	-1.004179
C	-4.536954	0.654256	-3.493009
C	-6.077162	-0.309694	-1.902636
C	-5.834224	0.277768	-3.143929
H	-2.465003	0.711513	-2.884715
H	-5.228880	-0.976553	-0.034064
H	-4.338422	1.099929	-4.470260
H	-7.090164	-0.615871	-1.631296
H	-6.656373	0.432165	-3.846436
C	3.392610	0.730822	-1.088635
C	3.892874	1.732834	-1.931445
C	4.141093	-0.443905	-0.903203
C	5.124888	1.568805	-2.564197
C	5.372769	-0.597778	-1.532012
C	5.868223	0.406844	-2.364875
H	3.318213	2.647603	-2.099555
H	3.756892	-1.243882	-0.262906
H	5.503999	2.356986	-3.219011
H	5.940733	-1.517940	-1.375208
H	6.831628	0.280283	-2.864118
C	1.226180	2.576951	-0.518556
C	1.919469	3.623886	0.105122
C	0.058180	2.866581	-1.233667
C	1.451094	4.932034	0.009258
C	-0.415065	4.174120	-1.325846
C	0.282125	5.208103	-0.703324
H	2.829815	3.410605	0.674545
H	-0.493453	2.040564	-1.700323
H	-0.907119	-4.788850	2.848500
H	-4.309073	-2.426124	4.042899
H	-2.802362	-4.372362	4.412515

^{3}B', -3927.82239, NImag=0

Co	0.001509	-0.581971	-0.523991
P	-2.284618	-0.507840	-0.335984
C	-2.919241	1.080488	-1.037130
C	-2.036424	2.174811	-1.025738
C	-4.195135	1.290701	-1.576953
C	-2.392205	3.420130	-1.535891
C	-4.568765	2.535142	-2.082738
C	-3.668774	3.600408	-2.064198
H	-4.911764	0.465198	-1.593072
H	-1.662347	4.232300	-1.514533
H	-5.571537	2.672947	-2.492838
H	-3.957082	4.574500	-2.465022
P	1.761711	0.730416	-0.047927
C	0.989863	2.016781	1.014514
C	-0.297850	2.450826	0.636023
C	1.511910	2.491078	2.222339
C	-1.054562	3.285520	1.453630
C	0.772365	3.343301	3.041995
C	-0.511939	3.726162	2.660142
O	-0.750261	1.961025	-0.565821
H	2.509706	2.168876	2.533630
H	-2.065487	3.572704	1.157330
H	1.196760	3.699013	3.982963
H	-1.108127	4.373886	3.307074
H	0.235443	-4.377821	0.495314
C	1.921564	-2.802186	-0.610610
C	2.442490	-2.205765	-1.778702
C	2.774024	-3.653765	0.121197
C	3.744526	-2.448859	-2.201504
C	4.072465	-3.905086	-0.314694
C	4.571024	-3.307589	-1.473991
H	1.780687	-1.552902	-2.360060
H	2.421435	-4.087769	1.060171
H	4.114642	-1.967867	-3.111697
H	4.716069	-4.561608	0.277995
H	5.594239	-3.503762	-1.802615
N	0.637765	-2.454520	-0.214699
C	-0.156853	-3.328402	0.429063
O	-1.259116	-3.050989	0.905510
C	-2.411879	-0.085410	1.447138
C	-3.502391	0.614837	1.978103
C	-1.299874	-0.338209	2.262056
C	-3.479453	1.056675	3.300115
C	-1.267522	0.124589	3.575500
C	-2.358142	0.821155	4.096111
H	-4.371989	0.826083	1.347597
H	-0.464067	-0.920508	1.854943
H	-4.337250	1.597230	3.707731
H	-0.389046	-0.062870	4.198235
H	-2.333967	1.182336	5.127214
C	-3.613553	-1.697108	-0.691792
C	-4.189458	-2.470139	0.323920
C	-3.985428	-1.933688	-2.023999
C	-5.144395	-3.435524	0.012766
C	-4.943494	-2.896774	-2.330467
C	-5.528428	-3.648186	-1.310784
H	-3.868854	-2.329665	1.358358
H	-3.521298	-1.357080	-2.830705
H	-5.585803	-4.033532	0.813412
H	-5.228573	-3.066260	-3.371519
H	-6.276587	-4.407525	-1.549933
C	3.082917	0.006737	0.970520
C	2.737177	-0.534848	2.220869
C	4.366076	-0.236606	0.462885
C	3.662138	-1.269827	2.955364
C	5.286866	-0.981804	1.197579
C	4.941573	-1.495936	2.445379
H	1.729002	-0.381569	2.619380
H	4.644997	0.139020	-0.525146
H	3.378225	-1.679025	3.927847
H	6.278572	-1.172029	0.780358
H	5.664113	-2.082824	3.017182
C	2.591647	1.707905	-1.352428
C	2.125619	1.571925	-2.664770
C	3.630679	2.609895	-1.084957
C	2.693396	2.314389	-3.699297
C	4.202644	3.346837	-2.118935
C	3.735623	3.198853	-3.426669
H	1.299642	0.879638	-2.863173
H	3.995667	2.731822	-0.060312

H	1.997561	5.742145	0.498128
H	-1.336129	4.381722	-1.875904
H	-0.087526	6.234211	-0.769066

^{3}TS_4, -4339.36635, NImag=1

Co	-0.044975000	-0.395643000	-0.212467000
P	2.112554000	0.522585000	-0.527254000
C	2.708335000	1.257118000	1.073004000
C	1.727208000	1.839760000	1.890822000
C	4.028421000	1.297895000	1.539129000
C	2.021301000	2.426699000	3.117736000
C	4.345254000	1.892814000	2.760310000
C	3.344869000	2.456764000	3.551349000
H	4.827581000	0.868867000	0.929827000
H	1.211562000	2.847800000	3.718373000
H	5.384660000	1.916930000	3.094907000
H	3.591715000	2.916391000	4.510796000
P	-2.038967000	0.600425000	0.632028000
C	-1.672833000	2.399587000	0.712210000
C	-0.374770000	2.772751000	1.111809000
C	-2.546789000	3.412045000	0.304112000
C	0.049844000	4.098269000	1.094431000
C	-2.138920000	4.746295000	0.285489000
C	-0.843025000	5.082632000	0.673088000
O	0.419356000	1.721170000	1.469331000
H	-3.559734000	3.149843000	-0.012077000
H	1.073425000	4.348970000	1.380610000
H	-2.835426000	5.522462000	-0.037424000
H	-0.513131000	6.123724000	0.642494000
H	0.070465000	-1.557563000	-4.035178000
C	-1.801172000	-1.635121000	-2.395630000
C	-2.478048000	-2.336792000	-1.377637000
C	-2.446350000	-1.524546000	-3.646536000
C	-3.740418000	-2.881422000	-1.591296000
C	-3.699909000	-2.092107000	-3.859853000
C	-4.363309000	-2.768207000	-2.835147000
H	-1.982320000	-2.440128000	-0.409425000
H	-1.974646000	-0.946907000	-4.445437000
H	-4.245072000	-3.404049000	-0.772778000
H	-4.177639000	-1.980365000	-4.837587000
H	-5.355853000	-3.193001000	-3.001233000
N	-0.571067000	-1.036274000	-2.118088000
C	0.338008000	-0.982009000	-3.109525000
O	1.417838000	-0.391331000	-3.063799000
C	0.721126000	-3.899937000	0.523279000
C	1.915801000	-3.745222000	1.518037000
C	1.133094000	-3.711636000	-0.925394000
O	-0.107218000	-2.754225000	0.890149000
C	-0.102441000	-5.154869000	0.701194000
O	2.000998000	-2.300962000	1.676167000
C	3.234294000	-4.271000000	0.997341000
C	1.612968000	-4.314502000	2.894676000
H	3.523222000	-3.800795000	0.050156000
H	3.178133000	-5.357693000	0.837317000
H	4.033157000	-4.082310000	1.728018000
H	0.646385000	-3.953379000	3.273504000
H	2.389784000	-3.994756000	3.601481000
H	1.591585000	-5.413061000	2.886072000
H	0.512937000	-6.051355000	0.536819000
H	-0.921685000	-5.173584000	-0.030227000
H	-0.544666000	-5.217586000	1.703013000
H	1.720525000	-2.789574000	-1.065379000
H	0.237687000	-3.630643000	-1.556308000
H	1.729318000	-4.560771000	-1.287019000
B	0.756308000	-1.805848000	1.392243000
H	0.363591000	-0.709954000	1.744571000
C	1.787333000	2.109541000	-1.400178000
C	0.548500000	2.295989000	-2.025426000
C	2.694179000	3.176318000	-1.354429000
C	0.215807000	3.529273000	-2.581427000
C	2.368587000	4.404909000	-1.927539000
C	1.125573000	4.585160000	-2.535230000
H	-0.158242000	1.459665000	-2.060535000
H	3.662964000	3.046463000	-0.861272000
H	-0.762102000	3.666324000	-3.050353000
H	3.086796000	5.227903000	-1.892461000
H	0.865433000	5.552568000	-2.972238000
C	3.659930000	-0.148705000	-1.219985000
C	4.324540000	-1.162165000	-0.513402000
C	4.161614000	0.257973000	-2.462010000
C	5.482203000	-1.741513000	-1.030685000
C	5.320269000	-0.321974000	-2.973445000
C	5.985244000	-1.320407000	-2.261461000
H	3.929310000	-1.493112000	0.451856000
H	3.627271000	1.014933000	-3.039288000
H	2.321539	2.200801	-4.720116
H	5.015780	4.044399	-1.904468
H	4.185834	3.779198	-4.235495

^{3}Int_3, -4339.36691, NImag=0

Co	-0.047357000	0.332884000	-0.114469000
P	-2.108752000	-0.753754000	-0.449850000
C	-2.653320000	-1.297289000	1.223199000
C	-1.635191000	-1.732606000	2.088558000
C	-3.954305000	-1.239765000	1.735076000
C	-1.889208000	-2.134198000	3.395799000
C	-4.227525000	-1.641087000	3.043232000
C	-3.200712000	-2.097981000	3.868851000
H	-4.765325000	-0.879623000	1.096511000
H	-1.062074000	-2.453222000	4.033582000
H	-5.251522000	-1.595771000	3.420370000
H	-3.414458000	-2.411460000	4.892958000
P	2.079071000	-0.527203000	0.500721000
C	1.788428000	-2.297978000	0.921401000
C	0.531003000	-2.654758000	1.446718000
C	2.715332000	-3.322999000	0.697586000
C	0.206861000	-3.980191000	1.730189000
C	2.410123000	-4.651616000	0.988323000
C	1.154426000	-4.974786000	1.499683000
O	-0.343699000	-1.615605000	1.612054000
H	3.691108000	-3.073276000	0.271369000
H	-0.787268000	-4.229510000	2.106166000
H	3.149875000	-5.433577000	0.806566000
H	0.898962000	-6.015104000	1.714282000
H	-0.003092000	1.825912000	-3.795263000
C	1.689380000	1.973753000	-1.966246000
C	2.208895000	2.698641000	-0.875809000
C	2.474632000	1.908012000	-3.136957000
C	3.437696000	3.347423000	-0.958844000
C	3.696415000	2.570472000	-3.217101000
C	4.190192000	3.297489000	-2.132809000
H	1.602071000	2.773171000	0.027810000
H	2.138522000	1.294898000	-3.976858000
H	3.808096000	3.903320000	-0.091931000
H	4.286250000	2.491514000	-4.134951000
H	5.155517000	3.805164000	-2.198454000
N	0.471658000	1.303610000	-1.833030000
C	-0.317646000	1.192411000	-2.922847000
O	-1.323896000	0.490726000	-3.016461000
C	-1.250009000	4.222772000	0.841036000
C	-2.603109000	3.524734000	1.195381000
C	-1.096156000	4.486907000	-0.648074000
O	-0.292650000	3.191291000	1.189040000
C	-0.946270000	5.464257000	1.648981000
O	-2.304797000	2.130611000	0.921848000
C	-3.779126000	3.963162000	0.351615000
C	-2.942715000	3.614513000	2.674535000
H	-3.598325000	3.823085000	-0.720442000
H	-4.001629000	5.026598000	0.523768000
H	-4.674258000	3.383916000	0.616646000
H	-2.086682000	3.325644000	3.299834000
H	-3.769096000	2.927538000	2.900591000
H	-3.253861000	4.628415000	2.962775000
H	-1.715785000	6.233193000	1.487232000
H	0.018754000	5.888734000	1.341669000
H	-0.890916000	5.250836000	2.723302000
H	-1.322963000	3.587163000	-1.238957000
H	-0.055539000	4.762431000	-0.866141000
H	-1.745619000	5.305639000	-0.987798000
B	-0.938294000	1.989193000	1.011363000
H	-0.373155000	0.961596000	1.454066000
C	-1.610499000	-2.386915000	-1.141841000
C	-2.178191000	-3.602476000	-0.734098000
C	-0.540573000	-2.412191000	-2.047814000
C	-1.694323000	-4.813650000	-1.227894000
C	-0.053585000	-3.624031000	-2.534248000
C	-0.628620000	-4.827477000	-2.126046000
H	-2.993680000	-3.608267000	-0.003762000
H	-0.099558000	-1.464226000	-2.371700000
H	-2.145770000	-5.752906000	-0.898131000
H	0.782349000	-3.628666000	-3.239098000
H	-0.242385000	-5.776772000	-2.504793000
C	-3.684534000	-0.337420000	-1.277308000
C	-4.669100000	-1.297544000	-1.542214000
C	-3.905216000	0.988626000	-1.662542000
C	-5.862491000	-0.932893000	-2.163560000
C	-5.100302000	1.354247000	-2.277184000
C	-6.081408000	0.395471000	-2.527941000
H	-4.504044000	-2.343359000	-1.266934000
H	-3.119549000	1.723927000	-1.484098000

H	5.991974000	-2.527835000	-0.467006000
H	5.701743000	0.003402000	-3.944247000
H	6.892151000	-1.773972000	-2.668500000
C	-3.693775000	0.576271000	-0.135216000
C	-4.876028000	0.324413000	0.570256000
C	-3.755889000	0.788200000	-1.520952000
C	-6.098325000	0.282237000	-0.101859000
C	-4.976647000	0.753405000	-2.186131000
C	-6.151658000	0.496548000	-1.477532000
H	-4.845788000	0.159806000	1.650656000
H	-2.832481000	0.969367000	-2.081779000
H	-7.015525000	0.082682000	0.457570000
H	-5.007523000	0.908268000	-3.267099000
H	-7.109412000	0.457114000	-2.001727000
C	-2.316150000	0.110066000	2.370724000
C	-2.140803000	0.978046000	3.454661000
C	-2.609818000	-1.240249000	2.621912000
C	-2.256712000	0.506163000	4.762429000
C	-2.738523000	-1.705202000	3.927274000
C	-2.556157000	-0.833511000	5.002639000
H	-1.913820000	2.033229000	3.276923000
H	-2.729466000	-1.933771000	1.783045000
H	-2.115457000	1.193855000	5.599805000
H	-2.973338000	-2.757221000	4.106789000
H	-2.646386000	-1.200252000	6.027715000

^{3}TS_5, -4339.35741, NImag=1

Co	-0.141947	0.166771	0.117089
P	-2.174735	-0.926536	-0.218703
C	-2.585105	-1.845430	1.322844
C	-1.532843	-2.179799	2.192251
C	-3.891514	-2.086176	1.771353
C	-1.758196	-2.707961	3.460579
C	-4.131238	-2.639315	3.028234
C	-3.067132	-2.945237	3.875220
H	-4.735120	-1.827828	1.126742
H	-0.909184	-2.918968	4.113646
H	-5.158286	-2.820765	3.351598
H	-3.252645	-3.360446	4.868115
P	1.996531	-0.557102	0.467838
C	1.895163	-2.336181	0.955368
C	0.723032	-2.804523	1.574257
C	2.905817	-3.265786	0.678925
C	0.574779	-4.150160	1.917325
C	2.774199	-4.609238	1.021698
C	1.605019	-5.045534	1.641342
O	-0.258770	-1.864382	1.765552
H	3.808733	-2.929663	0.161087
H	-0.350859	-4.504018	2.372941
H	3.577726	-5.312946	0.796466
H	1.481164	-6.097979	1.906866
H	-0.589620	2.698178	-2.947541
C	1.350563	2.209119	-1.525918
C	2.248415	2.824556	-0.635588
C	1.815828	1.922145	-2.825662
C	3.531818	3.176149	-1.047810
C	3.093171	2.293623	-3.235560
C	3.960225	2.935187	-2.352660
H	1.918064	3.065680	0.372248
H	1.171888	1.364609	-3.511839
H	4.203469	3.657837	-0.330926
H	3.420843	2.052113	-4.250372
H	4.966979	3.217381	-2.670152
N	0.038073	1.838238	-1.151160
C	-0.899200	1.979072	-2.142402
O	-1.984454	1.427205	-2.197083
C	-0.889799	4.529257	0.924001
C	-2.316712	3.877481	0.913498
C	-0.500170	5.127312	-0.420324
O	-0.046098	3.393456	1.187237
C	-0.672859	5.550239	2.022741
O	-2.050193	2.534814	0.482405
C	-3.293030	4.515665	-0.055326
C	-2.930205	3.787146	2.303877
H	-2.957375	4.415966	-1.095083
H	-3.436535	5.583681	0.167570
H	-4.275163	4.027671	0.019274
H	-2.230717	3.330695	3.017780
H	-3.825744	3.151568	2.263858
H	-3.230052	4.770908	2.692762
H	-1.376813	6.390030	1.925873
H	0.344312	5.960657	1.960657
H	-0.793688	5.110226	3.019887
H	-0.668468	4.425859	-1.247130
H	0.568794	5.380431	-0.414438

H	-6.622025000	-1.691232000	-2.368320000
H	-5.261323000	2.393531000	-2.575189000
H	-7.015396000	0.681596000	-3.017720000
C	3.389817000	-0.646515000	-0.762276000
C	3.128595000	-1.411304000	-1.911198000
C	4.579447000	0.087106000	-0.692125000
C	4.048614000	-1.459417000	-2.953202000
C	5.495233000	0.042821000	-1.742961000
C	5.236789000	-0.731254000	-2.871885000
H	2.197048000	-1.981478000	-1.979973000
H	4.789694000	0.709319000	0.182025000
H	3.834476000	-2.064892000	-3.837552000
H	6.415404000	0.628582000	-1.678331000
H	5.957003000	-0.762541000	-3.692860000
C	2.934866000	0.118527000	1.988697000
C	2.549587000	1.362094000	2.504292000
C	3.970187000	-0.589870000	2.615610000
C	3.197141000	1.893205000	3.620295000
C	4.613548000	-0.059090000	3.730468000
C	4.228763000	1.185422000	4.233357000
H	1.735152000	1.919827000	2.032992000
H	4.276140000	-1.565808000	2.226478000
H	2.888321000	2.865151000	4.011891000
H	5.419263000	-0.619326000	4.210904000
H	4.734341000	1.600810000	5.108451000

^{3}Int_4, -4339.35904, NImag=0

Co	0.028546	0.152672	0.133254
P	-2.010262	-0.904663	-0.250987
C	-2.303219	-2.231658	1.010505
C	-1.182728	-2.816234	1.619053
C	-3.562665	-2.691792	1.423288
C	-1.291317	-3.789686	2.608084
C	-3.689474	-3.676042	2.401919
C	-2.554889	-4.222180	3.001554
H	-4.462578	-2.268875	0.969936
H	-0.380298	-4.194242	3.054107
H	-4.683760	-4.015270	2.700366
H	-2.651747	-4.985281	3.776789
P	2.156878	-0.634146	0.426971
C	1.963103	-2.376011	-0.128841
C	0.811751	-3.049860	0.321000
C	2.776434	-3.023321	-1.064847
C	0.457596	-4.302974	-0.172903
C	2.442034	-4.284839	-1.558097
C	1.278541	-4.913464	-1.120528
O	0.072516	-2.367913	1.254059
H	3.680465	-2.524769	-1.423941
H	-0.459897	-4.787519	0.166927
H	3.088512	-4.770780	-2.291605
H	0.997432	-5.891276	-1.518439
H	-0.764764	2.953698	-2.646994
C	1.322159	2.594656	-1.229183
C	2.229019	2.836009	-0.180416
C	1.740928	2.913201	-2.536158
C	3.472216	3.406243	-0.426839
C	2.979213	3.508852	-2.770293
C	3.854467	3.767194	-1.719348
H	1.952933	2.569456	0.838947
H	1.112709	2.666816	-3.393939
H	4.155805	3.568009	0.410947
H	3.268400	3.746350	-3.797729
H	4.832465	4.216706	-1.905389
N	0.071969	1.980172	-0.972433
C	-0.862050	2.050219	-1.995237
O	-1.739731	1.239937	-2.203040
C	-1.144591	4.446370	1.047394
C	-2.474232	3.614155	0.997947
C	-0.851889	5.177798	-0.257361
O	-0.158741	3.426985	1.235720
C	-1.053540	5.422189	2.204702
O	-2.047588	2.362403	0.455817
C	-3.547604	4.186924	0.092399
C	-3.040638	3.354221	2.388458
H	-3.206501	4.249086	-0.948987
H	-3.858239	5.191243	0.419200
H	-4.433701	3.536362	0.104947
H	-2.277997	2.919524	3.050315
H	-3.870985	2.638815	2.314579
H	-3.428419	4.268519	2.860811
H	-1.863898	6.165519	2.162986
H	-0.099397	5.965509	2.165016
H	-1.102216	4.909533	3.172989
H	-0.949476	4.520287	-1.130901
H	0.181962	5.550489	-0.241560

H	-1.065333	6.045538	-0.634280
B	-0.700100	2.257536	0.698664
H	-0.399966	1.237442	1.399625
C	-1.500191	-2.192672	-1.361735
C	-1.168063	-3.497987	-0.979944
C	-1.203764	-1.770008	-2.671259
C	-0.524845	-4.356020	-1.872882
C	-0.585433	-2.638738	-3.566321
C	-0.230341	-3.929611	-3.166738
H	-1.419955	-3.856263	0.022031
H	-1.477189	-0.755486	-2.979818
H	-0.261004	-5.367486	-1.553423
H	-0.368740	-2.300512	-4.583023
H	0.269114	-4.604133	-3.866368
C	-3.834884	-0.583418	-0.899906
C	-4.552592	-1.565928	-1.593963
C	-4.412028	0.673665	-0.685338
C	-5.840068	-1.298605	-2.057273
C	-5.702096	0.932234	-1.143469
C	-6.417900	-0.049956	-1.828541
H	-4.104616	-2.548537	-1.772303
H	-3.822862	1.444026	-0.182263
H	-6.393141	-2.069224	-2.599776
H	-6.147831	1.916531	-0.977993
H	-7.426298	0.160424	-2.193482
C	3.112848	-0.703464	-0.974338
C	2.605025	-1.417776	-2.072307
C	4.385740	-0.135022	-1.064018
C	3.365350	-1.581258	-3.223962
C	5.146134	-0.298129	-2.223956
C	4.644058	-1.023030	-3.301220
H	1.602665	-1.856705	-2.014983
H	4.787382	0.449416	-0.232256
H	2.957576	-2.146595	-4.066156
H	6.138430	0.156047	-2.284167
H	5.244299	-1.148632	-4.205568
C	3.031015	0.150249	1.810832
C	2.588845	1.300685	2.474675
C	4.238794	-0.442929	2.207093
C	3.350553	1.858330	3.502171
C	4.997850	0.114630	3.232341
C	4.555334	1.269468	3.880211
H	1.640310	1.764366	2.188641
H	4.591897	-1.350109	1.707925
H	2.994138	2.757972	4.009203
H	5.938194	-0.355551	3.529914
H	5.150747	1.706329	4.685589

^{3}TS_6, -4339.34401, NImag=1

Co	0.191679000	0.359446000	-0.133731000
P	2.469435000	0.319917000	-0.015372000
C	2.613146000	-1.243674000	-0.964279000
C	1.862312000	-2.346294000	-0.510551000
C	3.280229000	-1.371740000	-2.190578000
C	1.785393000	-3.531586000	-1.237121000
C	3.207429000	-2.551095000	-2.928984000
C	2.457898000	-3.626778000	-2.453298000
H	3.852003000	-0.522609000	-2.574214000
H	1.182050000	-4.361862000	-0.860862000
H	3.727798000	-2.624844000	-3.885071000
H	2.386504000	-4.548760000	-3.035031000
P	-1.388650000	-1.252507000	-0.456577000
C	-1.124829000	-2.709021000	0.651678000
C	0.184144000	-2.991444000	1.085986000
C	-2.154513000	-3.508308000	1.169999000
C	0.456767000	-4.012824000	1.993444000
C	-1.894142000	-4.535146000	2.073096000
C	-0.586755000	-4.792083000	2.488944000
O	1.225268000	-2.174925000	0.698269000
H	-3.185913000	-3.313679000	0.861818000
H	1.491660000	-4.174655000	2.305604000
H	-2.718402000	-5.140656000	2.456342000
H	-0.379072000	-5.592731000	3.201291000
H	1.186033000	1.797806000	2.809710000
C	-1.151691000	1.113552000	2.534431000
C	-2.352043000	1.488333000	3.148633000
C	-0.561191000	-0.110998000	2.865480000
C	-2.967716000	0.627879000	4.054713000
C	-1.179643000	-0.964489000	3.777438000
C	-2.389571000	-0.604356000	4.369959000
H	-2.806998000	2.448144000	2.893759000
H	0.382614000	-0.399616000	2.388819000
H	-3.909142000	0.924128000	4.521996000
H	-0.715172000	-1.927099000	4.012019000
H	-2.880122000	-1.275994000	5.074675000

H	-1.524006	6.034969	-0.408462
B	-0.651498	2.238856	0.646762
H	-0.261689	1.253061	1.390810
C	-3.687015	-0.209627	-0.430437
C	-4.327589	-0.110647	-1.669131
C	-4.318378	0.313691	0.706283
C	-5.590039	0.474910	-1.763075
C	-5.583337	0.885408	0.613626
C	-6.224640	0.966437	-0.623957
H	-3.828953	-0.477470	-2.569097
H	-3.808216	0.273667	1.673637
H	-6.078942	0.548099	-2.737432
H	-6.067137	1.281424	1.510566
H	-7.215863	1.420010	-0.699834
C	-1.744933	-1.953501	-1.736276
C	-2.562478	-3.049869	-2.039116
C	-0.614708	-1.710468	-2.526892
C	-2.252761	-3.887001	-3.109124
C	-0.296667	-2.553554	-3.589396
C	-1.115892	-3.643655	-3.881292
H	-3.445074	-3.255596	-1.424973
H	0.024334	-0.849260	-2.295655
H	-2.897920	-4.738804	-3.337768
H	0.596903	-2.360090	-4.188159
H	-0.867546	-4.307287	-4.713165
C	3.676659	-0.123346	-0.451420
C	3.579028	0.110875	-1.831576
C	4.903604	0.089473	0.187324
C	4.689579	0.522763	-2.559977
C	6.013936	0.512803	-0.544428
C	5.912089	0.724677	-1.917247
H	2.616511	-0.025616	-2.337837
H	4.996896	-0.071306	1.264450
H	4.595076	0.706627	-3.632838
H	6.965792	0.677139	-0.033589
H	6.782186	1.058516	-2.487441
C	2.679019	-0.795746	2.174449
C	2.276527	0.187725	3.086274
C	3.456550	-1.871546	2.624224
C	2.664233	0.107575	4.423457
C	3.835228	-1.953913	3.962475
C	3.442092	-0.962615	4.863044
H	1.644702	1.014881	2.745162
H	3.768716	-2.648420	1.918993
H	2.347409	0.881359	5.126384
H	4.440597	-2.796604	4.305203
H	3.739091	-1.028925	5.912434

^{3}Int_5, -4339.31198, NImag=0

Co	0.013844	-0.468188	-0.398066
P	-2.256947	-0.730469	-0.229811
C	-2.832891	0.291361	1.208305
C	-1.923960	0.547136	2.245235
C	-4.087348	0.903730	1.288192
C	-2.244058	1.362438	3.328404
C	-4.432026	1.711439	2.371826
C	-3.511172	1.937563	3.393566
H	-4.807744	0.757574	0.478665
H	-1.491202	1.569071	4.092319
H	-5.420770	2.173375	2.411671
H	-3.769666	2.580393	4.238163
P	1.930080	-0.316264	0.805454
C	1.459075	-0.784629	2.527551
C	0.141375	-0.544647	2.958899
C	2.332541	-1.429176	3.406641
C	-0.303103	-0.971257	4.209741
C	1.909915	-1.837586	4.671488
C	0.591027	-1.616947	5.062166
O	-0.646252	0.087235	2.044343
H	3.358819	-1.631436	3.088476
H	-1.341291	-0.813500	4.505625
H	2.607256	-2.342490	5.342441
H	0.243584	-1.955980	6.040705
H	-0.146420	-2.012878	-4.019621
C	1.759702	-1.037083	-2.798993
C	2.519089	0.138424	-2.665755
C	2.346042	-2.132103	-3.465176
C	3.812975	0.207837	-3.176481
C	3.638347	-2.051999	-3.975743
C	4.385367	-0.882799	-3.832766
H	2.067413	1.001894	-2.170130
H	1.792737	-3.072410	-3.537419
H	4.380903	1.137377	-3.069337
H	4.074141	-2.922430	-4.473690
H	5.402064	-0.822788	-4.227302

N	-0.502296000	1.985362000	1.607170000
C	0.808365000	2.361614000	1.920370000
O	1.464141000	3.187988000	1.339549000
C	-3.032556000	3.088814000	-0.817944000
C	-1.981646000	4.276016000	-0.880438000
C	-4.453839000	3.526396000	-0.506875000
O	-2.559387000	2.291661000	0.293617000
C	-3.027491000	2.198807000	-2.048538000
O	-0.866243000	3.795891000	-0.099532000
C	-2.460371000	5.547192000	-0.196702000
C	-1.472463000	4.578070000	-2.275081000
H	-2.778450000	5.355645000	0.835285000
H	-3.297589000	6.014675000	-0.736305000
H	-1.633647000	6.270632000	-0.158714000
H	-0.994370000	3.698673000	-2.724556000
H	-0.721173000	5.379381000	-2.228121000
H	-2.285433000	4.916216000	-2.935051000
H	-3.339501000	2.745497000	-2.949355000
H	-3.733880000	1.372373000	-1.894990000
H	-2.031833000	1.765120000	-2.211793000
H	-4.526424000	4.071521000	0.442973000
H	-5.101432000	2.643915000	-0.436708000
H	-4.846656000	4.172107000	-1.306521000
B	-1.257582000	2.648223000	0.516562000
H	-0.125039000	1.453765000	-1.272944000
C	3.525269000	0.037528000	1.463598000
C	3.949620000	-1.230877000	1.878862000
C	3.875516000	1.155781000	2.241846000
C	4.698918000	-1.383068000	3.046096000
C	4.627994000	0.998021000	3.404768000
C	5.036113000	-0.269976000	3.815078000
H	3.713182000	-2.114279000	1.279032000
H	3.559642000	2.156196000	1.926916000
H	5.030196000	-2.378520000	3.348390000
H	4.894529000	1.879477000	3.994235000
H	5.626019000	-0.389801000	4.726519000
C	3.447620000	1.544213000	-0.951739000
C	4.845872000	1.455509000	-1.056120000
C	2.777356000	2.615469000	-1.553852000
C	5.557916000	2.416083000	-1.769533000
C	3.494971000	3.575911000	-2.263951000
C	4.880239000	3.478135000	-2.376518000
H	5.375859000	0.632060000	-0.567744000
H	1.688195000	2.683722000	-1.441968000
H	6.644919000	2.340637000	-1.850770000
H	2.965946000	4.414154000	-2.722277000
H	5.441409000	4.233687000	-2.931540000
C	-3.211678000	-1.098015000	-0.442336000
C	-3.813048000	-0.666848000	0.751037000
C	-4.014871000	-1.285747000	-1.574404000
C	-5.182223000	-0.443655000	0.814979000
C	-5.388203000	-1.054684000	-1.508842000
C	-5.978970000	-0.631940000	-0.318262000
H	-3.193025000	-0.506407000	1.634842000
H	-3.566965000	-1.608910000	-2.518993000
H	-5.630529000	-0.109374000	1.754297000
H	-6.004803000	-1.204847000	-2.400581000
H	-7.053835000	-0.448111000	-0.272917000
C	-1.042369000	-1.991912000	-2.104687000
C	-0.323863000	-1.239929000	-3.044350000
C	-1.442873000	-3.294876000	-2.429895000
C	-0.013512000	-1.789207000	-4.289355000
C	-1.136931000	-3.835553000	-3.676024000
C	-0.418424000	-3.084950000	-4.605722000
H	-0.009394000	-0.223241000	-2.782103000
H	-1.996599000	-3.892728000	-1.700205000
H	0.556271000	-1.199160000	-5.011865000
H	-1.454574000	-4.852408000	-3.920962000
H	-0.172180000	-3.512517000	-5.581356000

[1]Int_1, -3927.78980, NImag=0

Co	0.001205	-1.018432	-0.294750
P	1.069901	0.842278	-0.157352
C	1.695461	0.707032	1.572312
C	0.969717	-0.152394	2.406820
C	2.908951	1.209513	2.049988
C	1.447668	-0.566873	3.642547
C	3.386855	0.837198	3.306841
C	2.670027	-0.063746	4.091951
H	3.513253	1.858023	1.410220
H	0.873312	-1.283928	4.231502
H	4.344787	1.226105	3.658680
H	3.064094	-0.387529	5.057334
P	-2.190259	-0.596254	-0.279152
C	-2.474034	0.069242	1.402319
N	0.476901	-1.115418	-2.243657
C	-0.461614	-1.770933	-2.971062
O	-1.584331	-2.082441	-2.588473
C	0.167558	3.749833	-1.207075
C	-0.948576	3.721011	-0.107339
C	-0.384078	3.896186	-2.615576
O	0.732911	2.417649	-1.111510
C	1.270760	4.756300	-0.960828
O	-1.246978	2.309135	-0.006543
C	-2.224751	4.450031	-0.472382
C	-0.456809	4.162444	1.261110
H	-2.687563	4.039609	-1.378426
H	-2.037279	5.522443	-0.631850
H	-2.954841	4.353033	0.343131
H	0.454286	3.618766	1.548441
H	-1.230865	3.944816	2.010004
H	-0.239645	5.239673	1.296655
H	0.872357	5.781961	-0.948062
H	2.020653	4.697983	-1.761843
H	1.788291	4.569756	-0.011615
H	-1.182979	3.168287	-2.810995
H	0.417450	3.713171	-3.343609
H	-0.787171	4.902609	-2.796606
B	-0.183816	1.587432	-0.502648
H	0.041141	-1.811695	0.409569
C	-2.878052	-2.387884	0.279818
C	-2.151430	-3.533611	-0.068970
C	-4.045228	-2.538044	1.042634
C	-2.592211	-4.796161	0.318569
C	-4.486453	-3.803520	1.429200
C	-3.761887	-4.936487	1.065297
H	-1.232786	-3.421186	-0.646123
H	-4.616512	-1.659090	1.353285
H	-2.013212	-5.678960	0.037274
H	-5.397573	-3.900067	2.024608
H	-4.103561	-5.928381	1.371055
C	-3.382463	-0.161851	-1.559370
C	-2.886529	0.778453	-2.469338
C	-4.689773	-0.633576	-1.719487
C	-3.691327	1.271353	-3.492274
C	-5.495749	-0.143126	-2.747398
C	-5.003024	0.816203	-3.629905
H	-1.842384	1.095037	-2.386729
H	-5.084152	-1.400186	-1.046988
H	-3.286564	2.000977	-4.198610
H	-6.514190	-0.521980	-2.862147
H	-5.634742	1.196143	-4.436283
C	3.232991	-1.537280	0.402184
C	4.583350	-1.359758	0.738499
C	2.842933	-2.715958	-0.246857
C	5.521261	-2.342444	0.427723
C	3.782312	-3.699061	-0.548027
C	5.122902	-3.514031	-0.215430
H	4.907691	-0.450321	1.251286
H	1.792200	-2.845170	-0.524175
H	6.570302	-2.191356	0.693159
H	3.464463	-4.609165	-1.062397
H	5.860681	-4.281434	-0.461378
C	2.848331	1.249033	1.085967
C	2.548004	2.069412	2.181483
C	3.800775	1.693728	0.156521
C	3.190485	3.296640	2.349167
C	4.445566	2.915013	0.328251
C	4.143206	3.722509	1.425774
H	1.807419	1.747521	2.920087
H	4.050230	1.065898	-0.701888
H	2.945369	3.920116	3.212759
H	5.191975	3.238305	-0.401711
H	4.650633	4.680585	1.561136

[1]B', -3927.80135, NImag=0

Co	0.029997	0.404272	-0.378558
P	2.174967	0.319060	-0.042321
C	2.648697	-0.539504	-1.611884
C	1.629817	-1.301006	-2.189835
C	3.873471	-0.485019	-2.287914
C	1.776263	-1.973064	-3.395934
C	4.049488	-1.155185	-3.498851
C	3.004996	-1.895286	-4.053115
H	4.692794	0.104036	-1.865764
H	0.939859	-2.537531	-3.812591
H	5.008241	-1.093451	-4.018190
H	3.139353	-2.408302	-5.007583
P	-1.878498	-0.564637	-0.004619
C	-1.308209	-2.291235	-0.231935

C	-1.418345	-0.010865	2.325503
C	-3.652951	0.714094	1.802567
C	-1.538479	0.536368	3.603670
C	-3.783014	1.267511	3.072502
C	-2.720388	1.175429	3.969679
O	-0.246605	-0.645637	1.914321
H	-4.473744	0.802653	1.085130
H	-0.709636	0.480425	4.308958
H	-4.707960	1.771059	3.359639
H	-2.804665	1.605282	4.970206
H	0.105258	-1.034951	-1.749191
C	3.546650	-2.519717	-0.382655
C	3.975106	-1.634033	0.625167
C	4.460813	-2.847180	-1.404401
C	5.239022	-1.051886	0.575758
C	5.724875	-2.269312	-1.441431
C	6.121221	-1.354556	-0.461933
H	3.300523	-1.436155	1.460803
H	4.144052	-3.557812	-2.171649
H	5.543249	-0.359549	1.367225
H	6.412020	-2.531662	-2.251182
H	7.113036	-0.898146	-0.497794
N	2.305397	-3.115331	-0.367807
C	1.185923	-2.526736	-0.219620
O	-0.001052	-2.941032	-0.086796
C	-3.160075	-2.147840	-0.354723
C	-4.299688	-2.385864	0.423443
C	-2.732390	-3.128258	-1.260926
C	-5.008237	-3.578009	0.286454
C	-3.450945	-4.313249	-1.405087
C	-4.588437	-4.540505	-0.631702
H	-4.637840	-1.640640	1.148547
H	-1.819301	-2.960557	-1.837536
H	-5.893358	-3.756202	0.901784
H	-3.108246	-5.070250	-2.114016
H	-5.144685	-5.474986	-0.736932
C	-3.162130	0.520867	-1.356844
C	-3.172888	1.906803	-1.140428
C	-3.832026	0.010509	-2.479321
C	-3.851165	2.755076	-2.012826
C	-4.501010	0.863106	-3.354886
C	-4.517053	2.238060	-3.123519
H	-2.654200	2.330923	-0.275616
H	-3.838976	-1.066415	-2.668066
H	-3.854707	3.830976	-1.819205
H	-5.020044	0.446079	-4.221083
H	-5.048298	2.904778	-3.806628
C	0.204918	2.461275	-0.154942
C	-0.035067	3.110465	-1.375615
C	-0.302097	3.027950	1.022807
C	-0.749684	4.304607	-1.413454
C	-1.031362	4.216443	0.981142
C	-1.252757	4.860263	-0.235977
H	0.346099	2.677209	-2.305503
H	-0.118240	2.545401	1.987332
H	-0.923851	4.800140	-2.371699
H	-1.417497	4.646037	1.908916
H	-1.815734	5.796294	-0.267177
C	2.527161	1.190579	-1.193298
C	2.967345	0.191818	-2.068491
C	3.218879	2.409975	-1.131132
C	4.097534	0.400016	-2.857097
C	4.353024	2.610721	-1.913950
C	4.793604	1.604225	-2.775287
H	2.410280	-0.748065	-2.121129
H	2.862508	3.209849	-0.474112
H	4.436272	-0.388514	-3.532396
H	4.892682	3.559013	-1.856584
H	5.682644	1.764370	-3.390063

[1]Int_4, -4339.31497, NImag=0

Co	-0.030459	0.133273	0.060190
P	-1.963712	-0.985429	-0.455498
C	-2.526579	-1.084595	1.306227
C	-1.482615	-1.180165	2.227720
C	-3.826401	-1.017528	1.817610
C	-1.667503	-1.199242	3.600320
C	-4.045106	-1.031768	3.197835
C	-2.975145	-1.121759	4.086754
H	-4.674034	-0.945542	1.130598
H	-0.804600	-1.263482	4.265986
H	-5.065774	-0.969167	3.581788
H	-3.152339	-1.124172	5.164146
P	2.058623	-0.559039	0.215395
C	1.740515	-2.240814	0.878260
C	-0.121062	-2.464392	-0.958484
C	-1.872944	-3.414188	0.381322
C	0.505212	-3.699558	-1.065406
C	-1.263764	-4.665538	0.283587
C	-0.077349	-4.801548	-0.432915
O	0.397635	-1.293176	-1.519699
H	-2.791648	-3.293363	0.963160
H	1.448036	-3.805472	-1.602958
H	-1.708736	-5.530544	0.779281
H	0.418081	-5.772553	-0.497674
H	0.155388	3.399603	2.062742
C	-1.317912	2.801873	0.073951
C	-1.533159	2.789996	-1.317954
C	-2.213660	3.525528	0.882442
C	-2.595404	3.483989	-1.884777
C	-3.265152	4.235822	0.304385
C	-3.464775	4.220726	-1.076827
H	-0.826360	2.226956	-1.940815
H	-2.100315	3.500365	1.968961
H	-2.745761	3.453863	-2.966957
H	-3.951019	4.793115	0.947981
H	-4.296879	4.772298	-1.520371
N	-0.277219	2.021438	0.573170
C	0.402073	2.378655	1.676271
O	1.254912	1.684854	2.234588
C	-3.415669	-0.466927	-0.997532
C	-3.751296	-1.409366	-1.979029
C	-4.222585	0.673685	-0.850827
C	-4.875206	-1.222860	-2.784331
C	-5.345352	0.854673	-1.652051
C	-5.676152	-0.093402	-2.622438
H	-3.132845	-2.302015	-2.112323
H	-3.965729	1.430156	-0.100484
H	-5.128058	-1.969680	-3.541146
H	-5.961370	1.748016	-1.521331
H	-6.556089	0.050346	-3.253863
C	-2.503072	-0.512109	1.716851
C	-1.600120	-0.123621	2.717169
C	-3.816007	-0.851346	2.073824
C	-2.001856	-0.084169	4.050980
C	-4.213725	-0.809569	3.409259
C	-3.308521	-0.425470	4.399292
H	-0.577810	0.153866	2.441304
H	-4.534610	-1.145577	1.303030
H	-1.287546	0.224578	4.817962
H	-5.238851	-1.076320	3.677896
H	-3.625422	-0.388631	5.444499
C	3.345435	1.715538	0.007933
C	3.450024	2.540033	-1.122341
C	4.029388	2.076082	1.176046
C	4.252906	3.677651	-1.099112
C	4.832740	3.214594	1.196514
C	4.951361	4.014865	0.060622
H	2.892361	2.289554	-2.031006
H	3.910110	1.474260	2.079479
H	4.327537	4.307578	-1.988659
H	5.362259	3.483969	2.113440
H	5.579252	4.908710	0.081947
C	2.773029	-0.901193	1.190880
C	1.807418	-1.633824	1.889009
C	4.128278	-1.202231	1.376719
C	2.184856	-2.649095	2.764714
C	4.506470	-2.211956	2.259918
C	3.536118	-2.936901	2.954033
H	0.752081	-1.392978	1.719917
H	4.894973	-0.643587	0.830498
H	1.418704	-3.213847	3.302015
H	5.565838	-2.437665	2.404878
H	3.836857	-3.729821	3.643218

[1]Int_3, -4339.34567, NImag=0

Co	0.039181	-0.409953	-0.068521
P	1.375165	1.326682	-0.418161
C	2.289388	1.219420	1.197225
C	1.606226	0.604708	2.246430
C	3.629453	1.560215	1.420459
C	2.200521	0.293880	3.460427
C	4.244399	1.283709	2.641751
C	3.533517	0.647604	3.659358
H	4.206315	2.028852	0.619032
H	1.629787	-0.244291	4.218938
H	5.292184	1.552756	2.793104
H	4.022784	0.403598	4.605025
P	-2.147207	-0.020746	0.416058
C	-1.959063	1.075853	1.867038

C	0.540079	-2.367087	1.587713
C	2.518934	-3.390008	0.710668
C	0.097344	-3.573109	2.109040
C	2.093094	-4.618851	1.218390
C	0.888608	-4.708212	1.912416
O	-0.191886	-1.180050	1.681529
H	3.461750	-3.322840	0.159939
H	-0.859190	-3.638612	2.630755
H	2.704884	-5.510707	1.066874
H	0.545371	-5.669987	2.299541
H	-0.567316	2.786900	-2.846283
C	1.429910	2.080032	-1.551681
C	2.306488	2.814655	-0.740944
C	1.867491	1.683266	-2.827265
C	3.566546	3.168100	-1.220698
C	3.121223	2.056002	-3.303747
C	3.976160	2.812129	-2.505263
H	1.984234	3.139696	0.245451
H	1.218894	1.053255	-3.443515
H	4.233093	3.746494	-0.575242
H	3.435269	1.733581	-4.299500
H	4.963571	3.101631	-2.872642
N	0.099797	1.710130	-1.157510
C	-0.779569	1.844976	-2.280910
O	-1.633495	1.079283	-2.620854
C	-0.949167	4.525714	0.723973
C	-2.322254	3.782950	0.650639
C	-0.628152	5.272213	-0.564779
O	-0.035885	3.432830	0.856675
C	-0.790158	5.443124	1.919068
O	-1.981647	2.611923	-0.085990
C	-3.409425	4.530688	-0.095134
C	-2.817178	3.355034	2.028881
H	-3.136927	4.697545	-1.144885
H	-3.617333	5.505393	0.371444
H	-4.344720	3.952783	-0.087028
H	-2.029658	2.828313	2.587620
H	-3.663579	2.662264	1.914560
H	-3.159748	4.206298	2.635280
H	-1.559446	6.229968	1.920716
H	0.190979	5.937388	1.894207
H	-0.858015	4.889719	2.863763
H	-0.776366	4.631060	-1.445614
H	0.425054	5.585353	-0.555100
H	-1.247862	6.171863	-0.691898
B	-0.619386	2.289099	0.228283
H	-0.495130	1.329815	1.089833
C	-3.538293	-0.630581	-1.319262
C	-4.042730	-1.463169	-2.325094
C	-4.213182	0.564533	-1.026349
C	-5.209537	-1.119268	-3.008909
C	-5.382000	0.898076	-1.702858
C	-5.886221	0.057387	-2.696790
H	-3.522502	-2.388293	-2.585772
H	-3.792013	1.248779	-0.285866
H	-5.589100	-1.779461	-3.792649
H	-5.897213	1.831686	-1.461917
H	-6.800232	0.324532	-3.232611
C	-1.735526	-2.793193	-0.775758
C	-0.562330	-3.206364	-1.411274
C	-2.645564	-3.764443	-0.334704
C	-0.292439	-4.559845	-1.607183
C	-2.377776	-5.118463	-0.523986
C	-1.199581	-5.518503	-1.158482
H	0.151540	-2.433242	-1.717479
H	-3.568990	-3.457580	0.167187
H	0.636097	-4.866383	-2.096683
H	-3.090117	-5.868281	-0.170559
H	-0.988049	-6.581559	-1.298133
C	3.348536	-0.846824	-1.052596
C	4.558017	-0.141090	-1.074557
C	3.068686	-1.723941	-2.114447
C	5.466058	-0.317929	-2.118959
C	3.978012	-1.907307	-3.150463
C	5.183784	-1.201371	-3.157087
H	4.792374	0.567035	-0.276204
H	2.123543	-2.275433	-2.121888
H	6.400877	0.248620	-2.119699
H	3.743667	-2.602326	-3.960400
H	5.897247	-1.339832	-3.972865
C	3.027701	0.148854	1.631661
C	2.500447	1.245004	2.322071
C	4.212145	-0.441371	2.097279
C	3.158445	1.761484	3.439456
C	-0.733744	1.041568	2.544887
C	-2.941700	1.967145	2.316906
C	-0.521977	1.814092	3.686548
C	-2.733825	2.767039	3.436807
C	-1.528620	2.670963	4.128481
O	0.269906	0.234277	1.993366
H	-3.877629	2.045733	1.756041
H	0.432271	1.788053	4.210569
H	-3.508163	3.462114	3.766831
H	-1.350906	3.283056	5.015456
H	-0.743485	-0.165749	-3.874905
C	-1.132174	-1.935418	-2.243209
C	-0.628229	-3.236466	-2.078141
C	-2.461377	-1.783681	-2.676222
C	-1.442006	-4.342055	-2.309353
C	-3.269736	-2.895042	-2.909482
C	-2.769006	-4.181157	-2.716596
H	0.411673	-3.361441	-1.773219
H	-2.861781	-0.775513	-2.814826
H	-1.030776	-5.346875	-2.178289
H	-4.303474	-2.749490	-3.234578
H	-3.404122	-5.053194	-2.889411
N	-0.345561	-0.799784	-1.956351
C	-0.318094	0.160401	-2.892807
O	0.144398	1.296035	-2.777908
C	3.376602	-3.040813	-0.030644
C	2.939850	-3.126431	1.466243
C	4.444703	-1.984015	-0.261776
O	2.162252	-2.594628	-0.672615
C	3.794828	-4.360397	-0.644345
O	1.939097	-2.094899	1.549131
C	4.039619	-2.834875	2.464660
C	2.248851	-4.441622	1.798447
H	4.440313	-1.820838	2.342234
H	4.866970	-3.552913	2.361431
H	3.652451	-2.917519	3.490051
H	1.461302	-4.673025	1.066678
H	1.773060	-4.363853	2.785097
H	2.953879	-5.284700	1.825807
H	4.662037	-4.782791	-0.115217
H	4.083369	-4.215700	-1.694188
H	2.984031	-5.098750	-0.622042
H	4.147266	-1.013701	0.164447
H	4.598340	-1.839078	-1.338759
H	5.408248	-2.275968	0.179675
B	1.407304	-1.909575	0.275316
H	0.088322	-1.997789	0.243080
C	2.744963	1.333144	-1.631175
C	2.975398	0.176737	-2.384155
C	3.552527	2.458960	-1.841747
C	4.001304	0.146701	-3.326504
C	4.581055	2.424206	-2.782659
C	4.806668	1.267312	-3.527852
H	2.342848	-0.701574	-2.224643
H	3.370445	3.376702	-1.274190
H	4.168103	-0.760112	-3.913838
H	5.203778	3.308552	-2.938533
H	5.606987	1.242470	-4.271511
C	0.818880	3.086761	-0.390438
C	0.486036	3.693352	0.829425
C	0.603679	3.811709	-1.575132
C	-0.085938	4.963922	0.870125
C	0.049564	5.089085	-1.529902
C	-0.313795	5.665220	-0.312002
H	0.679822	3.175121	1.770939
H	0.857254	3.363471	-2.535625
H	-0.345738	5.406576	1.835217
H	-0.106209	5.638190	-2.462279
H	-0.760984	6.661799	-0.284588
C	-3.257679	0.944947	-0.666974
C	-2.682886	2.052963	-1.308077
C	-4.580655	0.592479	-0.964371
C	-3.424257	2.808186	-2.211120
C	-5.317719	1.347443	-1.877482
C	-4.744187	2.455914	-2.499612
H	-1.633895	2.301617	-1.119151
H	-5.035079	-0.285037	-0.495937
H	-2.957728	3.664258	-2.704509
H	-6.347667	1.062954	-2.106687
H	-5.323363	3.040165	-3.218711
C	-3.226196	-1.363710	1.071614
C	-4.303991	-1.117759	1.935555
C	-2.959995	-2.683485	0.687709
C	-5.100783	-2.164789	2.392970

C	4.867002	0.071159	3.214143
C	4.342602	1.178226	3.885346
H	1.559824	1.692496	1.981802
H	4.627408	-1.312283	1.579656
H	2.737890	2.623099	3.963845
H	5.789589	-0.396919	3.566620
H	4.857098	1.580051	4.761785

[1]Int_5, -4339.31720, NImag=0

Co	0.050665	0.266259	-0.304624
P	2.258293	0.510788	-0.199964
C	2.418565	0.187967	1.616595
C	1.283580	0.485934	2.375925
C	3.511182	-0.381749	2.274291
C	1.189719	0.208970	3.732698
C	3.452354	-0.650114	3.643035
C	2.295139	-0.361142	4.366149
H	4.409466	-0.633962	1.703432
H	0.261309	0.408128	4.271385
H	4.309228	-1.104515	4.144610
H	2.240129	-0.596553	5.431281
P	-1.963663	1.120093	-0.162195
C	-1.657293	2.324223	1.193350
C	-0.533291	2.097837	1.996677
C	-2.452302	3.437842	1.468181
C	-0.186049	2.955688	3.036446
C	-2.125824	4.308994	2.506708
C	-0.994161	4.065796	3.282737
O	0.206408	0.983645	1.645072
H	-3.332267	3.632341	0.849090
H	0.707278	2.774015	3.635797
H	-2.750207	5.182237	2.703968
H	-0.724526	4.749673	4.090360
H	0.702003	-0.373038	-4.057263
C	-0.614531	-1.711516	-2.477330
C	-0.014620	-2.662760	-3.326524
C	-1.898204	-1.998995	-1.990819
C	-0.691068	-3.823602	-3.693576
C	-2.569863	-3.160328	-2.354425
C	-1.974940	-4.084023	-3.215222
H	1.009854	-2.504076	-3.671833
H	-2.356474	-1.305431	-1.288706
H	-0.195672	-4.544428	-4.349574
H	-3.570449	-3.344785	-1.951181
H	-2.498696	-4.999594	-3.498637
N	0.056202	-0.537328	-2.100612
C	0.850826	0.034714	-3.026721
O	1.661815	0.940189	-2.837172
C	0.204672	-3.712529	1.219714
C	-0.971707	-3.091896	2.036241
C	1.519776	-3.686914	1.984311
O	0.335151	-2.777240	0.128693
C	-0.064781	-5.086333	0.644846
O	-0.818495	-1.679611	1.754416
C	-0.893856	-3.296702	3.534280
C	-2.331871	-3.515353	1.505748
H	0.023337	-2.870617	3.960532
H	-0.930734	-4.365950	3.792262
H	-1.748421	-2.807158	4.023648
H	-2.392584	-3.366937	0.417941
H	-3.117201	-2.904454	1.970151
H	-2.546779	-4.571810	1.722670
H	-0.276307	-5.818691	1.438702
H	0.815241	-5.439684	0.089215
H	-0.909146	-5.072102	-0.055529
H	1.703563	-2.691682	2.416192
H	2.349094	-3.909882	1.298318
H	1.542352	-4.426523	2.798139
B	-0.154318	-1.549538	0.537182
H	0.076281	1.771047	-0.791176
C	3.012574	2.178082	-0.331286
C	3.583214	2.627272	-1.531876
C	2.956548	3.060274	0.757222
C	4.089962	3.920883	-1.628709
C	3.451945	4.358596	0.651589
C	4.023028	4.793245	-0.542419
H	3.614286	1.963470	-2.395996
H	2.527249	2.736865	1.709115
H	4.534485	4.252742	-2.570130
H	3.394033	5.030027	1.511718
H	4.415827	5.809315	-0.626714
C	3.476410	-0.640299	-0.917731
C	3.026291	-1.899416	-1.338180
C	4.838030	-0.324198	-1.029803
C	-3.762707	-3.730919	1.138699
C	-4.833824	-3.474714	1.991909
H	-4.527672	-0.097728	2.259460
H	-2.112161	-2.893768	0.029838
H	-5.934487	-1.956545	3.067972
H	-3.541857	-4.752736	0.820388
H	-5.459900	-4.295296	2.350624

[1]Int_6, -4339.33251, NImag=0

Co	0.041096	-0.080099	-0.497583
P	-2.025213	-0.685157	-0.364430
C	-2.290891	-0.411622	1.442152
C	-1.134976	-0.268572	2.241183
C	-3.533164	-0.216937	2.057470
C	-1.226356	0.094920	3.582331
C	-3.638559	0.111462	3.407350
C	-2.479529	0.275141	4.161460
H	-4.442581	-0.298385	1.459117
H	-0.325680	0.287552	4.163544
H	-4.620805	0.260047	3.859553
H	-2.541770	0.570671	5.211177
P	2.050563	0.669860	-0.273785
C	2.377433	0.164615	1.461856
C	1.324366	-0.425703	2.183595
C	3.659622	0.124674	2.027824
C	1.556716	-1.102100	3.380751
C	3.892769	-0.490730	3.254047
C	2.841227	-1.124685	3.914861
O	0.075616	-0.423491	1.583776
H	4.500734	0.536452	1.463272
H	0.743471	-1.640418	3.867835
H	4.901499	-0.516471	3.670279
H	3.022208	-1.665356	4.846154
H	1.436158	-3.185897	-2.537782
C	1.062288	-3.039110	-0.100919
C	2.161845	-3.916392	-0.265282
C	0.222124	-3.294250	1.002970
C	2.395686	-4.967534	0.616729
C	0.461536	-4.343038	1.884375
C	1.554180	-5.191876	1.706141
H	2.855401	-3.753576	-1.091534
H	-0.652237	-2.664871	1.157343
H	3.260879	-5.616330	0.452373
H	-0.227877	-4.502767	2.719413
H	1.744158	-6.013579	2.400103
N	0.815093	-1.970611	-0.966273
C	1.132331	-2.136402	-2.273608
O	1.071024	-1.286774	-3.154376
C	-1.766041	3.705527	0.008288
C	-0.948798	3.557805	1.338999
C	-3.228729	3.318387	0.175408
O	-1.159762	2.716125	-0.852081
C	-1.654828	5.060415	-0.658991
O	-0.446435	2.207825	1.245792
C	-1.778155	3.672143	2.603660
C	0.244673	4.492852	1.418913
H	-2.557949	2.901850	2.656617
H	-2.258819	4.659522	2.674206
H	-1.134201	3.552119	3.486348
H	0.846484	4.461879	0.503042
H	0.891724	4.189447	2.253866
H	-0.065508	5.534012	1.589043
H	-2.043837	5.856558	-0.006901
H	-2.244071	5.070051	-1.586269
H	-0.617543	5.303384	-0.920535
H	-3.328278	2.327760	0.644402
H	-3.716426	3.267613	-0.807574
H	-3.777099	4.044942	0.791878
B	-0.558635	1.749134	-0.065124
H	-0.043481	0.322576	-1.885880
C	2.468206	2.440734	-0.463582
C	3.334568	3.138518	0.385756
C	1.917932	3.101866	-1.571915
C	3.655040	4.469871	0.125087
C	2.251342	4.428807	-1.837813
C	3.121238	5.114938	-0.990548
H	3.752913	2.649935	1.269009
H	1.210313	2.572555	-2.217450
H	4.325624	5.007261	0.799809
H	1.819348	4.931182	-2.706686
H	3.377900	6.157057	-1.194969
C	3.406753	-0.126532	-1.216188
C	3.730030	0.367034	-2.487217
C	4.028293	-1.297931	-0.768243

C	3.927082	-2.821691	-1.868602
C	5.733002	-1.252070	-1.560434
C	5.279120	-2.500972	-1.984508
H	1.971775	-2.164818	-1.230593
H	5.204660	0.652141	-0.700829
H	3.562384	-3.799323	-2.195446
H	6.791859	-0.995473	-1.643830
H	5.982001	-3.224348	-2.404999
C	-3.451482	0.251008	0.506301
C	-3.566227	0.044067	1.889148
C	-4.422432	-0.316519	-0.334379
C	-4.636123	-0.675208	2.416888
C	-5.485241	-1.047711	0.193018
C	-5.600729	-1.222668	1.571799
H	-2.806772	0.445187	2.565573
H	-4.353873	-0.180493	-1.417871
H	-4.711866	-0.814551	3.498360
H	-6.232536	-1.475501	-0.479822
H	-6.438810	-1.787994	1.986055
C	-2.640125	2.090070	-1.556636
C	-1.802326	2.384349	-2.641293
C	-3.961840	2.564626	-1.567644
C	-2.279170	3.138090	-3.712496
C	-4.430436	3.325653	-2.636300
C	-3.590380	3.610527	-3.712870
H	-0.765763	2.037544	-2.625122
H	-4.634898	2.335433	-0.736643
H	-1.615803	3.357284	-4.552116
H	-5.458410	3.695684	-2.628034
H	-3.960645	4.202181	-4.553615

^{3}Int_7, -4339.35125, NImag=0

Co	0.124053	-0.425815	0.047901
P	-0.277025	1.807251	0.553498
C	-1.917759	1.829699	1.395706
C	-3.065665	1.505546	0.650264
C	-2.059530	1.894982	2.788927
C	-4.297330	1.263772	1.256240
C	-3.287079	1.659648	3.407850
C	-4.405898	1.341383	2.642253
H	-1.185419	2.103715	3.409235
H	-5.158109	1.003401	0.635374
H	-3.360574	1.706712	4.496515
H	-5.366678	1.140287	3.121623
P	-1.965021	-1.379233	-0.211329
C	-3.319844	-0.841718	-1.334760
C	-3.610995	0.530735	-1.450296
C	-4.041118	-1.723001	-2.154743
C	-4.548109	1.005047	-2.366778
C	-4.991932	-1.260897	-3.062424
C	-5.237907	0.107044	-3.176704
O	-2.918817	1.456367	-0.710954
H	-3.839370	-2.795896	-2.089274
H	-4.717084	2.081935	-2.426905
H	-5.536258	-1.972182	-3.687245
H	-5.972500	0.477646	-3.895102
H	1.308517	-2.013549	-1.572490
C	2.817074	1.026389	-1.565013
C	3.480169	1.829440	-0.627729
C	2.406933	1.597135	-2.778467
C	3.704166	3.179159	-0.888181
C	2.638948	2.945552	-3.031299
C	3.279394	3.747523	-2.087379
H	3.828516	1.391085	0.305356
H	1.896720	0.981898	-3.519220
H	4.208189	3.790117	-0.134179
H	2.303928	3.376308	-3.978106
H	3.442639	4.809307	-2.286359
N	2.573622	-0.351081	-1.304133
C	1.294948	-0.905130	-1.573968
O	0.352194	-0.245929	-2.084453
C	5.284746	-2.014834	0.512980
C	4.124078	-3.067923	0.533523
C	5.925611	-1.757400	1.858497
O	4.598017	-0.808419	0.089679
C	6.338806	-2.318036	-0.538656
O	3.244635	-2.563352	-0.497011
C	3.337904	-3.056857	1.834019
C	4.540762	-4.475768	0.168920
H	3.030945	-2.038832	2.112681
H	3.911991	-3.493438	2.663444
H	2.415667	-3.639067	1.704581
H	4.971528	-4.529474	-0.837988
H	3.667891	-5.141947	0.193203
H	5.279749	-4.864214	0.884831
C	4.668271	-0.283647	-3.282124
C	4.970354	-1.946630	-1.565478
C	5.294487	-1.441847	-2.822903
H	3.230931	1.258746	-2.873593
H	3.765796	-1.728809	0.200747
H	4.902279	0.111779	-4.272860
H	5.443013	-2.861996	-1.199687
H	6.028716	-1.954570	-3.448621
C	-2.486773	-2.434495	-0.662038
C	-2.098789	-2.975731	-1.895585
C	-3.152026	-3.242399	0.266159
C	-2.367034	-4.309885	-2.188480
C	-3.423342	-4.577184	-0.033423
C	-3.026340	-5.113551	-1.257148
H	-1.568881	-2.348606	-2.620154
H	-3.440085	-2.837535	1.241458
H	-2.049440	-4.727535	-3.146717
H	-3.937892	-5.203626	0.699222
H	-3.227001	-6.162979	-1.484993
C	-3.348065	0.136084	-1.328486
C	-4.707897	-0.161308	-1.147351
C	-2.971684	0.976217	-2.383405
C	-5.674876	0.432547	-1.954056
C	-3.940698	1.549999	-3.205676
C	-5.292244	1.296560	-2.981506
H	-5.018638	-0.894054	-0.397490
H	-1.912447	1.175407	-2.552490
H	-6.730660	0.200200	-1.796285
H	-3.632610	2.199268	-4.028677
H	-6.050701	1.752635	-3.622464

^{3}TS_7, -4339.34254, NImag=1

Co	0.036548	0.114070	-0.138666
P	1.768082	1.623961	-0.035268
C	3.361560	0.849289	-0.506066
C	3.783215	-0.233401	0.286372
C	4.026990	1.061690	-1.719781
C	4.819300	-1.075612	-0.110654
C	5.071884	0.231516	-2.124751
C	5.462474	-0.838980	-1.323851
H	3.699400	1.865636	-2.382588
H	5.101571	-1.920163	0.522347
H	5.565253	0.410181	-3.082540
H	6.267341	-1.503973	-1.645402
P	0.973422	-1.953969	-0.077830
C	2.010235	-2.556404	1.334315
C	2.922320	-1.682652	1.954304
C	1.866572	-3.831532	1.903282
C	3.624614	-2.041508	3.102586
C	2.577183	-4.209553	3.040905
C	3.448757	-3.308997	3.651195
O	3.105726	-0.410956	1.462981
H	1.170189	-4.542080	1.450773
H	4.303267	-1.310963	3.547106
H	2.440634	-5.210383	3.456169
H	3.997307	-3.593072	4.551943
H	-2.352794	-1.236842	0.556977
C	-2.545406	2.120343	0.360705
C	-3.072625	2.915013	-0.670971
C	-1.617009	2.698456	1.244637
C	-2.695484	4.249177	-0.800592
C	-1.222571	4.026372	1.085114
C	-1.761514	4.812843	0.069042
H	-3.790395	2.477487	-1.365892
H	-1.227837	2.102795	2.067615
H	-3.126650	4.850801	-1.605650
H	-0.493818	4.448870	1.783500
H	-1.453476	5.854475	-0.049356
N	-2.924567	0.763055	0.479295
C	-1.903494	-0.239478	0.695999
O	-1.015283	-0.076368	1.611311
C	-6.484281	0.210709	-0.076321
C	-5.867590	-1.212707	-0.287318
C	-7.469934	0.636898	-1.142212
O	-5.317074	1.061121	-0.151982
C	-7.082588	0.387912	1.310115
O	-4.555190	-1.057825	0.287285
C	-5.675818	-1.557664	-1.756537
C	-6.587473	-2.331200	0.434350
H	-5.175527	-0.741645	-2.296787
H	-6.629896	-1.769068	-2.259609
H	-5.039449	-2.449053	-1.839752
H	-6.595014	-2.177613	1.520056
H	-6.086200	-3.288893	0.238006
H	-7.627703	-2.419154	0.087905

H	6.954941	-3.184606	-0.261448
H	7.002360	-1.450741	-0.651812
H	5.882480	-2.519959	-1.517502
H	5.198888	-1.385415	2.590644
H	6.721199	-1.006431	1.763341
H	6.378289	-2.676652	2.257809
B	3.476347	-1.215530	-0.579667
H	0.670302	-1.077566	1.408406
C	-0.304972	3.104152	-0.762371
C	0.121582	4.428020	-0.590714
C	-0.718596	2.699085	-2.042204
C	0.078281	5.335063	-1.649766
C	-0.772911	3.608379	-3.094121
C	-0.383747	4.933583	-2.900653
H	0.511196	4.766441	0.370214
H	-0.979018	1.654638	-2.211367
H	0.414014	6.363018	-1.490875
H	-1.105796	3.270786	-4.079169
H	-0.422257	5.646902	-3.727985
C	0.822132	2.478583	1.862122
C	0.599602	3.695787	2.526876
C	1.929643	1.706939	2.233036
C	1.489951	4.148255	3.497989
C	2.824456	2.160232	3.201784
C	2.611861	3.385941	3.828993
H	-0.292185	4.286578	2.299171
H	2.067788	0.729644	1.758830
H	1.303956	5.098407	4.004620
H	3.688811	1.547140	3.470225
H	3.310917	3.743445	4.589037
C	-1.420381	-2.976286	-0.914975
C	-1.017104	-4.009503	-0.055808
C	-1.162458	-3.099350	-2.290013
C	-0.383238	-5.142960	-0.561030
C	-0.537281	-4.238717	-2.791137
C	-0.142526	-5.262727	-1.929400
H	-1.188533	-3.917476	1.020802
H	-1.429612	-2.284435	-2.967926
H	-0.073960	-5.938100	0.122007
H	-0.345576	-4.320825	-3.863783
H	0.355487	-6.151244	-2.324443
C	-2.863111	-1.833175	1.323262
C	-4.148698	-2.392820	1.308642
C	-2.235206	-1.589808	2.550882
C	-4.792664	-2.705813	2.502915
C	-2.882595	-1.907124	3.745129
C	-4.159969	-2.463083	3.724088
H	-4.654196	-2.579048	0.356328
H	-1.230142	-1.152330	2.549857
H	-5.794542	-3.141789	2.481848
H	-2.385801	-1.708738	4.698300
H	-4.667900	-2.707706	4.660373

^{3}C, -4339.37030, NImag=0

Co	0.233639	0.111822	-0.582225
P	1.498725	-1.663559	-0.145498
C	3.186871	-1.319692	0.482366
C	3.932313	-0.346077	-0.206118
C	3.700456	-1.799325	1.692742
C	5.136954	0.141049	0.293226
C	4.907175	-1.320991	2.203168
C	5.620978	-0.349404	1.505215
H	3.131466	-2.541450	2.259655
H	5.681594	0.909390	-0.260642
H	5.282710	-1.700811	3.155725
H	6.561230	0.037335	1.905083
P	1.455451	1.891605	0.041260
C	2.757161	2.400970	-1.164164
C	3.567299	1.413600	-1.756915
C	2.912778	3.719806	-1.614628
C	4.486736	1.725549	-2.754927
C	3.839007	4.043236	-2.605112
C	4.623708	3.045207	-3.180192
O	3.410710	0.091578	-1.401288
H	2.286015	4.507571	-1.187487
H	5.079004	0.918043	-3.189815
H	3.938838	5.079468	-2.934873
H	5.342846	3.290988	-3.964631
H	-2.543304	1.568771	-0.078537
C	-3.057020	-1.736192	0.035279
C	-3.681400	-2.468708	1.058147
C	-2.186857	-2.410904	-0.837049
C	-3.440961	-3.832092	1.201578
C	-1.930519	-3.771251	-0.669010
C	-2.554980	-4.490641	0.347438
H	-8.019090	-0.175036	1.428168
H	-7.299901	1.450576	1.480009
H	-6.383553	0.060691	2.092175
H	-7.009924	0.665542	-2.137179
H	-7.853444	1.642526	-0.923999
H	-8.329243	-0.048792	-1.177583
B	-4.240193	0.281720	0.201768
H	-1.306223	-0.292374	-0.887376
C	2.018459	2.420855	1.604128
C	2.696074	3.629873	1.802540
C	1.434123	1.778947	2.705701
C	2.790764	4.185331	3.078097
C	1.532789	2.335105	3.978953
C	2.209401	3.540023	4.168710
H	3.146436	4.159884	0.961630
H	0.884064	0.846541	2.549864
H	3.319499	5.131377	3.217606
H	1.067845	1.826151	4.826627
H	2.280127	3.979721	5.166612
C	1.586351	2.993287	-1.239967
C	2.579009	3.945011	-1.529245
C	0.365776	3.070283	-1.922387
C	2.343722	4.954719	-2.458629
C	0.131176	4.079038	-2.855960
C	1.116993	5.025351	-3.122296
H	3.557668	3.883747	-1.045867
H	-0.414639	2.329523	-1.706013
H	3.125527	5.687468	-2.672783
H	-0.832549	4.123850	-3.368818
H	0.935686	5.817845	-3.852430
C	-0.371182	-3.198686	-0.093916
C	-0.726644	-3.903533	-1.251250
C	-1.176899	-3.327456	1.050333
C	-1.855520	-4.723424	-1.261616
C	-2.299599	-4.149820	1.037776
C	-2.643493	-4.851130	-0.119052
H	-0.120541	-3.810084	-2.156630
H	-0.933207	-2.749139	1.947294
H	-2.117902	-5.267548	-2.172363
H	-2.919451	-4.230911	1.934101
H	-3.527291	-5.493918	-0.129996
C	1.985045	-2.411900	-1.539687
C	2.748169	-3.585942	-1.605970
C	1.979226	-1.540914	-2.635031
C	3.486379	-3.882186	-2.748767
C	2.715754	-1.839315	-3.781216
C	3.470253	-3.009310	-3.838947
H	2.764335	-4.272379	-0.753382
H	1.390057	-0.616882	-2.577303
H	4.078106	-4.800011	-2.791435
H	2.706019	-1.148806	-4.628161
H	4.050856	-3.242873	-4.734809

^{3}TS_8, -4750.91985, NImag=1

Co	0.470510000	-0.029332000	-0.184591000
P	1.837978000	1.751572000	-0.180613000
C	3.626496000	1.427799000	-0.429937000
C	4.226215000	0.469992000	0.406474000
C	4.383470000	1.923390000	-1.497582000
C	5.520974000	0.009473000	0.187689000
C	5.682788000	1.471808000	-1.729073000
C	6.246831000	0.511974000	-0.890824000
H	3.938790000	2.657212000	-2.175398000
H	5.943134000	-0.749008000	0.851725000
H	6.250743000	1.863098000	-2.575775000
H	7.259162000	0.145442000	-1.076586000
P	1.870667000	-1.809538000	-0.322519000
C	2.807636000	-2.270214000	1.197116000
C	3.506194000	-1.265856000	1.898874000
C	2.746990000	-3.538858000	1.791109000
C	4.135331000	-1.525547000	3.113828000
C	3.375585000	-3.808071000	3.006244000
C	4.076530000	-2.802150000	3.667975000
O	3.468685000	0.039769000	1.464798000
H	2.178855000	-4.332304000	1.299822000
H	4.646344000	-0.703944000	3.619600000
H	3.307841000	-4.808249000	3.439645000
H	4.566977000	-3.003956000	4.622766000
H	-2.488390000	-0.439677000	-2.449952000
C	-3.359851000	2.270728000	-0.737641000
C	-4.516770000	3.001228000	-0.404204000
C	-2.114782000	2.910872000	-0.576501000
C	-4.421133000	4.306521000	0.070372000
C	-2.034191000	4.221770000	-0.114611000
C	-3.184350000	4.934179000	0.219237000

H	-4.367341	-1.954112	1.733927
H	-1.750565	-1.852060	-1.663000
H	-3.939949	-4.384220	2.002957
H	-1.241637	-4.275070	-1.354190
H	-2.354411	-5.557296	0.474384
N	-3.299796	-0.351744	-0.101382
C	-2.151133	0.545791	-0.254519
O	-1.454989	0.435255	-1.418302
C	-6.860146	0.313976	-0.301819
C	-6.267562	1.732982	-0.007202
C	-8.066393	-0.054642	0.534779
O	-5.762241	-0.551172	0.051429
C	-7.148927	0.099702	-1.779907
O	-4.866049	1.538133	-0.277878
C	-6.396593	2.125622	1.456980
C	-6.792745	2.835325	-0.901530
H	-6.043888	1.321698	2.118185
H	-7.433815	2.365039	1.730807
H	-5.779726	3.013087	1.651340
H	-6.564057	2.646517	-1.957080
H	-6.333382	3.795180	-0.629156
H	-7.882282	2.943303	-0.795083
H	-8.023564	0.673823	-2.116944
H	-7.349447	-0.964667	-1.959782
H	-6.288489	0.386298	-2.400370
H	-7.834738	-0.058965	1.606649
H	-8.419053	-1.059883	0.267890
H	-8.894851	0.648014	0.361502
B	-4.610941	0.192175	-0.105286
H	-1.483640	0.346410	0.659829
C	1.838262	-2.597203	-1.690820
C	2.947762	-3.435356	-1.864469
C	0.956581	-2.406582	-2.762620
C	3.145783	-4.100148	-3.073442
C	1.153197	-3.073012	-3.970789
C	2.245090	-3.926285	-4.125182
H	3.671308	-3.557037	-1.051997
H	0.116149	-1.712330	-2.643427
H	4.013045	-4.753214	-3.198383
H	0.456364	-2.915806	-4.797275
H	2.403728	-4.447396	-5.072349
C	0.889930	-2.916199	1.047639
C	1.323287	-4.247953	1.068135
C	-0.061161	-2.498888	1.987298
C	0.832216	-5.134288	2.025165
C	-0.546612	-3.381991	2.948681
C	-0.097077	-4.701285	2.971362
H	2.048736	-4.599742	0.329150
H	-0.444086	-1.472423	1.941798
H	1.176151	-6.171561	2.030389
H	-1.297283	-3.042669	3.666185
H	-0.483332	-5.399209	3.718246
C	0.423421	3.407934	0.153734
C	0.603671	4.417652	1.108881
C	-0.621485	3.526339	-0.776862
C	-0.233756	5.533082	1.120343
C	-1.450341	4.645917	-0.765085
C	-1.257691	5.652440	0.181372
H	1.400148	4.335043	1.853351
H	-0.804150	2.714160	-1.489812
H	-0.085385	6.312480	1.871855
H	-2.263786	4.720917	-1.490609
H	-1.913974	6.526009	0.195499
C	2.353727	1.891293	1.643530
C	3.460832	2.706807	1.913775
C	1.876703	1.039522	2.646736
C	4.064884	2.680265	3.169331
C	2.476539	1.016583	3.904162
C	3.571243	1.839028	4.167442
H	3.853983	3.368052	1.134525
H	1.032813	0.377048	2.420636
H	4.927995	3.319831	3.370295
H	2.094071	0.344417	4.676212
H	4.047649	1.818718	5.150577
H	-5.495904000	2.541609000	-0.522306000
H	-1.194589000	2.358887000	-0.771990000
H	-5.339822000	4.845236000	0.318739000
H	-1.046792000	4.680109000	-0.001179000
H	-3.118940000	5.960432000	0.587256000
N	-3.419029000	0.951111000	-1.218347000
C	-2.173375000	0.389454000	-1.785715000
O	-1.289893000	-0.029030000	-0.850217000
C	-6.558238000	-0.813427000	-0.565455000
C	-5.759494000	-1.810726000	-1.472664000
C	-7.989762000	-0.575121000	-0.996892000
O	-5.812626000	0.409518000	-0.725443000
C	-6.502894000	-1.181767000	0.908414000
O	-4.424023000	-1.276902000	-1.418194000
C	-6.206080000	-1.764277000	-2.926275000
C	-5.739407000	-3.238706000	-0.968761000
H	-6.240005000	-0.731787000	-3.300939000
H	-7.198481000	-2.214472000	-3.068950000
H	-5.488344000	-2.319558000	-3.544502000
H	-5.258921000	-3.317885000	0.014577000
H	-5.181533000	-3.878966000	-1.665344000
H	-6.759190000	-3.643454000	-0.889983000
H	-7.099708000	-2.076191000	1.135730000
H	-6.893908000	-0.348305000	1.507389000
H	-5.468299000	-1.366200000	1.226803000
H	-8.048162000	-0.154057000	-2.007441000
H	-8.478777000	0.132158000	-0.313776000
H	-8.566534000	-1.511495000	-0.977371000
B	-4.532240000	0.068995000	-1.115440000
H	-1.764717000	1.185727000	-2.450759000
C	1.792150000	2.794858000	1.326456000
C	2.917224000	3.407637000	1.891428000
C	0.545357000	2.956643000	1.944667000
C	2.789784000	4.181226000	3.044764000
C	0.417004000	3.736283000	3.090429000
C	1.540693000	4.350466000	3.643142000
H	3.900004000	3.278068000	1.427471000
H	-0.333814000	2.454874000	1.524483000
H	3.673407000	4.654472000	3.480291000
H	-0.563705000	3.847536000	3.559532000
H	1.445394000	4.955407000	4.548061000
C	1.474137000	2.965558000	-1.510882000
C	1.828413000	4.319371000	-1.441816000
C	0.768347000	2.503558000	-2.628516000
C	1.486823000	5.188705000	-2.476450000
C	0.430552000	3.370644000	-3.665448000
C	0.788806000	4.716056000	-3.588844000
H	2.368058000	4.697547000	-0.567716000
H	0.452279000	1.453510000	-2.653806000
H	1.760299000	6.244641000	-2.411117000
H	-0.131207000	2.998516000	-4.525561000
H	0.513394000	5.402323000	-4.393113000
C	0.932748000	-3.332025000	-0.760823000
C	1.532842000	-4.543310000	-1.136600000
C	-0.463535000	-3.226598000	-0.796312000
C	0.750075000	-5.633202000	-1.510880000
C	-1.245089000	-4.317623000	-1.177008000
C	-0.641936000	-5.523278000	-1.529168000
H	2.622868000	-4.636589000	-1.146973000
H	-0.938787000	-2.269697000	-0.555229000
H	1.229548000	-6.571527000	-1.800386000
H	-2.332802000	-4.208466000	-1.209642000
H	-1.252978000	-6.377092000	-1.832478000
C	3.167695000	-1.817240000	-1.625869000
C	4.319562000	-2.613892000	-1.575427000
C	2.946643000	-1.014950000	-2.751941000
C	5.216449000	-2.624228000	-2.641870000
C	3.842728000	-1.025907000	-3.818658000
C	4.976961000	-1.835136000	-3.767399000
H	4.523465000	-3.222768000	-0.688216000
H	2.062672000	-0.367022000	-2.775059000
H	6.111350000	-3.249716000	-2.592311000
H	3.658026000	-0.391760000	-4.689164000
H	5.682139000	-1.844009000	-4.602012000
C	-2.077055000	-0.190039000	3.234525000
C	-1.722810000	-1.571458000	2.598886000
C	-2.721982000	0.756713000	2.236998000
O	-0.759216000	0.357463000	3.528570000
C	-2.870416000	-0.272784000	4.518023000
O	-0.428332000	-1.290676000	1.975429000
C	-2.705301000	-2.043435000	1.555005000
C	-1.456620000	-2.655563000	3.629396000
H	-2.744698000	-1.362354000	0.694156000
H	-3.706746000	-2.124559000	2.004011000

^{3}Int_8, -4750.92447, NImag=0

Co	0.512494000	0.037640000	0.076785000
P	2.197347000	1.543682000	0.051819000
C	3.903794000	0.948242000	-0.271679000
C	4.354014000	-0.165259000	0.458984000
C	4.736676000	1.440480000	-1.283761000
C	5.598113000	-0.744755000	0.218533000
C	5.978512000	0.861367000	-1.543485000
C	6.411439000	-0.224889000	-0.785944000
H	4.400609000	2.285882000	-1.889905000
H	5.914251000	-1.606771000	0.810705000
H	6.606320000	1.260503000	-2.342837000
H	7.385451000	-0.679997000	-0.980791000
P	1.556527000	-1.892240000	-0.498477000
C	2.560393000	-2.751847000	0.784013000
C	3.396721000	-1.995334000	1.631121000
C	2.409779000	-4.113868000	1.084204000
C	4.049606000	-2.571069000	2.717855000
C	3.070195000	-4.700656000	2.162381000
C	3.889799000	-3.929262000	2.983567000
O	3.519268000	-0.634826000	1.444433000
H	1.746580000	-4.725584000	0.467880000
H	4.671329000	-1.932909000	3.349058000
H	2.931756000	-5.764478000	2.366519000
H	4.401209000	-4.380340000	3.836754000
H	-2.228986000	-0.628391000	-1.868224000
C	-3.141418000	2.465472000	-1.067897000
C	-4.240838000	3.318687000	-1.275987000
C	-1.909002000	3.053568000	-0.718804000
C	-4.105187000	4.697493000	-1.140000000
C	-1.783639000	4.435147000	-0.600260000
C	-2.878680000	5.272375000	-0.806174000
H	-5.203843000	2.893848000	-1.555363000
H	-1.047922000	2.417360000	-0.506923000
H	-4.977475000	5.333944000	-1.312378000
H	-0.808237000	4.854870000	-0.334178000
H	-2.779315000	6.355643000	-0.707537000
N	-3.244535000	1.072485000	-1.234829000
C	-1.982073000	0.329705000	-1.364482000
O	-1.371827000	0.136720000	-0.162047000
C	-6.553950000	-0.316652000	-0.568891000
C	-5.770039000	-1.527673000	-1.172548000
C	-7.929178000	-0.094735000	-1.159639000
O	-5.707712000	0.797155000	-0.920197000
C	-6.620774000	-0.371342000	0.949127000
O	-4.402669000	-1.084101000	-1.066983000
C	-6.063481000	-1.739436000	-2.650154000
C	-5.941906000	-2.823314000	-0.407559000
H	-5.978396000	-0.800264000	-3.214382000
H	-7.069002000	-2.150916000	-2.816763000
H	-5.332880000	-2.446219000	-3.066608000
H	-5.547675000	-2.752873000	0.613703000
H	-5.415811000	-3.643321000	-0.914699000
H	-7.004310000	-3.102829000	-0.349607000
H	-7.319391000	-1.141794000	1.304731000
H	-6.956123000	0.600500000	1.335192000
H	-5.630134000	-0.579462000	1.376425000
H	-7.883407000	0.107552000	-2.236393000
H	-8.413871000	0.766202000	-0.680097000
H	-8.571812000	-0.972767000	-0.998506000
B	-4.430080000	0.301324000	-1.077264000
H	-1.365042000	0.912013000	-2.092607000
C	2.355583000	2.451475000	1.636819000
C	3.569468000	2.683287000	2.294669000
C	1.165266000	2.917809000	2.212845000
C	3.590679000	3.377530000	3.504341000
C	1.190214000	3.614804000	3.417232000
C	2.403504000	3.846304000	4.066105000
H	4.505980000	2.320949000	1.860400000
H	0.206662000	2.713892000	1.723646000
H	4.542903000	3.552572000	4.011310000
H	0.252879000	3.964264000	3.856632000
H	-2.431824000	-3.042642000	1.189824000
H	-0.761755000	-2.313362000	4.409400000
H	-1.002360000	-3.523390000	3.131491000
H	-2.384369000	-2.989435000	4.114725000
H	-3.837690000	-0.766825000	4.343035000
H	-3.076618000	0.735758000	4.899855000
H	-2.335299000	-0.824461000	5.300642000
H	-2.169782000	0.763719000	1.283857000
H	-2.729264000	1.779120000	2.641843000
H	-3.763762000	0.479991000	2.015920000
B	0.103697000	-0.230135000	2.661700000
H	1.229659000	0.128931000	2.484898000

^{3}TS_9, -4750.91598, NImag=1

Co	0.581338000	-0.078012000	0.002160000
P	1.988369000	1.614342000	0.420740000
C	3.784587000	1.353474000	0.145163000
C	4.354881000	0.203519000	0.718845000
C	4.591890000	2.126780000	-0.697434000
C	5.684932000	-0.144791000	0.493123000
C	5.921808000	1.783340000	-0.939889000
C	6.469525000	0.653170000	-0.336668000
H	4.166042000	3.005799000	-1.188457000
H	6.092253000	-1.045316000	0.958656000
H	6.527988000	2.399840000	-1.607064000
H	7.511755000	0.380691000	-0.519153000
P	1.944839000	-1.669904000	-0.808196000
C	2.983632000	-2.608419000	0.391874000
C	3.618622000	-1.925546000	1.449566000
C	3.045411000	-4.009966000	0.404399000
C	4.275109000	-2.609233000	2.469520000
C	3.712734000	-4.701005000	1.414456000
C	4.324216000	-4.001445000	2.452644000
O	3.542141000	-0.551950000	1.530835000
H	2.546182000	-4.573343000	-0.388070000
H	4.735056000	-2.029090000	3.272066000
H	3.742653000	-5.792436000	1.393749000
H	4.837669000	-4.537147000	3.254125000
H	-2.637964000	-1.178353000	-1.221927000
C	-2.874707000	2.144418000	-0.808129000
C	-3.243192000	3.093878000	-1.770694000
C	-2.158653000	2.568821000	0.323467000
C	-2.904734000	4.436052000	-1.607619000
C	-1.800670000	3.908246000	0.467264000
C	-2.173593000	4.847712000	-0.493433000
H	-3.815036000	2.765732000	-2.641875000
H	-1.914269000	1.832192000	1.089839000
H	-3.208975000	5.165388000	-2.363463000
H	-1.232098000	4.221426000	1.348082000
H	-1.894245000	5.897564000	-0.374314000
N	-3.234109000	0.782069000	-0.966678000
C	-2.145887000	-0.197742000	-1.057392000
O	-1.320685000	-0.202408000	0.031047000
C	-6.839188000	0.457145000	-0.816768000
C	-6.390206000	-0.990213000	-1.223833000
C	-7.994434000	1.009626000	-1.624375000
O	-5.659401000	1.235434000	-1.095033000
C	-7.121980000	0.586175000	0.672064000
O	-4.972605000	-0.955597000	-0.973492000
C	-6.582415000	-1.265704000	-2.707349000
C	-7.002654000	-2.098246000	-0.392835000
H	-6.154839000	-0.460852000	-3.321311000
H	-7.643159000	-1.374372000	-2.973914000
H	-6.067292000	-2.198150000	-2.974118000
H	-6.732811000	-2.008317000	0.666909000
H	-6.644686000	-3.076289000	-0.742772000
H	-8.099671000	-2.094676000	-0.473870000
H	-8.046997000	0.069901000	0.965309000
H	-7.226707000	1.648285000	0.929932000
H	-6.294562000	0.180064000	1.269725000
H	-7.754042000	1.072340000	-2.692343000
H	-8.244187000	2.022390000	-1.281010000
H	-8.892126000	0.384846000	-1.506549000
B	-4.586069000	0.372258000	-1.021314000
H	-1.572399000	0.024471000	-1.992585000
C	1.942535000	2.244070000	2.143753000
C	3.049113000	2.797853000	2.800795000
C	0.725515000	2.137735000	2.829179000
C	2.931368000	3.250759000	4.114431000
C	0.608881000	2.592333000	4.140214000
C	1.712198000	3.151161000	4.785435000
H	4.012053000	2.870147000	2.285508000
H	-0.133697000	1.675881000	2.334688000
H	3.800335000	3.679902000	4.619568000
H	-0.346426000	2.489756000	4.660801000

H	2.423405000	4.387103000	5.015375000
C	2.015318000	2.918859000	-1.150353000
C	2.655402000	4.157150000	-0.995467000
C	1.160337000	2.731202000	-2.242214000
C	2.450430000	5.176047000	-1.923159000
C	0.954196000	3.748940000	-3.171674000
C	1.601104000	4.972977000	-3.012848000
H	3.314287000	4.324426000	-0.137508000
H	0.623873000	1.781365000	-2.340009000
H	2.950465000	6.138691000	-1.791625000
H	0.268723000	3.591558000	-4.007477000
H	1.433301000	5.777701000	-3.732492000
C	0.377703000	-3.177349000	-1.078259000
C	0.763185000	-4.257583000	-1.886715000
C	-0.975085000	-3.014538000	-0.749711000
C	-0.185884000	-5.171434000	-2.338909000
C	-1.922694000	-3.928619000	-1.210684000
C	-1.531035000	-5.008155000	-2.000344000
H	1.813257000	-4.380154000	-2.171507000
H	-1.283915000	-2.149796000	-0.153151000
H	0.123342000	-6.009569000	-2.968362000
H	-2.974854000	-3.773480000	-0.959300000
H	-2.274846000	-5.720575000	-2.366321000
C	2.662279000	-1.749358000	-1.953234000
C	3.886566000	-2.409211000	-2.100590000
C	2.219253000	-0.902167000	-2.979829000
C	4.652482000	-2.221766000	-3.251743000
C	2.979257000	-0.720660000	-4.131109000
C	4.202177000	-1.380002000	-4.267400000
H	4.249363000	-3.068619000	-1.305392000
H	1.259461000	-0.384311000	-2.867512000
H	5.612068000	-2.735431000	-3.352418000
H	2.619931000	-0.056378000	-4.920881000
H	4.806474000	-1.233721000	-5.165776000
C	-2.162602000	0.151437000	3.370199000
C	-2.070345000	-1.411947000	3.115986000
C	-3.152224000	0.867029000	2.467212000
O	-0.842201000	0.624078000	2.996830000
C	-2.403664000	0.534079000	4.817129000
O	-0.879433000	-1.559370000	2.302293000
C	-3.235723000	-1.980834000	2.331928000
C	-1.824581000	-2.221276000	4.377966000
H	-3.321875000	-1.511392000	1.342063000
H	-4.182244000	-1.843228000	2.877156000
H	-3.092350000	-3.060310000	2.180019000
H	-0.944598000	-1.857680000	4.924885000
H	-1.635788000	-3.268596000	4.107399000
H	-2.687734000	-2.195319000	5.057318000
H	-3.376233000	0.157692000	5.165738000
H	-2.417504000	1.627973000	4.912430000
H	-1.624896000	0.151693000	5.487634000
H	-2.954094000	0.643184000	1.410591000
H	-3.041650000	1.952447000	2.599976000
H	-4.189621000	0.604500000	2.718795000
B	-0.242411000	-0.360953000	2.281748000
H	0.900634000	-0.234071000	1.844382000

^{3}Int_9, -4750.93723, NImag=0

Co	0.630013000	0.103688000	-0.199132000
P	2.006864000	1.732934000	0.429939000
C	3.780892000	1.276610000	0.360131000
C	4.128769000	0.039318000	0.931695000
C	4.756724000	1.959765000	-0.373563000
C	5.390083000	-0.520427000	0.740934000
C	6.028472000	1.417272000	-0.556774000
C	6.336850000	0.172431000	-0.011851000
H	4.505574000	2.917042000	-0.839557000
H	5.618809000	-1.497899000	1.172318000
H	6.771968000	1.959125000	-1.145257000
H	7.323389000	-0.269037000	-0.171446000
P	1.911413000	-1.640521000	-0.857622000
C	2.536110000	-2.623918000	0.572725000
C	3.065829000	-1.948018000	1.688685000
C	2.419269000	-4.018121000	0.659823000
C	3.440310000	-2.628015000	2.844352000
C	2.801684000	-4.708896000	1.808841000
C	3.304944000	-4.013069000	2.906306000
O	3.162908000	-0.573808000	1.687433000
H	2.005177000	-4.572890000	-0.186228000
H	3.828649000	-2.050868000	3.685637000
H	2.696117000	-5.795153000	1.847051000
H	3.594599000	-4.547003000	3.814025000
H	-2.982430000	-1.541180000	-0.751046000
C	-2.749676000	1.801137000	-1.079507000
C	-2.942200000	2.544128000	-2.249895000
H	1.625834000	3.501275000	5.816958000
C	1.623131000	3.104530000	-0.585197000
C	2.120394000	4.381866000	-0.294465000
C	0.772285000	2.943939000	-1.686209000
C	1.799464000	5.465062000	-1.110862000
C	0.459499000	4.022371000	-2.510343000
C	0.978078000	5.284379000	-2.224790000
H	2.764071000	4.529368000	0.578696000
H	0.324033000	1.960782000	-1.876198000
H	2.191674000	6.457542000	-0.875539000
H	-0.213273000	3.880789000	-3.359129000
H	0.725960000	6.135979000	-2.861585000
C	1.061486000	-3.005476000	-1.714241000
C	1.624771000	-3.713408000	-2.785672000
C	-0.256948000	-3.285585000	-1.327227000
C	0.887830000	-4.693801000	-3.447801000
C	-0.988707000	-4.270241000	-1.989921000
C	-0.419778000	-4.975046000	-3.050098000
H	2.646869000	-3.495023000	-3.109484000
H	-0.710148000	-2.725880000	-0.502817000
H	1.335839000	-5.237618000	-4.283159000
H	-2.016314000	-4.477365000	-1.680101000
H	-0.998028000	-5.739986000	-3.574213000
C	3.116695000	-1.079975000	-2.089582000
C	4.411643000	-1.572260000	-2.283430000
C	2.644274000	-0.062385000	-2.929688000
C	5.213720000	-1.057508000	-3.302627000
C	3.439837000	0.445981000	-3.951894000
C	4.730016000	-0.052457000	-4.139207000
H	4.799202000	-2.358782000	-1.627470000
H	1.637943000	0.338718000	-2.763815000
H	6.227336000	-1.442693000	-3.440335000
H	3.055809000	1.241352000	-4.595463000
H	5.362569000	0.349292000	-4.934340000
C	-2.637697000	-1.152864000	3.119555000
C	-2.239351000	-2.604484000	2.632855000
C	-3.769274000	-0.541704000	2.312829000
O	-1.445626000	-0.381097000	2.853116000
C	-2.944241000	-1.053858000	4.600795000
O	-1.119043000	-2.371904000	1.753722000
C	-3.324033000	-3.314895000	1.845285000
C	-1.727359000	-3.494303000	3.754404000
H	-3.625289000	-2.748600000	0.953639000
H	-4.218595000	-3.481867000	2.464252000
H	-2.959871000	-4.298175000	1.515798000
H	-0.914929000	-3.007210000	4.310176000
H	-1.324231000	-4.421625000	3.326030000
H	-2.520812000	-3.763555000	4.465564000
H	-3.809013000	-1.679258000	4.866981000
H	-3.191847000	-0.015852000	4.860745000
H	-2.093351000	-1.358107000	5.221758000
H	-3.549606000	-0.560777000	1.239796000
H	-3.902447000	0.509971000	2.604815000
H	-4.718905000	-1.067841000	2.489166000
B	-0.719614000	-1.072260000	1.918588000
H	0.446162000	-0.728665000	1.721991000

^{3}TS_10, -4750.90476, NImag=1

Co	0.856443000	-0.188906000	-0.148889000
P	1.809733000	1.808467000	0.030773000
C	3.628723000	1.785906000	-0.182434000
C	4.329905000	0.852460000	0.601607000
C	4.329401000	2.452233000	-1.193836000
C	5.669107000	0.556059000	0.360872000
C	5.675533000	2.175609000	-1.434750000
C	6.337645000	1.218557000	-0.668140000
H	3.804533000	3.176028000	-1.823990000
H	6.173821000	-0.197514000	0.970477000
H	6.202102000	2.695190000	-2.238333000
H	7.385067000	0.981189000	-0.868916000
P	2.482595000	-1.662445000	-0.454692000
C	3.399146000	-2.077093000	1.095530000
C	3.835375000	-1.046071000	1.947986000
C	3.588652000	-3.395869000	1.532170000
C	4.425153000	-1.317521000	3.179915000
C	4.186520000	-3.678300000	2.759792000
C	4.601059000	-2.637676000	3.588588000
O	3.618876000	0.271233000	1.617407000
H	3.246896000	-4.220870000	0.900731000
H	4.729665000	-0.477253000	3.806816000
H	4.319111000	-4.716710000	3.071254000
H	5.060824000	-2.850359000	4.556328000
H	-2.733781000	-0.778327000	-2.254404000
C	-3.372122000	2.051295000	-0.659619000
C	-4.445072000	2.957005000	-0.658244000

C	-2.009609000	2.361337000	-0.027624000
C	-2.416311000	3.830928000	-2.363530000
C	-1.478255000	3.644156000	-0.150779000
C	-1.681804000	4.384472000	-1.315384000
H	-3.528702000	2.108999000	-3.063162000
H	-1.908268000	1.787617000	0.896917000
H	-2.585169000	4.405583000	-3.278212000
H	-0.908086000	4.073967000	0.678580000
H	-1.265539000	5.390962000	-1.405857000
N	-3.314017000	0.501017000	-0.943954000
C	-2.418822000	-0.638524000	-1.037941000
O	-1.274960000	-0.503449000	-0.256492000
C	-6.925593000	0.741830000	-0.709827000
C	-6.707942000	-0.763506000	-1.093076000
C	-7.982654000	1.454187000	-1.526649000
O	-5.639068000	1.324217000	-1.003127000
C	-7.184012000	0.933770000	0.776370000
O	-5.298871000	-0.944837000	-0.847150000
C	-6.942220000	-1.029424000	-2.572546000
C	-7.483954000	-1.749311000	-0.245985000
H	-6.399562000	-0.307335000	-3.198757000
H	-8.007617000	-0.980718000	-2.837980000
H	-6.574604000	-2.033027000	-2.824475000
H	-7.207808000	-1.682775000	0.813364000
H	-7.279969000	-2.776286000	-0.577739000
H	-8.566883000	-1.577777000	-0.334142000
H	-8.183410000	0.582190000	1.069039000
H	-7.111945000	2.001453000	1.022289000
H	-6.440482000	0.400043000	1.383770000
H	-7.737188000	1.464127000	-2.595277000
H	-8.072656000	2.498127000	-1.197971000
H	-8.965750000	0.977231000	-1.400177000
B	-4.717157000	0.304827000	-0.927326000
H	-2.066954000	-0.769493000	-2.080726000
C	1.823169000	2.389569000	2.131359000
C	2.863122000	3.052732000	2.798741000
C	0.605227000	2.184861000	2.792716000
C	2.674952000	3.534079000	4.093041000
C	0.419866000	2.671899000	4.086207000
C	1.450207000	3.350054000	4.736102000
H	3.832310000	3.183171000	2.306533000
H	-0.196359000	1.614422000	2.312474000
H	3.491333000	4.049490000	4.605061000
H	-0.535761000	2.506919000	4.589732000
H	1.304906000	3.725875000	5.751876000
C	1.934213000	3.204062000	-0.664599000
C	2.327049000	4.496654000	-0.295245000
C	1.430588000	2.994956000	-1.955789000
C	2.244899000	5.546508000	-1.209424000
C	1.362214000	4.038510000	-2.875320000
C	1.773967000	5.317496000	-2.503020000
H	2.696447000	4.687088000	0.716707000
H	1.059793000	1.998033000	-2.229964000
H	2.551744000	6.551485000	-0.909491000
H	0.961179000	3.857057000	-3.875175000
H	1.712449000	6.142533000	-3.216814000
C	0.928370000	-2.859921000	-1.812627000
C	1.176711000	-3.135599000	-3.164626000
C	-0.203598000	-3.424421000	-1.199470000
C	0.317567000	-3.965519000	-3.886187000
C	-1.050625000	-4.258778000	-1.923559000
C	-0.796221000	-4.531057000	-3.268980000
H	2.045593000	-2.700785000	-3.665692000
H	-0.438983000	-3.204393000	-0.152622000
H	0.524928000	-4.170496000	-4.939391000
H	-1.925322000	-4.689400000	-1.429152000
H	-1.467470000	-5.180557000	-3.836092000
C	3.407883000	-1.452621000	-1.906029000
C	4.351224000	-2.477765000	-2.064361000
C	3.582870000	-0.254185000	-2.603567000
C	5.441976000	-2.304493000	-2.912145000
C	4.672182000	-0.081108000	-3.456869000
C	5.602317000	-1.106627000	-3.612594000
H	4.226543000	-3.419922000	-1.520930000
H	2.860061000	0.555992000	-2.456296000
H	6.171968000	-3.109102000	-3.030278000
H	4.798373000	0.863856000	-3.991237000
H	6.459164000	-0.972804000	-4.277394000
C	-2.614005000	-0.857566000	2.962787000
C	-1.932257000	-2.259374000	2.806107000
C	-4.027145000	-0.836885000	2.393188000
O	-1.793185000	-0.030737000	2.144777000
C	-2.612332000	-0.315222000	4.379569000
O	-1.493219000	-2.221791000	1.452701000

C	-2.107610000	2.513320000	-0.261418000
C	-4.249362000	4.280107000	-0.270028000
C	-1.922475000	3.840001000	0.116508000
C	-2.990010000	4.735423000	0.116369000
H	-5.432923000	2.623387000	-0.970424000
H	-1.262385000	1.821085000	-0.210699000
H	-5.100086000	4.966502000	-0.282088000
H	-0.927951000	4.167391000	0.432035000
H	-2.841830000	5.774352000	0.418679000
N	-3.544149000	0.705930000	-1.068064000
C	-2.391865000	0.000864000	-1.559063000
O	-1.560507000	-0.639629000	-0.601882000
C	-6.995921000	-0.573610000	-0.973457000
C	-6.141629000	-1.783663000	-1.511080000
C	-8.162457000	-0.190865000	-1.862210000
O	-6.044166000	0.516230000	-0.979497000
C	-7.480887000	-0.755797000	0.454687000
O	-4.789138000	-1.385714000	-1.203120000
C	-6.218449000	-1.940092000	-3.022105000
C	-6.424301000	-3.104045000	-0.826896000
H	-5.994589000	-0.995096000	-3.536496000
H	-7.208053000	-2.283455000	-3.353291000
H	-5.475688000	-2.679966000	-3.348326000
H	-6.228425000	-3.056142000	0.251211000
H	-5.780855000	-3.889318000	-1.244771000
H	-7.470008000	-3.409637000	-0.976500000
H	-8.270407000	-1.517178000	0.518961000
H	-7.894815000	0.193235000	0.820512000
H	-6.670470000	-1.046280000	1.132659000
H	-7.838770000	0.099441000	-2.868404000
H	-8.702216000	0.661010000	-1.427952000
H	-8.873738000	-1.024474000	-1.954077000
B	-4.783902000	-0.018414000	-1.062907000
H	-1.752732000	0.709542000	-2.112084000
C	1.565144000	2.709378000	1.610170000
C	2.474433000	3.659862000	2.093247000
C	0.415755000	2.415827000	2.356053000
C	2.223893000	4.328823000	3.290495000
C	0.161172000	3.098689000	3.544575000
C	1.062351000	4.054647000	4.013279000
H	3.390163000	3.872646000	1.531711000
H	-0.268731000	1.634975000	2.003465000
H	2.940155000	5.065914000	3.662253000
H	-0.744234000	2.874199000	4.113912000
H	0.864917000	4.581430000	4.950243000
C	1.284013000	3.030421000	-1.241080000
C	1.402616000	4.420010000	-1.112441000
C	0.681188000	2.511954000	-2.395217000
C	0.929115000	5.265969000	-2.114290000
C	0.210770000	3.353751000	-3.400680000
C	0.331736000	4.735573000	-3.258112000
H	1.855417000	4.846929000	-0.212270000
H	0.569582000	1.423012000	-2.488621000
H	1.019956000	6.348712000	-1.998009000
H	-0.263337000	2.931752000	-4.290073000
H	-0.047244000	5.401679000	-4.036669000
C	1.721735000	-3.276413000	-0.888666000
C	2.177053000	-4.132796000	-1.899148000
C	0.556370000	-3.614699000	-0.181420000
C	1.486947000	-5.312589000	-2.183180000
C	-0.127066000	-4.792447000	-0.466402000
C	0.338503000	-5.647724000	-1.467055000
H	3.072877000	-3.880960000	-2.473097000
H	0.179133000	-2.930389000	0.584644000
H	1.850883000	-5.973350000	-2.974150000
H	-1.037588000	-5.028828000	0.090456000
H	-0.198887000	-6.571488000	-1.695834000
C	3.851714000	-1.512935000	-1.678091000
C	5.020236000	-2.286842000	-1.630030000
C	3.708546000	-0.567344000	-2.698423000
C	6.013386000	-2.126352000	-2.593307000
C	4.700174000	-0.406936000	-3.665412000
C	5.853620000	-1.187294000	-3.614473000
H	5.152813000	-3.022013000	-0.829469000
H	2.810369000	0.062033000	-2.710868000
H	6.919345000	-2.736133000	-2.547708000
H	4.576579000	0.341068000	-4.452610000
H	6.635238000	-1.059573000	-4.367463000
C	-2.914893000	-0.575433000	2.714804000
C	-2.316591000	-2.030051000	2.628639000
C	-4.411262000	-0.547733000	2.448671000
O	-2.302289000	0.092356000	1.596552000
C	-2.570169000	0.177077000	3.980721000
O	-2.017886000	-2.153728000	1.222291000

C	-2.867995000	-3.436777000	2.991137000
C	-0.708775000	-2.402277000	3.707722000
H	-3.669757000	-3.433218000	2.241822000
H	-3.326748000	-3.429140000	3.991449000
H	-2.317444000	-4.382158000	2.884218000
H	-0.051360000	-1.523213000	3.627188000
H	-0.127335000	-3.280601000	3.392087000
H	-0.979361000	-2.533318000	4.765884000
H	-3.149519000	-0.986407000	5.067141000
H	-3.113746000	0.662983000	4.412265000
H	-1.591491000	-0.177489000	4.758346000
H	-4.065727000	-1.296424000	1.395510000
H	-4.347846000	0.210468000	2.290061000
H	-4.752542000	-1.355138000	3.039758000
B	-1.108297000	-0.864744000	1.185057000
H	0.173743000	-0.667677000	1.337964000

^{3}Int_10, -4750.91957, NImag=0

Co	-0.603419000	0.148835000	-0.737371000
P	-1.899656000	1.754079000	0.045662000
C	-3.504265000	1.181837000	0.730339000
C	-4.284523000	0.353063000	-0.095339000
C	-3.899891000	1.330523000	2.065187000
C	-5.386518000	-0.341881000	0.398494000
C	-5.008263000	0.649370000	2.568607000
C	-5.740579000	-0.197257000	1.739080000
H	-3.310455000	1.965136000	2.732845000
H	-5.952167000	-0.998388000	-0.267221000
H	-5.287872000	0.766987000	3.617987000
H	-6.596725000	-0.750190000	2.132883000
P	-1.794077000	-1.713155000	-0.510482000
C	-3.135799000	-1.980617000	-1.751789000
C	-4.005381000	-0.921349000	-2.071778000
C	-3.266629000	-3.164592000	-2.492064000
C	-4.941754000	-1.028896000	-3.096751000
C	-4.209933000	-3.287330000	-3.511426000
C	-5.043285000	-2.214229000	-3.821453000
O	-3.910764000	0.280199000	-1.411402000
H	-2.603193000	-4.006267000	-2.273824000
H	-5.577480000	-0.168027000	-3.312275000
H	-4.285506000	-4.222779000	-4.070168000
H	-5.776404000	-2.297895000	-4.626905000
H	1.670275000	0.197994000	-2.407236000
C	4.718204000	-0.702333000	-1.559921000
C	5.977921000	-0.077674000	-1.569383000
C	4.680960000	-2.101414000	-1.693282000
C	7.146788000	-0.825982000	-1.674540000
C	5.856671000	-2.838157000	-1.808797000
C	7.102158000	-2.213712000	-1.792692000
H	6.042506000	1.005379000	-1.487999000
H	3.735706000	-2.640874000	-1.668418000
H	8.108076000	-0.305885000	-1.673992000
H	5.788386000	-3.925167000	-1.903107000
H	8.020809000	-2.797655000	-1.878884000
N	3.541793000	0.079655000	-1.440103000
C	2.255138000	-0.470772000	-1.759179000
O	1.425201000	-0.601676000	-0.589425000
C	3.930584000	3.326144000	0.193086000
C	2.665804000	3.524778000	-0.699465000
C	4.936860000	4.451924000	0.127726000
O	4.522517000	2.133112000	-0.385231000
C	3.575422000	2.987734000	1.633058000
O	2.313618000	2.150296000	-1.009557000
C	2.976627000	4.212840000	-2.019141000
C	1.511648000	4.202183000	-0.001742000
H	3.833679000	3.749048000	-2.527938000
H	3.196246000	5.280350000	-1.879947000
H	2.106179000	4.131852000	-2.684029000
H	1.204196000	3.660993000	0.898721000
H	0.639056000	4.264570000	-0.667273000
H	1.784624000	5.227776000	0.288403000
H	3.181396000	3.859011000	2.174973000
H	4.474688000	2.635821000	2.157586000
H	2.816067000	2.191156000	1.679846000
H	5.321890000	4.596249000	-0.888847000
H	5.792794000	4.237969000	0.781587000
H	4.485628000	5.396373000	0.464501000
B	3.488227000	1.437320000	-0.958685000
H	2.351976000	-1.444526000	-2.253210000
C	-2.387218000	3.075748000	-1.133237000
C	-3.569096000	3.818050000	-1.016570000
C	-1.528151000	3.322288000	-2.211192000
C	-3.872331000	4.810690000	-1.948031000
C	-1.824165000	4.325637000	-3.132152000
C	-2.996449000	5.071383000	-3.002234000
C	-3.292010000	-3.127182000	3.005837000
C	-1.017846000	-2.189963000	3.402330000
H	-4.172323000	-3.139206000	2.351091000
H	-3.631506000	-3.012751000	4.045941000
H	-2.803589000	-4.107561000	2.921765000
H	-0.285629000	-1.422950000	3.112312000
H	-0.573913000	-3.168023000	3.167140000
H	-1.184323000	-2.147939000	4.488242000
H	-2.975317000	-0.332270000	4.867595000
H	-3.002185000	1.187051000	3.944726000
H	-1.484781000	0.278846000	4.104752000
H	-4.636764000	-1.098878000	1.523786000
H	-4.742739000	0.491763000	2.309809000
H	-4.997118000	-0.989085000	3.267983000
B	-1.877694000	-0.880072000	0.726266000
H	0.371350000	-0.664207000	1.317716000

^{3}TS_11, -4750.88847, NImag=1

Co	-0.806162000	-0.008602000	-1.152363000
P	-1.601587000	1.889717000	-0.136540000
C	-3.370059000	1.799104000	0.341197000
C	-4.248187000	1.098571000	-0.505903000
C	-3.884628000	2.287404000	1.549631000
C	-5.591946000	0.922206000	-0.175552000
C	-5.222416000	2.104468000	1.895698000
C	-6.077114000	1.429453000	1.027013000
H	-3.219665000	2.807612000	2.243353000
H	-6.245593000	0.374705000	-0.858113000
H	-5.593580000	2.487736000	2.848399000
H	-7.128464000	1.285560000	1.287531000
P	-2.210093000	-1.610743000	-0.382534000
C	-3.613868000	-1.785914000	-1.560113000
C	-4.164262000	-0.619903000	-2.123275000
C	-4.056869000	-3.016207000	-2.063667000
C	-5.097950000	-0.673402000	-3.152873000
C	-5.006234000	-3.082257000	-3.082823000
C	-5.521876000	-1.910837000	-3.634325000
O	-3.729731000	0.616066000	-1.682789000
H	-3.634469000	-3.941301000	-1.661749000
H	-5.476280000	0.263258000	-3.567164000
H	-5.332228000	-4.055095000	-3.457036000
H	-6.253730000	-1.956771000	-4.443839000
H	1.643133000	0.809227000	-2.158850000
C	4.499260000	-0.979016000	-1.919148000
C	5.867562000	-0.679201000	-1.859682000
C	4.105542000	-2.289233000	-2.227835000
C	6.816725000	-1.673986000	-2.075810000
C	5.063478000	-3.273255000	-2.449978000
C	6.424363000	-2.979409000	-2.369524000
H	6.191799000	0.337496000	-1.641993000
H	3.050740000	-2.556101000	-2.250017000
H	7.877350000	-1.417600000	-2.022528000
H	4.734711000	-4.290410000	-2.678466000
H	7.170706000	-3.757799000	-2.541073000
N	3.542957000	0.056609000	-1.717491000
C	2.249917000	-0.088076000	-2.084575000
O	0.974703000	-0.374460000	-0.325763000
C	4.554600000	2.547668000	0.769902000
C	3.558077000	3.353051000	-0.126658000
C	5.830435000	3.281852000	1.112115000
O	4.881291000	1.411149000	-0.081235000
C	3.892539000	1.985694000	2.017425000
O	2.929102000	2.293079000	-0.896807000
C	4.256183000	4.265022000	-1.121281000
C	2.495810000	4.101428000	0.643143000
H	5.048065000	3.738626000	-1.672599000
H	4.703417000	5.138369000	-0.627120000
H	3.523672000	4.630873000	-1.853222000
H	1.858097000	3.417791000	1.215128000
H	1.848495000	4.670397000	-0.038565000
H	2.953780000	4.816483000	1.342846000
H	3.623577000	2.780061000	2.727747000
H	4.585935000	1.299718000	2.523137000
H	2.975734000	1.425649000	1.774250000
H	6.396810000	3.562739000	0.216192000
H	6.478086000	2.649008000	1.732823000
H	5.609438000	4.195745000	1.682121000
B	3.809002000	1.249995000	-0.908762000
H	1.927703000	-0.966927000	-2.639648000
C	-1.524012000	3.325430000	-1.275759000
C	-2.625772000	4.105415000	-1.642248000
C	-0.266114000	3.619359000	-1.825577000
C	-2.470618000	5.167779000	-2.534663000
C	-0.111896000	4.688302000	-2.703089000
C	-1.215796000	5.464974000	-3.062564000

H	-4.260747000	3.614566000	-0.192292000
H	-0.644873000	2.683097000	-2.328241000
H	-4.799616000	5.381452000	-1.852822000
H	-1.146633000	4.512079000	-3.969643000
H	-3.235856000	5.848366000	-3.732609000
C	-1.241858000	2.717450000	1.478735000
C	-1.567367000	4.050486000	1.759428000
C	-0.317158000	2.061520000	2.305008000
C	-0.985196000	4.709882000	2.842222000
C	0.254562000	2.716034000	3.395423000
C	-0.075154000	4.044830000	3.664658000
H	-2.272821000	4.586911000	1.118287000
H	-0.016913000	1.033881000	2.067011000
H	-1.243505000	5.752587000	3.044317000
H	0.979000000	2.191931000	4.025020000
H	0.380580000	4.564551000	4.511254000
C	-0.660410000	-3.113890000	-0.876535000
C	-0.395495000	-4.169006000	0.006442000
C	0.082663000	-3.031876000	-2.068189000
C	0.592974000	-5.111519000	-0.287840000
C	1.056126000	-3.980661000	-2.365395000
C	1.322010000	-5.021444000	-1.471351000
H	-0.965940000	-4.258992000	0.935424000
H	-0.106576000	-2.191389000	-2.747015000
H	0.789286000	-5.925077000	0.416120000
H	1.620355000	-3.904164000	-3.299465000
H	2.093380000	-5.760746000	-1.700566000
C	-2.599400000	-2.271253000	1.053288000
C	-3.545139000	-3.304059000	1.122181000
C	-2.229083000	-1.612221000	2.229631000
C	-4.096293000	-3.675444000	2.346314000
C	-2.777808000	-1.984559000	3.456838000
C	-3.711482000	-3.017300000	3.516833000
H	-3.852754000	-3.821063000	0.207263000
H	-1.504647000	-0.790683000	2.161964000
H	-4.832356000	-4.482355000	2.389736000
H	-2.484323000	-1.454869000	4.367600000
H	-4.148515000	-3.306668000	4.475841000
C	3.338723000	-2.148085000	1.972962000
C	2.066741000	-1.660746000	2.761129000
C	4.497938000	-1.165792000	2.044023000
O	2.870777000	-2.132268000	0.602910000
C	3.796358000	-3.549458000	2.309091000
O	1.395287000	-0.828604000	1.777006000
C	2.364692000	-0.804911000	3.972892000
C	1.127774000	-2.796726000	3.120102000
H	2.909683000	0.109873000	3.706236000
H	2.961899000	-1.361066000	4.709983000
H	1.426170000	-0.507303000	4.461601000
H	0.899944000	-3.415899000	2.241760000
H	0.178996000	-2.392292000	3.496886000
H	1.554778000	-3.443457000	3.899012000
H	4.082543000	-3.627318000	3.367986000
H	4.675458000	-3.808865000	1.703790000
H	3.017423000	-4.293228000	2.102194000
H	4.185097000	-0.149265000	1.760353000
H	5.280804000	-1.472591000	1.336574000
H	4.941053000	-1.123332000	3.048692000
B	1.880642000	-1.202180000	0.553195000
H	-0.672062000	0.272676000	-2.363104000

^{3}Int_11, -4750.95315, NImag=0

Co	-0.051156000	-0.134949000	-0.856701000
P	-0.568527000	-2.307727000	0.163808000
C	0.804157000	-3.076307000	1.103202000
C	2.038859000	-3.179036000	0.443857000
C	0.762998000	-3.394374000	2.466251000
C	3.206945000	-3.529449000	1.118179000
C	1.919424000	-3.765563000	3.150821000
C	3.139964000	-3.815144000	2.480568000
H	-0.182700000	-3.326133000	3.009268000
H	4.157920000	-3.566533000	0.582414000
H	1.867679000	-3.998620000	4.216379000
H	4.053418000	-4.080099000	3.018086000
P	2.327964000	0.065659000	-0.553308000
C	3.479581000	-1.106437000	-1.417855000
C	3.140363000	-2.465424000	-1.517575000
C	4.678554000	-0.708360000	-2.030884000
C	3.911832000	-3.373188000	-2.239153000
C	5.473110000	-1.610883000	-2.735369000
C	5.082031000	-2.943031000	-2.857430000
O	2.000888000	-2.922861000	-0.901974000
H	4.998280000	0.333770000	-1.965692000
H	3.579049000	-4.411543000	-2.294603000
H	6.399263000	-1.264813000	-3.198986000
H	-3.613511000	3.884889000	-1.226658000
H	0.600890000	3.004093000	-1.556218000
H	-3.338842000	5.768604000	-2.816696000
H	0.874110000	4.908827000	-3.121038000
H	-1.097554000	6.297327000	-3.760370000
C	-0.815198000	2.579320000	1.370121000
C	-0.911589000	3.926276000	1.749812000
C	-0.080374000	1.694157000	2.166265000
C	-0.301175000	4.369235000	2.921795000
C	0.526465000	2.138253000	3.340907000
C	0.415221000	3.475055000	3.721966000
H	-1.469115000	4.631309000	1.124360000
H	0.036641000	0.657086000	1.845502000
H	-0.383137000	5.419383000	3.213895000
H	1.101775000	1.431611000	3.946249000
H	0.892664000	3.827249000	4.640259000
C	-1.440085000	-3.275034000	-0.367204000
C	-1.930049000	-4.343684000	0.398604000
C	-0.267752000	-3.451248000	-1.115182000
C	-1.265291000	-5.568378000	0.404668000
C	0.399848000	-4.674484000	-1.100139000
C	-0.098063000	-5.734756000	-0.343227000
H	-2.833618000	-4.211510000	1.002019000
H	0.118579000	-2.604103000	-1.693410000
H	-1.654502000	-6.395226000	1.003959000
H	1.326918000	-4.793567000	-1.667399000
H	0.429276000	-6.692165000	-0.327658000
C	-3.008633000	-1.564210000	1.270364000
C	-4.379564000	-1.722301000	1.501617000
C	-2.162453000	-1.293538000	2.357391000
C	-4.895570000	-1.603469000	2.793241000
C	-2.677059000	-1.189161000	3.646325000
C	-4.048164000	-1.337762000	3.867282000
H	-5.053329000	-1.933598000	0.665241000
H	-1.086454000	-1.170404000	2.186816000
H	-5.970212000	-1.717712000	2.958747000
H	-2.003312000	-0.979933000	4.482163000
H	-4.455616000	-1.242990000	4.876770000
C	3.082871000	-2.685375000	1.373577000
C	2.027523000	-2.322720000	2.478343000
C	4.384422000	-1.910857000	1.521920000
O	2.440902000	-2.218585000	0.178876000
C	3.366593000	-4.167497000	1.236113000
O	1.380585000	-1.166017000	1.919736000
C	2.621241000	-1.946123000	3.819858000
C	0.973622000	-3.406451000	2.642126000
H	3.266800000	-1.061333000	3.745529000
H	3.213921000	-2.772828000	4.238869000
H	1.820268000	-1.715217000	4.536541000
H	0.541409000	-3.684015000	1.669864000
H	0.156548000	-3.040932000	3.279939000
H	1.382911000	-4.315171000	3.106574000
H	3.789713000	-4.577785000	2.165347000
H	4.099280000	-4.334436000	0.433798000
H	2.460853000	-4.734644000	0.987304000
H	4.198464000	-0.828325000	1.571543000
H	5.023013000	-2.092083000	0.645941000
H	4.947710000	-2.208827000	2.417972000
B	1.544441000	-1.212066000	0.528255000
H	-0.650936000	-0.391110000	-2.743050000

^{3}D, -4013.96929, NImag=0

Co	-0.250450000	-0.436946000	-1.022000000
P	1.697901000	-1.129300000	-0.201132000
C	2.553080000	-0.075395000	1.028667000
C	2.748426000	1.275625000	0.690927000
C	2.830780000	-0.463047000	2.345159000
C	3.202371000	2.205774000	1.622379000
C	3.284289000	0.458598000	3.288493000
C	3.468419000	1.791223000	2.926381000
H	2.665773000	-1.501859000	2.643553000
H	3.333066000	3.249149000	1.325958000
H	3.484276000	0.134022000	4.311809000
H	3.817411000	2.519361000	3.662262000
P	-0.507541000	1.618691000	-0.142707000
C	0.534955000	3.041583000	-0.677180000
C	1.915710000	2.850209000	-0.874979000
C	0.002045000	4.292925000	-1.020109000
C	2.725478000	3.855142000	-1.397884000
C	0.807432000	5.309623000	-1.530860000
C	2.169844000	5.089824000	-1.726036000
O	2.479753000	1.622158000	-0.611934000
H	-1.069817000	4.469036000	-0.895373000
H	3.786812000	3.646001000	-1.545903000
H	0.363898000	6.273979000	-1.787348000

H	5.691745000	-3.650103000	-3.424082000
H	-1.637050000	-0.586651000	-2.896949000
C	-1.525206000	2.685095000	-2.309411000
C	-0.159458000	2.988967000	-2.220960000
C	-2.430806000	3.743122000	-2.507165000
C	0.291301000	4.300631000	-2.340039000
C	-1.972225000	5.051549000	-2.616355000
C	-0.609427000	5.344124000	-2.539747000
H	0.553363000	2.186805000	-2.026345000
H	-3.495516000	3.530238000	-2.588262000
H	1.361846000	4.502859000	-2.253944000
H	-2.695707000	5.854950000	-2.778357000
H	-0.255933000	6.373768000	-2.630018000
N	-1.969141000	1.352877000	-2.235898000
C	-1.057421000	0.289639000	-2.582617000
O	-0.883566000	0.965742000	0.460789000
C	-5.005765000	1.141824000	-0.231141000
C	-4.882699000	-0.295106000	-0.832930000
C	-6.389038000	1.746705000	-0.324411000
O	-4.108004000	1.894846000	-1.079712000
C	-4.456024000	1.233113000	1.181932000
O	-3.503145000	-0.310262000	-1.278856000
C	-5.749442000	-0.493451000	-2.067188000
C	-5.105222000	-1.411709000	0.159620000
H	-5.618061000	0.325902000	-2.787867000
H	-6.816528000	-0.559085000	-1.812568000
H	-5.464616000	-1.429941000	-2.566982000
H	-4.411845000	-1.346909000	1.005018000
H	-4.961989000	-2.390407000	-0.320987000
H	-6.132544000	-1.379064000	0.552333000
H	-5.103460000	0.721830000	1.909345000
H	-4.368943000	2.287846000	1.473301000
H	-3.444608000	0.806028000	1.237076000
H	-6.730148000	1.837737000	-1.363009000
H	-6.391144000	2.752408000	0.116385000
H	-7.119080000	1.137828000	0.228951000
B	-3.166407000	1.004932000	-1.527930000
H	-0.414491000	0.609007000	-3.414452000
C	0.727711000	3.724743000	2.046134000
C	-0.527190000	3.451720000	2.944596000
C	0.526788000	4.912685000	1.118108000
O	0.780538000	2.541991000	1.234974000
C	2.022872000	3.869110000	2.823050000
O	-1.353251000	2.657526000	2.091062000
C	-1.283504000	4.695179000	3.364149000
C	-0.186641000	2.598759000	4.160909000
H	-1.676031000	5.240070000	2.497125000
H	-0.641691000	5.376474000	3.942802000
H	-2.138399000	4.422332000	3.998219000
H	0.391948000	1.711053000	3.864345000
H	-1.116933000	2.252909000	4.632631000
H	0.394719000	3.148336000	4.915326000
H	1.932968000	4.644335000	3.599129000
H	2.843506000	4.174202000	2.158203000
H	2.315085000	2.926854000	3.306854000
H	-0.421675000	4.832503000	0.567361000
H	1.337045000	4.932396000	0.375476000
H	0.536766000	5.869312000	1.660841000
B	-0.513551000	2.000523000	1.185588000
H	0.403849000	-0.958242000	-2.035289000
C	-1.090279000	-3.602637000	-1.019073000
C	-2.161229000	-3.302475000	-1.875194000
C	-0.478603000	-4.858417000	-1.107003000
C	-2.614129000	-4.249483000	-2.791306000
C	-0.929536000	-5.799101000	-2.032716000
C	-1.998211000	-5.498691000	-2.875737000
H	-2.648742000	-2.323914000	-1.810398000
H	0.352356000	-5.110432000	-0.442677000
H	-3.452257000	-4.006350000	-3.449432000
H	-0.443751000	-6.776303000	-2.090811000
H	-2.351053000	-6.237752000	-3.598994000
C	-1.885230000	-2.370608000	1.438906000
C	-2.034848000	-1.278162000	2.305487000
C	-2.669385000	-3.515365000	1.640988000
C	-2.945412000	-1.337631000	3.360495000
C	-3.582280000	-3.567426000	2.692661000
C	-3.720323000	-2.480047000	3.557046000
H	-1.460154000	-0.365467000	2.125573000
H	-2.563186000	-4.375800000	0.973741000
H	-3.059451000	-0.473071000	4.019823000
H	-4.189083000	-4.464417000	2.839291000
H	-4.436979000	-2.523416000	4.380951000
C	3.017644000	1.653345000	-1.159514000
C	3.508597000	2.640628000	-0.300397000
H	2.803416000	5.878542000	-2.137638000
O	-1.478858000	-1.098468000	-2.386607000
C	2.919452000	-1.298288000	-1.559170000
C	4.292953000	-1.071071000	-1.409265000
C	2.418282000	-1.658225000	-2.817899000
C	5.152505000	-1.220679000	-2.496334000
C	3.280450000	-1.813955000	-3.901550000
C	4.648841000	-1.596377000	-3.742031000
H	4.691721000	-0.765810000	-0.436452000
H	1.339282000	-1.808958000	-2.945252000
H	6.222971000	-1.039694000	-2.370988000
H	2.878949000	-2.096849000	-4.877356000
H	5.324586000	-1.711471000	-4.592903000
C	1.733673000	-2.782088000	0.596854000
C	2.918936000	-3.495430000	0.823826000
C	0.510531000	-3.348631000	0.977477000
C	2.881501000	-4.745142000	1.437581000
C	0.475833000	-4.598977000	1.595873000
C	1.659716000	-5.296991000	1.828018000
H	3.879208000	-3.069208000	0.516575000
H	-0.418168000	-2.806686000	0.764821000
H	3.810101000	-5.294830000	1.609577000
H	-0.482616000	-5.035087000	1.889128000
H	1.632310000	-6.278771000	2.306880000
C	-2.205694000	2.232663000	-0.478777000
C	-2.986092000	2.936179000	0.448142000
C	-2.759204000	1.899978000	-1.724841000
C	-4.293327000	3.304557000	0.131880000
C	-4.063159000	2.276597000	-2.040538000
C	-4.833674000	2.977202000	-1.111986000
H	-2.577349000	3.186785000	1.431508000
H	-2.175067000	1.305304000	-2.434660000
H	-4.895763000	3.846460000	0.865167000
H	-4.483693000	2.002079000	-3.010681000
H	-5.860661000	3.261198000	-1.354131000
C	-0.408521000	1.666104000	1.689381000
C	-0.115775000	2.814656000	2.434741000
C	-0.659068000	0.461007000	2.360919000
C	-0.091571000	2.761081000	3.827964000
C	-0.643871000	0.410922000	3.753090000
C	-0.360601000	1.562123000	4.488571000
H	0.098763000	3.757780000	1.921044000
H	-0.861377000	-0.440303000	1.768899000
H	0.140692000	3.661635000	4.401977000
H	-0.840248000	-0.534447000	4.265752000
H	-0.339900000	1.523151000	5.580346000
C	-4.248837000	-2.552458000	-0.659070000
C	-3.455715000	-1.815893000	0.477438000
C	-3.941149000	-4.043559000	-0.697130000
O	-3.714206000	-1.971442000	-1.854698000
C	-5.744920000	-2.318825000	-0.624482000
O	-2.192379000	-1.584725000	-0.171196000
C	-3.236765000	-2.640487000	1.729427000
C	-4.060493000	-0.466788000	0.832221000
H	-2.685479000	-3.565847000	1.521900000
H	-4.196175000	-2.911830000	2.194762000
H	-2.662939000	-2.065676000	2.471310000
H	-4.256461000	0.133023000	-0.067903000
H	-3.359289000	0.098062000	1.464386000
H	-5.003599000	-0.571924000	1.387580000
H	-6.179120000	-2.657170000	0.328172000
H	-6.233107000	-2.879188000	-1.433227000
H	-5.991085000	-1.258816000	-0.762380000
H	-2.856437000	-4.225984000	-0.680526000
H	-4.334555000	-4.469943000	-1.629312000
H	-4.395871000	-4.585421000	0.144655000
B	-2.424919000	-1.536212000	-1.588132000

C	3.035079000	1.888996000	-2.543888000
C	4.043041000	3.822291000	-0.815928000
C	3.576023000	3.063706000	-3.057080000
C	4.090987000	4.032085000	-2.192527000
H	3.470759000	2.482923000	0.778763000
H	2.630719000	1.135272000	-3.228331000
H	4.427577000	4.583232000	-0.131489000
H	3.588273000	3.227808000	-4.137001000
H	4.516769000	4.954718000	-2.593901000
C	2.923563000	-0.038685000	1.179770000
C	4.287273000	-0.020778000	1.503486000
C	1.980001000	-0.173117000	2.202952000
C	4.696314000	-0.125538000	2.830789000
C	2.390316000	-0.295262000	3.529458000
C	3.747471000	-0.267055000	3.845530000
H	5.035357000	0.077382000	0.710118000
H	0.915835000	-0.181091000	1.944575000
H	5.761211000	-0.104453000	3.074788000
H	1.642752000	-0.419993000	4.317600000
H	4.069847000	-0.361568000	4.885379000

^{3}TS_12, -4425.50564, NImag=1[a]

Co	0.082069000	-0.174174000	-0.597457000
P	-1.190119000	1.680802000	-0.684207000
C	-1.332602000	2.639719000	0.874000000
C	-1.755381000	1.946558000	2.021971000
C	-0.850306000	3.942898000	1.044867000
C	-1.694731000	2.515006000	3.290866000
C	-0.780736000	4.524707000	2.310699000
C	-1.197053000	3.809349000	3.431584000
H	-0.497712000	4.503791000	0.175301000
H	-2.022205000	1.935416000	4.157610000
H	-0.387916000	5.537729000	2.420917000
H	-1.133366000	4.257350000	4.426023000
P	0.552696000	-0.417600000	1.592556000
C	-0.766650000	-0.949009000	2.762445000
C	-2.028995000	-0.327885000	2.705177000
C	-0.633397000	-2.056692000	3.612094000
C	-3.105575000	-0.789626000	3.457976000
C	-1.703301000	-2.521238000	4.375641000
C	-2.943090000	-1.889422000	4.297127000
O	-2.261846000	0.690344000	1.810447000
H	0.326784000	-2.577057000	3.663860000
H	-4.067012000	-0.282435000	3.356207000
H	-1.567389000	-3.387287000	5.026959000
H	-3.788548000	-2.255009000	4.884093000
O	0.759895000	-1.213816000	-2.114581000
C	-2.920310000	1.425869000	-1.229722000
C	-4.040152000	1.878201000	-0.524726000
C	-3.106388000	0.679783000	-2.402539000
C	-5.324242000	1.585452000	-0.984044000
C	-4.388167000	0.398585000	-2.864564000
C	-5.501158000	0.846317000	-2.152603000
H	-3.910970000	2.458493000	0.393174000
H	-2.232423000	0.303085000	-2.947249000
H	-6.193185000	1.937617000	-0.422501000
H	-4.520929000	-0.189706000	-3.775313000
H	-6.508059000	0.613709000	-2.506884000
C	-0.622310000	2.967003000	-1.867948000
C	-1.473576000	3.976461000	-2.340366000
C	0.708175000	2.934417000	-2.304228000
C	-0.996834000	4.945068000	-3.220398000
C	1.183583000	3.908988000	-3.182775000
C	0.334296000	4.914941000	-3.640411000
H	-2.518058000	4.003527000	-2.014055000
H	1.366847000	2.126249000	-1.965655000
H	-1.668027000	5.727223000	-3.583556000
H	2.222553000	3.876128000	-3.521209000
H	0.706180000	5.673701000	-4.333288000
C	1.822686000	-1.733460000	1.792645000
C	2.796568000	-1.758601000	2.799281000
C	1.832583000	-2.733257000	0.811396000
C	3.753552000	-2.772649000	2.826699000
C	2.783861000	-3.751073000	0.844751000
C	3.747747000	-3.772071000	1.852927000
H	2.820491000	-0.975187000	3.562199000
H	1.099547000	-2.680135000	0.001364000
H	4.513397000	-2.778825000	3.612115000
H	2.786676000	-4.516715000	0.064275000
H	4.503496000	-4.560998000	1.874268000
C	1.347265000	1.003390000	2.441815000
C	1.366780000	1.171809000	3.832735000
C	2.000265000	1.942103000	1.631916000
C	2.045418000	2.247555000	4.402555000
C	2.682954000	3.014673000	2.203535000

^{3}Int_12, -4425.51212, NImag=0

Co	-0.142815000	0.411916000	-0.448996000
P	2.013314000	0.179596000	-1.048738000
C	3.197089000	-0.487529000	0.187568000
C	3.184177000	0.085644000	1.470900000
C	4.018379000	-1.603141000	-0.015378000
C	3.984214000	-0.405999000	2.500741000
C	4.814161000	-2.112507000	1.010229000
C	4.803785000	-1.506962000	2.264891000
H	4.022528000	-2.095127000	-0.991355000
H	3.948369000	0.069839000	3.483432000
H	5.438917000	-2.989162000	0.826627000
H	5.428412000	-1.897741000	3.071641000
P	-0.152196000	-0.532023000	1.623763000
C	0.496857000	0.472736000	3.024599000
C	1.654343000	1.255801000	2.841310000
C	-0.208262000	0.641556000	4.225476000
C	2.077613000	2.170919000	3.801108000
C	0.217960000	1.543210000	5.199313000
C	1.357600000	2.315612000	4.985236000
O	2.362463000	1.171778000	1.660750000
H	-1.121181000	0.064334000	4.393421000
H	2.971959000	2.763252000	3.597401000
H	-0.353092000	1.650115000	6.123972000
H	1.688580000	3.034306000	5.738176000
O	-1.940118000	0.639338000	-1.186045000
C	2.795409000	1.770403000	-1.528914000
C	4.106545000	2.133268000	-1.195947000
C	2.002562000	2.670260000	-2.253767000
C	4.615752000	3.370013000	-1.591501000
C	2.513523000	3.903180000	-2.649933000
C	3.822134000	4.256162000	-2.319452000
H	4.735214000	1.446693000	-0.620774000
H	0.966662000	2.411322000	-2.493948000
H	5.639642000	3.644121000	-1.325254000
H	1.877485000	4.596305000	-3.205789000
H	4.222254000	5.226707000	-2.622677000
C	2.330833000	-0.872230000	-2.520652000
C	3.537454000	-0.824732000	-3.233732000
C	1.315301000	-1.735980000	-2.952606000
C	3.734625000	-1.644070000	-4.342483000
C	1.518465000	-2.560694000	-4.059997000
C	2.726710000	-2.518347000	-4.753534000
H	4.329198000	-0.138174000	-2.917060000
H	0.350277000	-1.747169000	-2.431305000
H	4.678096000	-1.598539000	-4.891879000
H	0.721338000	-3.232072000	-4.388844000
H	2.881649000	-3.160003000	-5.624370000
C	-1.826325000	-1.008012000	2.212078000
C	-2.081629000	-2.153105000	2.979404000
C	-2.900370000	-0.199550000	1.811926000
C	-3.386952000	-2.479206000	3.344420000
C	-4.204549000	-0.531409000	2.175672000
C	-4.451034000	-1.671349000	2.940964000
H	-1.256642000	-2.803116000	3.286028000
H	-2.704871000	0.682785000	1.197553000
H	-3.575113000	-3.376016000	3.939981000
H	-5.033753000	0.097377000	1.840913000
H	-5.474444000	-1.936287000	3.218178000
C	0.737533000	-2.132338000	1.709032000
C	1.438035000	-2.601006000	2.825372000
C	0.679827000	-2.926331000	0.553818000
C	2.062555000	-3.848447000	2.788904000
C	1.296501000	-4.174393000	0.522642000

C	2.708887000	3.167369000	3.589496000
H	0.842583000	0.456190000	4.475160000
H	1.964978000	1.816688000	0.542685000
H	2.055088000	2.370191000	5.488561000
H	3.186849000	3.741981000	1.561418000
H	3.239686000	4.010642000	4.037984000
C	4.211203000	-0.579274000	-2.762918000
C	3.936759000	0.262964000	-1.465535000
C	4.162677000	0.272025000	-4.025095000
O	3.093336000	-1.474344000	-2.809929000
C	5.491202000	-1.388159000	-2.720497000
O	2.500765000	0.258009000	-1.418188000
C	4.426481000	1.696429000	-1.526337000
C	4.455709000	-0.412543000	-0.205725000
H	3.971261000	2.254581000	-2.353904000
H	5.519570000	1.737193000	-1.645317000
H	4.177538000	2.221181000	-0.592457000
H	4.129753000	-1.460327000	-0.149205000
H	4.062463000	0.107821000	0.680134000
H	5.553573000	-0.389991000	-0.149636000
H	6.368822000	-0.738074000	-2.587509000
H	5.621260000	-1.938547000	-3.662151000
H	5.477394000	-2.123732000	-1.906907000
H	3.251087000	0.886492000	-4.055412000
H	4.143909000	-0.386818000	-4.903331000
H	5.033001000	0.937777000	-4.116090000
B	2.029866000	-0.872467000	-2.149104000
H	-2.941732000	-1.019599000	0.185452000
B	-2.606001000	-1.981854000	-0.431884000
O	-3.399360000	-2.578000000	-1.360397000
O	-1.403920000	-2.613328000	-0.243098000
C	-2.590604000	-3.591539000	-2.014503000
C	-1.513582000	-3.903237000	-0.931673000
C	-3.477831000	-4.761139000	-2.376413000
H	-2.882543000	-5.592240000	-2.782046000
H	-4.045805000	-5.129707000	-1.513397000
H	-4.200524000	-4.461556000	-3.147137000
C	-1.983328000	-2.947963000	-3.249379000
H	-1.452992000	-3.684568000	-3.868407000
H	-2.780226000	-2.505065000	-3.862496000
H	-1.260733000	-2.166588000	-2.972732000
C	-1.989599000	-4.890494000	0.121116000
H	-1.282527000	-4.888470000	0.962763000
H	-2.041538000	-5.913560000	-0.277473000
H	-2.980480000	-4.621590000	0.514154000
C	-0.181340000	-4.327836000	-1.507947000
H	-0.332551000	-5.150265000	-2.223339000
H	0.480690000	-4.710331000	-0.719679000
H	0.322698000	-3.497868000	-2.021137000

[a]One extra very low imaginary frequency below *i*3cm^{-1} is present

^{3}TS_13, -4425.50761, NImag=1

Co	-0.112393000	0.394204000	-0.307332000
P	1.971986000	0.804334000	-0.969489000
C	3.350914000	0.044829000	-0.026556000
C	3.328578000	0.190934000	1.371627000
C	4.337380000	-0.781608000	-0.577746000
C	4.272519000	-0.431266000	2.186761000
C	5.281366000	-1.417594000	0.228052000
C	5.253482000	-1.233717000	1.608732000
H	4.356775000	-0.945743000	-1.658175000
H	4.224750000	-0.292547000	3.269211000
H	6.036096000	-2.062551000	-0.226877000
H	5.992570000	-1.725223000	2.245864000
P	0.146466000	-1.049138000	1.415389000
C	0.738980000	-0.404721000	3.035327000
C	1.732111000	0.594256000	3.065650000
C	0.126902000	-0.739810000	4.252391000
C	2.083415000	1.239956000	4.247736000
C	0.485080000	-0.110787000	5.443492000
C	1.457805000	0.886932000	5.441466000
O	2.341471000	0.991300000	1.894598000
H	-0.658977000	-1.499491000	4.263344000
H	2.846476000	2.019911000	4.208989000
H	-0.009961000	-0.394343000	6.374602000
H	1.731328000	1.394519000	6.369080000
O	-2.014014000	0.716200000	-0.754003000
C	2.385691000	2.592519000	-0.937125000
C	3.647815000	3.095178000	-0.596766000
C	1.355508000	3.489137000	-1.252206000
C	3.876093000	4.471001000	-0.583536000
C	1.586927000	4.862148000	-1.241838000
C	2.847825000	5.356152000	-0.906686000
H	4.457935000	2.407845000	-0.333518000
C	1.990022000	-4.637954000	1.641734000
H	1.501267000	-1.984448000	3.728221000
H	0.137171000	-2.550269000	-0.320728000
H	2.614071000	-4.203562000	3.663312000
H	1.245656000	-4.782189000	-0.385186000
H	2.482162000	-5.613277000	1.617398000
C	-3.981637000	-2.075853000	-2.242326000
C	-2.736868000	-2.810632000	-1.624789000
C	-3.904540000	-1.987854000	-3.760807000
O	-3.853352000	-0.745497000	-1.728088000
C	-5.319460000	-2.643604000	-1.813378000
O	-1.791859000	-1.737398000	-1.499909000
C	-2.134503000	-3.890427000	-2.501492000
C	-3.017661000	-3.355984000	-0.233462000
H	-1.803916000	-3.493612000	-3.469730000
H	-2.853979000	-4.701491000	-2.689019000
H	-1.258287000	-4.333532000	-2.004305000
H	-3.475848000	-2.589233000	0.405877000
H	-2.076217000	-3.667634000	0.242142000
H	-3.688140000	-4.227202000	-0.259354000
H	-5.417359000	-3.700177000	-2.104451000
H	-6.136045000	-2.087227000	-2.293515000
H	-5.461365000	-2.567527000	-0.727953000
H	-2.929391000	-1.598058000	-4.086725000
H	-4.675672000	-1.294937000	-4.123077000
H	-4.065756000	-2.961763000	-4.245178000
B	-2.507487000	-0.517652000	-1.451144000
H	0.259444000	2.127659000	0.183674000
B	-0.783032000	2.722432000	-0.070233000
O	-0.913357000	3.495108000	-1.176505000
O	-1.777094000	2.845038000	0.844385000
C	-2.229745000	4.102797000	-1.149419000
C	-2.795899000	3.715152000	0.289087000
C	-2.037024000	5.593350000	-1.362580000
H	-2.996506000	6.128878000	-1.341543000
H	-1.375711000	6.040401000	-0.610584000
H	-1.581261000	5.765145000	-2.346885000
C	-3.018483000	3.509783000	-2.303758000
H	-4.033799000	3.927380000	-2.352187000
H	-2.512178000	3.753045000	-3.247834000
H	-3.076132000	2.417810000	-2.224255000
C	-2.927290000	4.889580000	1.242992000
H	-3.230189000	4.522363000	2.232533000
H	-3.685814000	5.607786000	0.902414000
H	-1.977493000	5.424302000	1.368097000
C	-4.091199000	2.924933000	0.247547000
H	-4.907521000	3.518207000	-0.188125000
H	-4.386338000	2.654823000	1.271392000
H	-3.977153000	2.000145000	-0.333166000

^{3}Int_13, -4425.51638, NImag=0

Co	-0.038723000	0.365188000	0.052362000
P	-1.989378000	1.218052000	0.694924000
C	-3.396693000	0.051599000	0.797757000
C	-3.736394000	-0.638323000	-0.378734000
C	-4.037499000	-0.324679000	1.983832000
C	-4.689870000	-1.653581000	-0.383385000
C	-4.988515000	-1.345337000	1.994773000
C	-5.315163000	-2.004916000	0.811795000
H	-3.776313000	0.179473000	2.918103000
H	-4.927420000	-2.169295000	-1.316803000
H	-5.471181000	-1.626955000	2.932844000
H	-6.059562000	-2.804668000	0.814926000
P	-0.475201000	-1.642326000	-0.862226000
C	-1.578705000	-1.930809000	-2.310367000
C	-2.747261000	-1.161667000	-2.472502000
C	-1.244186000	-2.815747000	-3.346537000
C	-3.538699000	-1.266004000	-3.613808000
C	-2.037766000	-2.936577000	-4.485737000
C	-3.184873000	-2.157537000	-4.623585000
O	-3.092740000	-0.230829000	-1.520085000
H	-0.333856000	-3.414864000	-3.265367000
H	-4.423549000	-0.631284000	-3.693203000
H	-1.749346000	-3.635539000	-5.273556000
H	-3.804176000	-2.237833000	-5.519633000
O	1.901499000	0.799512000	0.342898000
C	-2.634882000	2.633824000	-0.269829000
C	-3.996802000	2.827536000	-0.531255000
C	-1.699214000	3.554405000	-0.765341000
C	-4.420505000	3.931465000	-1.270265000
C	-2.130471000	4.660893000	-1.494339000
C	-3.488688000	4.851150000	-1.750475000
H	-4.732833000	2.108466000	-0.157947000

H	0.355340000	3.114319000	-1.492452000
H	4.863500000	4.853825000	-0.313553000
H	0.768580000	5.545666000	-1.480463000
H	3.028044000	6.433761000	-0.888625000
C	2.352788000	0.333200000	-2.703808000
C	3.474880000	0.812574000	-3.394557000
C	1.461992000	-0.524903000	-3.362753000
C	3.715571000	0.419382000	-4.708872000
C	1.707650000	-0.922091000	-4.677557000
C	2.835202000	-0.454140000	-5.350147000
H	4.164879000	1.502038000	-2.897540000
H	0.555711000	-0.865211000	-2.847003000
H	4.592704000	0.799272000	-5.238337000
H	1.007590000	-1.592012000	-5.182910000
H	3.024555000	-0.760623000	-6.381750000
C	-1.378814000	-1.961683000	1.887070000
C	-1.391003000	-3.329695000	2.194017000
C	-2.590701000	-1.252271000	1.877910000
C	-2.590420000	-3.976548000	2.488809000
C	-3.787205000	-1.905170000	2.172173000
C	-3.791606000	-3.267098000	2.474893000
H	-0.457593000	-3.900109000	2.194284000
H	-2.600822000	-0.183123000	1.641480000
H	-2.586486000	-5.043846000	2.723925000
H	-4.724238000	-1.342880000	2.151258000
H	-4.731810000	-3.778017000	2.697252000
C	1.283545000	-2.418513000	0.978318000
C	2.146734000	-3.063909000	1.869354000
C	1.257115000	-2.824991000	-0.364379000
C	2.965055000	-4.103203000	1.424358000
C	2.065246000	-3.869586000	-0.804474000
C	2.923012000	-4.510458000	0.091389000
H	2.184844000	-2.747686000	2.917078000
H	0.590172000	-2.304697000	-1.062058000
H	3.644101000	-4.595723000	2.125105000
H	2.035407000	-4.174936000	-1.854129000
H	3.566922000	-5.323623000	-0.252219000
C	-3.842041000	-1.775920000	-2.517114000
C	-2.448624000	-2.466847000	-2.282390000
C	-3.961688000	-1.172514000	-3.909212000
O	-3.819673000	-0.685893000	-1.580592000
C	-5.036318000	-2.656778000	-2.215090000
O	-1.637215000	-1.359968000	-1.850505000
C	-1.822345000	-3.072187000	-3.522234000
C	-2.487962000	-3.486794000	-1.156796000
H	-1.654685000	-2.321402000	-4.304837000
H	-2.453944000	-3.870604000	-3.939222000
H	-0.848262000	-3.518514000	-3.271127000
H	-2.960129000	-3.068067000	-0.257851000
H	-1.463772000	-3.783744000	-0.888360000
H	-3.038579000	-4.394332000	-1.443103000
H	-5.036521000	-3.557415000	-2.846783000
H	-5.967674000	-2.109189000	-2.413116000
H	-5.053139000	-2.969350000	-1.163601000
H	-3.092732000	-0.542306000	-4.146486000
H	-4.855043000	-0.535489000	-3.953683000
H	-4.052211000	-1.941635000	-4.689460000
B	-2.493781000	-0.364452000	-1.342143000
H	-0.407525000	1.953119000	0.615723000
B	-1.607081000	2.215301000	0.430909000
O	-1.903960000	3.325760000	-0.330039000
O	-2.486438000	2.025905000	1.476471000
C	-3.288911000	3.638401000	-0.093352000
C	-3.592566000	2.928011000	1.295865000
C	-3.424577000	5.150049000	-0.059372000
H	-4.456012000	5.453374000	0.172540000
H	-2.754537000	5.609476000	0.677000000
H	-3.169031000	5.565161000	-1.043906000
C	-4.105731000	3.087164000	-1.254802000
H	-5.169746000	3.347290000	-1.160144000
H	-3.734700000	3.528403000	-2.190151000
H	-4.017322000	1.999112000	-1.344960000
C	-3.571505000	3.879366000	2.481815000
H	-3.651343000	3.299946000	3.411505000
H	-4.403699000	4.596955000	2.455546000
H	-2.629469000	4.441399000	2.525382000
C	-4.870434000	2.107973000	1.300089000
H	-5.754171000	2.733930000	1.106767000
H	-5.004970000	1.637037000	2.284539000
H	-4.836793000	1.309800000	0.546566000

^{3}TS_14, -4425.49462, NImag=1

Co	0.104997000	0.385489000	-0.078543000
P	-1.680897000	1.310124000	0.867575000
C	-3.140555000	0.201116000	0.905146000
H	-0.626804000	3.407080000	-0.589895000
H	-5.485199000	4.072851000	-1.472310000
H	-1.394557000	5.374757000	-1.872886000
H	-3.821924000	5.715297000	-2.330397000
C	-1.894138000	1.883184000	2.402566000
C	-2.850651000	2.756223000	2.938655000
C	-0.803530000	1.498118000	3.193363000
C	-2.726870000	3.218500000	4.246719000
C	-0.682217000	1.958010000	4.504146000
C	-1.644758000	2.816564000	5.032305000
H	-3.697177000	3.077439000	2.323303000
H	-0.030664000	0.844217000	2.770898000
H	-3.476202000	3.900528000	4.655742000
H	0.174454000	1.652408000	5.109168000
H	-1.547828000	3.183553000	6.056912000
C	1.056854000	-2.533647000	-1.344746000
C	1.242122000	-3.912753000	-1.166799000
C	2.104289000	-1.764417000	-1.871779000
C	2.448641000	-4.511587000	-1.525442000
C	3.313611000	-2.365669000	-2.218915000
C	3.487327000	-3.739007000	-2.049888000
H	0.438921000	-4.522270000	-0.740742000
H	1.992771000	-0.684826000	-2.013678000
H	2.583214000	-5.586993000	-1.384436000
H	4.123091000	-1.741583000	-2.606199000
H	4.436564000	-4.210363000	-2.317719000
C	-1.157420000	-2.716933000	0.457902000
C	-2.108038000	-3.724450000	0.263832000
C	-0.676258000	-2.472109000	1.754114000
C	-2.569541000	-4.473995000	1.346563000
C	-1.129145000	-3.228773000	2.831355000
C	-2.080884000	-4.230017000	2.629115000
H	-2.498379000	-3.919272000	-0.740399000
H	0.075719000	-1.688027000	1.914514000
H	-3.319051000	-5.253114000	1.185762000
H	-0.743486000	-3.029790000	3.834421000
H	-2.445665000	-4.817916000	3.474711000
C	4.835163000	-0.793189000	1.603837000
C	3.660209000	-1.559941000	2.311387000
C	5.462506000	0.266564000	2.496174000
O	4.157566000	-0.098794000	0.535297000
C	5.899300000	-1.688145000	1.005569000
O	2.534540000	-0.697718000	2.048792000
C	3.819345000	-1.718818000	3.808042000
C	3.361051000	-2.896813000	1.655545000
H	3.879969000	-0.750637000	4.319574000
H	4.723968000	-2.296042000	4.049343000
H	2.958347000	-2.261519000	4.222420000
H	3.262581000	-2.783820000	0.567601000
H	2.408993000	-3.292085000	2.037387000
H	4.143802000	-3.642510000	1.854790000
H	6.379257000	-2.302548000	1.781556000
H	6.679934000	-1.079305000	0.529979000
H	5.485515000	-2.355996000	0.239932000
H	4.697407000	0.918301000	2.941819000
H	6.129554000	0.900320000	1.896515000
H	6.054246000	-0.175945000	3.309771000
B	2.848391000	0.040785000	0.920870000
H	0.510947000	1.387747000	-1.278698000
B	1.716297000	1.694063000	-0.878915000
O	1.735789000	3.089034000	-0.561140000
O	2.701659000	1.437425000	-1.879381000
C	2.924907000	3.632222000	-1.131559000
C	3.147355000	2.698981000	-2.370153000
C	2.684603000	5.089447000	-1.474053000
H	3.536004000	5.517541000	-2.024895000
H	1.779675000	5.217882000	-2.081770000
H	2.551729000	5.678166000	-0.555421000
C	4.054602000	3.508817000	-0.113644000
H	4.979581000	3.997978000	-0.454542000
H	3.744824000	3.987769000	0.825997000
H	4.281407000	2.455138000	0.100851000
C	2.266185000	3.100147000	-3.548097000
H	2.280124000	2.300214000	-4.301186000
H	2.607531000	4.027681000	-4.031324000
H	1.222876000	3.239946000	-3.228663000
C	4.593293000	2.566702000	-2.805760000
H	5.025455000	3.544408000	-3.068397000
H	4.666180000	1.920935000	-3.692462000
H	5.204409000	2.112218000	-2.015487000

^{3}Int_14, -4750.91519, NImag=0

Co	-0.431328000	-0.016036000	-0.437667000
P	-1.139250000	1.954946000	0.397570000
C	-2.948179000	1.994288000	0.726339000

C	-3.571400000	-0.308932000	-0.332697000
C	-3.699304000	-0.345681000	2.065983000
C	-4.498189000	-1.344209000	-0.416921000
C	-4.632638000	-1.380766000	1.995873000
C	-5.022394000	-1.885032000	0.756963000
H	-3.376857000	0.025298000	3.042986000
H	-4.791651000	-1.728616000	-1.396988000
H	-5.044794000	-1.803651000	2.914755000
H	-5.739748000	-2.707028000	0.697535000
P	-0.573049000	-1.467561000	-1.083781000
C	-1.661618000	-1.349260000	-2.569302000
C	-2.756061000	-0.463622000	-2.561971000
C	-1.387671000	-2.021941000	-3.768755000
C	-3.537238000	-0.259397000	-3.696906000
C	-2.169672000	-1.831467000	-4.907129000
C	-3.244721000	-0.945381000	-4.873369000
O	-3.036195000	0.287164000	-1.445723000
H	-0.531825000	-2.700871000	-3.816338000
H	-4.364095000	0.450907000	-3.637092000
H	-1.929289000	-2.370927000	-5.825848000
H	-3.856172000	-0.782987000	-5.763810000
O	2.113535000	0.860996000	0.674244000
C	-2.328915000	2.876564000	0.170953000
C	-3.692412000	3.193034000	0.135868000
C	-1.398282000	3.785656000	-0.349952000
C	-4.120339000	4.407523000	-0.399306000
C	-1.828971000	5.005090000	-0.869565000
C	-3.188696000	5.317563000	-0.897937000
H	-4.426452000	2.481061000	0.527050000
H	-0.335516000	3.517061000	-0.356596000
H	-5.187158000	4.643706000	-0.427327000
H	-1.099018000	5.714535000	-1.267736000
H	-3.523894000	6.269868000	-1.316470000
C	-1.477481000	1.716136000	2.651285000
C	-2.269612000	2.645798000	3.337651000
C	-0.470236000	1.036134000	3.350046000
C	-2.069152000	2.876265000	4.697671000
C	-0.274926000	1.261788000	4.711949000
C	-1.074932000	2.181826000	5.388493000
H	-3.050396000	3.195073000	2.802621000
H	0.172290000	0.328737000	2.813217000
H	-2.692435000	3.604477000	5.222655000
H	0.513092000	0.723494000	5.245042000
H	-0.919184000	2.365427000	6.454405000
C	0.924372000	-2.313012000	-1.749876000
C	1.079155000	-3.699908000	-1.877886000
C	2.010219000	-1.479298000	-2.058561000
C	2.294594000	-4.236988000	-2.303404000
C	3.227647000	-2.016707000	-2.471254000
C	3.372519000	-3.399434000	-2.595560000
H	0.252524000	-4.370824000	-1.625605000
H	1.891530000	-0.394723000	-1.959077000
H	2.404102000	-5.320653000	-2.396110000
H	4.063294000	-1.343876000	-2.682320000
H	4.325923000	-3.827060000	-2.916393000
C	-1.380478000	-2.810374000	-0.110944000
C	-2.129638000	-3.853807000	-0.671934000
C	-1.232688000	-2.754903000	1.281128000
C	-2.698140000	-4.832459000	0.141379000
C	-1.795803000	-3.737241000	2.094729000
C	-2.528528000	-4.778317000	1.525742000
H	-2.276212000	-3.896138000	-1.756530000
H	-0.674278000	-1.917496000	1.718373000
H	-3.281094000	-5.641134000	-0.306965000
H	-1.677428000	-3.678303000	3.180061000
H	-2.978802000	-5.543884000	2.162472000
C	4.226396000	-1.591682000	2.185598000
C	2.797767000	-2.246335000	2.252415000
C	4.635293000	-0.940581000	3.496494000
O	4.041625000	-0.519826000	1.225425000
C	5.314478000	-2.511949000	1.678234000
O	1.937168000	-1.130135000	1.912913000
C	2.396209000	-2.763005000	3.616672000
C	2.591962000	-3.311702000	1.192301000
H	2.385279000	-1.968646000	4.372876000
H	3.081221000	-3.553946000	3.954803000
H	1.386888000	-3.194880000	3.568709000
H	2.898715000	-2.953380000	0.200422000
H	1.526425000	-3.576500000	1.137191000
H	3.159066000	-4.225672000	1.417780000
H	5.418835000	-3.391739000	2.329610000
H	6.278517000	-1.986518000	1.667507000
H	5.111260000	-2.857127000	0.657348000
H	3.848634000	-0.273821000	3.877256000
C	-3.762101000	1.683712000	-0.377896000
C	-3.566775000	2.161636000	1.969318000
C	-5.132205000	1.472405000	-0.243791000
C	-4.942300000	1.974304000	2.113976000
C	-5.717834000	1.611214000	1.013753000
H	-2.960768000	2.420936000	2.842123000
H	-5.725913000	1.199640000	-1.119809000
H	-5.407031000	2.099501000	3.094702000
H	-6.790627000	1.439349000	1.129296000
P	-2.225456000	-1.191989000	-0.954263000
C	-3.155244000	-0.606099000	-2.444931000
C	-3.489992000	0.753744000	-2.564688000
C	-3.491675000	-1.446188000	-3.515418000
C	-4.115312000	1.257692000	-3.702836000
C	-4.128491000	-0.955296000	-4.654776000
C	-4.436451000	0.400223000	-4.752463000
O	-3.122159000	1.644291000	-1.586657000
H	-3.238388000	-2.508679000	-3.461733000
H	-4.331644000	2.326957000	-3.747040000
H	-4.375952000	-1.636129000	-5.472244000
H	-4.925519000	0.793703000	-5.646414000
H	1.601358000	-1.950892000	-1.113807000
C	2.320112000	0.810000000	0.640235000
C	3.035019000	1.052574000	1.817675000
C	2.214763000	1.827805000	-0.317445000
C	3.607866000	2.306416000	2.036883000
C	2.784801000	3.075590000	-0.089256000
C	3.486141000	3.322246000	1.091716000
H	3.132733000	0.267933000	2.566727000
H	1.648985000	1.623517000	-1.231441000
H	4.152878000	2.486223000	2.967247000
H	2.668279000	3.862245000	-0.840125000
H	3.930702000	4.303409000	1.276119000
N	1.707991000	-0.460570000	0.345672000
C	2.265917000	-1.120216000	-0.839930000
O	3.535285000	-1.647412000	-0.530749000
C	1.298140000	-2.449020000	3.383052000
C	0.625748000	-3.347971000	2.295337000
C	0.530301000	-2.336278000	4.680713000
O	1.309535000	-1.152382000	2.732297000
C	2.749033000	-2.826794000	3.635465000
O	1.070483000	-2.714379000	1.071131000
C	-0.886178000	-3.246193000	2.335938000
C	1.078862000	-4.790095000	2.281861000
H	-1.203274000	-2.193906000	2.354621000
H	-1.313506000	-3.751294000	3.213408000
H	-1.312501000	-3.704279000	1.434616000
H	2.156034000	-4.877730000	2.096885000
H	0.558992000	-5.335908000	1.482902000
H	0.845075000	-5.284152000	3.236300000
H	2.834862000	-3.779912000	4.175527000
H	3.231284000	-2.049812000	4.243963000
H	3.309174000	-2.912626000	2.692667000
H	-0.461839000	-1.892454000	4.529835000
H	1.077486000	-1.703080000	5.392246000
H	0.400115000	-3.324479000	5.145266000
B	1.354129000	-1.411888000	1.387845000
H	2.311252000	-0.406774000	-1.674893000
C	-0.958275000	3.488925000	-0.609407000
C	-1.424535000	4.730808000	-0.156699000
C	-0.417896000	3.390721000	-1.895467000
C	-1.306980000	5.864210000	-0.959095000
C	-0.303611000	4.524461000	-2.699183000
C	-0.737814000	5.763784000	-2.229619000
H	-1.888882000	4.811540000	0.831565000
H	-0.125591000	2.398068000	-2.261605000
H	-1.669014000	6.828899000	-0.594683000
H	0.117129000	4.436679000	-3.704243000
H	-0.648493000	6.652228000	-2.860021000
C	-0.427713000	2.393410000	2.035916000
C	0.284534000	3.566633000	2.315800000
C	-0.512482000	1.414080000	3.039892000
C	0.863687000	3.765911000	3.569320000
C	0.054648000	1.616779000	4.293614000
C	0.743476000	2.799452000	4.564888000
H	0.407862000	4.330109000	1.544410000
H	-1.019517000	0.465096000	2.826073000
H	1.423502000	4.684974000	3.762031000
H	-0.026920000	0.839071000	5.056627000
H	1.197424000	2.959328000	5.545952000
C	-1.647043000	-2.845824000	-1.517166000
C	-2.101924000	-4.061166000	-0.989434000
C	-0.601389000	-2.870649000	-2.457204000
C	-1.515229000	-5.268106000	-1.374500000

H	5.537177000	-0.334957000	3.338299000
H	4.857605000	-1.686367000	4.272060000
B	2.712147000	-0.228707000	1.227478000
H	0.510324000	1.334416000	-1.352230000
B	2.470846000	1.763672000	-0.328602000
O	2.228961000	3.104515000	-0.202989000
O	3.356363000	1.439477000	-1.322580000
C	3.053250000	3.773663000	-1.181341000
C	3.466661000	2.611019000	-2.164177000
C	2.238581000	4.871900000	-1.831031000
H	2.809742000	5.367262000	-2.630055000
H	1.307783000	4.481699000	-2.260435000
H	1.973136000	5.634702000	-1.085841000
C	4.235442000	4.358091000	-0.424129000
H	4.898883000	4.940929000	-1.078390000
H	3.865616000	5.024290000	0.366531000
H	4.830844000	3.569721000	0.056665000
C	2.498959000	2.429755000	-3.322271000
H	2.760198000	1.512697000	-3.869225000
H	2.546057000	3.269251000	-4.030007000
H	1.467292000	2.311651000	-2.960329000
C	4.889607000	2.704127000	-2.674382000
H	5.039169000	3.630077000	-3.248824000
H	5.103832000	1.860166000	-3.343969000
H	5.624174000	2.678240000	-1.860760000

^{3}TS_15, -4750.87042, NImag=1

Co	-0.566439000	0.012475000	-0.430830000
P	-1.642344000	1.880820000	0.237550000
C	-3.355640000	1.526116000	0.810243000
C	-4.190681000	0.897119000	-0.129694000
C	-3.840013000	1.680928000	2.113467000
C	-5.433626000	0.377208000	0.224064000
C	-5.091479000	1.181577000	2.477221000
C	-5.877552000	0.515878000	1.538383000
H	-3.219399000	2.179311000	2.863414000
H	-6.040475000	-0.133383000	-0.527738000
H	-5.446484000	1.301974000	3.503245000
H	-6.847677000	0.103271000	1.825201000
P	-2.096481000	-1.579793000	-0.611174000
C	-3.338178000	-1.454632000	-1.975345000
C	-3.981115000	-0.227303000	-2.213723000
C	-3.623453000	-2.509960000	-2.853685000
C	-4.845921000	-0.049550000	-3.291222000
C	-4.498251000	-2.347888000	-3.927071000
C	-5.103768000	-1.112914000	-4.152816000
O	-3.716442000	0.857088000	-1.414894000
H	-3.138134000	-3.477977000	-2.701832000
H	-5.301416000	0.931907000	-3.436292000
H	-4.699138000	-3.189445000	-4.593624000
H	-5.780690000	-0.975512000	-4.999025000
H	1.162340000	-1.340975000	-1.661289000
C	1.945793000	1.458826000	0.050687000
C	2.410112000	1.916402000	1.292457000
C	1.743173000	2.391389000	-0.978149000
C	2.709134000	3.263918000	1.474000000
C	2.037642000	3.738104000	-0.782526000
C	2.535326000	4.184697000	0.441265000
H	2.545804000	1.209823000	2.109403000
H	1.326676000	2.061590000	-1.931460000
H	3.075183000	3.597159000	2.448672000
H	1.861784000	4.444289000	-1.598488000
H	2.764026000	5.241885000	0.595239000
N	1.599105000	0.084783000	-0.138689000
C	1.739986000	-0.446327000	-1.428746000
O	3.178896000	-1.337148000	-0.945594000
C	3.299958000	-2.015471000	2.409220000
C	1.864900000	-2.587450000	2.158060000
C	3.566805000	-1.578684000	3.834421000
O	3.297801000	-0.847935000	1.564766000
C	-0.023124000	-4.076103000	-2.843923000
C	-0.472110000	-5.280156000	-2.297952000
H	-2.920509000	-4.071109000	-0.264709000
H	-0.240406000	-1.921468000	-2.869025000
H	-1.880705000	-6.205990000	-0.947851000
H	0.789380000	-4.075804000	-3.574947000
H	-0.012695000	-6.225322000	-2.596932000
C	-3.649593000	-1.606641000	0.151879000
C	-4.814356000	-2.244833000	-0.299499000
C	-3.575122000	-1.215076000	1.490891000
C	-5.864355000	-2.504275000	0.578375000
C	-4.623226000	-1.472007000	2.373277000
C	-5.769040000	-2.121381000	1.918248000
H	-4.901016000	-2.539947000	-1.350177000
H	-2.682715000	-0.674006000	1.823550000
H	-6.765397000	-3.005364000	0.215546000
H	-4.550471000	-1.146672000	3.414372000
H	-6.596081000	-2.320590000	2.604261000
C	6.035266000	0.469229000	-1.942233000
C	6.859634000	-0.747660000	-1.393134000
C	6.058238000	1.664433000	-1.004267000
O	4.685865000	-0.051407000	-1.933725000
C	6.391422000	0.887447000	-3.351826000
O	5.904313000	-1.405472000	-0.532432000
C	8.074069000	-0.366197000	-0.575182000
C	7.237613000	-1.738074000	-2.483580000
H	7.800096000	0.218625000	0.310766000
H	8.782719000	0.223067000	-1.175382000
H	8.596704000	-1.268350000	-0.230222000
H	6.368585000	-2.005693000	-3.100644000
H	7.615996000	-2.659803000	-2.022297000
H	8.019966000	-1.342383000	-3.146092000
H	7.443786000	1.201206000	-3.413075000
H	5.770288000	1.738260000	-3.661706000
H	6.229071000	0.077719000	-4.073112000
H	5.793926000	1.375725000	0.023567000
H	5.315557000	2.401798000	-1.336151000
H	7.042202000	2.153595000	-0.985725000
B	4.663676000	-1.044158000	-0.986024000
H	-0.077527000	0.251111000	-2.006756000

^{3}Int_15, -4750.99121, NImag=0

Co	0.403510000	-0.053677000	-0.228158000
P	1.608634000	1.876439000	0.013365000
C	3.411962000	1.625373000	0.274385000
C	3.760697000	0.730601000	1.300807000
C	4.448861000	2.192950000	-0.474188000
C	5.075280000	0.316836000	1.499437000
C	5.773342000	1.805639000	-0.273384000
C	6.079548000	0.847331000	0.692074000
H	4.217354000	2.942743000	-1.234527000
H	5.303646000	-0.411754000	2.281112000
H	6.567044000	2.249114000	-0.878257000
H	7.112374000	0.521628000	0.836112000
P	1.814153000	-1.829264000	0.259419000
C	2.287126000	-2.022815000	2.034747000
C	2.724441000	-0.889544000	2.741854000
C	2.196479000	-3.230071000	2.741570000
C	3.058769000	-0.948846000	4.092211000
C	2.533686000	-3.302489000	4.092704000
C	2.964710000	-2.162842000	4.769766000
O	2.729584000	0.334831000	2.113769000
H	1.849912000	-4.128394000	2.223492000
H	3.381278000	-0.034309000	4.594264000
H	2.453743000	-4.255939000	4.619000000
H	3.223925000	-2.214917000	5.829401000
H	-1.164757000	-0.878020000	1.561426000
C	-2.199961000	1.898813000	0.016921000
C	-2.696308000	2.389104000	-1.212502000
C	-2.118944000	2.823354000	1.081244000
C	-3.062490000	3.721470000	-1.359618000
C	-2.465100000	4.163333000	0.913071000
C	-2.938974000	4.633848000	-0.309160000
H	-2.818851000	1.698067000	-2.042383000
H	-1.782891000	2.506731000	2.067647000
H	-3.451387000	4.053430000	-2.327152000
H	-2.371100000	4.842204000	1.765715000
H	-3.221695000	5.681302000	-0.435951000
N	-1.778524000	0.566939000	0.172272000
C	-1.482281000	0.175314000	1.543411000
O	-2.994807000	-1.622533000	0.170135000
C	-2.473969000	-1.198303000	-2.941871000
C	-0.960613000	-1.286230000	-2.584752000
C	-2.756424000	-0.533013000	-4.276065000
O	-2.977327000	-0.371477000	-1.904491000

C	4.389489000	-2.956110000	1.918099000
O	1.651459000	-2.267855000	0.778122000
C	0.803377000	-1.851644000	2.965821000
C	1.747049000	-4.083363000	2.358725000
H	0.926122000	-0.761969000	2.865441000
H	0.827486000	-2.106224000	4.035858000
H	-0.188781000	-2.118826000	2.572150000
H	2.364502000	-4.635131000	1.639182000
H	0.706279000	-4.406727000	2.220764000
H	2.053186000	-4.368565000	3.376549000
H	4.495379000	-3.835688000	2.569378000
H	5.349863000	-2.424113000	1.896871000
H	4.184693000	-3.298464000	0.894424000
H	2.884513000	-0.779235000	4.151838000
H	4.592276000	-1.195730000	3.928678000
H	3.460713000	-2.422121000	4.532785000
B	2.412303000	-1.115661000	0.521246000
H	2.033136000	0.187155000	-2.268664000
C	-1.952831000	3.276869000	-0.919520000
C	-2.763112000	4.363008000	-0.559838000
C	-1.423327000	3.219536000	-2.211986000
C	-3.004240000	5.394023000	-1.465653000
C	-1.666237000	4.250962000	-3.118617000
C	-2.449263000	5.342605000	-2.745377000
H	-3.214833000	4.399356000	0.436915000
H	-0.850134000	2.330401000	-2.498550000
H	-3.634821000	6.237868000	-1.174559000
H	-1.251258000	4.195232000	-4.128295000
H	-2.641302000	6.149589000	-3.457037000
C	-0.917853000	2.672143000	1.730850000
C	-0.618909000	4.030762000	1.875990000
C	-0.582939000	1.800690000	2.780636000
C	-0.031158000	4.505207000	3.050348000
C	-0.004315000	2.271638000	3.954267000
C	0.270404000	3.633528000	4.093953000
H	-0.828802000	4.729345000	1.062417000
H	-0.776007000	0.728149000	2.661061000
H	0.200906000	5.569405000	3.143073000
H	0.243369000	1.571793000	4.757263000
H	0.730270000	4.010736000	5.010648000
C	-1.173388000	-3.093068000	-1.079616000
C	-1.003440000	-4.176665000	-0.210126000
C	-0.472758000	-3.089025000	-2.298783000
C	-0.153748000	-5.229580000	-0.548936000
C	0.376791000	-4.139700000	-2.632157000
C	0.542706000	-5.213049000	-1.754904000
H	-1.533300000	-4.197325000	0.747011000
H	-0.594622000	-2.239796000	-2.980548000
H	-0.029493000	-6.066815000	0.142857000
H	0.915846000	-4.120229000	-3.582609000
H	1.213126000	-6.035637000	-2.014279000
C	-3.153439000	-2.166549000	0.781100000
C	-4.167865000	-3.121803000	0.625432000
C	-2.930480000	-1.617728000	2.046792000
C	-4.931257000	-3.523290000	1.718818000
C	-3.692616000	-2.017862000	3.143873000
C	-4.693814000	-2.972863000	2.980749000
H	-4.362081000	-3.554440000	-0.361095000
H	-2.156682000	-0.850119000	2.152836000
H	-5.718498000	-4.269917000	1.587551000
H	-3.511309000	-1.570488000	4.124520000
H	-5.297180000	-3.286493000	3.836174000
C	5.779303000	1.002745000	-1.588700000
C	6.593092000	-0.299922000	-1.275228000
C	5.625960000	1.898840000	-0.370863000
O	4.462012000	0.468212000	-1.876901000
C	6.264769000	1.786810000	-2.786020000
O	5.577007000	-1.168287000	-0.716154000
C	7.694081000	-0.121621000	-0.253125000
C	7.123847000	-0.976977000	-2.527913000
H	7.299415000	0.208930000	0.714914000
H	8.433658000	0.615882000	-0.597671000
H	8.219646000	-1.072494000	-0.092362000
H	6.337809000	-1.090707000	-3.287314000
H	7.491520000	-1.979812000	-2.273724000
H	7.954192000	-0.413412000	-2.975780000
H	7.298141000	2.131375000	-2.635068000
H	5.634484000	2.674151000	-2.933172000
H	6.228374000	1.194576000	-3.708281000
H	5.290598000	1.324854000	0.506058000
H	4.863534000	2.664335000	-0.572123000
H	6.566156000	2.407647000	-0.115694000
B	4.377325000	-0.705544000	-1.173898000
H	-0.426180000	0.240341000	-2.061346000
C	-3.140146000	-2.570217000	-2.879645000
O	-1.006740000	-1.354246000	-1.153321000
C	-0.209554000	-0.014178000	-2.959819000
C	-0.238670000	-2.502499000	-3.127178000
H	-0.730341000	0.890842000	-2.607393000
H	-0.035919000	0.089366000	-4.041468000
H	0.797744000	-0.047842000	-2.498420000
H	-0.630621000	-3.431691000	-2.693490000
H	0.835685000	-2.454998000	-2.889620000
H	-0.330438000	-2.559145000	-4.222587000
H	-2.857973000	-3.206127000	-3.732038000
H	-4.231330000	-2.441735000	-2.898246000
H	-2.883595000	-3.093224000	-1.948408000
H	-2.396695000	0.504452000	-4.297977000
H	-3.839157000	-0.509598000	-4.461327000
H	-2.287495000	-1.081356000	-5.107138000
B	-2.274879000	-0.685033000	-0.690041000
H	-2.350466000	0.260768000	2.223121000
C	1.342375000	3.216500000	1.261641000
C	1.607963000	4.561224000	0.966992000
C	0.956150000	2.882494000	2.566363000
C	1.448487000	5.547358000	1.938129000
C	0.806115000	3.867531000	3.540564000
C	1.041142000	5.205072000	3.226924000
H	1.941914000	4.847320000	-0.033817000
H	0.779260000	1.837456000	2.829605000
H	1.649838000	6.591021000	1.685062000
H	0.499214000	3.586230000	4.550851000
H	0.914223000	5.979161000	3.987342000
C	1.443174000	2.736825000	-1.591933000
C	0.370277000	3.625163000	-1.771752000
C	2.188849000	2.356437000	-2.720349000
C	0.074845000	4.137867000	-3.032726000
C	1.894466000	2.875182000	-3.979599000
C	0.837428000	3.770523000	-4.140743000
H	-0.254562000	3.913576000	-0.920496000
H	3.007407000	1.637684000	-2.621062000
H	-0.768339000	4.824177000	-3.142509000
H	2.492785000	2.570526000	-4.841821000
H	0.604687000	4.174384000	-5.128724000
C	1.064241000	-3.464879000	-0.096987000
C	1.688945000	-4.460286000	-0.858305000
C	-0.247061000	-3.681497000	0.354717000
C	1.019309000	-5.648781000	-1.153563000
C	-0.911394000	-4.868677000	0.065259000
C	-0.279631000	-5.856234000	-0.692797000
H	2.701471000	-4.307864000	-1.240952000
H	-0.775298000	-2.906517000	0.915647000
H	1.518076000	-6.414399000	-1.752803000
H	-1.937275000	-5.005160000	0.415302000
H	-0.804436000	-6.784478000	-0.931283000
C	3.465848000	-1.934236000	-0.541405000
C	4.489176000	-2.768419000	-0.069918000
C	3.710462000	-1.127093000	-1.656353000
C	5.726239000	-2.795504000	-0.709663000
C	4.948032000	-1.150566000	-2.296853000
C	5.958396000	-1.985799000	-1.822875000
H	4.316696000	-3.400577000	0.806970000
H	2.915446000	-0.458357000	-2.005290000
H	6.517053000	-3.449955000	-0.334957000
H	5.126707000	-0.504741000	-3.160426000
H	6.932148000	-2.002707000	-2.318132000
C	-5.995403000	0.064429000	1.011821000
C	-6.220561000	-1.345851000	1.660877000
C	-6.655186000	0.194729000	-0.353869000
O	-4.579795000	0.063582000	0.793095000
C	-6.355025000	1.242721000	1.891587000
O	-5.179103000	-2.135573000	1.054743000
C	-7.561606000	-1.974789000	1.348770000
C	-5.969989000	-1.338995000	3.161518000
H	-7.695125000	-2.130911000	0.271600000
H	-8.386490000	-1.344291000	1.712702000
H	-7.646873000	-2.954243000	1.838933000
H	-5.010493000	-0.859165000	3.402022000
H	-5.928297000	-2.373138000	3.529158000
H	-6.763373000	-0.812761000	3.711250000
H	-7.423683000	1.235215000	2.153360000
H	-6.143214000	2.181386000	1.360511000
H	-5.769589000	1.252249000	2.819492000
H	-6.410187000	-0.663534000	-0.995858000
H	-6.270286000	1.095371000	-0.851495000
H	-7.749495000	0.276138000	-0.284130000
B	-4.192787000	-1.258262000	0.645743000
H	-0.666169000	0.779986000	1.972735000

^{3}TS_16, -4750.97533, NImag=1

Co	-0.367388000	-0.022535000	0.044663000
P	-1.877862000	1.687726000	-0.043212000
C	-3.456921000	1.252196000	-0.879523000
C	-3.354037000	0.458271000	-2.034158000
C	-4.735453000	1.661668000	-0.482162000
C	-4.482514000	0.059648000	-2.749055000
C	-5.872325000	1.262442000	-1.183016000
C	-5.743766000	0.459044000	-2.314754000
H	-4.843673000	2.305524000	0.394587000
H	-4.366569000	-0.562185000	-3.639662000
H	-6.859368000	1.587197000	-0.847373000
H	-6.629682000	0.146455000	-2.872491000
P	-1.613803000	-1.891174000	-0.261778000
C	-1.705036000	-2.217951000	-2.078787000
C	-1.871532000	-1.137339000	-2.963622000
C	-1.462773000	-3.480161000	-2.639903000
C	-1.770457000	-1.295992000	-4.342898000
C	-1.377754000	-3.653459000	-4.020541000
C	-1.520267000	-2.560085000	-4.873224000
O	-2.083061000	0.127419000	-2.455344000
H	-1.323079000	-4.340722000	-1.980440000
H	-1.888586000	-0.418134000	-4.981329000
H	-1.186410000	-4.647620000	-4.429621000
H	-1.437295000	-2.688568000	-5.954631000
H	1.316516000	-1.116142000	-1.723272000
C	1.961629000	1.887376000	-0.455153000
C	1.584457000	2.736034000	0.611310000
C	2.807186000	2.455975000	-1.437089000
C	1.995772000	4.058097000	0.684457000
C	3.220562000	3.784094000	-1.355879000
C	2.818117000	4.606733000	-0.304992000
H	0.932524000	2.328362000	1.387043000
H	3.150295000	1.850187000	-2.278267000
H	1.666912000	4.674244000	1.528079000
H	3.871127000	4.184404000	-2.140310000
H	3.138539000	5.649330000	-0.253168000
N	1.475146000	0.594090000	-0.508008000
C	1.757381000	-0.105660000	-1.742217000
O	3.158631000	-1.436772000	0.379413000
C	2.256759000	-0.078496000	3.429457000
C	0.914605000	-0.804603000	3.036786000
C	2.068579000	1.214126000	4.197762000
O	2.858397000	0.210919000	2.160313000
C	3.217002000	-0.998103000	4.173452000
O	1.201969000	-1.317238000	1.724632000
C	-0.254290000	0.151740000	2.908069000
C	0.530783000	-1.974555000	3.922312000
H	0.008085000	1.002949000	2.266126000
H	-0.602662000	0.557392000	3.868674000
H	-1.105771000	-0.369940000	2.441974000
H	1.296917000	-2.759220000	3.919503000
H	-0.400464000	-2.430128000	3.554479000
H	0.362411000	-1.651380000	4.960421000
H	2.861733000	-1.246624000	5.183599000
H	4.191746000	-0.500784000	4.266200000
H	3.376305000	-1.936903000	3.623886000
H	1.495113000	1.954546000	3.626233000
H	3.046644000	1.660862000	4.420428000
H	1.552937000	1.035168000	5.153154000
B	2.378481000	-0.717234000	1.257854000
H	2.838572000	-0.249134000	-1.940826000
C	-1.451013000	3.189048000	-1.016817000
C	-2.081361000	4.425363000	-0.819861000
C	-0.492404000	3.066199000	-2.027718000
C	-1.728983000	5.525376000	-1.598473000
C	-0.145361000	4.165291000	-2.810336000
C	-0.756420000	5.398216000	-2.591253000
H	-2.848263000	4.533446000	-0.046759000
H	-0.008761000	2.100149000	-2.187929000
H	-2.217636000	6.488121000	-1.429519000
H	0.622610000	4.057738000	-3.579812000
H	-0.474803000	6.264533000	-3.194661000
C	-2.362916000	2.341339000	1.592990000
C	-1.628803000	3.389730000	2.172709000
C	-3.290190000	1.654053000	2.392331000
C	-1.829441000	3.745824000	3.505109000
C	-3.495155000	2.017577000	3.721485000
C	-2.764004000	3.063969000	4.284913000
H	-0.886718000	3.927513000	1.574945000
H	-3.853993000	0.816598000	1.971517000
H	-1.248832000	4.565132000	3.936414000
H	-4.229661000	1.474752000	4.322517000
H	-2.921646000	3.346807000	5.328285000

^{3}E, -3853.84209, NImag=0

Co	-0.013814000	-0.901428000	-0.752310000
P	-2.025913000	-0.253166000	-0.058849000
C	-2.164851000	1.572864000	-0.095637000
C	-1.385217000	2.298651000	0.823283000
C	-2.737089000	2.282234000	-1.159945000
C	-1.187140000	3.670789000	0.698352000
C	-2.547167000	3.657263000	-1.296759000
C	-1.770045000	4.349585000	-0.370494000
H	-3.314546000	1.744317000	-1.916341000
H	-0.562215000	4.192639000	1.427380000
H	-2.994623000	4.184537000	-2.142008000
H	-1.606844000	5.424114000	-0.480688000
P	1.421936000	0.682675000	-0.008308000
C	1.564265000	1.535088000	1.624847000
C	0.405182000	1.874910000	2.349554000
C	2.801609000	1.792974000	2.235262000
C	0.477422000	2.429084000	3.626099000
C	2.883379000	2.360042000	3.505605000
C	1.719601000	2.673852000	4.205989000
O	-0.838013000	1.575052000	1.849794000
H	3.721966000	1.534433000	1.704611000
H	-0.454660000	2.652675000	4.148786000
H	3.862119000	2.549354000	3.951432000
H	1.776275000	3.107568000	5.206785000
H	1.161460000	-1.213131000	-3.672912000
C	-2.476546000	-0.800002000	1.644352000
C	-3.779545000	-0.785201000	2.153377000
C	-1.439753000	-1.284943000	2.453250000
C	-4.037404000	-1.237960000	3.447214000
C	-1.696104000	-1.739273000	3.743531000
C	-2.998211000	-1.716096000	4.244118000
H	-4.608182000	-0.425014000	1.539107000
H	-0.416362000	-1.288512000	2.060338000
H	-5.059722000	-1.220387000	3.832570000
H	-0.875101000	-2.113987000	4.359642000
H	-3.203967000	-2.074578000	5.255533000
C	-3.445866000	-0.834342000	-1.067700000
C	-4.727956000	-0.263277000	-1.047966000
C	-3.215779000	-1.948708000	-1.886652000
C	-5.754771000	-0.802332000	-1.820101000
C	-4.246232000	-2.493143000	-2.652213000
C	-5.516711000	-1.921110000	-2.619897000
H	-4.923638000	0.621138000	-0.434166000
H	-2.209307000	-2.384855000	-1.923934000
H	-6.747443000	-0.346042000	-1.798266000
H	-4.051629000	-3.364550000	-3.281535000
H	-6.323743000	-2.342893000	-3.223707000
C	3.135652000	0.087026000	-0.271542000
C	4.029917000	0.669879000	-1.179800000
C	3.526998000	-1.071325000	0.418181000
C	5.293132000	0.113219000	-1.380602000
C	4.792608000	-1.617266000	0.223596000
C	5.679447000	-1.026576000	-0.676905000
H	3.740498000	1.562877000	-1.740115000
H	2.828727000	-1.563417000	1.104554000
H	5.979497000	0.576146000	-2.093869000
H	5.074531000	-2.523096000	0.765184000
H	6.668851000	-1.461259000	-0.837477000
C	1.277319000	2.092262000	-1.174741000
C	1.839620000	3.354564000	-0.942561000
C	0.577796000	1.870237000	-2.367754000
C	1.710912000	4.367491000	-1.890269000
C	0.451760000	2.881762000	-3.318352000
C	1.019419000	4.132406000	-3.079823000
H	2.382629000	3.544663000	-0.011288000
H	0.120312000	0.888871000	-2.552563000
H	2.154008000	5.348170000	-1.700192000
H	-0.098582000	2.693997000	-4.243189000
H	0.919773000	4.928734000	-3.821249000
N	0.889224000	-2.211403000	-1.857324000
C	1.643281000	-1.986536000	-3.055878000
H	2.684167000	-1.646118000	-2.864595000
C	1.349407000	-3.169218000	-0.997829000
C	2.540429000	-3.922244000	-1.158058000
C	0.603820000	-3.401189000	0.193461000
C	2.968117000	-4.796319000	-0.162546000
C	1.056425000	-4.254562000	1.189058000
C	2.252968000	-4.962332000	1.026179000
H	3.146670000	-3.792931000	-2.057125000
H	-0.382299000	-2.920036000	0.288543000
H	3.896547000	-5.355874000	-0.314964000
H	0.452724000	-4.394541000	2.091030000
H	2.604315000	-5.649614000	1.798363000

C	-0.863991000	-3.450081000	0.355040000
C	-1.575929000	-4.443350000	1.039514000
C	0.513956000	-3.619884000	0.154456000
C	-0.918202000	-5.577168000	1.520001000
C	1.165938000	-4.754522000	0.624164000
C	0.451322000	-5.734928000	1.314878000
H	-2.651971000	-4.338800000	1.201601000
H	1.095101000	-2.845868000	-0.353648000
H	-1.484637000	-6.342881000	2.055693000
H	2.241736000	-4.857700000	0.463707000
H	0.963582000	-6.621876000	1.695660000
C	-3.355465000	-2.055660000	0.300262000
C	-4.412700000	-2.417110000	-0.542800000
C	-3.633487000	-1.791704000	1.650034000
C	-5.717005000	-2.489976000	-0.053382000
C	-4.932403000	-1.881858000	2.143184000
C	-5.981652000	-2.222530000	1.288213000
H	-4.218345000	-2.638941000	-1.595907000
H	-2.818623000	-1.515080000	2.327631000
H	-6.532392000	-2.758906000	-0.729623000
H	-5.126911000	-1.677125000	3.199231000
H	-7.003726000	-2.281282000	1.669247000
C	6.212744000	0.117619000	-0.604399000
C	6.183602000	-1.191673000	-1.469497000
C	7.097769000	-0.012984000	0.626281000
O	4.854457000	0.203732000	-0.137830000
C	6.552128000	1.378327000	-1.370338000
O	5.145086000	-1.963090000	-0.829549000
C	7.470086000	-1.989103000	-1.452810000
C	5.736385000	-0.934492000	-2.900193000
H	7.731585000	-2.321102000	-0.441009000
H	8.305938000	-1.394351000	-1.849575000
H	7.369231000	-2.884828000	-2.080462000
H	4.815960000	-0.333340000	-2.929572000
H	5.525645000	-1.892145000	-3.394758000
H	6.505344000	-0.409183000	-3.483753000
H	7.560716000	1.315604000	-1.805363000
H	6.525056000	2.244920000	-0.696333000
H	5.834792000	1.573188000	-2.176485000
H	6.873622000	-0.933301000	1.184114000
H	6.908990000	0.835862000	1.296403000
H	8.166563000	-0.017976000	0.369697000
B	4.339787000	-1.065897000	-0.167046000
H	1.354393000	0.406944000	-2.642500000

^{3}TS_17, -4265.37429, NImag=1

Co	-0.234222000	0.425237000	-0.330910000
P	-1.237645000	-1.332074000	0.724135000
C	-0.160128000	-2.708268000	1.275309000
C	0.809489000	-3.115978000	0.340201000
C	-0.151124000	-3.310550000	2.536861000
C	1.812758000	-4.021146000	0.676040000
C	0.834569000	-4.236568000	2.879689000
C	1.824962000	-4.571441000	1.957288000
H	-0.917996000	-3.039756000	3.267876000
H	2.574960000	-4.289000000	-0.059297000
H	0.832634000	-4.691146000	3.872674000
H	2.612102000	-5.278674000	2.228653000
P	2.002764000	0.019574000	-0.401697000
C	2.512859000	-1.232163000	-1.663574000
C	1.752891000	-2.413082000	-1.749167000
C	3.593809000	-1.100899000	-2.546538000
C	2.020560000	-3.393184000	-2.701360000
C	3.878935000	-2.081975000	-3.495482000
C	3.085585000	-3.224341000	-3.582924000
O	0.672244000	-2.579537000	-0.914849000
H	4.233162000	-0.217073000	-2.488813000
H	1.382756000	-4.278790000	-2.733789000
H	4.727001000	-1.949245000	-4.170642000
H	3.298179000	-3.989480000	-4.332608000
H	0.879692000	0.969346000	-3.049413000
C	-2.479542000	-2.255871000	-0.266159000
C	-3.455511000	-3.061085000	0.336022000
C	-2.416084000	-2.182357000	-1.661555000
C	-4.375796000	-3.752947000	-0.448183000
C	-3.334288000	-2.879172000	-2.444283000
C	-4.319627000	-3.657601000	-1.839505000
H	-3.503352000	-3.139353000	1.426871000
H	-1.644347000	-1.562711000	-2.125125000
H	-5.141091000	-4.369735000	0.029386000
H	-3.287043000	-2.796803000	-3.532625000
H	-5.047624000	-4.193916000	-2.453099000
C	-2.153870000	-0.760974000	2.200461000
C	-3.491809000	-0.354498000	2.070345000
C	-1.482097000	-0.453245000	3.395284000
H	1.725375000	-2.891458000	-3.688749000

^{3}Int_16, -4265.38352, NImag=0

Co	-0.204426000	0.476342000	-0.382171000
P	-0.524173000	-1.608668000	0.611137000
C	0.966799000	-2.368963000	1.370574000
C	2.098008000	-2.436791000	0.538204000
C	1.112059000	-2.777486000	2.700404000
C	3.348023000	-2.809704000	1.025485000
C	2.353244000	-3.175073000	3.198294000
C	3.471812000	-3.168399000	2.366924000
H	0.242881000	-2.770132000	3.363186000
H	4.213468000	-2.815971000	0.358724000
H	2.446842000	-3.480961000	4.242544000
H	4.450751000	-3.455348000	2.757827000
P	2.087987000	0.789780000	-0.340861000
C	3.141508000	-0.215794000	-1.471975000
C	2.882503000	-1.595567000	-1.549378000
C	4.168426000	0.293555000	-2.279694000
C	3.580009000	-2.426698000	-2.422443000
C	4.883717000	-0.531780000	-3.145902000
C	4.582280000	-1.890665000	-3.227163000
O	1.877720000	-2.134385000	-0.783700000
H	4.412677000	1.357821000	-2.232345000
H	3.322161000	-3.487069000	-2.453270000
H	5.678207000	-0.107606000	-3.763472000
H	5.132238000	-2.537831000	-3.913821000
H	-0.099113000	2.300785000	-2.502198000
C	-1.075651000	-2.977059000	-0.480539000
C	-1.492270000	-4.212726000	0.031644000
C	-1.040444000	-2.786095000	-1.865689000
C	-1.903345000	-5.227580000	-0.830257000
C	-1.448612000	-3.802112000	-2.726835000
C	-1.888314000	-5.020131000	-2.210345000
H	-1.503140000	-4.380288000	1.113544000
H	-0.695527000	-1.825703000	-2.260078000
H	-2.236432000	-6.185185000	-0.422608000
H	-1.436827000	-3.632351000	-3.806021000
H	-2.218570000	-5.813930000	-2.884907000
C	-1.745092000	-1.555910000	1.972846000
C	-3.059496000	-2.014766000	1.809040000
C	-1.432487000	-0.837528000	3.138398000

C	-4.133139000	0.332920000	3.098523000
C	-2.127022000	0.225543000	4.426401000
C	-3.454964000	0.626630000	4.280649000
H	-4.032854000	-0.564181000	1.143903000
H	-0.433135000	-0.736491000	3.523358000
H	-5.173834000	0.641695000	2.971024000
H	-1.584003000	0.448106000	5.348144000
H	-3.958393000	1.165900000	5.086398000
C	3.034786000	1.500670000	-0.769278000
C	3.558686000	2.234045000	0.307164000
C	3.192375000	2.023576000	-2.063514000
C	4.238105000	3.431749000	0.095977000
C	3.883171000	3.214903000	-2.275452000
C	4.412496000	3.923263000	-1.196764000
H	3.426619000	1.870702000	1.329623000
H	2.779528000	1.494981000	-2.925404000
H	4.633305000	3.982933000	0.952607000
H	4.004170000	3.592464000	-3.293603000
H	4.953463000	4.857634000	-1.363922000
C	2.929332000	-0.663141000	1.049335000
C	4.273889000	-1.044649000	0.936920000
C	2.282786000	-0.827399000	2.274732000
C	4.948586000	-1.581016000	2.030253000
C	2.954172000	-1.365731000	3.371937000
C	4.289132000	-1.744539000	3.250574000
H	4.797993000	-0.922932000	-0.016120000
H	1.232082000	-0.541140000	2.353533000
H	5.996029000	-1.875866000	1.930387000
H	2.426694000	-1.497470000	4.320379000
H	4.818921000	-2.170741000	4.105903000
N	-0.971896000	0.947906000	-2.088956000
C	-0.189510000	0.917201000	-3.292643000
H	-0.330374000	-0.008795000	-3.893027000
C	-2.333158000	0.934161000	-2.273935000
C	-2.965529000	0.827807000	-3.540141000
C	-3.197128000	0.994111000	-1.146595000
C	-4.352450000	0.744095000	-3.652198000
C	-4.575171000	0.907537000	-1.272533000
C	-5.177229000	0.772244000	-2.528792000
H	-2.363350000	0.789998000	-4.449617000
H	-2.751178000	1.138020000	-0.156284000
H	-4.796532000	0.649831000	-4.648101000
H	-5.197297000	0.959834000	-0.372232000
H	-6.262545000	0.703555000	-2.626447000
H	-0.404679000	1.761572000	-3.979855000
C	0.081147000	4.396135000	0.621835000
C	-1.395013000	3.926464000	0.837674000
C	0.565203000	4.161802000	-0.798516000
O	0.829640000	3.475227000	1.469701000
C	0.368543000	5.809492000	1.073295000
O	-1.218299000	2.504272000	1.139705000
C	-2.277415000	4.075247000	-0.378564000
C	-2.044492000	4.532526000	2.069117000
H	-1.914637000	3.469986000	-1.218538000
H	-2.318282000	5.129185000	-0.691613000
H	-3.302144000	3.750030000	-0.156394000
H	-1.397094000	4.447028000	2.953349000
H	-2.978696000	3.997226000	2.285243000
H	-2.285501000	5.594019000	1.918497000
H	-0.242120000	6.529387000	0.509362000
H	1.424563000	6.052695000	0.893635000
H	0.169415000	5.949495000	2.142642000
H	0.346811000	3.132034000	-1.128007000
H	1.651830000	4.314021000	-0.844630000
H	0.091002000	4.852749000	-1.509155000
B	0.064146000	2.361118000	1.584409000
H	0.455891000	1.324537000	2.041712000

^{3}TS_18, -4265.38074, NImag=1

Co	-0.109157000	0.455375000	-0.416893000
P	-0.251117000	-1.695039000	0.402590000
C	1.282244000	-2.345105000	1.180154000
C	2.455593000	-2.245449000	0.411739000
C	1.408870000	-2.783298000	2.503039000
C	3.713866000	-2.488134000	0.957500000
C	2.660630000	-3.051457000	3.057210000
C	3.811754000	-2.881524000	2.291032000
H	0.513511000	-2.899812000	3.118628000
H	4.607063000	-2.366390000	0.340359000
H	2.734964000	-3.382184000	4.095373000
H	4.796713000	-3.065751000	2.726076000
P	2.097615000	0.987868000	-0.272707000
C	3.343995000	0.185741000	-1.371348000
C	3.255875000	-1.203616000	-1.565873000
C	4.348765000	0.872430000	-2.068558000
C	-4.026701000	-1.766716000	2.781825000
C	-2.392706000	-0.605780000	4.117809000
C	-3.697761000	-1.065669000	3.940516000
H	-3.337727000	-2.553213000	0.899738000
H	-0.422078000	-0.439410000	3.276935000
H	-5.047397000	-2.126456000	2.629077000
H	-2.123925000	-0.047770000	5.018254000
H	-4.456799000	-0.874652000	4.703058000
C	2.435608000	2.521016000	-0.837418000
C	2.595917000	3.511053000	0.143114000
C	2.371879000	2.915194000	-2.183656000
C	2.701428000	4.853881000	-0.213509000
C	2.487910000	4.257005000	-2.538233000
C	2.651511000	5.231682000	-1.554122000
H	2.633496000	3.230825000	1.199529000
H	2.229371000	2.164478000	-2.965938000
H	2.824336000	5.610002000	0.565307000
H	2.443703000	4.542360000	-3.591983000
H	2.736972000	6.284426000	-1.832694000
C	3.055765000	0.656784000	1.225053000
C	4.455030000	0.742720000	1.235201000
C	2.380131000	0.465154000	2.432314000
C	5.158128000	0.635763000	2.432160000
C	3.082445000	0.355770000	3.632008000
C	4.473054000	0.439609000	3.633222000
H	5.000329000	0.892184000	0.298302000
H	1.288772000	0.391039000	2.417219000
H	6.248687000	0.704067000	2.429071000
H	2.538858000	0.193553000	4.566366000
H	5.027195000	0.349699000	4.570566000
N	-1.331601000	0.703163000	-1.950958000
C	-0.776504000	1.564460000	-2.963045000
H	-0.191312000	1.028472000	-3.741365000
C	-2.489715000	0.043644000	-2.278087000
C	-2.941870000	-0.133108000	-3.610334000
C	-3.300688000	-0.505479000	-1.252849000
C	-4.098201000	-0.859778000	-3.886466000
C	-4.452220000	-1.223702000	-1.542039000
C	-4.863708000	-1.421384000	-2.864375000
H	-2.358954000	0.272551000	-4.440179000
H	-3.013155000	-0.310703000	-0.216430000
H	-4.403697000	-0.992712000	-4.928832000
H	-5.053286000	-1.621938000	-0.717342000
H	-5.770032000	-1.986953000	-3.090604000
H	-1.550592000	2.145842000	-3.501847000
C	-2.616692000	3.702809000	0.364821000
C	-3.351690000	2.727122000	1.352616000
C	-3.093421000	3.554383000	-1.069580000
O	-1.244911000	3.227492000	0.417846000
C	-2.634257000	5.156373000	0.786167000
O	-2.530400000	1.536980000	1.291920000
C	-4.762887000	2.359674000	0.946998000
C	-3.312739000	3.203411000	2.796325000
H	-4.790374000	1.863796000	-0.030987000
H	-5.406424000	3.251054000	0.907459000
H	-5.194293000	1.665885000	1.682080000
H	-2.290254000	3.463614000	3.104791000
H	-3.665821000	2.397456000	3.453430000
H	-3.954662000	4.081044000	2.957066000
H	-3.665644000	5.534148000	0.844987000
H	-2.096224000	5.767288000	0.049010000
H	-2.153336000	5.309895000	1.759669000
H	-3.093617000	2.502409000	-1.385226000
H	-2.415216000	4.104084000	-1.736316000
H	-4.105517000	3.961106000	-1.202967000
B	-1.307738000	1.911948000	0.801322000
H	-0.256443000	1.304081000	1.151550000

^{3}Int_17, -4265.39704, NImag=0

Co	-0.163825000	0.196801000	-0.573794000
P	-0.133681000	-1.854355000	0.401504000
C	1.374836000	-2.137605000	1.406277000
C	2.618847000	-1.969475000	0.773555000
C	1.369242000	-2.311982000	2.795543000
C	3.806813000	-1.913119000	1.499531000
C	2.552734000	-2.275400000	3.532119000
C	3.767239000	-2.058241000	2.885115000
H	0.416748000	-2.452312000	3.313396000
H	4.753708000	-1.751298000	0.979266000
H	2.521756000	-2.401096000	4.616445000
H	4.696057000	-2.005442000	3.457672000
P	1.907423000	1.022377000	-0.382655000
C	3.400153000	0.304003000	-1.194344000
C	3.536168000	-1.095511000	-1.223614000
C	4.386394000	1.059868000	-1.845802000

C	4.100094000	-1.877435000	-2.445149000
C	5.210271000	0.205874000	-2.938168000
C	5.078789000	-1.168084000	-3.136737000
O	2.280180000	-1.913856000	-0.910359000
H	4.454204000	1.952189000	-1.934729000
H	3.973043000	-2.954399000	-2.570244000
H	5.983764000	0.765954000	-3.467786000
H	5.743306000	-1.691743000	-3.827419000
H	-0.508937000	2.781464000	-1.763137000
C	-0.558766000	-2.942111000	-0.906301000
C	-0.551398000	-4.317975000	-0.642721000
C	-0.774536000	-2.496048000	-2.213871000
C	-0.785999000	-5.230125000	-1.669664000
C	-1.013248000	-3.407604000	-3.240505000
C	-1.023399000	-4.774732000	-2.968058000
H	-0.365845000	-4.676800000	0.374987000
H	-0.759301000	-1.420869000	-2.420647000
H	-0.783770000	-6.301894000	-1.456482000
H	-1.199231000	-3.044484000	-4.253981000
H	-1.213784000	-5.491362000	-3.770810000
C	-1.528793000	-2.030506000	1.674422000
C	-2.649719000	-2.835300000	1.432630000
C	-1.462917000	-1.325141000	2.885828000
C	-3.668639000	-2.938063000	2.379492000
C	-2.465070000	-1.448610000	3.842063000
C	-3.577129000	-2.252862000	3.589330000
H	-2.742966000	-3.369496000	0.483610000
H	-0.619809000	-0.652545000	3.076577000
H	-4.540399000	-3.561628000	2.166435000
H	-2.387906000	-0.896749000	4.782148000
H	-4.373568000	-2.339302000	4.332407000
C	2.240973000	2.761124000	-0.715973000
C	2.271294000	3.750697000	0.276185000
C	2.139903000	3.157052000	-2.059504000
C	2.217867000	5.100651000	-0.068617000
C	2.099356000	4.505444000	-2.401789000
C	2.137310000	5.482643000	-1.406318000
H	2.332442000	3.464979000	1.330052000
H	2.083278000	2.399916000	-2.848044000
H	2.239437000	5.858813000	0.717548000
H	2.026881000	4.794683000	-3.452867000
H	2.097362000	6.540808000	-1.674217000
C	2.949962000	0.916053000	1.358358000
C	4.323520000	1.160365000	1.494250000
C	2.197171000	0.610344000	2.495038000
C	4.926400000	1.100350000	2.747940000
C	2.800103000	0.547891000	3.750658000
C	4.165831000	0.792468000	3.878202000
H	4.926692000	1.397690000	0.612481000
H	1.127154000	0.412104000	2.375012000
H	5.997522000	1.293226000	2.845331000
H	2.200547000	0.297409000	4.629602000
H	4.642536000	0.740835000	4.860005000
N	-1.619690000	1.014643000	-1.575038000
C	-1.221132000	2.172127000	-2.341415000
H	-0.736533000	1.920185000	-3.307205000
C	-2.695511000	0.303134000	-2.056182000
C	-3.281477000	0.543045000	-3.324778000
C	-3.276206000	-0.726973000	-1.275975000
C	-4.355307000	-0.222050000	-3.779118000
C	-4.347848000	-1.475580000	-1.737070000
C	-4.902122000	-1.240123000	-3.000215000
H	-2.878469000	1.321225000	-3.975408000
H	-2.876932000	-0.899882000	-0.277354000
H	-4.768882000	-0.013830000	-4.770541000
H	-4.764619000	-2.257401000	-1.093381000
H	-5.743485000	-1.833715000	-3.363785000
H	-2.069346000	2.841421000	-2.581731000
C	-3.354135000	3.201406000	0.764433000
C	-3.735589000	1.915301000	1.589135000
C	-4.038911000	3.260638000	-0.590576000
O	-1.931946000	3.031735000	0.551692000
C	-3.566081000	4.505626000	1.506627000
O	-2.710393000	0.973978000	1.214172000
C	-5.084749000	1.317897000	1.248186000
C	-3.608663000	2.116080000	3.092508000
H	-5.154463000	1.042479000	0.188699000
H	-5.900334000	2.017006000	1.486579000
H	-5.240569000	0.401692000	1.835743000
H	-2.618812000	2.512967000	3.360173000
H	-3.728525000	1.147749000	3.597037000
H	-4.372873000	2.801492000	3.485362000
H	-4.625543000	4.639859000	1.770434000
H	-3.270981000	5.350932000	0.870526000
C	4.578495000	-1.718134000	-1.906246000
C	5.443635000	0.448341000	-2.517062000
C	5.533133000	-0.942637000	-2.559329000
O	2.598201000	-1.882397000	-0.598207000
H	4.318543000	2.151012000	-1.836441000
H	4.623507000	-2.808826000	-1.908838000
H	6.196894000	1.062858000	-3.014597000
H	6.352495000	-1.426806000	-3.095200000
H	-0.831433000	2.449211000	-2.171907000
C	-0.131080000	-3.253337000	-0.779859000
C	0.465018000	-4.488822000	-0.493852000
C	-0.742350000	-3.062889000	-2.025120000
C	0.431565000	-5.519563000	-1.430717000
C	-0.783403000	-4.097792000	-2.958180000
C	-0.197014000	-5.327298000	-2.662258000
H	0.959357000	-4.643557000	0.470645000
H	-1.198485000	-2.096327000	-2.263075000
H	0.898862000	-6.479792000	-1.198599000
H	-1.275309000	-3.936289000	-3.920324000
H	-0.224502000	-6.138155000	-3.394202000
C	-1.457760000	-2.284691000	1.598728000
C	-2.054208000	-3.549318000	1.668943000
C	-1.919725000	-1.266466000	2.446042000
C	-3.088395000	-3.791468000	2.573080000
C	-2.947547000	-1.512295000	3.352373000
C	-3.536371000	-2.775677000	3.416380000
H	-1.722606000	-4.349790000	1.002173000
H	-1.499031000	-0.258901000	2.360661000
H	-3.551707000	-4.780350000	2.612381000
H	-3.305866000	-0.706813000	3.998183000
H	-4.352281000	-2.965297000	4.117856000
C	1.798375000	2.701799000	-1.107096000
C	1.410099000	3.784582000	-0.306404000
C	1.883910000	2.886292000	-2.497202000
C	1.136248000	5.024934000	-0.878768000
C	1.619191000	4.129426000	-3.065021000
C	1.244349000	5.203638000	-2.256446000
H	1.297159000	3.651387000	0.773463000
H	2.151419000	2.044684000	-3.144169000
H	0.827942000	5.855990000	-0.240404000
H	1.697016000	4.257670000	-4.147364000
H	1.028969000	6.177042000	-2.702910000
C	2.516845000	1.345287000	1.324401000
C	3.801539000	1.849654000	1.568965000
C	1.665847000	1.092621000	2.404897000
C	4.222016000	2.099097000	2.872741000
C	2.087048000	1.343917000	3.710396000
C	3.364863000	1.846694000	3.946014000
H	4.479592000	2.048854000	0.733555000
H	0.665940000	0.692810000	2.207090000
H	5.224548000	2.494267000	3.053789000
H	1.413174000	1.137298000	4.545732000
H	3.697395000	2.042152000	4.968372000
N	-1.954551000	0.822152000	-1.470485000
C	-1.515942000	1.686729000	-2.560731000
H	-1.001521000	1.117946000	-3.354205000
C	-2.884760000	-0.176601000	-1.828605000
C	-3.251315000	-0.398327000	-3.170337000
C	-3.434046000	-1.035137000	-0.854126000
C	-4.099814000	-1.451290000	-3.518887000
C	-4.277743000	-2.077099000	-1.213575000
C	-4.615991000	-2.305665000	-2.550374000
H	-2.870916000	0.245724000	-3.962941000
H	-3.197084000	-0.869193000	0.193829000
H	-4.356298000	-1.596434000	-4.571969000
H	-4.677315000	-2.724306000	-0.427744000
H	-5.275818000	-3.130676000	-2.827107000
H	-2.358317000	2.227446000	-3.028178000
C	-3.076021000	3.539631000	0.381181000
C	-3.445814000	2.464582000	1.453170000
C	-4.128083000	3.622139000	-0.720181000
O	-1.877335000	3.001043000	-0.167579000
C	-2.783214000	4.919545000	0.936655000
O	-3.077302000	1.258430000	0.792172000
C	-4.916501000	2.392864000	1.810531000
C	-2.599181000	2.615095000	2.714767000
H	-5.529041000	2.134455000	0.938029000
H	-5.276756000	3.347637000	2.222714000
H	-5.084550000	1.615279000	2.569611000
H	-1.530316000	2.699409000	2.466017000
H	-2.730308000	1.728562000	3.351888000
H	-2.883898000	3.496319000	3.308391000
H	-3.648257000	5.325746000	1.482968000
H	-2.549686000	5.616216000	0.118736000

H	-2.970799000	4.558742000	2.425962000
H	-3.917062000	2.327882000	-1.156750000
H	-3.604056000	4.077801000	-1.182314000
H	-5.115320000	3.457360000	-0.486954000
B	-1.668344000	1.686176000	0.672182000
H	-0.479254000	1.386699000	0.987967000

^{3}TS_19, -4265.37577, NImag=1

Co	-0.078901000	-0.383530000	-0.565943000
P	1.862619000	-1.180306000	0.261653000
C	2.440708000	-0.127227000	1.644033000
C	2.797913000	1.190480000	1.310546000
C	2.386040000	-0.469841000	2.999083000
C	3.040749000	2.153539000	2.287007000
C	2.643554000	0.480215000	3.987453000
C	2.954977000	1.791404000	3.630496000
H	2.114008000	-1.490183000	3.283846000
H	3.285309000	3.176831000	1.992193000
H	2.585901000	0.197465000	5.040868000
H	3.133928000	2.544086000	4.401852000
P	-0.073298000	1.835953000	-0.243122000
C	1.258714000	3.067295000	-0.678983000
C	2.605382000	2.691759000	-0.524012000
C	1.022368000	4.355589000	-1.185921000
C	3.657860000	3.522036000	-0.905235000
C	2.065053000	5.203516000	-1.555304000
C	3.388063000	4.782640000	-1.429546000
O	2.915321000	1.448391000	-0.031010000
H	-0.005071000	4.709534000	-1.297050000
H	4.678956000	3.156936000	-0.777437000
H	1.838865000	6.198659000	-1.944736000
H	4.209652000	5.437415000	-1.728374000
H	-3.578910000	0.555080000	-2.512883000
C	3.378252000	-1.309993000	-0.768766000
C	4.664948000	-1.438771000	-0.229190000
C	3.233371000	-1.189243000	-2.153984000
C	5.779846000	-1.474509000	-1.064525000
C	4.346276000	-1.231111000	-2.992104000
C	5.621796000	-1.376819000	-2.448166000
H	4.794768000	-1.500149000	0.856365000
H	2.231114000	-1.045958000	-2.570666000
H	6.779392000	-1.573949000	-0.633803000
H	4.216968000	-1.138367000	-4.073543000
H	6.497220000	-1.403317000	-3.101668000
C	1.715960000	-2.832121000	1.056897000
C	2.678284000	-3.845193000	0.966424000
C	0.517147000	-3.096270000	1.739192000
C	2.450402000	-5.091605000	1.551503000
C	0.296136000	-4.337654000	2.330341000
C	1.262232000	-5.340956000	2.236489000
H	3.609150000	-3.672089000	0.420645000
H	-0.253955000	-2.315744000	1.761632000
H	3.207858000	-5.874805000	1.466515000
H	-0.642791000	-4.529181000	2.856547000
H	1.085599000	-6.318816000	2.691025000
C	-1.546818000	2.593152000	-1.038333000
C	-2.774506000	2.598008000	-0.363426000
C	-1.516438000	3.029798000	-2.373282000
C	-3.930776000	3.056730000	-0.992287000
C	-2.668210000	3.503248000	-2.995987000
C	-3.881231000	3.521632000	-2.304998000
H	-2.827945000	2.222557000	0.662272000
H	-0.576892000	2.999233000	-2.933984000
H	-4.879193000	3.042615000	-0.449943000
H	-2.620104000	3.852311000	-4.030587000
H	-4.786418000	3.889862000	-2.793735000
C	-0.332765000	2.323071000	1.528799000
C	-0.398382000	3.674065000	1.899261000
C	-0.470065000	1.342768000	2.515165000
C	-0.603084000	4.034138000	3.228890000
C	-0.668924000	1.704288000	3.847903000
C	-0.738373000	3.048160000	4.208370000
H	-0.290562000	4.455933000	1.141755000
H	-0.428534000	0.293235000	2.209527000
H	-0.657961000	5.090846000	3.502503000
H	-0.762823000	0.925173000	4.609466000
H	-0.895937000	3.331391000	5.252240000
N	-2.396078000	-1.079667000	-1.974755000
C	-2.778724000	-0.062198000	-2.932919000
H	-1.936163000	0.602614000	-3.175561000
C	-1.284000000	-1.871202000	-2.290086000
C	-0.605206000	-1.722417000	-3.523679000
C	-0.817743000	-2.870560000	-1.401096000
C	0.452348000	-2.563121000	-3.863218000
C	0.242347000	-3.701147000	-1.764176000
H	-1.919225000	4.906312000	1.613951000
H	-4.384685000	2.620933000	-1.097351000
H	-3.728281000	4.208539000	-1.559664000
H	-5.054767000	4.109037000	-0.381428000
B	-1.955929000	1.568307000	-0.042485000
H	-0.842638000	1.220297000	0.592636000

^{3}Int_18, -3853.79568, NImag=0

Co	-0.076510000	-0.656702000	-1.270206000
P	-1.401407000	0.838979000	-0.002713000
C	-0.399374000	1.947696000	1.068156000
C	0.435843000	1.327166000	2.012494000
C	-0.242886000	3.327103000	0.883494000
C	1.384984000	2.040474000	2.741171000
C	0.698081000	4.055101000	1.610261000
C	1.514544000	3.411669000	2.536321000
H	-0.832470000	3.841235000	0.122478000
H	2.028228000	1.514053000	3.450012000
H	0.809058000	5.126465000	1.429863000
H	2.265961000	3.972918000	3.096243000
P	1.969691000	-0.406999000	-0.296100000
C	2.341194000	-1.012426000	1.414518000
C	1.390347000	-0.792191000	2.429694000
C	3.474177000	-1.765925000	1.759783000
C	1.521184000	-1.353318000	3.697791000
C	3.628310000	-2.312756000	3.032734000
C	2.640967000	-2.124742000	3.998631000
O	0.276916000	-0.028284000	2.173403000
H	4.253515000	-1.934847000	1.012758000
H	0.739343000	-1.160606000	4.435106000
H	4.523387000	-2.893101000	3.266590000
H	2.748590000	-2.563891000	4.992820000
H	0.538475000	0.407341000	-2.306796000
C	-2.671705000	0.141311000	1.149241000
C	-3.880135000	0.758827000	1.496408000
C	-2.410297000	-1.138363000	1.658759000
C	-4.785686000	0.125228000	2.346837000
C	-3.312549000	-1.771456000	2.508203000
C	-4.503493000	-1.138630000	2.860353000
H	-4.143905000	1.736046000	1.091825000
H	-1.487502000	-1.645013000	1.365312000
H	-5.723588000	0.624669000	2.601883000
H	-3.090423000	-2.774983000	2.879585000
H	-5.217418000	-1.636421000	3.520977000
C	-2.321434000	2.017483000	-1.072691000
C	-3.055579000	3.119375000	-0.601640000
C	-2.268549000	1.799333000	-2.457103000
C	-3.738964000	3.952825000	-1.484563000
C	-2.954916000	2.630637000	-3.341522000
C	-3.696717000	3.705621000	-2.856974000
H	-3.076578000	3.348771000	0.466364000
H	-1.656746000	0.975393000	-2.840733000
H	-4.303698000	4.804381000	-1.097452000
H	-2.901711000	2.437935000	-4.415438000
H	-4.234268000	4.359300000	-3.548072000
C	3.129170000	-1.369428000	-1.345272000
C	3.763489000	-0.738102000	-2.425381000
C	3.282984000	-2.757734000	-1.199144000
C	4.542388000	-1.469544000	-3.319608000
C	4.066411000	-3.486470000	-2.091817000
C	4.699711000	-2.844746000	-3.155296000
H	3.642567000	0.338437000	-2.571769000
H	2.795686000	-3.279242000	-0.370918000
H	5.028997000	-0.957535000	-4.152954000
H	4.179036000	-4.564510000	-1.954702000
H	5.312054000	-3.416669000	-3.856118000
C	2.774100000	1.253036000	-0.292680000
C	3.987882000	1.449873000	0.383192000
C	2.215816000	2.314333000	-1.010417000
C	4.631946000	2.682789000	0.333520000
C	2.864508000	3.548834000	-1.060426000
C	4.071728000	3.736045000	-0.391915000
H	4.437384000	0.630700000	0.952155000
H	1.271312000	2.149347000	-1.538675000
H	5.578908000	2.821564000	0.860856000
H	2.415535000	4.370916000	-1.623808000
H	4.578849000	4.703233000	-0.433081000
N	-1.126056000	-2.274328000	-1.636361000
C	-0.106773000	-2.668901000	-0.849170000
H	-0.288496000	-3.075469000	0.164032000
C	-2.444247000	-2.488032000	-1.258117000
C	-2.831636000	-3.656443000	-0.571748000
C	-3.442916000	-1.564615000	-1.618072000
C	-4.161943000	-3.859866000	-0.217984000
C	-4.764306000	-1.766258000	-1.242902000

C	0.885710000	-3.561633000	-2.991956000
H	-0.927871000	-0.968801000	-4.241448000
H	-1.336589000	-3.032872000	-0.458373000
H	0.945856000	-2.426257000	-4.829367000
H	0.559735000	-4.476943000	-1.062504000
H	1.716246000	-4.216250000	-3.264229000
H	-3.135384000	-0.505809000	-3.878262000
C	-5.049297000	-0.835562000	0.487569000
C	-4.222221000	-2.030136000	1.078061000
C	-6.257101000	-1.295813000	-0.314549000
O	-4.122618000	-0.247626000	-0.446391000
C	-5.453306000	0.211861000	1.503578000
O	-3.336394000	-2.354532000	-0.016116000
C	-5.041330000	-3.259392000	1.410890000
C	-3.371698000	-1.619045000	2.269047000
H	-5.548470000	-3.667839000	0.528620000
H	-5.799770000	-3.030835000	2.174029000
H	-4.390298000	-4.047101000	1.813453000
H	-2.770918000	-0.727669000	2.041294000
H	-2.671770000	-2.430580000	2.512286000
H	-3.988541000	-1.424981000	3.158229000
H	-6.085979000	-0.226632000	2.289194000
H	-6.033631000	1.008453000	1.017955000
H	-4.581179000	0.674535000	1.982105000
H	-5.979228000	-2.064719000	-1.048866000
H	-6.675169000	-0.442468000	-0.865398000
H	-7.048496000	-1.705396000	0.328639000
B	-3.207087000	-1.219508000	-0.782361000

^{3}TS_20, -3853.78837, NImag=1

Co	0.181675000	0.413977000	-1.376628000
P	2.011103000	-0.291498000	-0.142778000
C	1.690628000	-2.049881000	0.254541000
C	0.708068000	-2.310285000	1.229300000
C	2.138287000	-3.128633000	-0.519907000
C	0.192393000	-3.587347000	1.435423000
C	1.638714000	-4.414456000	-0.315470000
C	0.664306000	-4.641179000	0.656336000
H	2.867916000	-2.955791000	-1.315256000
H	-0.583812000	-3.740013000	2.189271000
H	2.000221000	-5.239491000	-0.932894000
H	0.257098000	-5.644000000	0.803968000
P	-1.638043000	-0.399466000	-0.202954000
C	-1.978246000	-0.610261000	1.608924000
C	-0.949945000	-1.059162000	2.457204000
C	-3.222834000	-0.347803000	2.202175000
C	-1.141542000	-1.221974000	3.827860000
C	-3.429604000	-0.516183000	3.570171000
C	-2.387553000	-0.952024000	4.387069000
O	0.320600000	-1.226805000	1.962739000
H	-4.049897000	-0.000175000	1.577791000
H	-0.296286000	-1.548140000	4.437143000
H	-4.411208000	-0.301960000	3.998238000
H	-2.541112000	-1.077788000	5.460998000
H	-0.691014000	0.041937000	-2.608029000
C	2.460779000	0.563248000	1.422586000
C	3.738937000	0.495660000	1.987762000
C	1.481951000	1.350495000	2.043230000
C	4.025423000	1.186986000	3.164958000
C	1.767591000	2.039459000	3.217411000
C	3.041005000	1.957330000	3.782228000
H	4.524571000	-0.093701000	1.508299000
H	0.487134000	1.416693000	1.590230000
H	5.026539000	1.125397000	3.598140000
H	0.993444000	2.652560000	3.685287000
H	3.268950000	2.501943000	4.701678000
C	3.565828000	-0.260905000	-1.098691000
C	4.660996000	-1.107505000	-0.868630000
C	3.658528000	0.721025000	-2.097054000
C	5.822503000	-0.977913000	-1.627464000
C	4.826950000	0.854296000	-2.845755000
C	5.907210000	0.003322000	-2.615957000
H	4.605877000	-1.875951000	-0.091801000
H	2.804811000	1.387988000	-2.274076000
H	6.668076000	-1.645080000	-1.443682000
H	4.889944000	1.625598000	-3.616641000
H	6.819482000	0.103542000	-3.208788000
C	-3.102418000	0.541625000	-0.754142000
C	-3.901146000	0.110481000	-1.821399000
C	-3.320835000	1.818405000	-0.213837000
C	-4.908189000	0.933916000	-2.325072000
C	-4.335233000	2.632256000	-0.710193000
C	-5.131410000	2.192798000	-1.769077000
H	-3.730451000	-0.872945000	-2.268242000
H	-2.679537000	2.188408000	0.593851000
C	-5.135521000	-2.912205000	-0.534334000
H	-2.076588000	-4.410706000	-0.335920000
H	-3.152186000	-0.669087000	-2.172521000
H	-4.441525000	-4.772836000	0.314986000
H	-5.516141000	-1.017473000	-1.506110000
H	-6.176435000	-3.069400000	-0.243536000
H	0.800543000	-3.038744000	-1.346889000

H	-5.522707000	0.586831000	-3.159240000
H	-4.488717000	3.624075000	-0.278022000
H	-5.921260000	2.835331000	-2.165042000
C	-1.999112000	-2.127040000	-0.752832000
C	-3.080370000	-2.854391000	-0.233474000
C	-1.162628000	-2.741042000	-1.691229000
C	-3.320046000	-4.161498000	-0.650078000
C	-1.397480000	-4.052432000	-2.102748000
C	-2.477143000	-4.764772000	-1.585549000
H	-3.742868000	-2.394502000	0.505909000
H	-0.316791000	-2.179618000	-2.101071000
H	-4.169936000	-4.713652000	-0.241465000
H	-0.726185000	-4.519577000	-2.827628000
H	-2.663819000	-5.791882000	-1.908685000
N	0.347207000	2.344262000	-1.861830000
C	-0.537213000	1.746231000	-2.720283000
H	-1.619109000	1.969874000	-2.655997000
C	-0.022627000	3.389734000	-1.035972000
C	-1.176790000	4.181663000	-1.229360000
C	0.843132000	3.754779000	0.018693000
C	-1.472507000	5.235410000	-0.367220000
C	0.540361000	4.805593000	0.872786000
C	-0.630095000	5.552218000	0.698615000
H	-1.842094000	3.973134000	-2.070632000
H	1.768265000	3.185616000	0.140344000
H	-2.375849000	5.828185000	-0.541880000
H	1.233235000	5.052414000	1.682750000
H	-0.866334000	6.382735000	1.367353000
H	-0.204674000	1.622240000	-3.761625000

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