Supporting Information

Near-Ambient Temperature Dehydrogenative Synthesis of the Amide Bond: Mechanistic Insight and Application

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1. General Information

All dehydrogenation experiments were carried out under an inert atmosphere (with N$_2$ or Ar) using standard Schlenk techniques. Complexes RuHCl(CO)P$_{tBu}$NN$_{tBu}$H (1),$^1$ RuHCl(CO)P$_{tBu}$NN$_{tBu}$H (2),$^1$ RuHCl(CO)P$_{Ph}$NN$_{tBu}$H (3),$^2$ RuHCl(CO)P$_{Ph}$NN$_{Et}$ (4),$^3$ RuHClP$_{Bu}$NN$_{Bpy}$ (5),$^4$ RuHClP$_{Ph}$NN$_{Bpy}$ (6),$^5$ Mn(CO)$_2$BrP$_{Bu}$NN$_{Bpy}$ (7),$^6$ and Mn(CO)$_2$BrP$_{Bu}$NN$_{tBu}$H (8)$^7$ were prepared according to the previously reported procedures. All catalysts were weighed inside nitrogen filled glove box. Reagent grade amines, alcohols and hexyl hexanoate were purchased from commercial sources and used without further purification. All solvents were purified according to standard procedures under an argon atmosphere, sparged with argon, and stored over 4 Å molecular sieves. Liquid amines, alcohols and esters were purged with argon for half an hour prior to their use. 1,3,5-trimethylbenzene (mesitylene) and potassium tert-butoxide were purchased from commercial sources and used as received.

NMR spectra were recorded at room temperature on a Bruker AMX-300 (300 MHz) or AMX-400 (400 MHz) or AMX-500 (500 MHz) spectrometers. Chemical shifts of the NMR spectra are reported relative to residual signals of CDCl$_3$ ($^1$H NMR: $\delta = 7.26$ ppm, $^{13}$C NMR: $\delta = 77.16$ ppm), benzene-D$_6$ ($^1$H NMR: $\delta = 7.16$ ppm, $^{13}$C NMR: $\delta = 128.06$ ppm), CD$_2$Cl$_2$ ($^1$H NMR: $\delta = 5.32$ ppm, $^{13}$C NMR: $\delta = 54.00$ ppm) or the internal standard mesitylene. $^{31}$P{$^1$H} NMR chemical shifts are reported in ppm downfield from H$_3$PO$_4$ and referenced to an external 85% solution of phosphoric acid in D$_2$O. GC–MS was carried out on HP 6890 / 5973 (MS detector) instruments equipped with a 30 m column (Restek 5MS, 0.32 mm internal diameter) with a 5% phenylmethylsilicone coating (0.25 mm) and helium as carrier gas. GC was carried out on HP 6890 or Agilent 7890B Series GC System with N$_2$ or Helium as carrier gas. IR spectra were recorded on a Nicolet FTIR spectrophotometer (KBr, thin Film). Optical rotations were measured in a PerkinElmar 341 series polarimeter with sodium lamp.

![Figure S1](image-url) Complexes screened for near-ambient temperature dehydrogenative amide synthesis in this study.
2. $^1$H and $^{31}$P{$^1$H} NMR spectra of selected complexes

**Figure S2.** $^1$H (top, 300 MHz) and $^{31}$P{$^1$H} (bottom, 121 MHz) NMR spectra of complex 1 in $\text{C}_6\text{D}_6$. 
Figure S3. $^1$H (top, 300 MHz) and $^{31}$P{$^1$H} (bottom, 121 MHz) NMR spectra of complex 2 in C$_6$D$_6$. 

S4
3. Standard procedure for the dehydrogenative coupling

\[
\begin{array}{c}
\text{Catalyst} \\
\text{t-BuOK} \\
\text{Solvent, reflux}
\end{array}
\]

In a N₂ glove box, 5 µmol of ruthenium catalyst and 10 µmol of t-BuOK were dissolved in 1 mL of dry solvent (diethyl ether or methyl tert-butyl ether (MTBE) or toluene) in a 5 mL vial. The solution was stirred for 5 mins after which a solution of pre-dissolved alcohol (0.5 mmol) and amine (0.55 mmol) in 1 mL dry solvent was added to the initial solution. The resulting solution was transferred to a Schlenk tube. The tube was sealed, taken out of the box, and was connected to a condenser (ethylene glycol/ water: T = 1 °C) under argon flow. The Schlenk tube was subsequently dipped into a preheated oil bath (50 °C for Et₂O; 70 °C for MTBE; and 130 °C for toluene as solvent) and the solution was refluxed under argon flow for the given time. Afterwards, the reaction solution was cooled to room temperature. A known amount of mesitylene was added to the solution as an internal standard. For some reactions where amide precipitation from solution was observed, THF was added to produce a homogeneous solution. A sample of the resulting solution was then analyzed by GC-MS and ¹H NMR with CDCl₃ as the deuterated solvent. NMR yields were calculated from integration ratios between amide characteristics peaks and mesitylene methyl protons peak (δ ~ 2.2 ppm). The amides were isolated as described below.

*For Table 2, entries 2, 4, 16*

The solvent, mesitylene standard, and any unreacted alcohol and amine were removed in vacuo to afford almost pure amide. The resulting solid was washed with pentane and subsequently recrystallized in cold ethyl acetate / hexane solvent mixture.

*For Table 2, entries 1,3,5,7,11,13*

For amides which were viscous oils, after removing all the volatile solvent and reactants the remaining oily substance was extracted with hexane. Afterwards the hexane was removed in vacuo to obtain pure amides.

*For Table 2, entry18, diamide*

White precipitation of the amide was observed during the reaction. The amide was isolated by filtering the solid from the solution after the reaction and then was washed with pentane to afford pure amide.

The chiral amides from Table 2, entries 19-20 were purified via column chromatography (ethyl acetate/ hexane)
**Figure S4.** Schematic representation of the reaction setup

**Figure S5.** Detection of H₂ gas after the reaction in a closed vessel. Helium was used as the carrier gas.
4. $^1$H NMR spectra of selected crude reaction mixtures

**Figure S6.** $^1$H NMR spectra of the crude reaction mixture after dehydrogenative synthesis of N-benzyllhexanamide (Table 2, entry 2) in CDCl$_3$.

**Figure S7.** $^1$H NMR spectra of the crude reaction mixture after dehydrogenative synthesis of N-benzylbenzamide (Table 2, entry 4) in CDCl$_3$. THF was added after the reaction to dissolve precipitating amide. Acetone impurity from NMR tube.
5. Mechanistic reactions

5.1. Binding of different substrates to the dearomatized/ deprotonated PNNH complexes

A scheme summarizing the different binding modes of different substrates to the dearomatized/deprotonated ruthenium PNNH complexes is shown below, as observed during the course of this study.

**Scheme S1**
5.2. Synthesis of complex 1d

In a 20 mL vial, 30 mg (63 µmol) of complex 1 was dissolved in 1 mL diethylether. 14.1 mg of t-BuOK was then added to the solution upon which the solution color changed to violet from light yellow. The solution was stirred for 5 mins after which 26 mg of 1-hexanol (pre-dissolved in 1 mL Et₂O) was added to the solution. Subsequently, the resulting green colored solution was filtered through a short Celite® pad and transferred to a J. Young NMR tube. The tube was then heated at 45 °C for half an hour and the green solution turned yellow. Afterwards, the tube was taken back inside the box and the solvent and excess hexanol was removed in vacuum to afford complex 1d.C₆H₁₃OH. For 1d.C₁₃H₁₉NO, 4 eq of amine was also added alongside 4 eq of 1-hexanol with rest of the procedure being unchanged. ¹H and ³¹P NMR spectra suggests that at room temperature, 1d exist as two isomers in 9:1 ratio. Single crystals of 1d suitable for XRD analysis were grown by dissolving 1d in a mixture of THF/pentane followed by slow evaporation of the solvent.

³¹P{¹H} NMR (1d.C₆H₁₃OH) (97 MHz, Benzene-d₆): δ 119.5 (s) (major, 91%); 120.18 (s) (minor, 9%)

¹H NMR (1d.C₆H₁₃OH) (400 MHz, Benzene-d₆) (major): δ 6.93 (t, J = 8.0 Hz, 1H), 6.57 (dd, J = 8.4, 3.0 Hz, 2H), 4.64 (dd, J = 8.5, 4.1 Hz, 1H), 4.22 (s, 1H), 4.15 (s, 1H), 3.98 (t, J = 6.4 Hz, 2H), 2.97 (d, J = 8.6 Hz, 2H), 2.03 – 1.90 (m, 1H), 1.85 (p, J = 6.7 Hz, 2H), 1.62 (dddt, J = 27.0, 16.1, 7.9, 3.8 Hz, 2H), 1.55 – 1.39 (m, 11H), 1.35 (d, J = 12.9 Hz, 9H), 1.30 (d, J = 13.0 Hz, 9H), 1.22 – 1.12 (m, 4H), 1.09 (s, 9H), 1.06 – 0.88 (m, 4H), 0.74 – 0.55 (m, 1H), -15.12 (d, J = 28.6 Hz, 1H).

¹³C NMR (1d.C₆H₁₃OH) (126 MHz, Toluene-d₈) (major): δ 208.18 (d, J = 15.6 Hz), 161.90 (d, J = 2.7 Hz), 159.98 (d, J = 4.3 Hz), 134.88, 118.35, 118.12 (d, J = 8.4 Hz), 77.64, 70.66, 61.96, 54.12, 38.16, 37.83 (d, J = 11.0 Hz), 36.98 (d, J = 19.6 Hz), 33.83, 32.58, 32.21, 30.05 (d, J = 3.2 Hz), 29.14 (d, J = 4.6 Hz), 28.40, 26.38, 26.20, 22.96, 14.14, 14.06.

IR (thin film, KBr) = 1900 cm⁻¹ (vCO).
Figure S8. $^1$H NMR spectrum of complex 1d.C$_6$H$_{13}$OH in C$_6$D$_6$.

Figure S9. $^1$H($^{31}$P) NMR spectra of complex 1d.C$_6$H$_{13}$OH in C$_6$D$_6$. 
Figure S10. $^{13}$C($^1$H) NMR spectrum of complex 1d.$C_6H_{13}$OH in Tol-d$_8$.

Figure S11. DEPTQ 135 NMR spectrum of complex 1d.$C_6H_{13}$OH in $C_6$D$_6$. 
Figure S12. $^1$H-$^{13}$C HSQC NMR spectrum of complex 1d.C$_6$H$_{13}$OH in C$_6$D$_6$.

Figure S13. $^1$H-$^1$H COSY NMR spectrum of complex 1d.C$_6$H$_{13}$OH in C$_6$D$_6$. 
Figure S14. $^{31}$P{$^1$H} NMR spectrum of complex 1d.C$_6$H$_{13}$OH in C$_6$D$_6$.

Figure S15. IR spectrum of complex 1d.C$_6$H$_{13}$OH (thin film, KBr).
5.3. Synthesis of complex 9

5.3.1. Synthesis of the ligand

In a 20 mL vial, 100 mg of the precursor was dissolved in 1 mL propylamine. 4 mL dioxane was added to the solution and the resulting mixture was heating at 100 °C in an oil bath with stirring for 16 h inside a closed Schlenk flask. Afterwards, the flask was cooled to room temperature followed by the removal of flask atmosphere through vacuum. The flask was then filled with argon and was heated at 100 °C for an additional 30 min. Afterwards, the flask was cooled down to room temperature and the dioxane and excess amine were removed under vacuum. 10 mL pentane was added to the remaining sticky white solid, stirred and the resulting solution was filtered through a short Celite® pad. The remaining solid was washed again with 10 mL pentane, which was also filtered. Both pentane solutions were combined from which the removal of pentane afforded the desired ligand as a colorless oily liquid with 78% yield.

$^{31}$P NMR (202 MHz, Toluene-d$_8$) δ 35.77 (s).

$^1$H NMR (500 MHz, Toluene-d$_8$) δ 7.24 (t, $J = 7.7$ Hz, 1H), 7.20 (d, $J = 7.3$ Hz, 1H), 6.92 (d, $J = 7.4$ Hz, 1H), 3.85 (s, 2H, NHCH$_2$Py), 3.05 (bs, 2H, PCH$_2$Py), 2.51 (t, $J = 6.8$ Hz, 2H, NHCH$_2$CH$_2$), 2.13 (s, 1H, NH), 1.48 (sextet, $J = 7.0$ Hz, 2H, NHCH$_2$CH$_2$CH$_3$), 1.13 (bd, $J = 10.5$ Hz, 18H, PC(CH$_3$)$_3$), 0.93 (t, $J = 7.6$ Hz, 3H, NHCH$_2$CH$_2$CH$_3$).

$^{13}$C NMR (126 MHz, Toluene-d$_8$) δ 161.53 (d, $J = 15.0$ Hz, Py-C2), 159.84 (s, Py-C6), 135.63 (s, Py-C4), 121.59 (d, $JC,P = 9.4$ Hz, Py-C3), 118.35 (d, $J = 1.8$ Hz, Py-C5), 55.45 (s, NHCH$_2$Py), 51.38 (s, NCH$_2$CH$_2$CH$_3$), 31.95 (d, $JC,P = 26.0$ Hz, PC(CH$_3$)$_3$), 31.51 (d, $JC,P = 24.3$ Hz, PCH$_2$Py), 29.45 (d, $JC,P = 13.8$ Hz, PC(CH$_3$)$_3$), 23.51 (s, NHCH$_2$CH$_2$CH$_3$), 11.69 (s, NHCH$_2$CH$_2$CH$_3$).
5.3.2. Synthesis of the complex

In a 20 mL vial, 120 mg (0.126 mmol) of RuHCl(CO)(PPh₃)₃ was suspended in 3 mL THF. A solution of 55 mg PNNH(n-Pr) ligand (0.178 mmol) in 5 mL THF was added dropwise to the stirring suspension. The resulting solution was transferred to a pressure tube and heated at 66 °C for 3 hours. THF was then removed from the yellow solution under vacuum till the solution volume became 2 mL. Afterwards, 10 mL of pentane was slowly added to the solution while stirring resulting in the formation of pale yellow precipitates. The supernatant was decanted, and the pale yellow solid was washed with pentane (2x10 mL) and ether (2x5 mL) to afford complex 9 in 72% (43 mg) yield.

³¹P NMR (202 MHz, Methylene Chloride-­d₂) δ 108.74 (s).

¹H NMR (500 MHz, Methylene Chloride-­d₂) δ 7.68 (t, J = 7.8 Hz, 1H), 7.39 (d, J = 7.9 Hz, 1H), 7.19 (d, J = 7.8 Hz, 1H), 4.58 (dt, J = 15.2, 4.0 Hz, 1H), 4.31 (bs, 1H), 4.11 (dd, J = 15.2, 10.5 Hz, 1H), 3.68 (dd, J = 16.7, 7.7 Hz, 1H), 3.59 – 3.42 (m, 1H), 3.27 – 3.08 (m, 1H), 3.06 – 2.93 (m, 1H), 2.03 – 1.84 (m, 1H), 1.45 (d, J = 13.4 Hz, 9H), 1.19 (d, J = 13.0 Hz, 9H), 1.05 (t, J = 7.5 Hz, 3H), -15.77 (d, J = 23.4 Hz, 1H)

¹³C NMR (126 MHz, Methylene Chloride-­d₂) δ 208.17 (dd, J = 15.5, 3.0 Hz), 160.83 (d, J = 4.2 Hz), 158.64 (d, J = 2.3 Hz), 137.14, 120.99 (d, J = 9.1 Hz), 118.06, 60.95, 59.41, 36.65 (d, J = 16.3 Hz), 29.92 (d, J = 4.1 Hz), 28.26, 22.73, 11.19.

IR (thin film, KBr) = 1898 cm⁻¹ (νCO)
Figure S16. $^{31}$P{$^1$H} NMR spectrum of complex 9 in CD$_2$Cl$_2$.

Figure S17. $^1$H NMR spectrum of complex 9 in CD$_2$Cl$_2$. 
Figure S18. DEPTQ 135 NMR spectrum of complex 9 in CD$_2$Cl$_2$.

Figure S19. $^1$H-$^{13}$C HSQC NMR spectrum of complex 9 in CD$_2$Cl$_2$. 
5.4. NMR observations

\textit{a) Reaction of complex 1 with t-BuOK, and hexanol}

\textbf{Figure S20.} Reaction of complex 1 with t-BuOK, and hexanol in Et$_2$O as observed in $^{31}$P{\textsuperscript{1}H}(top) and \textsuperscript{1}H (bottom, hydride region) NMR. [R = t-Bu; R$_1$ = C$_5$H$_{11}$]
b) Reaction of complex 1 with t-BuOK, benzylamine and hexanol

Figure S21. Reaction of complex 1 with t-BuOK, benzylamine and hexanol in Et₂O as observed in $^{31}$P{¹H} and ¹H (hydride region) NMR. [R = t-Bu]
c) Reaction of complex 4 with t-BuOK, benzylamine and hexanol

Figure S22. Reaction of complex 4 with t-BuOK, benzylamine and hexanol in Et₂O as observed in \(^{31}\)P\(_{\{1\}H}\) NMR.
d) aldehyde exchange experiments

Exchange of bound hexanal with benzaldehyde

Figure S23. Exchange of the bound aldehyde of 1d with free benzaldehyde in solution as observed in $^1$H and $^{31}$P($^1$H) NMR.
Exchange of bound benzaldehyde with hexanal

Figure S24. Exchange of bound benzaldehyde with p-Cl benzaldehyde. The complex 1d’ was synthesized by heating a diethyl ether solution the alkoxy complex at 45 °C for 1 hour. The free benzaldehyde is observed in the solution after adding excess p-Cl benzaldehyde. ¹H spectrum is shown only for the hydride and aldehyde region for clarity.
Exchange of bound benzaldehyde with p-Cl benzaldehyde

Figure S25. Exchange of bound benzaldehyde with hexanal. The complex 1d’ was synthesized by heating a diethyl ether solution the alkoxy complex at 45 °C for 15 min, which only resulted in partial conversion (rest of the alkoxy complex is seen in the spectrum). The free benzaldehyde is observed in the solution after adding excess hexanal. $^1$H spectrum is shown only for the hydride and aldehyde region for clarity.
e) Formation of the amidate complex from 1d after addition of amine and regeneration of the aldehyde bound complex upon addition of alcohol

Figure S26. Formation of the amidate (and amido in minor amounts) complex from the aldehyde complex upon addition of amine and mild heating (panel 2), and the regeneration of 1d upon addition of alcohol and mild heating (panel 3), as observed from $^{31}$P$^1$H NMR. #unidentified species.
**Figure S27.** $^1$H NMR spectrum of sample containing 1c, 1d, and 1h (1c/1d/1h ~ 6/6/7). The NH proton of 1h is very downfield due to hydrogen bonding. N arm, P arm, and NH protons of the ligand are shown in left inset. Hydride region magnified in right inset.
6. X ray crystallography

Key bond lengths (Å) and angles (°): Ru(1)-P(1) 2.2576(5), Ru(1)-O(2) 2.2380(15), Ru(1)-N(1)2.0850(19),Ru(1)-N(2)2.2010(17), Ru(1)-C(26)(carbonyl) 1.818(2), O(2)-C(8) 1.394(3), C(7)-C(8) 1.570(3); P(1)-Ru(1)-H 81.5(11), O(2)-Ru(1)-P(1) 105.13(4), O(2)-Ru(1)-H 168.8(11), N(1)-Ru(1)-P(1) 81.81(5), N(1)-Ru(1)-O(2) 81.74(7), N(2)-Ru(1)-O(2) 72.92(6), C(8)-O(2)-Ru(1) 113.36(13), O(2)-C(8)-C(7) 109.38(18).

Data were collected on a Rigaku Xtalab Pro diffractometer dual source equipped with Dectris Pilatus 200K detector and microfocus, with CuKα (λ=1.54184 Å). The data were processed with CrysAlis PRO. Structure was solved by direct methods with SHELXT. Data were refined as Full-matrix least-squares refinement based on F² with SHELXL and OLEX2. All non-hydrogen atoms were further refined with anisotropic displacement coefficients. Hydrogen atoms were assigned isotropic displacement coefficients, and their coordinates were allowed to ride on their respective carbons. Hydride was located in the electron density map. Crystallographic data and refinement parameters are summarized in Supplementary Table S1.
Table S1. Crystal data and structure refinement for 1d.C_{13}H_{19}NO.

| Property                        | Value                                      |
|---------------------------------|--------------------------------------------|
| **1d.C_{13}H_{19}NO**           |                                            |
| **Empirical formula**           | C_{39}H_{66}N_{3}O_{3}P Ru                 |
| **Formula weight**              | 756.98 g/mol                               |
| **Temperature**                 | 100.01(10) K                              |
| **Wavelength**                  | 1.54184 Å                                 |
| **Crystal system**              | Monoclinic                                 |
| **Space group**                 | C2/c                                       |
| **Unit cell dimensions**        | a = 38.7143(4) Å, α = 90°                 |
|                                 | b = 11.06422(11) Å, β = 94.3975(8)°       |
|                                 | c = 18.64152(18) Å, γ = 90°               |
| **Volume**                      | 7961.47(14) Å^3                           |
| **Z**                           | 8                                          |
| **Density (calculated)**        | 1.263 Mg/m^3                               |
| **Absorption coefficient**      | 3.855 mm^-1                                |
| **F(000)**                      | 3232                                       |
| **Crystal size**                | 0.065 x 0.03 x 0.011 mm                    |
| **Theta angle for data collection** | 4.157 to 68.243 deg.                      |
| **Limiting indices**            | -45<=h<=46, -13<=k<=13, -21<=l<=22         |
| **Reflections collected/ unique** | 58215 / 7298 [R(int) = 0.0654]             |
| **Completeness to theta = 67.684** | 100.0 %                                    |
| **Absorption correction**       | Gaussian                                   |
| **Max. and min, transmission**  | 1.000 and 0.926                           |
| **Refinement method**           | Full-matrix least-squares on F^2           |
| **Data/ restraints/ parameters** | 7298 / 0 / 461                             |
| **Goodness-of-fit on F^2**      | 1.053                                      |
| **Final R indices [I>2σ(I)]**   | R1 = 0.0329, wR2 = 0.0870                  |
| **R indices (all data)**        | R1 = 0.0352, wR2 = 0.0884                  |
| **Largest diff. peak and hole** | 0.919 and -0.712 e.A^3                    |
7. Procedure for the dehydrogenative synthesis of pharmaceuticals

Moclobemide: 5 µmol of catalyst 1 and 10 µmol of t-BuOK were mixed in a 5 mL vial and 1 mL MTBE was added. The resulting brown solution was stirred for 5 min. In a separate 5 mL vial, 0.5 mmol of p-chlorobenzyl alcohol and 0.6 mmol of 4-(2-aminoethyl)morpholine (CAS# 2038-03-1) were dissolved in 1 mL MTBE. The latter solution was then added to the former brown solution at which the color disappeared to give a light red solution. The whole solution was then transferred to a 20 mL Schlenk flask with a side arm. The flask was sealed, taken outside the box, and connected to a condenser (1 °C, EG/H2O). The solution was then refluxed for 60 h under argon flow (bath temperature 70 °C). After the given time, the flask was cooled down to room temperature, and a known amount of mesitylene was added to the solution as a standard. A portion of the solution was analyzed by 1H NMR with CDCl3 as the solvent to determine the NMR yield. The CDCl3 solution was then added back to the parent solution and pure moclobemide was obtained from the crude solution by removing the solvent in vacuo, followed by recrystallization in a cold diethylether-pentane solvent mixture (85%). Alternatively, moclobemide can also be purified by flash column chromatography (MeOH 1-2% in CH2Cl2) and obtained as a white powder (88% yield).

1H NMR (400 MHz, CDCl3) δ 7.69 (d, J = 8.5 Hz, 2H), 7.38 (d, J = 8.4 Hz, 2H), 6.83 (t, J = 5.1 Hz, 1H), 3.70 (t, J = 4.6 Hz, 4H), 3.51 (q, J = 5.7 Hz, 2H), 2.57 (t, J = 6.1 Hz, 2H), 2.47 (s, 4H).

13C{1H} NMR (101 MHz, CDCl3) δ 166.35, 137.60, 132.98, 128.80, 128.38, 66.98, 56.85, 53.34, 36.14.

Itopride: 5 µmol of catalyst 1 and 10 µmol of t-BuOK were mixed in a 5 mL vial and 1 mL MTBE was added. The resulting dark brown solution was stirred for 5 min. In a separate 5 mL vial, 0.5 mmol of 3,4-dimethoxybenzyl alcohol and 0.6 mmol of 4-[2-(dimethylamino)ethoxy]benzylamine (CAS# 20059-73-8) were dissolved in 1 mL MTBE. The latter solution was then added to the former dark brown solution at which the brown color disappeared to give a light red solution. The whole solution was then transferred to a 20 mL Schlenk flask with a side arm. The flask was sealed, taken outside the box, and connected to a condenser (1 °C, EG/H2O). The solution was then refluxed for 60 h under argon flow (bath temperature 70 °C). After the given time, the flask was cooled down to room temperature, and a known amount of mesitylene was added to the solution as a standard. A portion of the solution was analyzed by 1H NMR with CDCl3 as the deuterated solvent to determine the NMR yield. The NMR solution was then added back to the parent solution and pentane was added.
to the solution. Formation of a white precipitate was observed which was filtered, washed with copious amounts of pentane and diethyl ether and dried to afford pure itopride in 92% yield.

$^1$H NMR (500 MHz, CDCl$_3$) δ 7.53 (d, $J = 1.8$ Hz, 1H), 7.39 (dd, $J = 8.3$, 1.9 Hz, 1H), 7.33 (d, $J = 8.5$ Hz, 2H), 6.96 (d, $J = 8.6$ Hz, 2H), 6.90 (d, $J = 8.4$ Hz, 1H), 6.77 (t, $J = 5.1$ Hz, 1H), 4.62 (d, $J = 5.6$ Hz, 2H), 4.12 (t, $J = 5.7$ Hz, 2H), 3.97 (d, $J = 1.7$ Hz, 6H), 2.80 (t, $J = 5.7$ Hz, 2H), 2.41 (s, 6H).

$^{13}$C NMR (126 MHz, CDCl$_3$) δ 166.94, 158.26, 151.69, 148.92, 130.61, 129.20, 127.06, 119.47, 114.73, 110.68, 110.23, 65.98, 58.23, 55.97, 55.96, 45.84, 43.57.

Trimethobenzamide: 5 µmol of catalyst 1 and 10 µmol of $t$-BuOK were mixed in a 5 mL vial and 1 mL MTBE was added. The resulting dark brown solution was stirred for 5 min. In a separate 5 mL vial, 0.5 mmol of 3,4,5-trimethoxybenzyl alcohol and 0.6 mmol of 4-[2-(dimethylamino)ethoxy]benzylamine (CAS# 20059-73-8) were dissolved in 1 mL MTBE. The latter solution was then added to the former dark brown solution at which the brown color disappeared to give a light red solution. The whole solution was then transferred to a 20 mL Schlenk flask with a side arm. The flask was sealed, taken outside the box, and connected to a condenser (1 °C, EG/H$_2$O). The solution was then refluxed for 60 h under argon flow (bath temperature 70 °C). After the given time, the flask was cooled down to room temperature, and pentane was added to the solution. Formation of white precipitate was observed which was filtered, washed with copious amounts of pentane and diethyl ether, and dried to afford pure trimethobenzamide in 94% yield.

$^1$H NMR (300 MHz, CDCl$_3$) δ 7.26 (d, $J = 8.1$ Hz, 2H), 7.05 (s, 2H), 6.89 (d, $J = 8.3$ Hz, 2H), 6.74 (d, $J = 5.8$ Hz, 1H), 4.54 (d, $J = 5.6$ Hz, 2H), 4.06 (t, $J = 5.7$ Hz, 2H), 3.87 (s, 3H), 3.86 (s, 6H), 2.73 (t, $J = 5.7$ Hz, 2H), 2.34 (s, 6H).

$^{13}$C NMR (75 MHz, CDCl$_3$) δ 167.02, 158.32, 153.12, 140.83, 130.43, 129.85, 129.23, 114.73, 104.44, 66.01, 60.87, 58.25, 56.26, 45.87, 43.65.
**N, N-Diethyl-meta-toluamide (DEET):** 10 µmol of catalyst 1 and 20 µmol of t-BuOK were mixed in a 5 mL vial and 1 mL dioxane was added. The resulting violet solution was stirred for 5 min. In a separate 5 mL vial 0.5 mmol of 3-methylbenzyl alcohol and 5 mmol of diethylamine were dissolved in 1 mL dioxane. The latter solution was then added to the former violet solution at which the violet color disappeared to give a light red solution. The resulting solution was then transferred to a 50 mL Schlenk tube. 0.5 mmol of powdered K$_3$PO$_4$ was subsequently added to the reaction flask. Afterwards, the tube was sealed and heated at a bath temperature of 130 °C for 60 h. The generated gas mixture was released in the 6th, 28th and 50th hour. After the given time, the reaction mixture was cooled down to room temperature and filtered via a short Celite pad to remove the K$_3$PO$_4$ affording a light yellow color solution. A known amount of mesitylene was added to the solution and a part of the solution was analyzed by $^1$H NMR with CDCl$_3$ as the deuterated solvent to determine the NMR yield (32%). The product was not isolated due to low yield.
Figure S28. $^1$H (top, 400 MHz) and $^{13}$C{$^1$H} (bottom, 101 MHz) NMR spectra of isolated N-heptylhexanamide (T2, E1) in CDCl$_3$. 
Figure S29. $^1$H (top, 500 MHz) and $^{13}$C($^1$H) (bottom, 125 MHz) NMR spectra of isolated N-benzylhexanamide (T2, E2) in CDCl$_3$. 
Figure S30. $^1$H (top, 400 MHz) and $^{13}$C($^1$H) (bottom, 101 MHz) NMR spectra of isolated N-heptylbenzamide (T2, E3) in CDCl$_3$. 
Figure S31. $^1$H (top, 400 MHz) and $^{13}$C($^1$H) (bottom, 101 MHz) NMR spectra of isolated N-benzylbenzamide (T2, E4) in CDCl$_3$. 
Figure S32. $^1$H (top, 400 MHz) and $^{13}$C($^1$H) (bottom, 101 MHz) NMR spectra of isolated N-furfurylhexanamide (T2, E5) in CDCl$_3$. 
Figure S33. $^1$H (top, 400 MHz) and $^{13}$C$^1$H (bottom, 101 MHz) NMR spectra of isolated N-hexanoylmorpholine (T2, E7) in CDCl$_3$. 
Figure S34. $^1$H (top, 400 MHz) and $^{13}$C($^1$H) (bottom, 101 MHz) NMR spectra of isolated N-heptyl-methoxyacetamide (T2, E11) in CDCl$_3$. 
Figure S35. $^1$H (top, 400 MHz) and $^{13}$C$[^1]$H (bottom, 101 MHz) NMR spectra of isolated N-heptyl-isovaleramide (T2, E13) in CDCl$_3$. acetone from the NMR tube.
Figure S36. $^1$H (top, 400 MHz) and $^{13}$C($^1$H) (bottom, 101 MHz) NMR spectra of isolated N-phenylhexanamide (T2, E16) in CDCl$_3$. *acetone from the NMR tube.
Figure S37. $^1$H (top, 400 MHz) and $^{13}$C [$^1$H] (bottom, 101 MHz) NMR spectra of isolated N,N'-Diacetylethylenediamine (T2, E18) in DMSO-d$_6$. 
Figure S38. $^1$H (top, 400 MHz) and $^{13}$C($^1$H) (bottom, 101 MHz) NMR spectra of isolated moclobemide (Scheme 6) in CDCl$_3$. 

S41
Figure S39. $^1$H (top, 500 MHz) and $^{13}$C($^1$H) (bottom, 126 MHz) NMR spectra of isolated itopride (Scheme 6) in CDCl$_3$. 

S42
Figure S40. $^1$H (top, 300 MHz) and $^{13}$C($^1$H) (bottom, 75 MHz) NMR spectra of isolated trimethobenzamide (Scheme 6) in CDCl$_3$. 
Figure S41. $^1$H (top, 300 MHz) and $^{13}$C($^1$H) (bottom, 75 MHz) NMR spectra of isolated (S)-N-benzyl-2-methylbutanamide in CDCl$_3$. [\(\alpha\)]$_{589}^{20}$ measured = 13.4 (c = 1g/100 mL).\textsuperscript{11}
Figure S42. $^1$H (top, 300 MHz) and $^{13}$C{$^1$H} (bottom, 75 MHz) NMR spectra of isolated (R)-N-(sec-butyl)benzamide in CDCl$_3$. $[\alpha]_{589}^{20}$ measured = 20.0 ($c = 1$g/100 mL).$^{12}$
9. Computational details

All geometries were optimized using Truhlar’s M06-L functional,\textsuperscript{13} the triple-\(\xi\) def2-TZVP basis set\textsuperscript{14} and W06 density fitting to increase computational efficiency\textsuperscript{15} as well as Grimme’s D3(0) empirical dispersion correction.\textsuperscript{16} Frequency calculations at this level of theory were run in order to confirm stationary points and transition states, as well as to compute thermodynamic properties. Single point energies of the optimized structures were computed using the range-separated meta-GGA hybrid functional \(\omega\)B97M-V of the Head-Gordon group\textsuperscript{17} including dispersion correction,\textsuperscript{18} together with the triple-\(\xi\) def2-TZVPP basis set\textsuperscript{14} and the corresponding auxiliary basis sets, def2/J\textsuperscript{15} and def2-TZVPP/C,\textsuperscript{19} for RIJCOSX density fitting. To take the influence of the solvent into account, single point calculations were performed with the integral equation formalism variant (IEFPCM) of the PCM model in the SMD variation of Truhlar and co-workers, with diethyl ether. Gibbs free energies were computed by adding the free energy correction terms from the frequency calculations to the single point energies according to

\[
G^{\omega\text{B97M-V}}_{\text{SMD}} = E^{\omega\text{B97M-V}}_{\text{el/SMD}} + G^{\text{M06-L}_f}_{\text{freq/gas}}
\]  

Free energy values (\(G^0\)) were then corrected to account for changes in standard states (\(G^0\rightarrow G^{0'}\)). Specifically, all species were corrected for the condensed phase (1 atm to 1M), with the exception of \(H_2\) (maintained at 1 atm standard state). Optimizations and frequency calculations were done using the Gaussian 16 software suite in the C.01 revision.\textsuperscript{20} Single point calculations were performed using Gaussian 16\textsuperscript{20} or the ORCA Software in the 4.2.1 release.\textsuperscript{21}
Alternate concerted reaction pathway not computed in this study

Scheme S2

Alternate concerted reaction pathway not computed in this study

Scheme S2
Computed Structures, First Three Frequencies, Coordinates

Note: Only relevant hydrogen atoms shown for clarity.

Color Scheme: ruthenium (pink), phosphorus (orange), nitrogen (blue), carbon (grey), hydrogen (green)

1b

First three frequencies

|   | 1    | 2    | 3    |
|---|------|------|------|
| Freqencies | 34.6601 | 43.2879 | 48.8900 |
| Red. masses | 3.9936 | 3.3395 | 3.1858 |
| Frc.consts | 0.0028 | 0.0037 | 0.0045 |
| IR Inten | 0.2880 | 0.2219 | 0.1714 |

Coordinates

44  -0.369067000  -1.156958000  -0.107984000
15  -0.467441000  1.044484000   0.211016000
  7  -0.647441000  -3.403975000   0.309066000
  8   0.895548000  -0.949682000  -2.810344000
  6  -2.688028000  -1.324489000   4.177710000
  7  -1.410226000  -1.197596000   1.755802000
  6  -1.886045000   1.139709000   1.412390000
  1  -1.885606000   2.045368000   2.022804000
  6  -1.974151000  -0.086703000   2.260357000
  6  -2.615370000  -0.124328000   3.489335000
  1  -3.057055000   0.776999000   3.891970000
  6  -2.117735000  -2.461123000   3.631281000
  1  -2.162046000  -3.412804000   4.143902000
  6  -1.470204000  -2.364326000   2.409613000
  6  -0.728440000  -3.502044000   1.782766000
  1  -1.148930000  -4.454306000   2.114068000
  1  -2.987960000  -3.435790000   2.147113000
  6   0.978041000   1.794530000   1.171085000
  6   2.269706000   1.430732000   0.437907000
  1   2.346604000   0.350194000   0.327421000
Int 2

First three frequencies

|   |   |   |
|---|---|---|
| 1 | A |   |
| 2 | A |   |
| 3 | A |   |
| Frequencies -- | 22.2050 | 41.5483 | 45.9340 |
| Red. masses -- | 3.7004 | 4.5126 | 5.4340 |
| Frc consts -- | 0.0011 | 0.0046 | 0.0068 |

Coordinates

|   |   |   |
|---|---|---|
|   |   |   |
| 44 | -0.352248000 | -0.842417000 | 0.038152000 |
| 15 | -0.412739000 | 1.411742000 | -0.104997000 |
| 7  | -0.629529000 | -2.900167000 | 0.847847000 |
| 8  | 1.526998000 | -1.063454000 | -2.281550000 |
| 6  | -2.977054000 | -0.181809000 | 4.050638000 |
| 7  | -1.718012000 | -0.517803000 | 1.640246000 |
| 6  | -1.815891000 | 1.813343000 | 1.044347000 |
| 1  | -1.716043000 | 2.788669000 | 1.522442000 |
| 6  | -2.062724000 | 0.722987000 | 2.036173000 |
| 6  | -2.684514000 | 0.918140000 | 3.257279000 |
| 1  | -2.937892000 | 1.919795000 | 3.576711000 |
| 6  | -2.692382000 | -1.453590000 | 3.588045000 |
| 1  | -2.934831000 | -2.331161000 | 4.170852000 |
| 6  | -2.071957000 | -1.595668000 | 2.356467000 |
| 6  | -1.827991000 | -2.912892000 | 1.699826000 |
| 1  | -2.709077000 | -3.141242000 | 1.088577000 |
| 1  | -1.760595000 | -3.687754000 | 2.467071000 |
| 6  | 1.052665000 | 2.335755000 | 0.663771000 |
| 6  | 2.337291000 | 1.757564000 | 0.070888000 |
| 1  | 3.201594000 | 2.214384000 | 0.557626000 |
| 1  | 2.427251000 | 1.940726000 | -0.998720000 |
| 1  | 2.394137000 | 0.681440000 | 0.229863000 |
| 6  | 1.019932000 | 2.021327000 | 2.160950000 |
| 1  | 0.222687000 | 2.558314000 | 2.676090000 |
| 1  | 1.962613000 | 2.331843000 | 2.615519000 |
| 1  | 0.898906000 | 0.957670000 | 2.359615000 |
| 6  | 1.046617000 | 3.851937000 | 0.508871000 |
| 1  | 1.176664000 | 4.177222000 | -0.521194000 |
|   |         |         |         |         |
|---|---------|---------|---------|---------|
| 1 | 6       | 3       | 1       | 0       |
|   | -0.935748000 | 2.276787000 | -1.704189000 | -0.935748000 |
| 6 | -1.570528000 | 0.441832000 | -2.697822000 | -1.985324000 |
| 6 | -2.363177000 | 1.915898000 | -3.267037000 | -2.363177000 |
| 6 | -2.837730000 | 1.183984000 | -1.737011000 | -2.837730000 |
| 6 | -1.558738000 | 3.656958000 | -1.489269000 | -1.558738000 |
| 6 | -1.861184000 | 0.136124000 | -2.458363000 | -1.861184000 |
|   | -1.879815000 | 4.266332000 | -1.704189000 | -1.879815000 |
Int 3

First three frequencies

|   | 1          | 2          | 3          |
|---|------------|------------|------------|
| Freqs | 39.0330    | 49.6880    | 61.3649    |
| Reds. masses | 4.2263     | 4.7554     | 4.3068     |
| Frc. consts | 0.0038     | 0.0069     | 0.0096     |
| IR Inten | 0.7168     | 1.6185     | 2.1183     |

Coordinates

|   |          |            |            |
|---|----------|------------|------------|
| 44 | -0.101565| -0.632260  | -0.608338  |
| 1  | -0.641421| -1.900634  | -1.454600  |
| 15 | -2.179828| -0.042038  | 0.030359   |
| 8  | -0.190702| 0.900898   | -3.177959  |
| 7  | 1.962109 | -1.606144  | -0.440290  |
| 7  | -0.172433| -1.745915  | 1.209561   |
| 6  | -2.045512| -0.369432  | 1.842510   |
| 6  | -1.094537| -1.474205  | 2.148040   |
| 6  | -1.104778| -2.188568  | 3.338952   |
| 1  | -1.852551| -1.966533  | 4.087270   |
| 6  | -0.134295| -3.145924  | 3.563055   |
| 1  | -0.119024| -3.696550  | 4.494493   |
| 6  | 0.830520 | -3.387106  | 2.596199   |
| 1  | 1.610729 | -4.119686  | 2.750610   |
| 6  | 0.776941 | -2.668625  | 1.416419   |
| 6  | 1.720770 | -2.874644  | 0.274463   |
| 1  | 2.644655 | -3.329875  | 0.641066   |
| 1  | 1.272675 | -3.573556  | -0.437886  |
| 6  | -0.133272| 0.316233   | -2.173317  |
| 6  | -2.713789| 1.764253   | 0.009248   |
| 6  | -1.456278| 2.591364   | 0.265241   |
| 1  | -1.732219| 3.647526   | 0.304246   |
| 1  | -0.990104| 2.333746   | 1.219687   |
| 1  | -0.710458| 2.467713   | -0.518599  |
| 6  | -3.251675| 2.128919   | -1.390150  |
-3.385922000  3.210954000  -1.446568000
-2.563218000  1.846017000  -2.186303000
-4.219774000  1.674529000  -1.596687000
-3.742524000  2.118187000  1.065582000
-4.684628000  1.587854000  -0.960748000
-3.359010000  1.942030000  2.069588000
-3.964211000  3.185150000  -0.995975000
-3.579498000  -1.161547000  0.566451000
-3.564862000  -1.216990000  -2.093310000
-3.795931000  -0.257101000  -2.550970000
-2.593555000  -1.542148000  -2.463260000
-4.315742000  -1.932020000  -2.436055000
-4.964332000  -0.754920000  -0.974830000
-5.009956000  -0.662134000  1.010974000
-5.306982000  0.180710000  -0.512774000
-3.275030000  -2.563000000  -0.030912000
-2.274905000  -2.890685000  -0.309012000
-3.370970000  -2.620560000  1.054223000
-3.990971000  -3.269620000  -0.455737000
2.909060000  -1.696492000  -1.605393000
3.293670000  -0.265838000  -1.949859000
2.418054000  0.334420000  -2.188426000
3.813860000  0.210798000  -1.116767000
3.961320000  -0.251069000  -2.809674000
-3.066603000  -0.507107000  2.340938000
1.234170000  0.966834000  1.636401000
0.627613000  0.679487000  0.593374000
0.465386000  1.003244000  2.658906000
1.938944000  2.255803000  1.216087000
2.647720000  2.544580000  1.992675000
1.222205000  3.068317000  1.106625000
2.004175000  0.130909000  1.633688000
-1.566727000  0.529190000  2.259900000
2.479240000  2.136166000  0.273912000
2.389219000  -0.968610000  0.237891000
4.168969000  -2.474069000  -1.229087000
3.974438000  -3.535885000  -1.083343000
4.904890000  -2.390120000  -2.027188000
4.624314000  -2.079470000  -0.319163000
2.210841000  -2.361695000  -2.778681000
2.895296000  -2.430378000  -3.623552000
1.887310000  -3.374667000  -2.538763000
1.334759000  -1.794425000  -3.085639000
TS1

First three frequencies

|    | 1                      | 2                      | 3                      |
|----|------------------------|------------------------|------------------------|
| 1  | 1                      | 2                      | 3                      |
| A  | A                      | A                      | A                      |
| Frequncies | -428.8623 | 37.3502 | 49.4442 |
| Red. masses  | 2.1631 | 4.2658 | 4.7410 |
| Frc consts  | 0.2344 | 0.0035 | 0.0068 |
| IR Inten   | 1111.6610 | 0.3269 | 1.2909 |

Coordinates

|   |   |   |   |
|---|---|---|---|
| 44 | -0.101565000 | -0.632260000 | -0.608338000 |
| 1  | -0.641421000 | -1.900634000 | -1.454640000 |
| 15 | -2.179828000 | -0.042038000 | 0.030359000 |
| 8  | -0.190702000 | 0.900898000  | -3.177959000 |
| 7  | 1.962109000  | -1.606144000 | -0.440290000 |
| 7  | -0.172431000 | -1.745915000 | 1.209561000  |
| 6  | -2.045512000 | -0.369432000 | 1.842510000  |
| 6  | -1.094537000 | -1.474205000 | 2.148084000  |
| 6  | -1.104778000 | -2.188568000 | 3.338520000  |
| 1  | -1.852551000 | -1.966533000 | 4.087270000  |
| 6  | -0.134295000 | -3.145924000 | 3.563055000  |
| 1  | -0.119024000 | -3.696550000 | 4.494493000  |
| 6  | 0.830520000  | -3.387106000 | 2.596199000  |
| 1  | 1.610729000  | -4.119686000 | 2.750610000  |
| 6  | 0.776941000  | -2.668625000 | 1.416419000  |
| 6  | 1.720770000  | -2.874644000 | 0.274463000  |
| 1  | 2.644655000  | -3.329875000 | 0.641066000  |
| 1  | 1.272675000  | -3.573556000 | -0.437886000 |
| 6  | -0.133272000 | 0.316233000  | -2.173317000 |
| 6  | -2.713789000 | 1.764253000  | -0.009248000 |
| 6  | -1.456278000 | 2.591364000  | 0.265241000  |
| 1  | -1.732219000 | 3.647526000  | 0.304246000  |
| 1  | -0.990104000 | 2.333746000  | 1.219687000  |
| 1  | -0.710458000 | 2.467713000  | -0.518599000 |
|   |      X       |      Y       |      Z       |
|---|-------------|-------------|-------------|
|   | -3.25167500 | 2.12891900  | -1.39015000 |
| 1 | -3.38592200 | 3.21095400  | -1.44656800 |
| 1 | -2.56321800 | 1.84601700  | -2.18630300 |
| 1 | -4.21977400 | 1.67452900  | -1.59668700 |
| 6 | -3.74252400 | 2.11818700  | 1.06558200  |
| 1 | -4.68462800 | 1.58785400  | 0.96074800  |
| 1 | -3.35901000 | 1.94203000  | 2.06958800  |
| 1 | -3.96421100 | 3.18515000  | 0.99597500  |
| 6 | -3.57949800 | -0.56645100 | -1.16154700 |
| 6 | -3.56486200 | -2.09333100 | -1.25710100 |
| 1 | -3.79593100 | -2.55099700 | -1.54214800 |
| 1 | -2.93555000 | -2.46328600 | -1.93202000 |
| 6 | -4.31574200 | -2.43605500 | -1.93202000 |
|   | -4.96433200 | -0.07486300 | -2.55099700 |
| 1 | -5.68492500 | -0.36096000 | -1.52448300 |
| 1 | -5.00995600 | 1.01097400  | -0.66213400 |
| 1 | -5.30698200 | -0.51277400 | 0.18071000  |
| 6 | -3.27573000 | -0.03091200 | -2.56300000 |
| 1 | -2.27409500 | -0.30902000 | -2.89068500 |
| 1 | -3.37099700 | 1.05422300  | -2.62025600 |
| 1 | -3.99097100 | -0.45573700 | -3.26992100 |
| 6 | 2.90906000  | -1.60539300 | -1.69649200 |
| 6 | 3.29367000  | -1.94985900 | -0.26538800 |
| 1 | 2.41805400  | -2.18842600 | 0.33442000  |
| 1 | 3.81386000  | -1.11676700 | 0.21079800  |
| 1 | 3.96132000  | -2.80967400 | -0.25106900 |
| 6 | 3.00660300  | 2.34093800  | -0.50710700 |
| 6 | 1.23417000  | 1.63640100  | 0.96683400  |
| 1 | 0.62761300  | 0.59337400  | 0.67948700  |
| 8 | 0.46538600  | 2.65890600  | 1.00324400  |
| 6 | 1.93894400  | 1.21608700  | 2.25580300  |
| 1 | 2.64772000  | 1.99267500  | 2.54445800  |
| 1 | 1.22222500  | 1.10662500  | 3.06831700  |
| 1 | 2.00417500  | 1.63368800  | 0.13090900  |
| 1 | 1.56672700  | 2.25990000  | 0.52919000  |
| 1 | 2.47924000  | 0.27391200  | 2.13616600  |
| 1 | 2.38921900  | 0.23789100  | -0.96861000 |
| 6 | 4.16896900  | -1.22908700 | -2.47406900 |
| 1 | 3.97443800  | -1.08334300 | -3.55388500 |
| 1 | 4.90489000  | -2.02718800 | -2.39012000 |
| 1 | 4.62431400  | -0.31916300 | -2.07947000 |
| 6 | 2.21084100  | -2.77868100 | -2.36169500 |
| 1 | 2.89529600  | -3.62355200 | -2.43037800 |
| 1 | 1.88731000  | -2.53876300 | -3.37466700 |
| 1 | 1.33475900  | -3.08563900 | -1.79442500 |
First three frequencies

|     | 1                      | 2                      | 3                      |
|-----|------------------------|------------------------|------------------------|
| A   | -436.0669              | 22.1130                | 33.4792                |
| A   | 2.2481                 | 3.7135                 | 3.4662                 |
| A   | 0.2519                 | 0.0011                 | 0.0023                 |
| A   | 1106.6903              | 0.1362                 | 0.0671                 |

Coordinates

|     | 0.311397000 | -0.831691000 | 0.071887000 |
|-----|-------------|--------------|-------------|
| 15  | -0.380718000| 1.404858000  | -0.078337000|
| 6   | -0.612353000| -2.925553000 | 0.888843000 |
| 8   | 1.587901000 | -1.059382000 | -2.228727000|
| 6   | -3.027657000 | -0.186809000 | 4.041585000  |
| 7   | -1.695695000 | -0.519429000 | 1.666318000  |
| 6   | -1.782237000 | 1.811714000  | 1.072972000  |
| 6   | -1.677317000 | 2.783744000  | 1.557022000  |
| 6   | -2.049465000 | 0.718929000  | 2.055974000  |
| 6   | -2.706475000 | 0.912434000  | 3.260841000  |
| 1   | -2.966600000 | 1.914338000  | 3.574483000  |
| 6   | -2.734622000 | -1.458548000 | 3.579814000  |
| 1   | -1.300326000 | -2.338163000 | 4.148388000  |
| 6   | -2.077823000 | -1.595633000 | 2.367627000  |
| 6   | -1.830247000 | -2.916615000 | 1.713324000  |
| 1   | -2.687785000 | -3.123385000 | 1.063754000  |
| 1   | -1.808765000 | -3.700039000 | 2.475149000  |
| 6   | 1.080103000  | 2.358626000  | 0.674949000  |
| 6   | 2.369855000  | 1.803708000  | 0.071895000  |
| 1   | 3.230184000  | 2.259676000  | 0.567344000  |
| 1   | 2.458431000  | 2.009723000  | -0.993541000 |
| 1   | 2.429539000  | 0.724743000  | 0.208363000  |
6 1.070782000 2.049884000 2.173299000
1 0.265523000 2.567686000 2.695832000
1 2.009992000 2.386050000 2.617520000
1 0.975188000 0.981853000 2.361051000
6 1.047051000 3.874428000 0.517469000
1 1.165435000 4.199506000 -0.514061000
1 1.876554000 4.305040000 1.083477000
1 0.131198000 4.314462000 0.914370000
6 1.047051000 3.874428000 0.517469000
1 1.165435000 4.199506000 -0.514061000
1 1.876554000 4.305040000 1.083477000
1 0.131198000 4.314462000 0.914370000
6 1.047051000 3.874428000 0.517469000
1 1.165435000 4.199506000 -0.514061000
1 1.876554000 4.305040000 1.083477000
1 0.131198000 4.314462000 0.914370000
First three frequencies

\begin{align*}
\text{Frequencies} & \quad 45.5135 \quad 48.7827 \quad 66.4632 \\
\text{Red. masses} & \quad 5.3563 \quad 3.6089 \quad 5.6567 \\
\text{Frc consts} & \quad 0.0065 \quad 0.0051 \quad 0.0147 \\
\text{IR Inten} & \quad 1.2990 \quad 0.2361 \quad 1.0997 \\
\end{align*}

Coordinates

\begin{align*}
44 & \quad -0.358366000 \quad -1.142921000 \quad -0.176958000 \\
15 & \quad -0.453208000 \quad 1.046383000 \quad 0.193181000 \\
7 & \quad -0.609723000 \quad -3.399756000 \quad 0.202864000 \\
8 & \quad 1.046092000 \quad -0.935724000 \quad -2.815067000 \\
6 & \quad -2.654112000 \quad -1.430749000 \quad 4.108097000 \\
7 & \quad -1.364407000 \quad -1.224884000 \quad 1.692396000 \\
6 & \quad -1.871541000 \quad 1.109413000 \quad 1.400949000 \\
1 & \quad -1.887316000 \quad 2.003180000 \quad 2.028721000 \\
6 & \quad -1.948884000 \quad -0.134831000 \quad 2.222220000 \\
6 & \quad -2.594932000 \quad -0.214344000 \quad 3.446577000 \\
1 & \quad -3.054061000 \quad 0.670099000 \quad 3.867298000 \\
6 & \quad -2.055867000 \quad -2.543981000 \quad 3.540262000 \\
1 & \quad -2.082432000 \quad -3.507680000 \quad 4.031563000 \\
6 & \quad -1.402221000 \quad -2.404335000 \quad 2.328185000 \\
6 & \quad -0.605030000 \quad -3.489047000 \quad 1.676947000 \\
1 & \quad -0.919881000 \quad -4.469599000 \quad 2.044695000 \\
1 & \quad 0.435139000 \quad -3.337174000 \quad 1.981979000 \\
6 & \quad 0.984980000 \quad 1.804655000 \quad 1.175951000 \\
6 & \quad 2.290088000 \quad 1.507307000 \quad 0.438784000 \\
\end{align*}
|   | 1 | 2.390056000 | 0.437714000 | 0.255853000 |
|   | 1 | 3.133490000 | 1.831424000 | 1.052583000 |
|   | 1 | 2.363318000 | 2.025337000 | -0.515535000 |
|   | 6 | 1.026094000 | 1.066321000 | 2.516890000 |
|   | 1 | 0.181821000 | 1.324106000 | 3.158168000 |
|   | 1 | 1.936490000 | 1.352336000 | 3.052260000 |
|   | 1 | 1.048645000 | -0.014421000 | 2.371821000 |
|   | 6 | 0.874415000 | 3.296998000 | 1.465513000 |
|   | 1 | 0.960796000 | 3.910603000 | 0.570827000 |
|   | 1 | 1.688814000 | 3.591645000 | 2.131859000 |
|   | 1 | -1.553522000 | 0.704608000 | 2.562934000 |
|   | 6 | -1.010798000 | 2.268437000 | -1.140446000 |
|   | 6 | -2.005782000 | 1.551107000 | -2.052968000 |
|   | 1 | -2.365999000 | 2.260973000 | -2.801617000 |
|   | 1 | -2.868794000 | 1.168515000 | -1.508480000 |
|   | 6 | -1.709221000 | 3.510833000 | -0.585066000 |
|   | 1 | -2.622019000 | 3.259708000 | -0.045228000 |
|   | 1 | -2.004542000 | 4.150268000 | -1.419885000 |
|   | 1 | -1.084008000 | 4.109134000 | 0.070438000 |
|   | 6 | 0.191564000 | 2.680265000 | -1.988563000 |
|   | 1 | 0.885690000 | 3.323215000 | -1.450102000 |
|   | 1 | -0.157738000 | 3.240348000 | -2.858512000 |
|   | 1 | 0.742159000 | 1.815409000 | -2.358510000 |
|   | 1 | 0.296043000 | 1.293622000 | -0.118310000 |
|   | 6 | -1.652239000 | -4.224520000 | -0.500182000 |
|   | 6 | -1.410550000 | -5.711388000 | -0.249355000 |
|   | 1 | -0.415950000 | -6.016920000 | -0.583916000 |
|   | 1 | -2.134907000 | -6.307112000 | -0.803391000 |
|   | 1 | -1.512296000 | -5.983551000 | 0.800841000 |
|   | 6 | -1.516591000 | -3.933690000 | -1.985248000 |
|   | 1 | -1.716655000 | -2.883845000 | -2.186564000 |
|   | 1 | -2.203586000 | -4.550440000 | -2.556915000 |
|   | 1 | -0.500917000 | -4.155219000 | -2.335447000 |
|   | 6 | -3.028434000 | -3.811948000 | -0.007910000 |
|   | 1 | -3.189365000 | -4.087481000 | 1.035521000 |
|   | 1 | -3.797288000 | -4.310326000 | -0.596580000 |
|   | 1 | -3.155654000 | -2.734089000 | -0.116824000 |
|   | 6 | 0.504487000 | -1.029219000 | -1.788077000 |
|   | 1 | -3.164132000 | -1.509664000 | 5.059062000 |
|   | 1 | 1.122975000 | -1.448774000 | 0.643580000 |
|   | 1 | -2.763929000 | 1.151431000 | 0.768020000 |
|   | 1 | -1.899682000 | -1.016933000 | -0.871167000 |
First three frequencies

|     | 1       | 2       | 3       |
|-----|---------|---------|---------|
| Freq.  | 31.9365 | 44.1770 | 53.1675 |
| Red. m. | 3.9347  | 3.5347  | 3.9008  |
| Frc const | 0.0024  | 0.0041  | 0.0065  |
| IR Inten | 0.0538  | 0.3910  | 0.1451  |

Coordinates

44  -0.175027000  -0.874080000  -0.227645000
15  -0.506565000  1.267076000  0.334734000
  -0.342273000  -3.150690000  -0.102874000
  1.053252000  -0.283531000  -2.887317000
  2.473974000  -1.744750000  3.994638000
  1.209905000  -1.221242000  1.618785000
  1.918803000  1.077922000  1.530663000
  2.010403000  1.909288000  2.232710000
  1.875663000  -0.234249000  2.241160000
  2.510319000  -0.470749000  3.451124000
  3.033558000  0.333929000  3.949495000
  1.814334000  -2.756527000  3.319369000
  1.782886000  -3.764738000  3.710440000
  1.180636000  -2.461863000  2.121935000
  0.383845000  -3.453325000  1.338080000
  0.736435000  -4.466900000  1.546878000
  0.648655000  -3.378934000  1.691244000
  0.829541000  2.088107000  1.389464000

S60
|   |   |   |   |   |
|---|---|---|---|---|
| 6 | 2.143700000 | 2.029206000 | 0.615794000 |
| 1 | 2.332428000 | 1.011127000 | 0.282552000 |
| 6 | 2.159390000 | 2.689799000 | -0.248695000 |
| 1 | 0.979925000 | 1.197087000 | 2.627693000 |
| 1 | 0.105857000 | 1.241830000 | 3.279711000 |
| 6 | 1.183626000 | 0.160267000 | 2.350405000 |
| 1 | 0.546524000 | 3.514643000 | 1.842939000 |
| 1 | 0.550423000 | 4.228933000 | 1.021010000 |
| 6 | 1.329972000 | 3.825895000 | 2.538216000 |
| 1 | -0.402586000 | 3.607668000 | 2.373348000 |
| 6 | -1.203055000 | 2.515644000 | -0.902359000 |
| 1 | -1.562211000 | 1.041012000 | -2.472210000 |
| 6 | -0.583656000 | 3.139742000 | -1.698510000 |
| 1 | 0.541710000 | 3.822457000 | -1.099377000 |
| 1 | 0.630602000 | -3.339862000 | -0.404403000 |
| 6 | -1.259649000 | -3.928682000 | -0.958227000 |
| 1 | -0.936369000 | -5.582763000 | -1.281388000 |
| 1 | -1.009831000 | -5.839755000 | -0.843970000 |
| 6 | -1.117132000 | -3.432085000 | -2.386708000 |
| 1 | -1.429012000 | -2.935280000 | -2.475782000 |
| 1 | -0.711339000 | -4.038358000 | -3.070190000 |
| 6 | -0.073789000 | -3.499267000 | -2.700548000 |
| 1 | -2.817299000 | -3.697332000 | -0.485807000 |
| 6 | -2.883080000 | -4.102152000 | 0.513397000 |
| 1 | -3.418215000 | -4.185476000 | -1.157560000 |
| 6 | -2.934794000 | -2.629743000 | -0.469479000 |
| 1 | 0.592186000 | -0.521513000 | -1.842503000 |
| 6 | -2.968996000 | -1.948564000 | 4.935290000 |
| 1 | -2.819899000 | 1.093215000 | 0.909532000 |
| 1 | -1.636914000 | -0.750208000 | -0.896262000 |
| 8 | 1.652234000 | -1.426512000 | 0.924315000 |
| 6 | 2.760783000 | -2.026481000 | 0.431856000 |
| 1 | 3.251358000 | -2.612570000 | 1.236381000 |
| 6 | 3.802046000 | -1.058750000 | -0.121028000 |
| 1 | 4.119001000 | -0.353167000 | 0.646132000 |
| 1 | 3.378015000 | -0.489314000 | -0.951872000 |
| 1 | 4.690476000 | -1.580139000 | -0.485282000 |
| 7 | 2.458472000 | -3.059792000 | -0.629616000 |
|   | 1       | 2       | 3       |
|---|---------|---------|---------|
|   | Frequency | Red. masses | Frf const | IR Inten |
| 1 | -2.492089 | 3.376707  | 4.427402  | 3.044362 |
| 6 | -2.586185 | -4.193101 | -3.879513 | -5.203134 |
| 1 | -1.527625 | -0.655709 | 0.554839  | 0.422885 |
| 1 | -2.492089 | 3.376707  | 4.427402  | 3.044362 |
| 6 | -2.586185 | -4.193101 | -3.879513 | -5.203134 |
| 1 | -1.527625 | -0.655709 | 0.554839  | 0.422885 |

**TS3**

![TS3 Image]

**First three frequencies**

|   | 1       | 2       | 3       |
|---|---------|---------|---------|
|   | A       | A       | A       |
| Frequencies | -628.9627 | 24.2961 | 42.5423 |
| Red. masses | 1.8114   | 3.7489  | 3.5225  |
| Frf const  | 0.4455   | 0.0013  | 0.0038  |
| IR Inten  | 2357.4464 | 0.3683  | 0.4843  |

**Coordinates**

|   | -0.308031 | -0.912469 | 0.142530 |
|---|-----------|-----------|----------|
| 15| -0.407754 | 1.332740  | 0.049372 |
| 7 | -0.680631 | -3.026629 | 0.828318 |
| 8 | 1.748896  | -1.008195 | -2.028654 |
| 6 | -3.310539 | -0.366010 | 3.919357 |
| 7 | -1.809243 | -0.658881 | 1.641573 |
| 6 | -1.959259 | 1.659036  | 1.014815 |
| 1 | -1.982196 | 2.644108  | 1.483147 |
| 6 | -2.250550 | 0.565591  | 1.989588 |

S62
First three frequencies

|     | 1          | 2          | 3          |
|-----|------------|------------|------------|
| A   | -484.7245  | 29.0918    | 42.4845    |
| A   | 4.1131     | 4.4006     |            |
| A   | 0.0021     | 0.0047     |            |
| A   | 1.1867     | 2.7602     |            |
| Coordinates |
|-------------|
| 44 -0.070946000 -0.748359000 -0.760916000 |
| 1 -0.715360000 -2.022039000 -1.551688000 |
| 15 -2.089966000 -0.066292000 -0.043402000 |
| 8 -0.201717000 0.762032000 -3.342984000 |
| 7 1.902314000 -1.924212000 -0.710200000 |
| 7 -0.119763000 0.762032000 1.073716000 |
| 6 -1.831864000 0.288762000 1.775326000 |
| 6 -0.951905000 2.061252000 3.270551000 |
| 6 -0.936428000 -2.139325000 -3.066482000 |
| 6 -0.128086000 0.180571000 0.564874000 |
| 6 1.342730000 -1.417448000 3.577070000 |
| 1 2.448901000 -3.727460000 -0.321060000 |
| 6 0.201317000 3.728495000 1.977707000 |
| 6 -1.605626000 3.623247000 -0.097132000 |
| 1 -0.779892000 2.354220000 0.810299000 |
| 1 -0.690394000 2.382043000 -0.953429000 |
| 6 -3.296790000 -1.522060000 1.649390000 |
| 6 -1.342730000 3.074960000 -0.100699000 |
| 1 -2.692072000 1.641748000 -2.356677000 |
| 1 -4.285518000 1.548760000 -1.597720000 |
| 6 -3.530931000 2.183225000 0.968570000 |
| 1 -4.467482000 1.635811000 1.027647000 |
| 1 -3.028528000 2.109855000 1.932330000 |
| 1 -3.780928000 3.236171000 0.823045000 |
| 6 -3.546490000 -1.200597000 -0.465574000 |
| 6 -3.661815000 -1.339719000 -1.982981000 |
| 1 -3.943173000 -0.409888000 2.472115000 |
| 1 -2.722082000 -1.680428000 -2.415783000 |
| 1 -4.431057000 -2.078116000 -2.219088000 |
| 6 -4.879653000 -0.744775000 0.118766000 |
| 1 -5.633080000 -1.513208000 -0.069255000 |
| 1 -4.832414000 -0.601646000 1.199129000 |
| 1 -5.244889000 0.175847000 -0.331656000 |
| 6 -3.226815000 -2.580960000 0.113315000 |
| 1 -2.263664000 -2.951114800 -0.237556000 |
| 1 -3.227434000 -2.583010000 1.204042000 |
| 1 -3.994821000 -3.286566000 -0.209558000 |
| 6 2.754290000 -2.109250000 -1.935931000 |
| 6 3.224122000 -0.718936000 -2.337993000 |
| 1 2.382823000 -0.062914000 -2.550688000 |
| 1 3.819095000 -0.257572000 -1.547506000 |
1  3.846155000  -0.775530000  -3.229748000
1  -2.752312000  -0.324654000  2.361002000
6  1.438206000  1.193505000  1.374617000
1  0.803938000  0.535219000  0.350806000
8  0.644420000  1.409438000  2.332376000
6  2.593282000  0.237237000  1.670660000
1  2.232080000  -0.724399000  2.040464000
1  3.195123000  0.689955000  2.459540000
1  -1.263439000  0.601882000  2.087575000
1  3.254523000  0.101610000  0.811364000
1  2.449269000  -1.349104000  -0.073755000
6  3.972415000  -2.976153000  -1.622457000
1  3.705845000  -4.015248000  -1.433164000
1  4.657615000  -2.971041000  -2.468669000
1  4.517720000  -2.597229000  -0.755906000
6  1.929943000  -2.734973000  -3.046647000
1  2.546244000  -2.855212000  -3.936871000
1  1.557642000  -3.722393000  -2.773477000
1  1.074132000  -2.111222000  -3.296063000
7  1.956079000  2.360144000  0.626269000
1  1.720641000  2.304363000  -0.352663000
6  1.649695000  3.666022000  1.187156000
1  1.846963000  4.401689000  0.404072000
1  0.594107000  3.772164000  1.463358000
6  2.502100000  3.957253000  2.403780000
1  3.563283000  3.895958000  2.161593000
1  2.289309000  3.234285000  3.190457000
1  2.297338000  4.951772000  2.800670000

2b (Bn alkoxy complex)

First three frequencies
|   | 1          | 2          | 3          |
|---|------------|------------|------------|
|   | **A**      | **A**      | **A**      |
| Frequencies | **19.5928** | 27.6589    | 35.6768    |
| Red. masses  | **5.1137**  | 4.5670     | 3.7471     |
| Frc consts  | **0.0012**  | 0.0021     | 0.0028     |
| IR Inten    | **0.3535**  | 0.1547     | 0.0660     |

Coordinates

| 44 | -0.122338000 | -1.214339000 | -0.114591000 |
| 15 | -0.433737000 | 0.969972000  | 0.195729000  |
| 7  | -0.305611000 | -3.451750000 | 0.274030000  |
| 8  | 1.199589000  | -0.881250000 | -2.776630000 |
| 6  | -2.556934000 | -1.609626000 | 4.092010000  |
| 7  | -1.216671000 | -1.354292000 | 1.715431000  |
| 6  | -1.887998000 | 0.931665000  | 1.358812000  |
| 1  | -1.984905000 | 1.831873000  | 1.969514000  |
| 6  | -1.891375000 | -0.300390000 | 2.203504000  |
| 6  | -2.564879000 | -0.402676000 | 3.412331000  |
| 1  | -3.095043000 | 0.454221000  | 3.805188000  |
| 6  | -1.874056000 | -2.690950000 | 3.559887000  |
| 1  | -1.853189000 | -3.647131000 | 4.065604000  |
| 6  | -1.195036000 | -2.527791000 | 2.363846000  |
| 6  | -0.332341000 | -3.580833000 | 1.744696000  |
| 1  | -0.637143000 | -4.580260000 | 2.068139000  |
| 6  | 0.688830000  | -3.388562000 | 2.081833000  |
| 6  | 0.908818000  | 1.852053000  | 1.193150000  |
| 6  | 2.248184000  | 1.597283000  | 0.500025000  |
| 1  | 2.421880000  | 0.526077000  | 0.407575000  |
| 1  | 3.052626000  | 2.021966000  | 1.105311000  |
| 1  | 2.308140000  | 2.051317000  | -0.487733000 |
| 6  | 0.949362000  | 1.158964000  | 2.559403000  |
| 1  | 0.056462000  | 1.361446000  | 3.153821000  |
| 1  | 1.799318000  | 1.552706000  | 3.121806000  |
| 1  | 1.096680000  | 0.083005000  | 2.453179000  |
| 6  | 0.702746000  | 3.345206000  | 1.418945000  |
| 1  | 0.770017000  | 3.930543000  | 0.503525000  |
| 1  | 1.485501000  | 3.710124000  | 2.088333000  |
| 1  | -0.252204000 | 3.567213000  | 1.898229000  |
| 6  | -1.055968000 | 2.094223000  | -1.188190000 |
| 6  | -1.971945000 | 1.271592000  | -2.094584000 |
| 1  | -1.440620000 | 0.458974000  | -2.582179000 |
| 1  | -2.383895000 | 1.928490000  | -2.864174000 |
| 1  | -2.807934000 | 0.829380000  | -1.551681000 |
| 6  | -1.860359000 | 3.292646000  | -0.681252000 |
| 1  | -2.764196000 | 2.986738000  | -0.154630000 |
| 1  | -2.182686000 | 3.887351000  | -1.538658000 |
| 1  | -1.296238000 | 3.951266000  | -0.028116000 |
| 6  | 0.127923000  | 2.577302000  | -2.024625000 |
| 1  | 0.762059000  | 3.279711000  | -1.486876000 |
| 1  | -0.246552000 | 3.093383000  | -2.911091000 |
| 1  | 0.747872000  | 1.749472000  | -2.367857000 |
|   |       |       |       |       |
|---|-------|-------|-------|-------|
| 1 | 0.556799000 | -3.874078000 | -0.056048000 |       |
| 2 | -1.458173000 | -4.092699000 | -0.399176000 |       |
| 3 | 0.710187000  | -1.030561000 | -1.730720000 |       |
| 4 | -3.085640000 | -1.707708000 |  5.031147000 |       |
| 5 | -2.767640000 |  0.899020000 |  0.708283000 |       |
| 6 | -1.551424000 | -1.216016000 | -0.891757000 |       |
| 7 | 1.607206000  | -1.552823000 |  1.177533000 |       |
| 8 | 2.717021000  | -2.144475000 |  0.627921000 |       |
| 9 | 3.120022000  | -1.575899000 | -0.235440000 |       |
| 10| 2.508451000  | -3.157374000 |  0.200077000 |       |
| 11| 3.814387000  | -2.296707000 |  1.664976000 |       |
| 12| 3.467520000  | -2.900077000 |  2.505620000 |       |
| 13| 4.091911000  | -1.318025000 |  2.059432000 |       |
| 14| 4.708378000  | -2.767150000 |  1.252287000 |       |
| 15| -2.354321000 | -3.576248000 | -0.052898000 |       |
| 16| -1.360911000 | -3.866062000 | -1.460481000 |       |
| 17| -1.563326000 | -5.570748000 | -0.161328000 |       |
| 18| -2.488637000 | -6.089054000 |  0.740051000 |       |
| 19| -0.704090000  | -6.452066000 | -0.814250000 |       |
| 20| -2.556476000 | -7.452496000 |  0.984800000 |       |
| 21| -0.766967000  | -7.814304000 | -0.572113000 |       |
| 22| -1.694144000 | -8.317714000 |  0.329439000 |       |
| 23| -3.164404000 | -5.410460000 |  1.250577000 |       |
| 24| 0.015871000  | -6.063512000 | -1.526979000 |       |
| 25| -3.284045000 | -7.839637000 |  1.686583000 |       |
| 26| -0.096043000  | -8.486056000 | -1.091791000 |       |
| 27| -1.746290000 | -9.382262000 |  0.516862000 |       |

**TS3_{Bn} (Bn NH assisted amide formation)**
First three frequencies

|       | 1            | 2            | 3            |
|-------|--------------|--------------|--------------|
| Freq. | -641.8570    | 21.8936      | 27.5828      |
| Mass. | 1.9232       | 4.2675       | 3.9952       |
| Frc.  | 0.4668       | 0.0012       | 0.0018       |
| IR Int. | 2430.3007   | 0.4409       | 0.4119       |

Coordinates

|       |             |             |             |
|-------|-------------|-------------|-------------|
|       | 44          | -0.424481000 | -0.878848000 | 0.113742000 |
|       | 15          | -0.417190000 | 1.376118000  | 0.062093000  |
|       | 7           | -0.873464000 | -2.945828000 | 0.732121000  |
|       | 8           | 1.593139000  | -1.191096000 | -2.078437000 |
|       | 6           | -3.335534000 | -0.322572000 | 3.940698000  |
|       | 7           | -1.889608000 | -0.593497000 | 1.629994000  |
|       | 6           | -1.911763000 | 1.753220000  | 1.103007000  |
|       | 1           | -1.853710000 | 2.715864000  | 1.612960000  |
|       | 6           | -2.247495000 | 0.637691000  | 2.040165000  |
|       | 6           | -2.959665000 | 0.799666000  | 3.217367000  |
|       | 1           | -3.219976000 | 1.793554000  | 3.555308000  |
|       | 6           | -3.052007000 | -1.583551000 | 3.443627000  |
|       | 1           | -3.371388000 | -2.477196000 | 3.961808000  |
|       | 6           | -2.337554000 | -1.690515000 | 2.261754000  |
|       | 6           | -2.095202000 | -2.980250000 | 1.547412000  |
|       | 1           | -2.949558000 | -3.146641000 | 0.879667000  |
|       | 1           | -2.082105000 | -3.817847000 | 2.251018000  |
|       | 6           | 0.971715000  | 2.250156000  | 1.016864000  |
|       | 6           | 2.303078000  | 1.660980000  | 0.548793000  |
|       | 1           | 3.118695000  | 2.086662000  | 1.141668000  |
|       | 1           | 2.514681000  | 1.876356000  | -0.498582000 |
|       | 1           | 2.310001000  | 0.583161000  | 0.674400000  |
|       | 6           | 0.766002000  | 1.856237000  | 2.479078000  |
|       | 1           | -0.057433000 | 2.398112000  | 2.945320000  |
|       | 1           | 1.666722000  | 2.086733000  | 3.053121000  |
|       | 1           | 0.571223000  | 0.788525000  | 2.573295000  |
|       | 6           | 1.008343000  | 3.770807000  | 0.938480000  |
|       | 1           | 1.255238000  | 4.143071000  | -0.05373000  |
|       | 1           | 1.780339000  | 4.140513000  | 1.617710000  |
|       | 1           | 0.067572000  | 4.224965000  | 1.251814000  |
|       | 6           | -0.768710000 | 2.328621000  | -1.532725000 |
|       | 6           | -1.755536000 | 1.503618000  | -2.359207000 |
|       | 1           | -1.331882000 | 0.548868000  | -2.659566000 |
|       | 1           | -2.019451000 | 2.066505000  | -3.257209000 |
|       | 1           | -2.678634000 | 1.291280000  | -1.818385000 |
|       | 6           | -1.389021000 | 3.708649000  | -1.311579000 |
|       | 1           | -2.339622000 | 3.652979000  | -0.781106000 |
|       | 1           | -1.599161000 | 4.159237000  | -2.283887000 |
|       | 1           | -0.743639000 | 4.396265000  | -0.774697000 |
|       | 6           | 0.525888000  | 2.456286000  | -2.334227000 |
|       | 1           | 0.299420000  | 2.857019000  | -3.324282000 |
|       | 1           | 1.010593000  | 1.490623000  | -2.478291000 |
| 1 | -0.081546000 | -3.110355000 | 1.407402000 |
| 6 | 0.816420000 | -1.086417000 | -1.219733000 |
| 1 | -3.872201000 | -0.212786000 | 4.873816000 |
| 1 | -1.620492000 | -0.913566000 | 0.395310000 |
| 1 | -2.743641000 | 1.831884000 | 2.238690000 |
| 8 | 1.004679000 | -1.180059000 | 3.403200000 |
| 1 | 3.628720000 | -2.404306000 | 1.437210000 |
| 1 | 3.361043000 | -1.257932000 | 1.046702000 |
| 6 | 2.883690000 | -2.196993000 | 1.356540000 |
| 1 | 3.628720000 | -2.816343000 | 1.863053000 |
| 1 | 3.361043000 | -1.257932000 | 1.046702000 |
| 6 | 2.888369000 | -3.052425000 | 2.562670000 |
| 1 | 2.469006000 | -0.317642000 | 3.108559000 |
| 1 | 0.963393000 | -0.960070000 | 4.365251000 |
| 1 | 1.122684000 | 0.018017000 | 4.825668000 |
| 1 | -0.005674000 | 0.902863000 | 3.842563000 |
| 6 | 0.896086000 | 2.096660000 | 5.433552000 |
| 1 | 1.122684000 | 0.018017000 | 4.825668000 |
| 1 | 0.963393000 | -0.960070000 | 4.365251000 |
| 1 | 1.122684000 | 0.018017000 | 4.825668000 |
| 1 | -0.005674000 | 0.902863000 | 3.842563000 |
| 6 | 0.896086000 | 2.096660000 | 5.433552000 |
| 1 | 1.826995000 | -2.073404000 | 5.997736000 |
| 1 | 0.730155000 | -3.002503000 | 4.977924000 |
| 1 | 0.842250000 | -1.824628000 | 6.133152000 |
| 6 | -0.846178000 | 0.019164000 | 0.288596000 |
| 1 | -1.596890000 | 0.902863000 | 3.842563000 |
| 1 | 0.128048000 | -3.933973000 | -0.776794000 |
| 6 | -2.051907000 | 0.249020000 | 0.776794000 |
| 6 | -1.054388000 | 0.539501000 | 0.260844000 |
| 1 | 0.514335000 | -5.223006000 | 1.719333000 |
| 1 | -2.680641000 | -5.851559000 | -1.053814000 |
| 1 | -3.025250000 | -8.124639000 | -0.153352000 |
| 6 | -2.246320000 | -7.494378000 | 0.256732000 |
| 6 | -1.446490000 | 0.957990000 | 1.288916000 |
| 1 | -1.596955000 | -8.952792000 | 1.688319000 |
| 1 | -0.453018000 | -7.139658000 | 1.810243000 |
| 1 | 0.172804000 | -7.496064000 | 2.618600000 |

4b (Et₂ alkoxy complex)
First three frequencies

|    | 1         | 2         | 3         |
|----|-----------|-----------|-----------|
| A  | 38.8837   | 52.0653   | 58.3056   |
| A  | 3.7196    | 3.6611    | 4.8652    |
| A  | 0.0033    | 0.0058    | 0.0097    |
| A  | 0.2796    | 0.0060    | 1.3507    |

Coordinates

|    |          |          |          |
|----|----------|----------|----------|
|    | -0.165135000 | -1.234756000 | -0.294029000 |
| 15 | -0.386652000   | 0.949439000   | 0.097021000   |
|    | -0.596193000   | -3.522462000   | -0.051183000   |
| 8  | 1.240227000    | -0.881105000   | -2.909289000   |
| 6  | -2.421423000   | -1.649748000   | 4.005258000    |
| 7  | -1.239869000   | -1.398209000   | 1.547089000    |
| 6  | -1.820436000   | 0.919518000    | 1.284384000    |
| 1  | -1.885678000   | 1.811086000    | 1.911259000    |
| 6  | -1.828473000   | -0.327527000   | 2.104768000    |
| 6  | -2.242722000   | -0.427087000   | 3.352673000    |
| 1  | -2.885952000   | 0.443002000    | 3.799534000    |
| 6  | -1.843698000   | -2.749716000   | 3.396001000    |
| 1  | -1.846552000   | -3.720922000   | 3.872392000    |
| 6  | -1.254966000   | -2.592884000   | 2.150697000    |
| 6  | -0.571000000   | -3.702934000   | 1.417230000    |
| 1  | -0.988101000   | -4.671999000   | 1.716588000    |
| 1  | 0.484460000    | -3.660134000   | 1.703598000    |
| 6  | 0.972318000    | 1.786911000    | 1.113233000    |
| 6  | 2.300872000    | 1.593514000    | 0.385526000    |
| 1  | 2.461347000    | 0.544289000    | 0.146750000    |
| 1  | 3.119396000    | 1.920685000    | 1.030717000    |
| 1  | 2.364981000    | 2.166937000    | -0.537148000   |
| 6  | 1.034802000    | 1.011241000    | 2.433668000    |
| 1  | 0.164323000    | 1.202288000    | 3.063702000    |
|   | 1.909970000 | 1.347364000 | 2.994958000 |
|---|-------------|-------------|-------------|
|   | 1.140813000 | -0.063540000 | 2.259904000 |
|   | 0.763590000 | 3.262693000 | 3.588083000 |
|   | 0.824144000 | 3.902158000 | 0.552266000 |
|   | 1.551289000 | 3.588083000 | 2.115747000 |
|   | -0.187138000 | 3.453845000 | 1.930724000 |
|   | -0.998375000 | 2.136874000 | -1.242282000 |
|   | -1.925535000 | 1.371652000 | -2.185921000 |
|   | -1.405113000 | 0.578153000 | -2.715780000 |
|   | -2.330313000 | 2.071579000 | -2.920672000 |
|   | -2.765940000 | 0.914548000 | -1.499570000 |
|   | -1.869095000 | -3.976922000 | -0.661247000 |
|   | 0.706783000 | -1.034660000 | -1.886360000 |
|   | 2.830454000 | -1.926735000 | 0.630232000 |
|   | 3.096678000 | -1.287822000 | -0.233634000 |
|   | 3.079008000 | -2.953325000 | 0.278625000 |
|   | 3.768812000 | -1.603659000 | 1.779936000 |
|   | 3.597580000 | -2.231544000 | 2.642103000 |
|   | 3.654066000 | -0.565258000 | 2.094131000 |
|   | 4.814430000 | -1.763734000 | 1.509851000 |
|   | 1.792698000 | -3.731345000 | -1.721415000 |
|   | 1.930430000 | -5.070005000 | -0.587078000 |
|   | -3.132750000 | -3.383683000 | -0.088319000 |
|   | -3.120039000 | -2.296186000 | -0.138270000 |
|   | -3.983150000 | -3.738771000 | -0.668476000 |
|   | -3.304263000 | -3.685709000 | 0.944784000 |
|   | 0.540115000 | -4.247761000 | -0.680485000 |
|   | 0.463550000 | -4.060297000 | -1.752629000 |
|   | 1.440582000 | -3.748853000 | -0.331369000 |
|   | 0.626978000 | -5.736810000 | -0.407330000 |
|   | -0.237072000 | -6.293353000 | -0.767729000 |
|   | 0.748078000 | -5.950960000 | 0.654291000 |
|   | 1.501387000 | -6.141459000 | -0.914001000 |
First three frequencies

|    | 1          | 2          | 3          |
|----|------------|------------|------------|
| Frequencies | -537.7785  | 36.4810    | 49.7572    |
| Red. masses  | 2.1207     | 3.7039     | 4.8252     |
| Frc consts   | 0.3614     | 0.0029     | 0.0070     |
| IR Inten     | 2243.4448  | 0.7927     | 0.8197     |

Coordinates

|    |            |            |            |
|----|------------|------------|------------|
| 44 | -1.11208500| 0.68569100| -0.41296000|
| 1  | -1.94674300| 0.57983600| -1.79803800|
| 15 | -2.34432600| -1.05017600| 0.31396000|
| 8  | -3.02610100| 2.79351900| 0.51441400|
| 7  | 0.43804100 | 1.85015700| -1.68984300|
| 7  | 0.22541400 | -0.85578600| -1.02182400|
| 6  | -1.02852800| -2.34573700| 0.39358000|
| 6  | 0.02168000 | -2.13016800| -0.64348700|
| 6  | 0.81828100 | -3.14357900| -1.15975500|
| 1  | 0.64814300 | -4.16625600| -0.85288100|
| 6  | 1.82280700 | -2.82513900| -2.05744900|
| 1  | 2.43780200 | -3.60662500| -2.48444600|
| 6  | 2.05864600 | -1.49829700| -2.38017800|
| 1  | 2.86943300 | -1.21490300| -3.03774100|
| 6  | 1.25374800 | -0.52327700| -1.81444400|
| 6  | 1.58565000 | 0.93346900 | -1.87464600|
| 1  | 2.25344200 | 1.09352600 | -1.02093600|
| 1  | 2.14072400 | 1.16986800 | -2.78893700|
| 6  | -2.27461300| 1.98006300 | 0.15523700|
| 6  | -3.12688800| -1.09203900| 2.03129500|
| 6  | -2.24600500| -0.22954000| 2.93312500|
1   -2.640306000  -0.269745000  3.951494000
1   -1.209810000  -0.573440000  2.951565000
1   -2.529670000   0.811419000  2.612899000
6   -4.520702000  -0.468675000  1.998415000
1   -4.512612000   0.516665000  2.951565000
1   -5.258176000  -1.084835000  1.487431000
6   -3.181780000  -2.495023000  2.635777000
1   -3.770593000  -3.201248000  2.056708000
1   -4.512612000  -2.252967000  0.811419000
6   -3.573394000  -1.757930000 -0.948808000
6   -4.566906000  -0.678451000 -1.375372000
1   -5.214227000  -0.356197000 -0.562985000
1   -4.050156000   0.197596000 -1.764142000
1   -5.208204000  -1.072144000 -2.167004000
6   -4.329437000  -2.987875000 -0.452668000
1   -4.918263000  -3.397799000 -1.276488000
1   -3.658494000  -3.779624000 -0.117043000
1   -5.023569000  -2.764971000  0.354132000
6   -2.769774000  -2.185075000 -2.180131000
1   -2.142577000  -1.378294000 -2.558521000
1   -2.140492000  -3.052875000 -1.979206000
1   -3.463590000  -2.469455000 -2.973786000
6   -0.111869000   2.184950000  0.354132000
1   -0.439348000   1.239511000 -3.465086000
1   0.706387000  2.556628000  3.661916000
6   -1.245107000   3.176546000 -3.018999000
1   -2.054108000   2.839830000 -2.374037000
1   -0.927063000  4.164978000  2.689289000
6   -0.111869000   3.285925000 -4.027607000
6   0.870602000  3.056282000 -0.933917000
1   -0.024892000   3.637948000 -0.718389000
1   1.238310000   2.681614000  0.022457000
6   1.917513000   3.915067000 -1.612213000
1   2.193161000  4.740895000  0.958724000
6   2.828857000  3.356629000 -1.827147000
1   1.560504000  4.348578000  2.546247000
1   -1.403689000   3.370412000 -0.390670000
6   1.063726000   0.335509000  1.955537000
1   0.114399000   0.666156000  1.038847000
8   0.857467000   0.845060000  2.356311000
6   0.822514000  1.505235000  2.908706000
1   1.535671000  1.441224000  3.734151000
1   -0.180121000  1.460129000  3.322147000
7   2.323250000  0.565087000  1.214981000
1   2.859192000  1.285470000  1.684568000
6   3.144280000  -0.624355000  1.040829000
1   3.368278000  -1.110565000  1.998298000
1   2.560836000  -1.362410000  0.487284000
6   4.421799000  -0.296694000  0.303320000

S74
Ethylamine

Coordinates

Hydrogen

Frequency
IR Inten  --  0.0000

Coordinates

1  -3.519951000  0.215525000  0.000000000
1  -2.775939000  0.206181000  0.000000000

Acetaldehyde

|   |   |   |
|---|---|---|
|1  |A  |   |
|2  |A  |   |
|3  |A  |   |

Frequencies -- 154.3049  506.9440  767.3056
Red. masses -- 1.2367  2.4776  1.1213
Frc consta -- 0.0173  0.3752  0.3890
IR Inten -- 0.4429  11.7396  0.3559

Coordinates

|   |   |   |   |
|---|---|---|---|
|1  |3.494242000 0.601354000 -0.016792000
|6  |4.223765000 -0.700487000 0.003778000
|1  |2.547466000 0.518307000 -0.542768000
|1  |4.115023000 1.363965000 -0.489731000
|1  |3.321817000 0.943236000 1.004921000
|8  |3.829055000 -1.719751000 -0.492568000
|1  |5.206026000 -0.671724000 0.533159000

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