Supporting Information

Catalytic Oxidative Deamination by Water with H₂ Liberation

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General information

All reactions were performed under an atmosphere of purified nitrogen in an MBraun glovebox, or by using standard Schlenk techniques, unless otherwise noted. All commercially available reagents were used as received. 1,4-Dioxane was purified prior to use by refluxing and distilling over Na/benzophenone under an argon atmosphere. Water was purified on a Synergy UV Water Purification System, and was degassed prior to use by bubbling argon for at least 20 min. Complexes $[\text{Ru}]^1$, $[\text{Ru}]^2$, and $N$-alkyl acetamides$^3$ were synthesized according to reported procedures. GC–MS analysis was carried out on an Agilent Technologies 7820A chromatograph (flame ionization detector and thermal conductivity detector) equipped with a 5975 Series Mass Selective Detector, using helium as the carrier gas. Each of the conversions and yields were determined as an average of two runs, based on GC analysis using an Agilent Technologies 7890B chromatograph (flame ionization detector) with nitrogen as the carrier gas. Hydrogen gas was detected by GC analysis on an HP 6890 chromatograph (TCD detector) with nitrogen as the carrier gas. High resolution electrospray ionization mass spectrometry (HR-ESI-MS) was carried out on a Waters Xevo G2-XS QTof mass spectrometer at the Department of Chemical Research Support, Weizmann Institute of Science. NMR spectra were recorded using Bruker Advance III 300 MHz, Advance III 400 MHz, or Advance III HD-500 MHz spectrometers at 293 K. $^1$H NMR chemical shifts are referenced to the residual hydrogen signal of the deuterated solvent, and the $^{13}$C NMR chemical shifts are referenced to the $^{13}$C signal of the deuterated solvent. $^{31}$P NMR chemical shifts are reported relative to H$_3$PO$_4$, and referenced to an external sample of 85% aqueous phosphoric acid ($\delta = 0.0$ ppm). Abbreviations used in the description of the NMR data are as follows: Ar, aryl; br, broad; s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet.
Synthesis and characterization of complexes

Complex [Ru]-3: A THF solution of NaBEt₃H was prepared by adding 113 μl of 1.0 M NaBEt₃H (0.112 mmol) in toluene to 1.7 mL of THF. The afforded solution was added dropwise to a stirring suspension of 66.9 mg (0.111 mmol) of [Ru]-2 in 1.7 mL of THF. The resulting mixture was stirred at room temperature for 0.5 h, and the solvent was then removed under vacuum. The solid residue was washed twice with 3 mL of n-pentane to remove a dark impurity, and the remaining orange solids were extracted twice with 1.7 mL of benzene. The combined benzene extracts were filtered via a glass wool plug, and then frozen. The resulting solid solution was then placed under vacuum to remove the solvent, affording 60.5 mg (0.106 mmol; 96% yield) of [Ru]-3 as a flocculent orange powder. NMR data for this complex in C₆D₆ were reported previously.¹³¹P{¹H} NMR (162 MHz, dioxane-d₆): 75.63 (s). ¹H NMR (400 MHz, dioxane-d₆): 7.00 (d, 3JHH = 7.1 Hz, 2H, Ar-H), 6.87 (d, 3JHH = 7.2 Hz, 2H, Ar-H), 6.67 (t, 3JHH = 7.3 Hz, 2H, Ar-H), 3.62 (d, 2JHH = 14.2 Hz, 1H, dihydroacridine ArCH(H)Ar), 3.15 (d, 2JHH = 14.3 Hz, 1H, dihydroacridine ArCH(H)Ar), 2.96 (m, 4H, ArCH₂P), 2.38 (m, 2H, PCH(CH₃)₂), 1.56 (m, 2H, PCH(CH₃)₂), 1.33 (q, 3JHH = 6.8 Hz, 6H, PCH(CH₃)₂), 1.27 (q, 3JHH = 7.3 Hz, 6H, PCH(CH₃)₂), 0.72 (q, 3JHH = 7.2 Hz, 6H, PCH(CH₃)₂), -20.84 (t, 2JHH = 22.1 Hz, 1H, Ru-H).

Complex [Ru]-4: 4.4 mg (0.008 mmol) of [Ru]-3 were dissolved in 0.53 mL of dioxane-d₆. To the resulting solution were then added 8.7 mg of 9.6 wt% benzylamine (0.008 mmol) in dioxane-d₆. The color of the solution immediately changed from orange to brownish-yellow. ¹H and ³¹P NMR spectra of the resulting mixture indicated quantitative formation of [Ru]-4. ³¹P{¹H} NMR (162 MHz, dioxane-d₆): 76.39 (s). ¹H NMR (400 MHz, dioxane-d₆): 7.25 (m, 2H, benzylamine Ar₀₉₆₋ₓ-H), 7.18 (m, 1H, benzylamine Ar₃₆₋ₓ-H), 7.09 (d, 3JHH = 7.3 Hz, 2H, benzylamine Ar₉₋ₓ-H), 6.80 (d, 3JHH = 7.2 Hz, 4H, dihydroacridine Ar-H), 6.52 (t, 3JHH = 7.2 Hz, 2H, dihydroacridine Ar-H), 3.69 (t, 3JHH = 7.9 Hz, 2H, ArCH₂N), 3.64 (d, 2JHH = 16.2 Hz, 1H, dihydroacridine ArCH(H)Ar), 3.27 (d, 2JHH = 16.0 Hz, 1H, dihydroacridine ArCH(H)Ar), 3.04 (d, 2JHH = 11.8 Hz, 2H, ArCH(H)P), 2.97 (m, 2JHH = 11.9 Hz, 2H, ArCH(H)P), 2.53 (m, 2H, PCH(CH₃)₂), 2.13 (br s, 2H, NH₂), 1.49 (m, 2H, PCH(CH₃)₂), 1.37 (q, 3JHH = 7.0 Hz, 6H, PCH(CH₃)₂), 1.32 (q, 3JHH = 6.8 Hz, 6H, PCH(CH₃)₂), 1.19 (q, 3JHH = 7.5 Hz, 6H, PCH(CH₃)₂), 1.12 (q, 3JHH = 6.9 Hz, 6H, PCH(CH₃)₂), -15.02 (t, 2JHH = 25.0 Hz, 1H).
Ru-H). $^{13}$C $^1$H} (101 MHz, dioxane-$d_8$): 210.6 (t, $^2$J$_{PC}$ = 14.2 Hz, RuCO), 153.0 (t, $^3$J$_{PC}$ = 2.8 Hz, dihydroacridine C$_A$N(C$_A$), 143.8 (s, benzylamine C$_{ipso}$), 129.3 (s, benzylamine C$_{Ar-H}$), 128.5 (s, benzylamine C$_{Ar-H}$), 127.8 (s, benzylamine C$_{Ar-H}$), 127.6 (s, dihydroacridine C$_{Ar-H}$), 126.6 (s, dihydroacridine C$_{Ar-H}$), 126.3 (s, C$_{Ar-CH_2}$), 123.1 (s, C$_{Ar-CH_2}$), 117.6 (s, dihydroacridine C$_{Ar-H}$), 51.0 (br s, ArCH$_2$N), 36.4 (s, dihydroacridine ArCH$_2$Ar), 31.9 (vt, $^1$J$_{PC}$ + $^3$J$_{PC}$ = 21.3 Hz, ArCH$_2$P), 27.4 (vt, $^1$J$_{PC}$ + $^3$J$_{PC}$ = 29.7 Hz, PCH(CH$_3$)$_2$), 25.3 (vt, $^1$J$_{PC}$ + $^3$J$_{PC}$ = 11.6 Hz, PCH(CH$_3$)$_2$), 21.6 (s, PCH(CH$_3$)$_2$), 20.1 (vt, $^1$J$_{PC}$ + $^3$J$_{PC}$ = 5.7 Hz, PCH(CH$_3$)$_2$), 20.0 (s, PCH(CH$_3$)$_2$), 17.3 (s, PCH(CH$_3$)$_3$). The $^{13}$C $^1$H} NMR data were obtained from a DEPTQ experiment. Assignment of the $^1$H and $^{13}$C $^1$H} NMR signals was confirmed by $^1$H $^{31}$P}, $^1$H-$^1$H COSY, $^1$H-$^{13}$C HSQC and $^1$H-$^{13}$C HMBC experiments. The absolute configuration of the complex in dioxane-$d_8$ was corroborated by an $^1$H-$^1$H NOESY experiment. The relevant observed NOESY correlations are illustrated below:

**Complex [Ru]-5**: A solution of 5.3 mg (0.043 mmol) of benzoic acid in 0.57 mL of C$_6$H$_6$ was added to a stirring suspension containing 24.7 mg (0.043 mmol) of [Ru]-3 in 0.91 mL of C$_6$H$_6$. An immediate color change ensued, from dark orange to light orange-yellow. The afforded mixture was loaded into a pressure flask, and stirred a

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dihydroacridine $C_{ArC}\text{N}_{Ar}$), 134.1 (s, benzoate $C_{ipso}$), 131.9 (s, benzoate $C_{Ar-H}$), 130.0 (s, $C_{Ar\text{CH}_2C_{Ar}}$), 128.8 (s, benzoate $C_{Ar-H}$), 128.0 (s, benzoate $C_{Ar-H}$), 127.5 (s, dihydroacridine $C_{Ar-H}$), 126.5 (s, dihydroacridine $C_{Ar-H}$), 122.3 (s, $C_{Ar\text{CH}_2P}$), 118.7 (s, dihydroacridine $C_{Ar-H}$), 34.4 (s, dihydroacridine ArCH$_2$Ar), 29.8 (m, PCH(CH$_3$)$_2$), 28.4 (m, ArCH$_2$P), 26.3 (m, PCH(CH$_3$)$_2$), 20.7 (s, PCH(CH$_3$)$_2$), 19.8 (s, PCH(CH$_3$)$_2$), 19.1 (s, PCH(CH$_3$)$_2$), 19.0 (m, PCH(CH$_3$)$_2$). The $^{13}C\{^1H\}$ NMR data were obtained from a DEPTQ experiment. Assignment of the $^1H$ and $^{13}C\{^1H\}$ NMR signals was confirmed by $^1H\{^{31}P\}$, $^1H-^1H$ COSY, $^1H-^{13}C$ HSQC and $^1H-^{13}C$ HMBC experiments. HRMS (ESI) calculated for $C_{35}H_{46}NO_3P_2Ru$ [M+H]$^+$: 692.1996; found: 692.1981. $^{31}P\{^1H\}$ NMR (202 MHz, dioxane-$d_8$): 88.16 (s). $^1H$ NMR (500 MHz, dioxane-$d_8$): 7.51 (d, $^3J_{HH} = 7.7$ Hz, 2H, benzoate Ar-$H$), 7.39 (t, $^3J_{HH} = 7.5$ Hz, 1H, benzoate Ar-$H$), 7.23 (t, $^3J_{HH} = 7.7$ Hz, 2H, benzoate Ar-$H$), 6.87 (d, $^3J_{HH} = 7.3$ Hz, 2H, dihydroacridine Ar-$H$), 6.72 (d, $^3J_{HH} = 7.2$ Hz, 2H, dihydroacridine Ar-$H$), 6.57 (t, $^3J_{HH} = 7.4$ Hz, 2H, dihydroacridine Ar-$H$), 3.28 (d, $^2J_{HH} = 16.8$ Hz, 1H, dihydroacridine ArCHHA$\text{Ar}$), 3.16 (d, $^2J_{HH} = 16.8$ Hz, 1H, dihydroacridine ArCHHA$\text{Ar}$), 3.16 (m, 2H, ArCHHP), 2.69 (dd, $^2J_{HH} = 12.4$ Hz, $^2J_{PH} = 6.8$ Hz, 2H, ArCHHP), 2.39 (m, 2H, PCH(CH$_3$)$_2$), 1.89 (m, 2H, PCH(CH$_3$)$_2$), 1.50-1.43 (m, 18H, PCH(CH$_3$)$_2$), 1.39 (dd, $^2J_{PH} = 11.1$ Hz, $^3J_{HH} = 7.3$ Hz, 6H, PCH(CH$_3$)$_2$). The absolute configuration of the complex in dioxane-$d_8$ was corroborated by an $^1H-^1H$ NOESY experiment. The relevant observed NOESY correlation is illustrated below:
Synthesis and characterization of the organic products

**Butyric acid (2a):** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), *n*-butylamine (49 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a yellow oil in 95% yield (41.7 mg).

**1H NMR (400 MHz, CDCl₃):** δ 10.62 (br s, 1H), 2.35 (t, *J* = 7.4 Hz, 2H), 1.68 (h, *J* = 7.4 Hz, 2H), 0.98 (t, *J* = 7.4 Hz, 3H).

**13C{1H} NMR (101 MHz, CDCl₃):** δ 180.0, 35.9, 18.1, 13.6.

**Determination of H₂ and NH₃ generated during the reaction:** After cooling the reaction mixture to room temperature, the headspace was analyzed by GC with a TCD detector, using N₂ as the carrier gas. As shown in Figure S1, only H₂ was detected by GC while no other gases were present in detectable amounts. In a parallel experiment, the evolved gas was quantified by displacing water in an inverted graduated cylinder filled with water. About 24 mL of gas were collected, amounting to 98% yield based on full conversion of *n*-butylamine to butyrate. The reaction mixture was then acidified with 4 M HCl (3.0 mL). As shown in Figure S2, NH₄⁺ was detected as a characteristic triplet at 7.10 ppm in the ¹H NMR spectrum of the reaction mixture. Following similar procedures and analytical methods, H₂ and NH₄⁺ were also detected upon the oxidative deamination of other amines and amides.

**Figure S1.** GC analysis of the gas evolved during the oxidative deamination of *n*-butylamine

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Hexanoic acid (2b): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), \(n\)-hexylamine (57 \(\mu\)L, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na\(_2\)SO\(_4\) and all volatiles were removed under vacuum. The product was obtained as a yellow oil in 86% yield (50.0 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 11.01 (br s, 1H), 2.35 (t, \(J = 7.5\) Hz, 2H), 1.71–1.59 (m, 2H), 1.41–1.23 (m, 4H), 0.91 (t, \(J = 6.8\) Hz, 3H). \(^{13}\)C\(\{^1\text{H}\}\) NMR (126 MHz, CDCl\(_3\)): \(\delta\) 180.4, 34.1, 31.2, 24.3, 22.3, 13.8.

Octanoic acid (2c): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), \(n\)-octylamine (82 \(\mu\)L, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na\(_2\)SO\(_4\) and all volatiles were removed under vacuum. The product was obtained as a yellow oil in 98% yield (70.7 mg). \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) 11.33 (br s, 1H), 2.34 (t, \(J = 7.5\) Hz, 2H), 1.71–1.59 (m, 2H), 1.41–1.23 (m, 4H), 0.91 (t, \(J = 6.8\) Hz, 3H). \(^{13}\)C\(\{^1\text{H}\}\) NMR (126 MHz, CDCl\(_3\)): \(\delta\) 180.4, 34.1, 31.2, 24.3, 22.3, 13.8.
6,6-Dimethylbicyclo[3.1.1]heptane-2-carboxylic acid (2d): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), cis-myrtanylamine (84 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a brown oil in 71% yield (52.7 mg).

1H NMR (400 MHz, CDCl₃): δ 10.98 (brs, 1H), 2.94 (t, J = 8.8 Hz, 1H), 2.23 – 2.03 (m, 3H), 1.93 – 1.82 (m, 3H), 1.76 (td, J = 8.7, 4.6 Hz, 1H), 1.54 (d, J = 10.0 Hz, 1H), 1.24 (s, 3H), 0.88 (s, 3H).

13C{1H} NMR (101 MHz, CDCl₃): δ 183.0, 43.7, 41.2, 40.1, 39.2, 26.4, 24.2, 23.7, 20.3, 16.6.

5-Norbornane-2-carboxylic acid (2e): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 5-norbornene-2-methylamine (62 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as an orange oil in 65% yield (49.4 mg, a mixture of two stereoisomers). 1H NMR (400 MHz, CDCl₃): δ 9.47 (brs, 1H), 2.57 – 2.52 (m, 1H), 2.36 (dd, J = 9.2, 5.3 Hz, 1H), 2.33 – 2.25 (m, 1H), 1.88 – 1.79 (m, 1H), 1.57 – 1.43 (m, 4H), 1.30 – 1.23 (m, 1H), 1.22 – 1.16 (m, 2H). 13C{1H} NMR (101 MHz, CDCl₃): δ 182.3, 46.3, 40.9, 36.5, 36.0, 34.0, 29.4, 28.6.

2-Methoxyacetate (2f): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (6.0 mg, 0.010 mmol), NaOH (40.0 mg, 1.0 mmol), 2-methoxyethylamine (43 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was
sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. The reaction mixture was analyzed by \(^1\)H NMR spectroscopy with a long delay time (10 s), using pyridine as an internal standard (quantitative yield).

2-Phenylacetic acid (2g):

A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 2-phenethylamine (63 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a yellow solid in 98% yield (66.7 mg). \(^1\)H NMR (500 MHz, CDCl₃): \(\delta\) 8.70 (b s, 1H), 7.40 – 7.22 (m, 5H), 3.65 (s, 2H).

\(^{13}\)C\{\(^1\)H\} NMR (126 MHz, CDCl₃): \(\delta\) 177.4, 133.2, 129.4, 128.6, 127.3, 41.0.

2-(1H-indol-3-yl)acetic acid (2h):

A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), tryptamine (73 mg, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a brown solid in 75% yield (65.7 mg). \(^1\)H NMR (400 MHz, DMSO-d₆): \(\delta\) 12.09 (br s, 1H), 10.89 (s, 1H), 7.49 (d, \(J = 7.9\) Hz, 1H), 7.34 (d, \(J = 8.1\) Hz, 1H), 7.24-7.19 (m, 1H), 7.07 (t, \(J = 7.5\) Hz, 1H), 6.97 (t, \(J = 7.4\) Hz, 1H), 3.63 (s, 2H). \(^{13}\)C\{\(^1\)H\} NMR (101 MHz, DMSO-d₆): \(\delta\) 173.2, 136.1, 127.2, 123.9, 121.0, 118.6, 118.4, 111.4, 107.7, 31.0.
Benzoic acid (2i): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), benzylamine (55 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a pale-yellow solid in 98% yield (59.7 mg).

\[
\begin{align*}
\text{O} & \quad \text{MeO} \\
\text{OH} & \quad \text{H}
\end{align*}
\]

1H NMR (400 MHz, DMSO-d₆): δ 12.72 (br s, 1H), 7.95 (d, J = 7.4 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H). 13C {1H} NMR (101 MHz, DMSO-d₆): δ 167.3, 132.9, 130.8, 129.3, 128.6. In two control experiments, excess Hg (230 mg) or NEt₃ (70 μL) was added at the beginning of the reaction. Following the same reaction procedure as described above, the product, benzoic acid, was isolated in 97% yield in both cases (59.0 and 59.4 mg, respectively).

4-Methoxybenzoic acid (2j): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 4-methoxybenzylamine (49 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a pale-yellow solid in 95% yield (72.1 mg).

\[
\begin{align*}
\text{O} & \quad \text{MeO} \\
\text{OH} & \quad \text{H}
\end{align*}
\]

1H NMR (500 MHz, DMSO-d₆): δ 12.55 (br s, 1H), 7.90 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.9 Hz, 2H), 3.83 (s, 3H). 13C {1H} NMR (126 MHz, DMSO-d₆): δ 167.1, 162.9, 131.4, 123.1, 113.9, 55.5.

4-(Trifluoromethyl)benzoic acid (2k): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 4-(trifluoromethyl)benzylamine (71 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath...
temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a pale-yellow solid in 87% yield (82.6 mg). ¹H NMR (400 MHz, DMSO-d₆): δ 8.13 (d, J = 8.1 Hz, 1H), 7.87 (d, J = 8.3 Hz, 1H). ¹³C{¹H} NMR (101 MHz, DMSO-d₆): δ 166.3, 135.1, 132.4 (q, J_C-F = 31.9 Hz), 130.2, 125.7 (q, J_C-F = 3.8 Hz), 123.9 (q, J_C-F = 273.5 Hz).

4-Chlorobenzoic acid (2l): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 4-chlorobenzylamine (61 µL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a yellow solid in 93% yield (71.7 mg). ¹H NMR (500 MHz, DMSO-d₆): δ 13.16 (br s, 1H), 7.95 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 8.5 Hz, 2H). ¹³C{¹H} NMR (126 MHz, DMSO-d₆): δ 166.5, 137.9, 131.2, 129.8, 128.8.

4-aminobenzoate (2m): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 4-(aminomethyl)aniline (57 µL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. The reaction mixture was analyzed by ¹H NMR spectroscopy with a long delay time (10 s), using pyridine as an internal standard (98% yield).
Furan-2-carboxylic acid (2n): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex \([\text{Ru-2]}\) (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 2-aminomethylfuran (46 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all volatiles were removed under vacuum. The product was obtained as a yellow solid in 81% yield (45.4 mg). ¹H NMR (400 MHz, DMSO-d₆): δ 12.96 (br s, 1H), 7.91 (s, 1H), 7.20 (s, 1H), 6.64 (s, 1H). ¹³C{¹H} NMR (101 MHz, DMSO-d₆): δ 159.3, 147.1, 144.9, 117.7, 112.1.

Nicotinate (2o): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex \([\text{Ru-2]}\) (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 3-aminomethylpyridine (51 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. The reaction mixture was analyzed by ¹H NMR with long a delay time (10 s), using pyridine as an internal standard (89% yield).

Isophthalic acid (2p): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex \([\text{Ru-2]}\) (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 1,3-phenylenedimethanamine (33 μL, 0.25 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na₂SO₄ and all
Volatile molecules were removed under vacuum. The product was obtained as a pale-yellow solid in 99% yield (41.1 mg). $^1$H NMR (500 MHz, DMSO-$d_6$): $\delta$ 13.23 (br s, 2H), 8.48 (t, $J = 1.6$ Hz, 1H), 8.16 (dd, $J = 7.7$, 1.7 Hz, 2H), 7.64 (t, $J = 7.7$ Hz, 1H). $^{13}$C($^1$H) NMR (126 MHz, DMSO-$d_6$): $\delta$ 166.7, 133.5, 131.3, 130.0, 129.2.

**Adipic acid (2q):** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (6.0 mg, 0.010 mmol), NaOH (40.0 mg, 1.0 mmol), 1,6-hexanediamine (29.0 mg, 0.25 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na$_2$SO$_4$ and all volatile molecules were removed under vacuum. The product was obtained as a pale-yellow solid in 65% yield (23.8 mg). The same product was obtained from the oxidative deamination of hexamethylenimine (50% yield) or caprolactam (68% yield). $^1$H NMR (500 MHz, DMSO-$d_6$): $\delta$ 11.96 (br s, 2H), 2.20 (t, $J = 6.6$ Hz, 4H), 1.53 – 1.45 (m, 4H). $^{13}$C($^1$H) NMR (126 MHz, DMSO-$d_6$): $\delta$ 174.4, 33.5, 24.1.

**Glutaric acid (2r):** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), 5-amino-1-pentanol (25.8 mg, 0.25 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na$_2$SO$_4$ and all volatile molecules were removed under vacuum. The product was obtained as a pale-yellow solid in 52% yield (17.3 mg). The same product could be obtained from the oxidative deamination of piperidine (30% yield) or δ-valerolactam (59% yield). $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 12.08 (br s, 2H), 2.20 (t, $J = 6.6$ Hz, 4H), 1.53 – 1.45 (m, 4H). $^{13}$C($^1$H) NMR (101 MHz, DMSO-$d_6$): $\delta$ 174.1, 32.8, 20.0.

**Octan-2-one (3w):** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), 2-aminoocetane (84 μL, 0.50 mmol), 2.0 mL of
dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (94% yield).

Pentan-3-one (3x):11 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), 3-aminopentane (58 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (74% yield).

Cyclopentanone (3y):12 A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), cyclopentanamine (49 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (84% yield).

Cyclohexanone (3z):12 A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), cyclohexanamine (57 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (81% yield).
Cycloheptanone (3aa): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), cycloheptanamine (64 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (90% yield).

Cyclooctanone (3ab): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), cyclooctanamine (68 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (73% yield).

Acetophenone (3ac): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), 1-phenylethylamine (64 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (86% yield).

Acetophenone (3ad): A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), 1-(4-methoxyphenyl)ethylamine (74 μL, 0.50 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture...
was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (98% yield).

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\text{1-(Naphthalen-1-yl)ethan-1-one (3ae):}^{13}
\]

A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 (3.0 mg, 0.0050 mmol), 1-(1-naphthyl)ethylamine (40 μL, 0.25 mmol), 2.0 mL of dioxane, and 0.50 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Water (4.0 mL) was then added to the reaction mixture and ethyl acetate (3 × 4.0 mL) was used to extract the organic compounds. The combined organic extracts were analyzed by GC (FID detector), using mesitylene as an internal standard (59% yield).

**Procedures for mechanistic experiments**

**Catalytic deamination of benzylamine in the absence of base:** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 or [Ru]-3 (0.0050 mmol), benzylamine (55 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts were analyzed by GC (FID detector) using mesitylene as an internal standard to determine the yields of benzyl alcohol and N-benzylidenebenzylamine. In the next step, the aqueous phase was acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were also analyzed by GC (FID detector) using mesitylene as an internal standard to determine the yield of benzoic acid.

**Effect of different bases on the catalytic deamination of benzylamine:** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-2 or [Ru]-3 (0.0050 mmol), benzylamine (55 μL, 0.50 mmol), base (1.0 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled to room temperature.
Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts were analyzed by GC (FID detector) using mesitylene as an internal standard to determine the yields of benzyl alcohol and \(N\)-benzylidenebenzylamine. In the next step, the aqueous phase was acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were also analyzed by GC (FID detector) using mesitylene as an internal standard to determine the yield of benzoic acid. The reaction results with the bases including \(\text{NEt}_3\), \(\text{Na}_2\text{CO}_3\), \(\text{K}_3\text{PO}_4\) and \(\text{NaOH}\) are shown in Table S1.

**Table S1. Effect of Different Bases on the Catalytic Oxidative Deamination of Benzylamine**

| entry | base           | yield (%) | 2i | 4i | 6i |
|-------|----------------|-----------|----|----|----|
| 1     | none           |           | 24 | 50 | 8  |
| 2     | \(\text{NEt}_3\) |           | 21 | 47 | 3  |
| 3     | \(\text{Na}_2\text{CO}_3\) |       | 16 | 50 | 6  |
| 4     | \(\text{K}_3\text{PO}_4\) |         | 74 | 20 | n.d. |
| 5     | \(\text{NaOH}\)  |           | 99 | n.d. | n.d. |

**Catalytic oxidation of benzyl alcohol by water:** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex \([\text{Ru}]\)-3 (2.9 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), benzyl alcohol (52 \(\mu\)L, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over \(\text{Na}_2\text{SO}_4\) and all volatiles were removed under vacuum. The product, benzoic acid, was obtained as a pale-yellow solid in 99% yield (60.7 mg).

**Catalytic oxidative deamination of \(N\)-benzylidenebenzylamine by water:** A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex \([\text{Ru}]\)-3 (2.9 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), \(N\)-benzylidenebenzylamine (47 \(\mu\)L, 0.25 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over \(\text{Na}_2\text{SO}_4\) and all volatiles were removed under vacuum. The product, benzoic acid, was obtained as a pale-yellow solid in 96% yield (58.5 mg).
Catalytic oxidation of benzaldehyde by water: A 50 mL thick-glass pressure tube, equipped with a stirring bar, was charged with complex [Ru]-3 (2.9 mg, 0.0050 mmol), NaOH (40.0 mg, 1.0 mmol), benzaldehyde (51 μL, 0.50 mmol), 2.0 mL of dioxane, and 2.0 mL of water. The tube was sealed, and the reaction mixture was stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). After 48 h, the reaction mixture was cooled down to room temperature and the generated gas was carefully released in a hood. Saturated brine (5.0 mL) was then added to the reaction mixture, and the mixture was extracted with ethyl acetate (3 × 5.0 mL). The aqueous phase was then acidified with 4 M HCl (3.0 mL) and extracted with ethyl acetate (3 × 5.0 mL). The combined organic extracts from the acidified aqueous phase were dried over Na$_2$SO$_4$ and all volatiles were removed under vacuum. The product, benzoic acid, was obtained as a pale-yellow solid in 99% yield (60.7 mg).

Determination of the kinetic profile of benzylamine dehydrogenation: A series of 50 mL thick-glass pressure tubes, equipped with a stirring bar, was charged with complex [Ru]-3 (2.9 mg, 0.0050 mmol), benzylamine (55 μL, 0.50 mmol), water (18 μL, 0.50 mmol), and 2.0 mL of dioxane. An additional series of pressure tubes was set up as described above, but in the absence of water. All tubes were sealed, and the reaction mixtures were then stirred and heated at 150 °C (silicon oil bath temperature, solvent reflux). The tubes were removed from the heating bath at different designated time intervals, i.e., after 3, 6, 12, 18 and 24 h. After cooling to room temperature, the reaction mixtures were then subjected to GC analysis, using biphenyl as the internal standard.
Copies of NMR Spectra

$^{31}$P($^1$H) NMR (162 MHz, dioxane-$d_6$)

$^1$H NMR (400 MHz, dioxane-$d_6$)
$^{13}$C$^{1}H$ DEPTQ NMR (101 MHz, dioxane-$d_{8}$)

$^{1}H$-$^{1}H$ COSY NMR (400 MHz, dioxane-$d_{8}$)
$^1$H-$^{13}$C HSQC NMR (400 MHz, dioxane-$d_8$)

$^1$H-$^{13}$C HMBC NMR (400 MHz, dioxane-$d_8$)
$^1$H-$^1$H NOESY NMR (400 MHz, dioxane-d$_8$)

$^{31}$P($^1$H) NMR (162 MHz, C$_6$D$_6$)
$^1$H NMR (400 MHz, C$_6$D$_6$)

$^{13}$C($^1$H) DEPTQ NMR (101 MHz, C$_6$D$_6$)
$^1$H-$^1$H COSY NMR (400 MHz, C$_6$D$_6$)

$^1$H-$^{13}$C HSQC NMR (400 MHz, C$_6$D$_6$)
$^1$H-$^{13}$C HMBC NMR (400 MHz, C$_6$D$_6$)

$^{31}$P{$^1$H} NMR (202 MHz, dioxane-$d_8$)
$^1$H NMR (500 MHz, dioxane-$d_8$)

$^1$H-$^1$H NOESY NMR (500 MHz, dioxane-$d_8$)
\[ ^1\text{H NMR} (400 \text{ MHz, CDCl}_3) \]

\[ ^{13}\text{C NMR} (101 \text{ MHz, CDCl}_3) \]
$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^{1}$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)
2h

$^1$H NMR (400 MHz, DMSO-$d_6$)

$^{13}$C NMR (101 MHz, DMSO-$d_6$)
$^1$H NMR (400 MHz, DMSO-$d_6$)

$^{13}$C NMR (101 MHz, DMSO-$d_6$)
$^1$H NMR (500 MHz, DMSO-$d_6$)

$^{13}$C NMR (126 MHz, DMSO-$d_6$)

S35
$^1$H NMR (400 MHz, DMSO-$d_6$)

$^{13}$C NMR (101 MHz, DMSO-$d_6$)
$^1$H NMR (500 MHz, DMSO-$d_6$)

$^{13}$C NMR (126 MHz, DMSO-$d_6$)
$^1$H NMR (400 MHz, DMSO-$d_6$)

$^{13}$C NMR (101 MHz, DMSO-$d_6$)
$^1$H NMR (500 MHz, DMSO-$d_6$)

$^{13}$C NMR (126 MHz, DMSO-$d_6$)
$^1$H NMR (500 MHz, DMSO-$d_6$)

$^{13}$C NMR (126 MHz, DMSO-$d_6$)

COOH

COOH
$^1$H NMR (400 MHz, DMSO-$d_6$)

\[ \text{COOH} \]
\[ \text{COOH} \]

$^{13}$C NMR (101 MHz, DMSO-$d_6$)
Crystallographic analysis of [Ru]-5

Crystals of [Ru]-5 were grown from a saturated pentane solution at -30 °C. Diffraction data for one of these crystals were collected at 100 K with Cu Kα radiation (λ = 1.54184 Å), on a Rigaku XtaLab Pro diffractometer, equipped with microfocus and a Dectris Pilatus 200K detector. The structure was solved by direct methods using 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. Crystallographic data and refinement parameters are summarized in Table S2.

Table S2. Crystallographic data for complex [Ru]-5

| Property                        | Value                                      |
|---------------------------------|--------------------------------------------|
| CCDC number                     | 2023878                                    |
| Empirical formula               | 2C₃H₄NO₃P₂Ru+C₃H₁₂                         |
| Crystal dimensions (mm)         | 0.039 x 0.028 x 0.024                      |
| Formula weight (g/mol)          | 1453.60                                    |
| T (K)                           | 100(2)                                     |
| Wavelength (Å)                  | 1.54184                                    |
| Crystal system                  | Monoclinic                                 |
| Space group                     | P2₁/n                                     |
| a (Å)                           | 25.7295(3)                                 |
| b (Å)                           | 11.2014(1)                                 |
| c (Å)                           | 25.9806(3)                                 |
| α (°)                           | 90                                         |
| β (°)                           | 109.322(1)                                 |
| γ (°)                           | 90                                         |
| Volume (Å³)                     | 7066.02(14)                                |
| Z                               | 4                                          |
| ρcal (mg/m³)                    | 1.366                                      |
| μ (mm⁻¹)                        | 4.727                                      |
Figure S3. X-ray crystal structure of [Ru]-5 (thermal ellipsoids set at 50% probability level, isopropyl groups are presented as wireframe, and hydrogen atoms are omitted for clarity). Selected bond distances (Å) and angles (°) for [Ru]-5: Ru1-N1 2.163(2), Ru1-C35 1.833(3), Ru1-O2 2.2248(18), Ru1-O3 2.1673(18), Ru1-P1 2.2936(7), Ru1-P2 2.2941(7), O2-C28 1.271(3), O3-C28 1.267(3), N1-Ru1-C35 177.17(10), P1-Ru1-P2 106.27(2), O2-Ru1-O3 60.07(7), P1-Ru1-O2 151.68(5), P2-Ru1-O3 159.79(5), P1-Ru1-N1 87.92(6).
Computational details

All geometries were optimized using Truhlar’s M06-L functional, the triple-ξ def2-TZVP basis set and W06 density fitting to increase computational efficiency, as well as Grimme’s D3(0) empirical dispersion correction. To take the influence of the solvent into account, optimizations were performed with the integral equation formalism variant (IEFPCM) of the PCM model in the SMD variation of Truhlar and co-workers, with a 1:1 water/dioxane mixture (\( \epsilon = 40.28245 \), \( \epsilon_{\text{inf}} = 1.89979 \)). Frequency calculations at this level of theory at 423.15K 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 including dispersion correction, together with the triple-ξ def2-TZVPP basis set and the corresponding auxiliary basis sets, def2/J and def2-TZVPP/C for RIJCOSX density fitting. The single point calculations include the same solvation (SMD) approach as described above in the optimizations. Gibbs free energies were computed by adding the free energy correction term from the frequency calculation to the single point energy according to:

\[
G_{\omega \text{B97M-V SMD}} = E_{\omega \text{B97M-V elSMD}} + G_{\text{corr M06-L freq SMD}}
\]

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 at 423.15K), with the exception of \( \text{H}_2 \) (maintained at 1 atm standard state) and water (1 atm to 27.75M at 423.15K). Optimizations and frequency calculations were done using the Gaussian 16 software suite in the C.01 revision. Single point calculations were performed using the ORCA Software in the 4.2.1 release.

Free energy diagram:
Energy values (Hartrees) and imaginary frequencies (cm⁻¹):

|                | $E^\text{M06-}^{au}$ | $G^\text{o} \text{ freq/SMD}$ | Imaginary Frequency |
|----------------|-----------------------|-------------------------------|---------------------|
|                | $el/SMD$              | (1 atm, 423.15K)              |                     |
| **mer-[Ru]-3** | -1999.26270290704     | 0.51485                       |                     |
| **fac-[Ru]-3** | -1999.25112921153     | 0.518434                      |                     |
| INT1           | -2075.72182197317     | 0.539052                      |                     |
| INT2           | -2074.52002276128     | 0.521987                      |                     |
| INT3           | -2401.46478513765     | 0.657525                      |                     |
| INT4           | -2401.44162146400     | 0.652585                      |                     |
| INT5 INT6 INT7 | -2324.97870410119     | 0.633346                      |                     |
| TS1            | -2075.68455030215     | 0.539836 -1162.3272           |                     |
| TS2            | -2326.13221735081     | 0.643038 -895.8696            |                     |
| TS3            | -2401.44248623527     | 0.653345 -804.0563            |                     |
| TS4            | -2324.97234687098     | 0.628221 -561.2405            |                     |
| Water          | -76.445699461786      | -0.005837                     |                     |
| 1i             | -326.898833228635     | 0.096054                      |                     |
| 1-Phenylethane-1-imine | -325.692951307968     | 0.074648                      |                     |
| Hydrogen       | -1.158892721333       | -0.008092                     |                     |

Atomic coordinates:

**mer-[Ru]-3:**

|          | $x$       | $y$       | $z$       |
|----------|-----------|-----------|-----------|
| Ru       | -0.275616000 | 6.318234000 | 1.352914000 |
| P        | -1.852198000 | 7.542998000 | 0.151635000 |
| P        | 1.644530000  | 5.957582000 | 2.632845000 |
| O        | -2.158425000 | 5.645525000 | 3.557758000 |
| N        | 0.963442000  | 6.116792000 | -0.511800000 |
| C        | -1.409897000 | 5.968689000 | 2.718797000 |
| C        | -1.530622000 | 10.154854000 | 1.159965000 |
| C        | -3.211069000 | 8.703682000 | 2.312735000 |
| C        | -2.554897000 | 9.044569000 | 0.984325000 |
| C        | -4.087612000 | 7.513292000 | -1.618629000 |
| C        | -3.086250000 | 5.295539000 | -0.976686000 |
| C        | -3.369399000 | 6.725305000 | -0.535310000 |
| C        | 3.519141000  | 4.195581000 | 3.854920000 |
| C        | 1.189336000  | 3.304220000 | 3.412228000 |
| C        | 2.293337000  | 4.249900000 | 2.958360000 |
| C        | 0.983048000  | 6.279110000 | 5.358107000 |
| C        | 1.539703000  | 8.356863000 | 4.088920000 |
| C        | 1.822403000  | 6.869653000 | 4.236674000 |
| Atomic Symbol | Atomic Position | Atomic Position | Atomic Position | Atomic Position | Atomic Position | Atomic Position | Atomic Position | Atomic Position | Atomic Position | Atomic Position |
|---------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C             | 0.359542000     | 6.130090000     | -1.779943000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 2.214415000     | 5.480352000     | -0.487752000    |                 |                 |                 |                 |                 |                 |                 |
| C             | -0.914746000    | 8.258391000     | -1.253404000    |                 |                 |                 |                 |                 |                 |                 |
| C             | -0.487422000    | 7.186822000     | -2.195478000    |                 |                 |                 |                 |                 |                 |                 |
| C             | -0.977003000    | 7.211985000     | -3.498630000    |                 |                 |                 |                 |                 |                 |                 |
| C             | -0.681802000    | 6.219085000     | -4.419015000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 0.106319000     | 5.155105000     | -4.007581000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 0.604156000     | 5.098901000     | -2.715103000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 1.396702000     | 3.935563000     | -2.226371000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 2.525228000     | 4.443749000     | -1.396359000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 3.797952000     | 3.899087000     | -1.471741000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 4.803698000     | 4.324411000     | -0.616945000    |                 |                 |                 |                 |                 |                 |                 |
| C             | 4.492700000     | 5.277987000     | 0.339656000     |                 |                 |                 |                 |                 |                 |                 |
| C             | 3.228264000     | 5.853911000     | 0.430176000     |                 |                 |                 |                 |                 |                 |                 |
| C             | 2.939287000     | 6.747544000     | 1.584907000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -0.675069000    | 9.822434000     | 1.751698000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -1.155102000    | 10.534585000    | 0.211360000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -1.984433000    | 10.993706000    | 1.690272000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -3.767662000    | 9.564634000     | 2.686359000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -3.908337000    | 7.868777000     | 2.240857000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -2.462046000    | 8.448165000     | 3.063586000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -3.327281000    | 9.402446000     | 0.296244000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -5.033609000    | 7.030584000     | -1.870997000    |                 |                 |                 |                 |                 |                 |                 |
| H             | -4.315941000    | 8.535370000     | -1.318224000    |                 |                 |                 |                 |                 |                 |                 |
| H             | -3.493480000    | 7.557833000     | -2.531805000    |                 |                 |                 |                 |                 |                 |                 |
| H             | -2.499928000    | 5.268850000     | -1.895916000    |                 |                 |                 |                 |                 |                 |                 |
| H             | -2.538346000    | 4.737464000     | -0.214624000    |                 |                 |                 |                 |                 |                 |                 |
| H             | -4.020576000    | 4.766406000     | -1.171481000    |                 |                 |                 |                 |                 |                 |                 |
| H             | -4.017091000    | 6.677002000     | 0.348105000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 3.943393000     | 3.189689000     | 3.853964000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 4.300768000     | 4.880885000     | 3.525001000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 3.275274000     | 4.441458000     | 4.889246000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 0.805590000     | 3.553576000     | 4.401670000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 0.346549000     | 3.313810000     | 2.719353000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 1.566859000     | 2.281453000     | 3.460809000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 2.592814000     | 3.930631000     | 1.954596000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -0.079381000    | 6.296943000     | 5.112387000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 1.256716000     | 5.252331000     | 5.593657000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 1.114806000     | 6.866980000     | 6.268299000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 1.843267000     | 8.879925000     | 4.997343000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 2.071817000     | 8.812707000     | 3.254112000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 0.473898000     | 8.542269000     | 3.948262000     |                 |                 |                 |                 |                 |                 |                 |
| H             | 2.881151000     | 6.749003000     | 4.489637000     |                 |                 |                 |                 |                 |                 |                 |
| H             | -0.056869000    | 8.754164000     | -0.789686000    |                 |                 |                 |                 |                 |                 |                 |

S46
|  | X     | Y     | Z     |
|---|-------|-------|-------|
| H | -1.502882000 | 9.019243000 | -1.770660000 |
| H | -1.603426000 | 8.048478000 | -3.788814000 |
| H | -1.066874000 | 6.270106000 | -5.429367000 |
| H | 0.335301000  | 4.342648000 | -4.689175000 |
| H | 0.751680000  | 3.297854000 | -1.601019000 |
| H | 1.745511000  | 3.308554000 | -3.047151000 |
| H | 3.987254000  | 3.117181000 | -2.199672000 |
| H | 5.799462000  | 3.903934000 | -0.674828000 |
| H | 5.245577000  | 5.593877000 | 1.053788000  |
| H | 3.846624000  | 6.945354000 | 2.158972000  |
| H | 2.516502000  | 7.707458000 | 1.277351000  |
| H | -0.050909000 | 7.749587000 | 1.942729000  |

fac-[Ru]-3:

|  | X     | Y     | Z     |
|---|-------|-------|-------|
| H | 0.698609000 | 8.624298000 | 5.363443000 |
| P | -2.356218000 | 7.714541000 | 2.806985000 |
| P | 0.486103000  | 6.145084000 | 4.963616000 |
| O | -2.304538000 | 7.829335000 | 6.892610000 |
| N | 0.747745000  | 8.356968000 | 2.717657000 |
| C | -1.576282000 | 7.892267000 | 1.149925000 |
| H | -0.916678000 | 7.025929000 | 1.048764000 |
| H | -2.338242000 | 7.825471000 | 0.370669000 |
| C | -0.784789000 | 9.148896000 | 1.015786000 |
| C | -1.151379000 | 10.123653000 | 0.093424000 |
| H | -2.051912000 | 9.969819000 | -0.492303000 |
| C | -0.368983000 | 11.250637000 | -0.117225000 |
| H | -0.661165000 | 11.990772000 | -0.851266000 |
| C | 0.802375000  | 11.406170000 | 0.614359000 |
| H | 1.433561000  | 12.274223000 | 0.454186000 |
| C | 1.174066000  | 10.474229000 | 1.571942000 |
| C | 0.377327000  | 9.333574000 | 1.799740000 |
| C | 2.393589000  | 10.638753000 | 2.427720000 |
| H | 3.119453000  | 11.306833000 | 1.961270000 |
| H | 2.102150000  | 11.129162000 | 3.369432000 |
| C | 3.000070000  | 9.308167000 | 2.756240000 |
| C | 4.360752000  | 9.125231000 | 2.954835000 |
| H | 5.033113000  | 9.962257000 | 2.796388000 |
| C | 4.860105000  | 7.901061000 | 3.384371000 |
| H | 5.921997000  | 7.768422000 | 3.548067000 |
| C | 3.979898000  | 6.849828000 | 3.607206000 |
| H | 4.355966000  | 5.888363000 | 3.940990000 |
| C | 2.614555000  | 6.992146000 | 3.384587000 |
| C | 2.108228000  | 8.237363000 | 2.953100000 |
| C | 1.676817000  | 5.849070000 | 3.590402000 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 2.22906600 | 4.92909100 | 3.78371500 |
| H    | 1.05434700 | 5.68695200 | 2.70491300 |
| C    | -3.44391600| 6.22986200 | 2.59227800 |
| H    | -4.23232700| 6.54279500 | 1.90276500 |
| C    | -4.08865900| 5.83926600 | 3.91305400 |
| H    | -3.34285800| 5.55839100 | 4.65847900 |
| H    | -4.75325000| 4.98499200 | 3.77373700 |
| H    | -4.68165400| 6.65178500 | 4.33339400 |
| C    | -2.69524500| 5.07541400 | 1.93806900 |
| H    | -2.49194500| 5.26988300 | 0.88621900 |
| H    | -3.29310700| 4.16422800 | 1.99295700 |
| H    | -1.73850000| 4.86602200 | 2.41897800 |
| C    | -3.50176900| 9.18367500 | 2.82295400 |
| H    | -2.84896200| 9.96966500 | 2.42659600 |
| C    | -3.92281700| 9.60688200 | 4.22148400 |
| H    | -4.49466700| 8.83164200 | 4.73270300 |
| H    | -4.55552600| 10.49481500| 4.16810600 |
| H    | -3.06330000| 9.85098200 | 4.84512300 |
| C    | -4.69792000| 9.05658900 | 1.89342600 |
| H    | -4.42098700| 8.72489500 | 0.89232200 |
| H    | -5.19412700| 10.02337000| 1.79165900 |
| H    | -5.43629900| 8.35586800 | 2.28619000 |
| C    | 1.61269000 | 6.19578500 | 6.43832700 |
| H    | 2.34515300 | 6.93815900 | 6.09926100 |
| C    | 0.97886600 | 6.73395900 | 7.71120600 |
| H    | 0.52020700 | 7.70878000 | 7.55680400 |
| H    | 1.74679800 | 6.84881200 | 8.47811300 |
| H    | 0.22127200 | 6.06197800 | 8.11276800 |
| C    | 2.35316800 | 4.89174200 | 6.70261600 |
| H    | 1.69169300 | 4.12284200 | 7.10138200 |
| H    | 3.13140900 | 5.06266000 | 7.44856000 |
| H    | 2.83888900 | 4.49036500 | 5.81422900 |
| C    | -0.54795100| 4.60701300 | 5.05531600 |
| H    | -1.34581700| 4.84633600 | 4.34963900 |
| C    | -1.19776900| 4.41124900 | 6.41746500 |
| H    | -0.47572400| 4.09385300 | 7.16961400 |
| H    | -1.95683200| 3.63004400 | 6.34941700 |
| H    | -1.68842900| 5.31253900 | 6.78218700 |
| C    | 0.12566300 | 3.33149500 | 4.56908200 |
| H    | 0.47409200 | 3.41146600 | 3.54072400 |
| H    | -0.59516800| 2.51226000 | 4.60367700 |
| H    | 0.97205700 | 3.04360100 | 5.19099000 |
| C    | -1.62199000| 7.89793600 | 5.94816800 |
| Ru   | -0.55610800| 8.05100000 | 4.47532800 |
| INT1:          |                  |                  |                  |
|---------------|------------------|------------------|------------------|
| H             | 0.701353000      | 8.673856000      | 5.352573000      |
| P             | -2.374633000     | 7.734428000      | 2.847680000      |
| P             | 0.424080000      | 6.148020000      | 4.944699000      |
| O             | -2.310859000     | 7.936893000      | 6.915883000      |
| N             | 0.742314000      | 8.336312000      | 2.677616000      |
| C             | -1.614172000     | 7.977623000      | 1.186740000      |
| H             | -0.954576000     | 7.116128000      | 1.053310000      |
| H             | -2.388481000     | 7.930634000      | 0.418805000      |
| C             | -0.816260000     | 9.230128000      | 1.068602000      |
| C             | -1.207396000     | 10.259706000     | 0.220219000      |
| H             | -2.141418000     | 10.158947000     | -0.322890000     |
| C             | -0.408374000     | 11.379738000     | 0.029422000      |
| H             | -0.721676000     | 12.166714000     | -0.644548000     |
| C             | 0.803717000      | 11.470901000     | 0.702336000      |
| H             | 1.443669000      | 12.334931000     | 0.556424000      |
| C             | 1.205351000      | 10.480644000     | 1.589120000      |
| C             | 0.391655000      | 9.347316000      | 1.798087000      |
| C             | 2.462846000      | 10.583065000     | 2.406290000      |
| H             | 3.202516000      | 11.215211000     | 1.905916000      |
| H             | 2.230713000      | 11.093899000     | 3.348489000      |
| C             | 3.021066000      | 9.227925000      | 2.718566000      |
| C             | 4.375822000      | 9.002320000      | 2.913610000      |
| H             | 5.073250000      | 9.818781000      | 2.755757000      |
| C             | 4.839313000      | 7.762500000      | 3.338939000      |
| C             | 5.897332000      | 7.597495000      | 3.498263000      |
| C             | 3.928296000      | 6.738350000      | 3.563821000      |
| C             | 4.275684000      | 5.765814000      | 3.896651000      |
| C             | 2.567397000      | 6.923118000      | 3.345340000      |
| C             | 2.098250000      | 8.182865000      | 2.914216000      |
| C             | 1.591949000      | 5.813438000      | 3.556533000      |
| H             | 2.113477000      | 4.874325000      | 3.741757000      |
| H             | 0.956631000      | 5.678090900      | 2.675841000      |
| C             | -3.339521000     | 6.172532000      | 2.588542000      |
| H             | -4.112038000     | 6.420962000      | 1.856388000      |
| C             | -4.030453000     | 5.742032000      | 3.874181000      |
| H             | -3.327384000     | 5.619419000      | 4.699493000      |
| H             | -4.541519000     | 4.788374000      | 3.731334000      |
| H             | -4.777303000     | 6.469321000      | 4.191591000      |
| C             | -2.462782000     | 5.084186000      | 1.975569000      |
| H             | -2.325688000     | 5.238884000      | 0.906528000      |
| H             | -2.924249000     | 4.104241000      | 2.109069000      |
| H             | -1.467674000     | 5.039938000      | 2.420744000      |
C   -3.648354000    9.094480000    2.861173000
H   -3.054702000    9.956543000    2.537440000
C   -4.189552000    9.409406000    4.246703000
H   -4.733487000    8.567520000    4.676705000
H   -4.886457000   10.248060000    4.191106000
H   -3.395783000    9.685105000    4.936927000
C   -4.778425000    8.902699000    1.861350000
H   -4.424107000    8.644643000    0.863260000
C   -5.354548000    9.825584000    1.773573000
H   -5.470261000   10.131280000    2.183815000
C   1.587300000    6.205446000    6.394192000
H   2.312713000    6.943425000    6.031202000
C    0.989267000   6.757258000    7.678882000
H    0.526865000   7.730865000    7.528395000
H    1.777778000   6.879635000    8.422546000
H    0.243464000   6.090409000    8.109787000
C    2.333529000   4.904226000    6.655490000
H    1.682443000   4.142389000    7.084176000
H    3.133440000   5.083375000    7.376386000
H    2.792637000   4.488537000    5.759630000
C   -0.608339000   4.609958000    5.091563000
H   -1.422053000   4.826988000    4.399569000
C   -1.230146000   4.452244000    6.471678000
H   -0.496656000   4.141453000    7.215281000
H   -2.001755000   3.681008000    6.437712000
H   -1.700412000   5.368803000    6.826315000
C    0.048826000   3.320113000    4.621739000
H    0.373649000   3.374392000    3.583829000
H   -0.674689000   2.505267000    4.691610000
H    0.908396000   3.041546000    5.229442000
C   -1.638272000   7.994194000    5.963847000
Ru  -0.586032000   8.117295000    4.485783000
O   -1.090089000   10.424639000    4.122268000
H   -0.600291000   10.869365000    4.826695000
H   -0.642154000   10.694064000    3.303733000

INT2:
O     0.967396000    9.138912000    5.359373000
P    -2.274871000    7.689116000    2.875282000
P     0.412081000    6.133454000    4.884986000
O    -2.413812000    7.797519000    6.773807000
N     0.755244000    8.364872000    2.686982000
C   -1.555829000    7.884194000    1.190283000
H   -0.889619000    7.026884000    1.058864000
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| C    | -2.353132000 | 7.804548000  | 0.448926000  |
| C    | -0.786693000 | 9.150415000  | 1.017650000  |
| C    | -1.168276000 | 10.114201000 | 0.090923000  |
| H    | -2.079430000 | 9.959734000  | -0.477970000 |
| C    | -0.380980000 | 11.234132000 | -0.144474000 |
| H    | -0.681506000 | 11.968227000 | -0.881279000 |
| C    | 0.806733000  | 11.391330000 | 0.561650000  |
| H    | 1.438958000  | 11.253543000 | 0.375139000  |
| C    | 1.194623000  | 10.469428000 | 1.523030000  |
| C    | 0.389719000  | 9.341081000  | 1.775946000  |
| H    | 2.436807000  | 10.630388000 | 2.348858000  |
| H    | 3.174408000  | 11.248999000 | 1.833436000  |
| C    | 2.184935000  | 11.177305000 | 3.268642000  |
| C    | 3.012112000  | 9.298583000  | 2.731545000  |
| C    | 4.365973000  | 9.102445000  | 2.959065000  |
| H    | 5.052567000  | 9.927129000  | 2.795593000  |
| C    | 4.844424000  | 7.881136000  | 3.422699000  |
| H    | 5.901686000  | 7.741493000  | 3.609484000  |
| C    | 3.951402000  | 6.838573000  | 3.636281000  |
| H    | 4.313262000  | 5.875428000  | 3.980791000  |
| C    | 2.593331000  | 6.993613000  | 3.382351000  |
| C    | 2.106943000  | 8.242071000  | 2.940374000  |
| C    | 1.639687000  | 5.854891000  | 3.543823000  |
| H    | 2.177352000  | 4.927492000  | 3.742103000  |
| H    | 1.047018000  | 5.710891000  | 2.635437000  |
| C    | -3.373313000 | 6.213395000  | 2.664303000  |
| H    | -4.161932000 | 6.550143000  | 1.987033000  |
| C    | -4.024033000 | 5.822855000  | 3.982035000  |
| H    | -3.289177000 | 5.557535000  | 4.742490000  |
| H    | -4.679485000 | 4.961850000  | 3.841723000  |
| H    | -4.628808000 | 6.634681000  | 4.386751000  |
| C    | -2.647660000 | 5.064283000  | 1.971593000  |
| H    | -2.524940000 | 5.256630000  | 0.906907000  |
| H    | -3.220917000 | 4.141583000  | 2.074065000  |
| H    | -1.653037000 | 4.877064000  | 2.377361000  |
| C    | -3.426008000 | 9.161325000  | 2.898573000  |
| H    | -2.768357000 | 9.944600000  | 2.504565000  |
| C    | -3.875788000 | 9.604502000  | 4.281062000  |
| H    | -4.435513000 | 8.828914000  | 4.804544000  |
| H    | -4.530986000 | 10.473115000 | 4.192851000  |
| H    | -3.034876000 | 9.893405000  | 4.909679000  |
| C    | -4.611137000 | 9.032170000  | 1.953239000  |
| H    | -4.328252000 | 8.681075000  | 0.960865000  |
| H    | -5.091577000 | 10.004355000 | 1.830432000  |
H   -5.364164000  8.348791000  2.348721000
C    1.507774000  6.253854000  6.377516000
H    2.188926000  7.044846000  6.045667000
C    0.837762000  6.744107000  7.651443000
H    0.278939000  7.665108000  7.501793000
H   1.601841000  6.945346000  8.404317000
H    0.156956000  6.007130000  8.074857000
C    2.313885000  4.989901000  6.646474000
H    1.688969000  4.184731000  7.033056000
H   3.069757000  5.201060000  7.405211000
H    2.835155000  4.618200000  5.765810000
C   -0.595662000  4.583899000  4.999435000
H   -1.400587000  4.786538000  4.293948000
C   -1.233986000  4.388469000  6.367178000
H   -0.504096000  4.080168000  7.115121000
H   -1.984957000  3.599240000  6.304533000
H   -1.732694000  5.285388000  6.731934000
C    0.116140000  3.323059000  4.528843000
H    0.447068000  3.394926000  3.494189000
H   -0.576214000  2.481456000  4.590532000
H    0.980480000  3.075999000  5.144050000
C   -1.691455000  7.911944000  5.866537000
Ru  -0.566124000  8.100474000  4.437118000
H    0.774145000  9.235530000  6.297538000

INT3:
O    1.360982000  0.747325000  1.244053000
P   -2.002353000 -0.522675000 -1.307485000
P    0.766759000 -2.128745000  0.651825000
O   -2.171808000 -0.664043000  2.537252000
N    1.061632000  0.174373000 -1.509989000
C   -1.248465000 -0.324047000 -2.978277000
H   -0.550472000 -1.160840000 -3.066048000
H   -2.017176000 -0.447523000 -3.741904000
C   -0.502515000  0.955079000 -3.156660000
C   -0.909357000  1.927351000 -4.063791000
H   -1.821247000  1.766948000 -4.629031000
C   -0.146384000  3.067001000 -4.287453000
C   -0.469995000  3.807973000 -5.007357000
C    1.043107000  3.236829000 -3.587560000
H    1.648903000  4.122133000 -3.752806000
C    1.461359000  2.300921000 -2.652852000
C    0.688858000  1.145176000 -2.419547000
C    2.681224000  2.490748000 -1.801552000
S53
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -0.12326500 | -3.75948600 | 0.67425000 |
| H    | -0.90988600 | -3.60234200 | -0.06228200 |
| C    | -0.80028000 | -4.02207000 | 2.01237600 |
| H    | -0.08036500 | -4.31310900 | 2.77701700 |
| H    | -1.51334800 | -4.84224000 | 1.91041600 |
| H    | -1.34791600 | -3.15528100 | 2.38285800 |
| C    | 0.67860200  | -4.96687400 | 0.20830500 |
| H    | 1.03785800  | -4.85511200 | -0.81360000 |
| H    | 0.03665000  | -5.84992200 | 0.22953700 |
| H    | 1.53630900  | -5.17622400 | 0.84569400 |
| C    | -1.44093100 | -0.40868400 | 1.66250200 |
| Ru   | -0.31614900 | -0.09981000 | 0.27017100 |
| N    | -0.60814100 | 2.13334200  | 0.02953900 |
| H    | -0.77950700 | 2.41735000  | -0.93087300 |
| H    | 0.38401100  | 2.29454900  | 0.22263200 |
| C    | -1.41682500 | 2.97739200  | 0.93419000 |
| H    | -1.41364200 | 4.00548800  | 0.55794300 |
| H    | -2.44842200 | 2.62919600  | 0.90789200 |
| C    | -0.89571400 | 2.95724100  | 2.33993600 |
| C    | 0.36354000  | 3.48505400  | 2.63024800 |
| C    | -1.64665800 | 2.41833500  | 3.37841200 |
| C    | 0.86541900  | 3.45295800  | 3.92108800 |
| C    | -1.14856500 | 2.38502300  | 4.67484500 |
| C    | 0.11082700  | 2.89724000  | 4.94812400 |
| H    | 0.95813300  | 3.91531700  | 1.83082400 |
| H    | -2.62800300 | 2.01169700  | 3.16482100 |
| H    | 1.84612300  | 3.86280300  | 4.12864100 |
| H    | -1.74552800 | 1.95558600  | 5.47002200 |
| H    | 0.50298400  | 2.86970100  | 5.95708200 |
| H    | 1.09487400  | 0.96412300  | 2.14413700 |

**INT4:**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| O    | 1.40969600  | 0.92899800 | 1.34632400 |
| P    | -2.01481200 | -0.46698500 | -1.30037300 |
| P    | 0.73663200  | -2.18734700 | 0.59159200 |
| O    | -2.22774400 | -0.67076200 | 2.50214100 |
| N    | 1.04329400  | 0.18305300 | -1.49507000 |
| C    | -1.26079900 | -0.27181700 | -2.96834000 |
| H    | -0.58017800 | -1.12191200 | -3.06076500 |
| H    | -2.04043000 | -0.38317500 | -3.72287500 |
| C    | -0.49075700 | 0.99142600  | -3.15393800 |
| C    | -0.86263800 | 1.95860200  | -4.08082500 |
| H    | -1.76610000 | 1.80925000  | -4.66221000 |
| C    | -0.07296700 | 3.07988200  | -4.30429500 |

S54
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| H    | -0.368959 | 3.817916  | -5.038934 |
| C    | 1.106354  | 3.236201  | -3.584610 |
| H    | 1.730856  | 4.108781  | -3.747289 |
| C    | 1.491127  | 2.301066  | -2.634865 |
| C    | 0.695279  | 1.162620  | -2.406960 |
| C    | 2.701426  | 2.468907  | -1.766112 |
| C    | 3.442010  | 3.120059  | -2.234323 |
| H    | 2.400744  | 2.984115  | -0.840254 |
| C    | 3.291874  | 1.138687  | -1.405382 |
| C    | 4.647451  | 0.960940  | -1.175253 |
| H    | 5.318607  | 1.803309  | -1.309198 |
| C    | 5.145233  | -0.266502 | -0.751631 |
| H    | 6.203500  | -0.394370 | -0.562197 |
| C    | 4.269363  | -1.331107 | -0.587960 |
| H    | 4.646355  | -2.301923 | -0.283402 |
| C    | 2.908981  | -1.193986 | -0.845636 |
| H    | 2.399121  | 0.061583  | -1.237216 |
| C    | 1.991253  | -2.366603 | -0.745311 |
| H    | 2.563869  | -3.281162 | -0.592130 |
| C    | 1.412952  | -2.484177 | -1.667231 |
| H    | 2.954102  | -2.061318 | -1.451410 |
| C    | -3.855065 | -1.792352 | -2.011802 |
| C    | -3.388108 | -2.600735 | -0.096399 |
| H    | -2.541635 | -2.754290 | 0.568745  |
| H    | -3.891281 | -3.561209 | -0.220975 |
| H    | -4.076577 | -1.932475 | 0.415848  |
| C    | -2.187192 | -3.092094 | -2.272749 |
| H    | -2.187728 | -2.846042 | -3.333151 |
| H    | -2.647418 | -4.075185 | -2.162592 |
| H    | -1.144254 | -3.183557 | -1.964524 |
| C    | -3.352568 | 0.828372  | -1.295471 |
| H    | -2.790489 | 1.758497  | -1.177199 |
| C    | -4.312696 | 0.692039  | -0.121419 |
| H    | -5.012766 | -0.129049 | -0.281538 |
| H    | -4.906454 | 1.602362  | -0.024744 |
| H    | -3.812337 | 0.524000  | 0.830942  |
| C    | -4.139329 | 0.917053  | -2.596358 |
| H    | -3.522424 | 1.197270  | -3.446655 |
| H    | -4.915211 | 1.677979  | -2.494699 |
| H    | -4.643048 | -0.019960 | -2.838664 |
| C    | 1.839671  | -2.027617 | 2.085850  |
| H    | 2.475334  | -1.196946 | 1.762900  |
| C    | 1.137445  | -1.587301 | 3.363369  |
| H    | 0.481314  | -0.730254 | 3.214887  |

S55
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| H     | 1.88175700| -1.30404000| 4.110242000|
| H     | 0.534888000| -2.383263000| 3.799264000|
| C     | 2.743608000| -3.222064000| 2.356386000|
| H     | 2.187565000| -4.069340000| 2.757664000|
| H     | 3.493557000| -2.949186000| 3.101804000|
| H     | 3.277547000| -3.560190000| 1.469368000|
| C     | -0.092454000| -3.851760000| 0.677231000|
| H     | -0.897329000| -3.753353000| -0.050487000|
| C     | -0.737571000| -4.087240000| 2.035979000|
| H     | -0.003392000| -4.340610000| 2.794210000|
| C     | 2.743608000| -3.222064000| 2.356386000|
| C     | 0.028832000| -1.035903000| -3.068471000|

**INT5:**

| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| P     | -1.832187000| -0.401127000| -1.127173000|
| P     | 0.905255000| -2.215584000| 0.491447000|
| O     | -1.746579000| -0.577926000| 2.679057000|
| N     | 1.189613000| 0.117179000| -1.616075000|
| C     | -1.253583000| -0.157838000| -2.858009000|
| H     | -0.638341000| -1.035903000| -3.068471000|

S56
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -2.121199  | -0.191251 | -3.518524 |
| C    | -0.443886  | 1.071137  | -3.081028 |
| C    | -0.864348  | 2.101053  | -3.912643 |
| H    | -1.845436  | 2.038374  | -4.371964 |
| C    | -0.029819  | 3.177296  | -4.193501 |
| H    | -0.362680  | 3.967886  | -4.853958 |
| C    | 1.241152   | 3.220657  | -3.631495 |
| H    | 1.902259   | 4.053301  | -3.849456 |
| C    | 1.674406   | 2.225907  | -2.76483 |
| C    | 0.826579   | 1.142448  | -2.46821 |
| C    | 2.997680   | 2.278058  | -2.05672 |
| H    | 3.731893   | 2.845863  | -2.63188 |
| H    | 2.875598   | 2.834556  | -1.11547 |
| C    | 3.504081   | 0.899568  | -1.74512 |
| C    | 4.857481   | 0.606431  | -1.66689 |
| H    | 5.577020   | 1.392125  | -1.87150 |
| C    | 5.295572   | -0.66493  | -1.31439 |
| H    | 6.354200   | -0.881414 | -1.24725 |
| C    | 4.359215   | -1.659195 | -1.06453 |
| H    | 4.686561   | -2.662706 | -0.81373 |
| C    | 2.994805   | -1.408166 | -1.16514 |
| C    | 2.549739   | -0.106512 | -1.48739 |
| C    | 1.998361   | -2.503784 | -0.96834 |
| H    | 2.508605   | -3.461629 | -0.86794 |
| H    | 1.323507   | -2.571170 | -1.82760 |
| C    | -2.830979  | -1.953167 | -1.27565 |
| H    | -3.698591  | -1.665040 | -1.87541 |
| C    | -3.329883  | -2.425734 | 0.080611 |
| H    | -2.513167  | -2.577193 | 0.786404 |
| H    | -3.861285  | -3.373398 | -0.02063 |
| H    | -4.017498  | -1.709740 | 0.529834 |
| C    | -2.068616  | -3.022555 | -2.05286 |
| H    | -2.111673  | -2.841820 | -3.12561 |
| H    | -2.500580  | -4.007149 | -1.86755 |
| H    | -1.012659  | -3.071089 | -1.78069 |
| C    | -3.070610  | 0.981514  | -0.96446 |
| H    | -2.466833  | 1.838028  | -1.27942 |
| C    | -3.554777  | 1.253734  | 0.449623 |
| H    | -4.164717  | 0.436621  | 0.835853 |
| H    | -4.175880  | 2.151627  | 0.457994 |
| H    | -2.735437  | 1.416131  | 1.145096 |
| C    | -4.255398  | 0.863127  | -1.91370 |
| H    | -3.967871  | 0.643688  | -2.94093 |
| H    | -4.807204  | 1.804515  | -1.92534 |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| H | -4.950477000 | 0.089207000 | -1.585302000 |
| C | 2.195908000  | -2.028421000 | 1.828829000 |
| H | 2.817987000  | -1.242470000 | 3.010848000 |
| C | 1.679827000  | -1.477248000 | 3.148998000 |
| H | 1.124929000  | -0.550684000 | 3.808102000 |
| H | 2.522483000  | -1.585302000 | 2.561424000 |
| H | 1.034301000  | -2.179162000 | 2.671430000 |
| C | 3.081770000  | -3.246596000 | 2.046041000 |
| H | 2.549077000  | -4.046014000 | 2.293630000 |
| H | 3.934353000  | -2.973536000 | 2.578418000 |
| H | 3.478246000  | -3.652897000 | 1.116359000 |
| C | 0.021748000  | -3.831263000 | 0.774811000 |
| H | -0.871933000 | -3.725267000 | 0.160304000 |
| C | -0.447641000 | -3.969062000 | 2.216298000 |
| H | 0.377789000  | -4.188809000 | 2.892947000 |
| H | -1.158434000 | -4.793768000 | 2.293630000 |
| H | -0.947874000 | -3.070689000 | 2.578418000 |
| C | 0.743721000  | -5.080142000 | 0.291860000 |
| H | 0.929735000  | -5.057202000 | -0.781158000 |
| H | 0.121424000  | -5.954544000 | 0.492911000 |
| H | 1.696372000  | -5.238300000 | 0.795415000 |
| C | -1.094544000 | -0.348163000 | 1.741053000 |
| Ru| -0.073529000 | -0.087258000 | 0.247139000 |
| N | 0.200520000  | 1.916147000  | 0.359222000 |
| H | 0.536173000  | 2.319471000  | -0.509672000 |
| C | -0.445786000 | 2.973809000  | 1.108259000 |
| H | 0.134243000  | 3.898496000  | 0.975551000 |
| H | -1.446545000 | 3.216036000  | 0.717845000 |
| C | -0.562749000 | 2.708452000  | 2.583441000 |
| C | 0.511211000  | 2.184402000  | 3.301688000 |
| C | -1.728891000 | 3.022997000  | 3.276145000 |
| C | 0.420016000  | 1.974667000  | 4.668900000 |
| C | -1.825451000 | 2.818039000  | 4.646206000 |
| C | -0.751122000 | 2.289579000  | 5.347715000 |
| H | 1.424437000  | 1.934956000  | 2.772827000 |
| H | -2.573058000 | 3.430650000  | 2.729719000 |
| H | 1.265499000  | 1.563198000  | 5.207931000 |
| H | -2.743861000 | 3.065057000  | 5.164903000 |
| H | -0.824675000 | 2.122919000  | 6.415246000 |

**INT6:**

|  | X       | Y       | Z       |
|---|---------|---------|---------|
| P | -2.425494000 | 7.904217000  | 2.719739000 |
| P | 0.284344000  | 6.548400000  | 5.116023000 |
| O | -2.562114000 | 8.472143000  | 6.751671000 |
|   |          |          |          |
|---|----------|----------|----------|
| N | 0.720616000 | 8.534687000 | 2.641808000 |
| C | -1.562714000 | 8.002031000 | 1.098783000 |
| H | -0.892853000 | 7.138290000 | 0.872527000 |
| C | -2.288711000 | 7.853820000 | 0.297281000 |
| C | -0.758850000 | 9.234462000 | -0.403618000 |
| H | -1.117284000 | 10.150982000 | -0.106834000 |
| C | -2.033138000 | 9.985259000 | -0.665222000 |
| C | -0.306790000 | 11.240167000 | 0.282898000 |
| H | -0.592642000 | 11.942979000 | -1.175951000 |
| C | 0.889731000 | 11.394069000 | 0.045256000 |
| C | 1.549185000 | 12.222850000 | 1.290461000 |
| C | 1.261191000 | 10.512214000 | 1.627898000 |
| C | 2.533203000 | 10.704908000 | 2.063137000 |
| H | 3.309099000 | 11.134127000 | 1.423895000 |
| H | 2.379050000 | 11.458328000 | 2.849345000 |
| C | 3.009429000 | 9.425694000 | 3.021028000 |
| C | 4.343819000 | 9.240439000 | 2.788536000 |
| H | 5.053927000 | 10.027811000 | 2.942118000 |
| C | 4.773205000 | 8.084520000 | 3.659852000 |
| H | 5.814820000 | 7.956014000 | 3.925123000 |
| C | 3.846908000 | 7.089784000 | 3.941616000 |
| H | 4.165339000 | 6.169653000 | 4.420350000 |
| H | 2.508579000 | 7.230135000 | 3.592405000 |
| C | 4.061965000 | 8.422068000 | 2.974550000 |
| C | 1.542205000 | 6.121741000 | 3.844904000 |
| H | 2.069786000 | 5.216808000 | 4.147376000 |
| H | 0.967890000 | 5.892474000 | 2.942118000 |
| C | -3.239620000 | 6.242127000 | 2.595808000 |
| H | -3.983006000 | 6.338664000 | 1.800633000 |
| C | -3.979332000 | 5.901406000 | 3.884341000 |
| H | -3.367452000 | 6.059874000 | 4.773826000 |
| H | -4.293164000 | 4.856024000 | 3.881092000 |
| H | -4.875764000 | 6.509140000 | 4.001075000 |
| C | -2.242391000 | 5.172707000 | 2.151396000 |
| H | -2.112520000 | 5.179302000 | 1.070372000 |
| H | -2.595289000 | 4.179317000 | 2.433871000 |
| H | -1.250894000 | 5.303371000 | 2.587757000 |
| C | -3.811489000 | 9.127701000 | 2.514659000 |
| H | -3.264251000 | 10.023800000 | 2.205683000 |
| C | -4.542436000 | 9.446324000 | 3.810746000 |
| H | -5.157033000 | 8.609680000 | 4.143835000 |
| H | -5.211210000 | 10.296051000 | 3.663203000 |
| H | -3.868274000 | 9.697020000 | 4.628248000 |
INT7:
| Symbol | X-coordinate  | Y-coordinate  | Z-coordinate  |
|--------|---------------|---------------|---------------|
| H      | 0.503862000   | 8.559881000   | 5.489575000   |
| P      | -2.423842000  | 7.655246000   | 2.818570000   |
| P      | 0.338135000   | 6.065613000   | 4.938696000   |
| O      | -2.572837000  | 7.612646000   | 6.855081000   |
| N      | 0.681037000   | 8.379061000   | 2.785509000   |
| C      | -1.593296000  | 7.942911000   | 1.198752000   |
| H      | -0.894371000  | 7.108061000   | 1.099734000   |
| H      | -2.323151000  | 7.865920000   | 0.391107000   |
| C      | -0.836169000  | 9.223804000   | 1.116583000   |
| C      | -1.230893000  | 10.240910000  | 0.255671000   |
| H      | -2.140714000  | 10.112404000  | -0.321406000  |
| C      | -0.461844000  | 11.387211000  | 0.093638000   |
| H      | -0.775926000  | 12.166047000  | -0.589523000  |
| C      | 0.726656000   | 11.509658000  | 0.804039000   |
| H      | 1.346470000   | 12.391721000  | 0.678382000   |
| C      | 1.129843000   | 10.529794000  | 1.700533000   |
| C      | 0.340809000   | 9.376354000   | 1.889164000   |
| C      | 2.360387000   | 10.674858000  | 2.545638000   |
| H      | 3.106522000   | 11.299883000  | 2.050370000   |
| H      | 2.097929000   | 11.216892000  | 3.466249000   |
| C      | 2.931118100   | 9.339257000   | 2.918833000   |
| C      | 4.281942000   | 9.157011000   | 3.178243000   |
| H      | 4.958535000   | 9.966333000   | 3.051928000   |
| C      | 4.767535000   | 9.731679000   | 3.619649000   |
| H      | 5.821580000   | 7.801394000   | 3.829697000   |
| C      | 3.882944000   | 6.873322000   | 3.781341000   |
| H      | 4.248609000   | 5.905446000   | 4.108517000   |
| C      | 2.528725000   | 7.013907000   | 3.497887000   |
| C      | 2.030845000   | 8.266535000   | 3.074295000   |
| C      | 1.598037000   | 5.853096000   | 3.609339000   |
| H      | 2.156580000   | 4.932282000   | 3.777366000   |
| H      | 1.019579000   | 5.731824000   | 2.687976000   |
| C      | -3.317020000  | 6.058871000   | 2.501795000   |
| H      | -4.102935000  | 6.295892000   | 1.780386000   |
| C      | -3.981782000  | 5.553025000   | 3.773918000   |
| H      | -3.265876000  | 5.422471000   | 4.586265000   |
| H      | -4.462303000  | 4.589074000   | 3.597361000   |
| H      | -4.748314000  | 6.240854000   | 4.130078000   |
| C      | -2.395285000  | 5.030981000   | 1.851646000   |
| H      | -2.272713000  | 5.223306000   | 0.786918000   |
| H      | -2.808937000  | 4.026646000   | 1.958769000   |
| H      | -1.395767000  | 5.020957000   | 2.289460000   |
| C      | -3.762815000  | 8.954074000   | 2.769530000   |
| H      | -3.179850000  | 9.859916000   | 2.560714000   |
|    | X    | Y    | Z    |
|----|------|------|------|
| C  | -4.480902000 | 9.149396000 | 4.097948000 |
| H  | -5.165813000 | 8.327027000 | 4.305869000 |
| H  | -5.077231000 | 10.063474000 | 4.073364000 |
| H  | -3.800460000 | 9.220388000 | 4.946117000 |
| C  | -4.771360000 | 8.795176000 | 1.641830000 |
| H  | -4.304448000 | 8.623697000 | 0.672622000 |
| H  | -5.377363000 | 9.699009000 | 1.556279000 |
| H  | -5.456415000 | 7.968749000 | 1.835630000 |
| C  | 1.426403000 | 6.110079000 | 6.450589000 |
| H  | 2.123823000 | 6.905029000 | 6.160070000 |
| C  | 0.737482000 | 6.566885000 | 7.727455000 |
| H  | 0.214951000 | 7.512402000 | 7.594377000 |
| H  | 1.483258000 | 6.710854000 | 8.511883000 |
| H  | 0.021147000 | 5.834587000 | 8.097920000 |
| C  | 2.235619000 | 4.844545000 | 6.695625000 |
| H  | 1.611429000 | 4.029067000 | 7.061107000 |
| H  | 2.990125000 | 5.036169000 | 7.461183000 |
| H  | 2.758761000 | 4.494073000 | 5.806908000 |
| C  | -0.591709000 | 4.453295000 | 4.965517000 |
| H  | -1.378419000 | 4.641898000 | 4.235854000 |
| C  | -1.279537000 | 4.206551000 | 6.300684000 |
| H  | -0.572360000 | 3.904611000 | 7.073064000 |
| H  | -2.006626000 | 3.398973000 | 6.195991000 |
| H  | -1.815442000 | 5.084309000 | 6.661400000 |
| C  | 0.168876000 | 3.224334000 | 4.489282000 |
| H  | 0.543192000 | 3.338260000 | 3.472810000 |
| H  | -0.504007000 | 2.364053000 | 4.490057000 |
| H  | 1.011924000 | 2.974202000 | 5.131607000 |
| C  | -1.852702000 | 7.789878000 | 5.952315000 |
| Ru | -0.741986000 | 8.052186000 | 4.540973000 |
| N  | -1.232971000 | 10.279206000 | 4.317403000 |
| H  | -2.233125000 | 10.424620000 | 4.416481000 |
| H  | -1.023026000 | 10.554798000 | 3.360482000 |
| C  | -0.552720000 | 11.227723000 | 5.231923000 |
| H  | 0.515483000 | 11.020979000 | 5.195393000 |
| H  | -0.707459000 | 12.250064000 | 4.871396000 |
| C  | -1.066332000 | 11.101571000 | 6.632854000 |
| C  | -2.380009000 | 11.463744000 | 6.929962000 |
| C  | -0.259336000 | 10.616937000 | 7.657801000 |
| C  | -2.877274000 | 11.335900000 | 8.217685000 |
| C  | -0.752419000 | 10.490917000 | 8.949645000 |
| C  | -2.063307000 | 10.847430000 | 9.232024000 |
| H  | -3.016538000 | 11.853465000 | 6.141575000 |
| H  | 0.763895000 | 10.335076000 | 7.436056000 |
|    |    |    |    |
|----|----|----|----|
| H  | -3.899316000 | 11.622619000 | 8.432380000 |
| H  | -0.111269000 | 10.110373000 | 9.735453000 |
| H  | -2.449419000 | 10.748772000 | 10.238850000 |

**TS1:**

|    |    |    |    |
|----|----|----|----|
| H  | 0.570356000 | 9.103583000 | 5.367297000 |
| P  | -2.398206000 | 7.801841000 | 2.834580000 |
| P  | 0.303987000 | 6.190143000 | 4.827585000 |
| O  | -2.559639000 | 7.861909000 | 6.745414000 |
| N  | 0.651895000 | 8.444495000 | 2.658047000 |
| C  | -1.653787000 | 8.013408000 | 1.165543000 |
| H  | -0.985845000 | 7.157105000 | 1.041207000 |
| H  | -2.442797000 | 7.935193000 | 0.415823000 |
| C  | -0.879162000 | 9.276650000 | 1.007038000 |
| C  | -1.262089000 | 10.266962000 | 0.110338000 |
| H  | -2.181724000 | 10.138237000 | -0.450795000 |
| C  | -0.465983000 | 11.385394000 | -0.103491000 |
| H  | -0.769068000 | 12.142547000 | -0.815361000 |
| C  | 0.729488000 | 11.515739000 | 0.593637000 |
| H  | 1.363393000 | 12.380777000 | 0.428435000 |
| C  | 1.119481000 | 10.563965000 | 1.525943000 |
| C  | 0.309361000 | 9.434807000 | 1.753253000 |
| C  | 2.357817000 | 10.700980000 | 2.362813000 |
| H  | 3.104689000 | 11.321917000 | 1.865821000 |
| H  | 2.103437000 | 11.237242000 | 3.289182000 |
| C  | 2.919929000 | 9.356696000 | 2.724998000 |
| C  | 4.273898000 | 9.142991000 | 2.936856000 |
| H  | 4.966423000 | 9.964506000 | 2.784414000 |
| C  | 4.743928000 | 7.906260000 | 3.364433000 |
| H  | 5.801384000 | 7.751992000 | 3.537552000 |
| C  | 3.843243000 | 6.868157000 | 3.562415000 |
| H  | 4.198668000 | 5.893933000 | 3.881055000 |
| C  | 2.483612000 | 7.039996000 | 3.325182000 |
| C  | 2.005381000 | 8.302159000 | 2.913292000 |
| C  | 1.522767000 | 5.906611000 | 3.475907000 |
| H  | 2.057410000 | 4.974470000 | 3.657996000 |
| H  | 0.925015000 | 5.780102000 | 2.568066000 |
| C  | -3.409368000 | 6.268110000 | 2.635432000 |
| H  | -4.218918000 | 6.554650000 | 1.959117000 |
| C  | -4.030014000 | 5.845114000 | 3.958246000 |
| H  | -3.278110000 | 5.671820000 | 4.728413000 |
| H  | -4.594859000 | 4.920110000 | 3.832752000 |
| H  | -4.715946000 | 6.600429000 | 4.341138000 |
| C  | -2.611762000 | 5.163254000 | 1.948621000 |
| Element | X  | Y  | Z     |
|---------|----|----|-------|
| H       | -2.527079000 | 5.342100000 | 0.877991000 |
| H       | -3.108296000 | 4.201192000 | 2.083358000 |
| H       | -1.596901000 | 5.064831000 | 2.336011000 |
| C       | -3.604350000 | 9.217067000 | 2.864348000 |
| H       | -2.961246000 | 10.046295000 | 2.548015000 |
| C       | -4.147510000 | 9.570637000 | 4.238666000 |
| H       | -4.709231000 | 8.750937000 | 4.687205000 |
| H       | -4.830871000 | 10.417616000 | 4.151127000 |
| C       | -3.349198000 | 9.860862000 | 4.917220000 |
| H       | -4.731278000 | 9.070776000 | 1.851597000 |
| H       | -4.384830000 | 8.777626000 | 0.860948000 |
| H       | -5.252678000 | 10.023484000 | 1.745516000 |
| H       | -5.468261000 | 8.336241000 | 2.179717000 |
| C       | 1.434863000 | 6.352933000 | 6.296996000 |
| H       | 2.120574000 | 7.126195000 | 5.929810000 |
| C       | 0.784340000 | 6.895845000 | 7.559520000 |
| H       | 0.284382000 | 7.846909000 | 7.386192000 |
| H       | 1.552394000 | 7.065025000 | 8.316665000 |
| H       | 0.059880000 | 6.203936000 | 7.987120000 |
| C       | 2.255702000 | 5.105933000 | 6.596479000 |
| H       | 1.644996000 | 4.316303000 | 7.034055000 |
| H       | 0.303906000 | 5.349348000 | 7.322184000 |
| H       | 2.749733000 | 4.699503000 | 5.715156000 |
| C       | -0.648221000 | 4.605226000 | 4.987781000 |
| H       | -1.462307000 | 4.756291000 | 4.279522000 |
| C       | -1.279622000 | 4.443064000 | 6.363187000 |
| H       | -0.540913000 | 4.187443000 | 7.122295000 |
| H       | -2.008379000 | 3.631271000 | 6.334562000 |
| H       | -1.803653000 | 5.339762000 | 6.692552000 |
| C       | 0.093534000 | 3.348116000 | 4.556769000 |
| H       | 0.411712000 | 3.393311000 | 3.516332000 |
| H       | -0.574278000 | 2.490035000 | 4.653772000 |
| H       | 0.970854000 | 3.146697000 | 5.169787000 |
| C       | -1.852115000 | 7.995122000 | 5.833172000 |
| Ru      | -0.721553000 | 8.213506000 | 4.410463000 |
| O       | -0.974785000 | 10.443996000 | 4.334901000 |
| H       | 0.052174000 | 9.813217000 | 5.005044000 |
| H       | -0.602098000 | 10.716331000 | 3.485210000 |

**TS2:**

| Element | X  | Y  | Z     |
|---------|----|----|-------|
| H       | 0.543803000 | 8.735523000 | 5.542040000 |
| P       | -2.388371000 | 7.640701000 | 2.877082000 |
| P       | 0.322217000 | 5.953055000 | 4.869904000 |
| O       | -2.607831000 | 7.502565000 | 6.831007000 |
|  | X                  | Y                  | Z                  |
|---|--------------------|--------------------|--------------------|
| N | 0.677212000        | 8.336914000        | 2.836497000        |
| C | -1.588429000       | 8.020255000        | 1.263091000        |
| H | -0.900315000       | 7.188866000        | 1.091110000        |
| C | -2.348906000       | 7.993575000        | 0.480841000        |
| C | -0.828300000       | 9.301072000        | 1.237688000        |
| C | -1.217845000       | 10.373027000       | 0.444116000        |
| H | -2.129839000       | 10.289902000       | -0.138101000       |
| C | -0.440701000       | 11.522276000       | 0.361561000        |
| H | -0.749745000       | 12.346389000       | -0.268827000       |
| C | 0.744599000        | 11.596998000       | 1.084178000        |
| H | 1.362706000        | 12.487078000       | 1.024406000        |
| C | 1.141844000        | 10.556120000       | 1.912968000        |
| C | 0.347818000        | 9.398960000        | 2.011946000        |
| C | 2.353311000        | 10.633414000       | 2.794412000        |
| H | 3.103957000        | 11.310594000       | 2.382330000        |
| H | 2.058996000        | 11.077754000       | 3.758586000        |
| C | 2.927183000        | 9.272402000        | 3.054919000        |
| C | 4.277527000        | 9.063294000        | 3.292083000        |
| H | 4.958901000        | 9.905646000        | 3.229010000        |
| C | 4.756649000        | 7.803513000        | 3.633542000        |
| H | 5.811184000        | 7.651195000        | 3.825322000        |
| C | 3.867156000        | 6.741531000        | 3.725216000        |
| H | 4.227893000        | 5.751308000        | 3.982383000        |
| C | 2.511839000        | 6.911322000        | 3.461753000        |
| C | 2.024376000        | 8.193055000        | 3.126970000        |
| C | 1.564995000        | 5.758968000        | 3.521349000        |
| H | 2.108868000        | 4.823715000        | 3.653318000        |
| H | 0.981350000        | 5.683722000        | 2.598761000        |
| C | -3.242302000       | 6.041895000        | 2.511913000        |
| H | -4.008889000       | 6.290078000        | 1.773491000        |
| C | -3.943930000       | 5.501387000        | 3.749713000        |
| H | -3.266882000       | 5.398001000        | 4.598547000        |
| H | -4.371240000       | 4.518200000        | 3.546027000        |
| H | -4.757981000       | 6.154005000        | 4.064230000        |
| C | -2.282793000       | 5.049048000        | 1.859069000        |
| H | -2.177000000       | 5.244164000        | 0.793117000        |
| H | -2.652418000       | 4.028606000        | 1.971855000        |
| H | -1.279917000       | 5.083910000        | 2.287217000        |
| C | -3.728466000       | 8.926927000        | 2.933547000        |
| H | -3.157365000       | 9.835064000        | 2.711069000        |
| C | -4.360685000       | 9.113566000        | 4.301963000        |
| H | -4.892303000       | 8.222256000        | 4.636741000        |
| H | -5.087853000       | 9.927089000        | 4.263523000        |
| H | -3.620350000       | 9.369190000        | 5.054908000        |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -4.794242 | 8.748403  | 1.862287  |
| H | -4.381170 | 8.584677  | 0.867319  |
| H | -5.415008 | 9.644627  | 1.812211  |
| H | -5.457019 | 7.912693  | 2.092289  |
| C | 1.436201  | 6.047605  | 6.359791  |
| H | 2.115215  | 6.848137  | 6.041440  |
| C | 0.765375  | 6.519499  | 7.640477  |
| H | 0.241310  | 7.463900  | 7.502930  |
| H | 1.523755  | 6.676480  | 8.409687  |
| H | 0.055565  | 5.792857  | 8.033279  |
| C | 2.270680  | 4.798895  | 6.606433  |
| H | 1.666317  | 3.980320  | 6.997307  |
| H | 3.038410  | 5.014358  | 7.351467  |
| H | 2.778245  | 4.443355  | 5.710649  |
| C | -0.602065 | 4.341450  | 4.939294  |
| H | -1.412700 | 4.511239  | 4.231703  |
| C | -1.246691 | 4.105048  | 6.297590  |
| H | -0.514000 | 3.824600  | 7.053780  |
| H | -1.964145 | 3.286011  | 6.222629  |
| H | -1.786855 | 4.978976  | 6.660767  |
| C | 0.162889  | 3.118222  | 4.455701  |
| H | 0.498348  | 3.222781  | 3.424771  |
| H | -0.494500 | 2.247336  | 4.494725  |
| H | 1.032630  | 2.894688  | 5.071814  |
| C | -1.894779 | 7.688099  | 5.930739  |
| Ru| -0.750202 | 7.995534  | 4.538975  |
| N | -1.121518 | 10.199128 | 4.468150  |
| H | 0.053364  | 9.447806  | 5.208357  |
| H | -0.538431 | 10.724514 | 3.824777  |
| C | -1.549878 | 11.050420 | 5.569997  |
| H | -2.258705 | 11.807369 | 5.203806  |
| H | -2.100884 | 10.440273 | 6.290467  |
| C | -0.406960 | 11.735573 | 6.269194  |
| C | 0.185227  | 11.174408 | 7.400920  |
| C | 0.151783  | 12.898488 | 5.737349  |
| C | 1.310042  | 11.748514 | 7.976937  |
| C | 1.273906  | 13.477751 | 6.311403  |
| C | 1.859759  | 12.901293 | 7.431627  |
| H | -0.247475 | 10.276916 | 7.831788  |
| H | -0.300987 | 13.347976 | 4.858745  |
| H | 1.755779  | 11.298458 | 8.855840  |
| H | 1.692334  | 14.382085 | 5.886221  |
| H | 2.735826  | 13.352103 | 7.880846  |
TS3:

O  1.069448000  9.155957000  5.484309000
P -2.370929000  7.727204000  2.996675000
P  0.399299000  6.028278000  4.849066000
O  2.474552000  7.542784000  6.821995000
N  0.679752000  8.358390000  2.725050000
C -1.657879000  7.895718000  1.308085000
H -2.370929000  7.727204000  2.996675000
P  0.399299000  6.028278000  4.849066000
C -1.280373000  10.115009000  0.164693000
H -2.201752000  9.967029000  -0.388218000
C -0.799991000  11.960413000  -0.826411000
O  0.713830000  11.380567000  0.588330000
H  1.341518000  12.244672000  0.395542000
C  1.179450000  10.453407000  1.538061000
C  0.316798000  9.326453000  1.804355000
C  2.356620000  10.617254000  2.366800000
H  3.089571000  11.253385000  1.867118000
H  2.091183000  11.145779000  3.295401000
C  2.941706000  9.284404000  2.726349000
C  4.301537000  9.090577000  2.914046000
H  4.979668000  9.921701000  2.745327000
C  4.795956000  7.623920000  3.340210000
H  5.850810000  7.722066000  3.496221000
C  3.911296000  6.813130000  3.549616000
H  4.284688000  5.841737000  3.856815000
C  2.545144000  6.966502000  3.334866000
H  2.040724000  8.222879000  2.940122000
C  1.613725000  5.809475000  3.481932000
C  2.176743000  4.889087000  3.635866000
H  1.008042000  5.683948000  2.578775000
C  3.347166000  6.154023000  2.875476000
H  4.244988000  6.432763000  2.315327000
C  3.783966000  5.646763000  4.248153000
H  2.936537000  5.475217000  4.902078000
H  4.318406000  4.701046000  4.240831000
C  4.447032000  6.343779000  4.749975000
C  2.606549000  5.095496000  2.064739000
H  2.618565000  5.321366000  0.999910000
C  3.079011000  4.121343000  2.199870000
H  1.560524000  4.994661000  2.359190000
C  3.665132000  9.064234000  3.015496000
S68

H  -3.055787000  9.973291000  3.043101000
C  -4.545582000  9.032031000  4.256770000
H  -5.277774000  8.225825000  4.196523000
H  -5.106174000  9.964913000  4.337334000
H  -3.984084000  9.941886000  1.865144000
C  -4.537166000  9.119821000  1.768534000
H  -3.970074000  9.290857000  0.856640000
H  -5.248689000  9.964913000  1.637210000
C  1.541730000  6.199112000  6.310737000
H  2.174329000  7.020018000  5.956901000
C  0.882813000  6.665377000  7.601827000
H  0.251789000  7.542906000  7.464116000
H  1.653867000  6.928966000  8.328438000
H  0.266777000  5.890567000  8.056810000
C  2.437652000  4.996448000  6.571972000
H  1.883046000  4.163694000  7.004639000
H  3.214376000  5.270745000  7.288260000
H  2.938724000  4.636354000  5.674583000
C  -0.458542000  4.383197000  4.982713000
H  -1.280460000  4.487036000  4.274994000
C  -1.073064000  4.175957000  6.360146000
H  -0.317037000  3.932668000  7.106318000
H  -1.776528000  3.342070000  6.328094000
H  -1.619072000  5.051690000  6.711919000
C  0.349171000  3.171544000  4.540000000
H  0.650614000  3.237098000  3.495539000
H  -0.267147000  2.276075000  4.642090000
H  1.244421000  3.017884000  5.140216000
C  -1.778469000  7.801281000  5.923059000
Ru  -0.679551000  8.103577000  4.500995000
N  -0.815186000  10.284040000  4.397035000
H  -0.808403000  10.612632000  3.437691000
H  0.423330000  9.949789000  5.045950000
C  -1.729677000  11.118643000  5.169929000
H  -1.643354000  12.153695000  4.813947000
H  -2.782548000  10.845390000  5.030533000
C  -1.424349000  11.099745000  6.643425000
C  -0.188409000  11.545962000  7.117105000
C  -2.359139000  10.648850000  7.569529000
C  0.110607000  11.518009000  8.470156000
C  -2.067365000  10.620551000  8.927537000
C  -0.829136000  11.049342000  9.381555000
H  0.546310000  11.916802000  6.409553000
|     |       |       |       |
|-----|-------|-------|-------|
| H   | -3.324427000 | 10.303434000 | 7.216232000 |
| H   | 1.075431000  | 11.867593000 | 8.817049000 |
| H   | -2.807434000 | 10.257188000 | 9.630209000 |
| H   | -0.597016000 | 11.024953000 | 10.438995000 |
| H   | 0.948235000  | 9.232631000  | 6.439910000 |

**TS4:**

|     |       |       |       |
|-----|-------|-------|-------|
| P   | -2.454343000 | 7.836564000 | 2.649420000 |
| P   | 0.229859000  | 6.542721000  | 5.064913000  |
| O   | -2.815728000 | 8.296709000  | 6.547635000  |
| N   | 0.655526000  | 8.526580000  | 2.593850000  |
| C   | -1.578791000 | 7.879781000  | 1.033940000  |
| H   | -0.891234000 | 7.030976000  | 1.070244000  |
| H   | -2.297077000 | 7.693652000  | 0.233425000  |
| C   | -0.809778000 | 9.130735000  | 0.783564000  |
| C   | -1.178789000 | 10.006069000 | -0.230412000 |
| H   | -2.076156000 | 9.792478000  | -0.802170000 |
| C   | -0.398142000 | 11.110778000 | -0.545322000 |
| H   | -0.689345000 | 11.778737000 | -1.345993000 |
| C   | 0.776313000  | 11.327074000 | 0.163229000  |
| H   | 1.411306000  | 12.171888000 | -0.084577000 |
| C   | 1.153408000  | 10.492100000 | 1.206605000  |
| C   | 0.345479000  | 9.392873000  | 1.556773000  |
| C   | 2.392571000  | 10.762146000 | 2.007881000  |
| H   | 3.172651000  | 11.192839000 | 1.374533000  |
| H   | 2.186029000  | 11.542728000 | 2.754217000  |
| C   | 2.897515000  | 9.526681000  | 2.694768000  |
| C   | 4.225165000  | 9.414986000  | 3.085044000  |
| H   | 4.904658000  | 10.231105000 | 2.860502000  |
| C   | 4.685770000  | 8.294239000  | 3.763361000  |
| H   | 5.721205000  | 8.223195000  | 4.071039000  |
| C   | 3.801124000  | 7.256975000  | 4.023802000  |
| H   | 4.147833000  | 6.359969000  | 4.526132000  |
| C   | 2.471583000  | 7.322632000  | 3.621872000  |
| C   | 1.988174000  | 8.483482000  | 2.972159000  |
| C   | 1.558900000  | 6.164364000  | 3.850322000  |
| H   | 2.126905000  | 5.296431000  | 4.185904000  |
| H   | 1.037138000  | 5.890853000  | 2.928094000  |
| C   | -3.349462000 | 6.217568000  | 2.568947000  |
| H   | -4.122062000 | 6.349004000  | 1.806915000  |
| C   | -4.034081000 | 5.907729000  | 3.891459000  |
| H   | -3.323063000 | 5.865632000  | 4.717530000  |
| H   | -4.539530000 | 4.941905000  | 3.840593000  |
| H   | -4.782528000 | 6.657468000  | 4.146791000  |

S69
C  -1.034848000  12.043417000  8.070812000
C   1.359634000  11.911179000  7.926092000
C  -0.215392000  12.238655000  8.642424000
H  -2.127656000  11.367916000  6.358872000
H   2.137988000  11.116339000  6.086999000
H   0.297647000  12.646542000  9.641919000

Water:
O  -1.120191000  0.000000000  -0.070599000
H  -1.120191000  0.756126000   0.525818000
H  -1.120191000  0.756126000  -0.525818000

1i:
N  -0.828890000  -0.009859000  -0.893455000
H  -0.823732000   0.983247000  -0.696437000
H  -1.712384000  -0.188577000  -1.358742000
C  -0.785088000  -0.740766000   0.364379000
H   0.106830000  -0.415442000   0.908442000
H  -1.627405000  -0.188577000  -1.358742000
C  -0.807360000  -3.058071000   1.309244000
C  -0.502380000  -4.212910000  -1.184543000
C  -0.737308000  -4.436043000   1.189939000
C  -0.584325000  -5.021471000  -0.061746000
H  -0.497470000  -2.204480000  -1.942013000
H  -0.932961000  -2.607157000   2.288062000
H  -0.386085000  -4.657766000  -2.165539000
H  -0.804999000  -5.057134000   2.074878000
H  -0.533171000  -6.098833000  -0.157929000

1-Phenylethane-1-imine:
N  -1.020470000  -0.064366000  -0.894671000
H  -0.166102000   0.469212000  -1.042203000
C  -1.005499000  -0.609586000   0.256295000
H  -0.169174000  -0.493421000   0.956389000
C  -2.100081000  -1.442263000   0.756388000
C  -3.243652000  -1.693251000  -0.007389000
C  -2.000418000  -2.004120000   2.030845000
C  -4.259005000  -2.484517000   0.495832000
C  -3.018975000  -2.794955000   2.535274000
C  -4.149369000  -3.037419000   1.768328000

S71
|  | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -3.320276 | -1.258714 | -0.996477 |
| H | -1.113217 | -1.806295 | 2.622975  |
| H | -5.142190 | -2.675253 | -0.100935 |
| H | -2.931438 | -3.223875 | 3.525409  |
| H | -4.946881 | -3.656895 | 2.159241  |

**Hydrogen:**

|  | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | 0.053636  | -0.004747 | 0.000000  |
| H | 0.795664  | -0.070413 | 0.000000  |
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