Supporting Information

Highly Selective Directed Iridium-Catalyzed Hydrogen Isotope Exchange Reactions of Aliphatic Amides
Mégane Valero, Remo Weck, Stefan Güssregen, Jens Atzrodt,* and Volker Derdau

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Experimental

General

Commercially available chemicals and solvents were used as received. Deuterium (99.9\%D) was purchased in from Sigma Aldrich in 12l bottles. $^1$H and $^{13}$C NMR spectra were obtained on Bruker Avance 300 and 400 spectrometers (Bruker, Rheinstetten, Germany). The chemical shifts ($\delta$) are expressed in ppm and are given relative to the residual proton signal of dmoso-d6 ($\delta$ 2.50 ppm) or chloroform-d ($\delta$ 7.26 ppm). NMR assignments were made using additional 2D NMR experiments. The listed $^1$H NMR spectra show sequential the substrate before reaction and two spectra of the substrate after HIE reaction with catalyst 1. $^3$H-NMR spectra were recorded on a Bruker Avance 500 spectrometer (Bruker, Rheinstetten, Germany) equipped with a tritium specific SEX-probe (533 MHz). HRMS was provided via a Bruker micro-TOF-QII in positive ESI mode. Calibration was achieved against a sodium formate injection. A Dionex Ultimate 3000 RSLC system was used as an inlet to the MS, employing a flow of 0.5 mL min$^{-1}$ of 0.044 \% TFA in 50\% acetonitrile (aq.).

Silica-gel column chromatography was carried out with SiO$_2$ (Merck, 0.063-0.200 mesh). The purity of the products was determined by an LC-MS system with a Symmetry Shield RP18 column, 3.9x150 mm with a gradient program under the following conditions: mobile phase A: water (900 mL), acetonitrile (100 mL), TFA (1 mL); mobile phase B: water (100 mL), acetonitrile (900 mL), TFA (0.75 mL); flow 1.5 mL/min; detection UV 254 nm and UV 210 nm.

General HIE protocol (Method A):

All screenings were performed in a Radleys synthesis station for parallel solution phase chemistry. Therefore into a flask a stirring bar, the substrate (1 eq, 500 µL), the catalyst (10 mol\%, 0.1eq. 500µL) were added. After the vial was sealed with open connection to the gas inlet and then evacuated until slight bubbling of the solution and then refilled with deuterium gas from a balloon for three times, the vial was closed and put into the preheated synthesis station. The reaction was stirred (500 rpm) under D$_2$ atmosphere (1 atm) for the appropriate time and temperature. The crude reaction mixture was purified by silica gel chromatography and analyzed by NMR.

Fig. S1: Radleys synthesis station for parallel solution phase chemistry.
Commercially available catalysts

A
CAS 34801-95-1

B
CAS 369657-32-9

C
CAS 1194050-23-1

D
CAS 1019852-99-3

E
CAS 64536-78-3

F
CAS 2071645-61-7

1
CAS 1019852-99-3
A) Catalyst Screening

The following catalysts A-F and 1 were used in the screening at 25°C (DCM) and 50°C in isopropyl acetate.

Table 1: Catalyst screening in the HIE reaction of amide 4.\textsuperscript{a,b}

\[
\begin{array}{cccc}
\text{Entry} & \text{Catalyst} & \text{Solvent} & \text{T°C} & \text{D/molecule} \\
1 & A & \text{Dichloromethane} & \text{RT} & 0 \\
2 & B & \text{Dichloromethane} & \text{RT} & 0 \\
3 & C & \text{Dichloromethane} & \text{RT} & 0 \\
4 & D & \text{Dichloromethane} & \text{RT} & 0 \\
5 & 1 & \text{Dichloromethane} & \text{RT} & 0 \\
6 & E & \text{Dichloromethane} & \text{RT} & 0 \\
7 & F & \text{Dichloromethane} & \text{RT} & 0 \\
8 & A & \text{Isopropyl acetate} & \text{50°C} & 0 \\
9 & B & \text{Isopropyl acetate} & \text{50°C} & 0.8 \\
10 & C & \text{Isopropyl acetate} & \text{50°C} & 0 \\
11 & D & \text{Isopropyl acetate} & \text{50°C} & 0.6 \\
12 & 1 & \text{Isopropyl acetate} & \text{50°C} & 2.0 \\
13 & E & \text{Isopropyl acetate} & \text{50°C} & 0.5 \\
14 & F & \text{Isopropyl acetate} & \text{50°C} & 0 \\
\end{array}
\]
Solvent screening of catalyst 1 in the HIE reaction of 4-[(4-methyl)dithio]-4-methyl-N-(benzyl)-pentanamide 4

For the screening of different solvents, 4-[(4-methyl)dithio]-4-methyl-N-(benzyl)-pentanamide 4 in solvent (14 μmol, 500 μL, 1 eq.), the catalyst 1 (2.4 mg, 1.4 μmol, 10 mol%, 0.1 eq.) and the different solvents were used. All reactions were performed according to the general method A at 50°C for 3 h.

Table 2: Solvent screening of catalyst 1 in the HIE reaction of amide 4. a,b

| Entry | Solvent          | D/molecule |
|-------|------------------|------------|
| 1     | chloroform       | 1.1        |
| 2     | MTBE             | 0.5        |
| 3     | ethanol          | 1.2        |
| 4     | MeTHF            | 0.5        |
| 5     | isopropylacetate | 2.0        |
| 6     | chlorobenzene    | 1.8        |

aConditions: substrate 4 (4.0 mg, 14 μmol), catalyst 1 (2.4 mg, 1.4 μmol, 10 mol%), solvent (1 mL), D₂ (1atm), 50°C, 3 h. bPosition determined by ¹H NMR and percentage of deuterium incorporation analysed by LC-MS.
**General procedure for parameter screening:** For the screening of catalyst ratio and temperature amides 2-4 in isopropyl acetate (2.5 µmol, 500 µL, 1 eq.), the catalyst 1 (10-50 mol%) were used. All reactions were performed according to the general method A for 3 h.

**Table 3:** Evaluation of catalyst loading and temperature in the HIE reaction of amides 2-4 and catalyst 1,\(^a,b\)

![Chemical structures](attachment:image.png)

| Substrate | catalyst 1 | Temp. | D/molecule |
|-----------|------------|-------|------------|
| 2         | 50%        | 22°C  | 2          |
| 3         | 50%        | 22°C  | 2          |
| 4         | 50%        | 22°C  | 2          |
| 2         | 25%        | 22°C  | 2          |
| 3         | 25%        | 22°C  | 2          |
| 4         | 25%        | 22°C  | 1,9        |
| 2         | 25%        | 50°C  | 2          |
| 3         | 25%        | 50°C  | 2          |
| 4         | 25%        | 50°C  | 2          |
| 2         | 10%        | 80°C  | 2          |
| 3         | 10%        | 80°C  | 2          |
| 4         | 10%        | 80°C  | 2          |
| 2         | 5%         | 80°C  | 0,5        |
| 3         | 5%         | 80°C  | 0,7        |
| 4         | 5%         | 80°C  | 0,6        |

\(^a\)Conditions: Isopropyl acetate 1mL, 2.5 µmol substrate 2-4, D₂ 1 atm, 3h; \(^b\)Positions determined by \(^1\)H-NMR and percentage of deuterium incorporation determined by LC-MS
4-[(4-methyl)dithio]-4-methyl-\(N\)-(propyl)-pentanamide 2

\[
\text{Molecular Weight } = 235.4130 \\
\text{Molecular Formula } = \text{C}_{10}\text{H}_{21}\text{NOS}_2
\]

**Method A:** 3.00 mg (13.0 \(\mu\)mol) 2; 2.3 mg (1.3 \(\mu\)mol) catalyst 1, 3h

\(^1\text{H NMR (300 MHz, CDCl}_3\):} \ \delta 5.56 (br s, 1H, \(\text{NH}\)), 3.17 (dd, \(^3\text{J} = 6.9 \text{ Hz}, ^3\text{J} = 6.9 \text{ Hz}, 2\text{H}), 2.35 (s, 3\text{H}, \text{SCH}_3), 2.23-2.18 (m, 2\text{H}), 1.91-1.86 (m, 2\text{H}), 1.51 (dt, \(^3\text{J} = 6.9 \text{ Hz}, ^3\text{J} = 7.5 \text{ Hz}, 2\text{H}), 1.23 (s, 6\text{H}, \text{CH}_3), 0.88 (t, \(^3\text{J} = 7.5 \text{ Hz}, 3\text{H}) \text{ ppm. Incorporation expected at } \delta 1.91-1.86 \text{ (red arrow). Determined against integral at } \delta 2.35 \text{ (blue arrow).}

**HRMS (positive ESI):** \(m/z\) calculated for \(\text{C}_{10}\text{H}_{21}\text{NOS}_2 [\text{M+H}]^+: 236.1137\); found: 263.1139.

**Yield:** 2.60 mg, 11.0 \(\mu\)mol, 88%; 99\%D for \(\delta 1.91-1.86\).
4-[(4-methyl)dithio]-4-methyl-N-(diethyl)-pentanamide 3

\[
\begin{align*}
\text{Molecular Weight} & = 249.4401 \\
\text{Molecular Formula} & = C_{11}H_{23}NOS_2
\end{align*}
\]

**Method A:** 3.00 mg (12.0 \(\mu\)mol) 3; 2.1 mg (1.2 \(\mu\)mol) catalyst 1, 3h

\(^1\text{H NMR (300 MHz, CDCl}_3\)): 3.33-3.22 (m, 4H), 2.34 (s, 3H, SCH\(_3\)), 2.27-2.24 (m, 2H), 1.87-1.80 (m, 2H) 1.25 (s, 6H), 1.15 (t, \(^3\text{J} = 7.2 \text{ Hz}, 3\text{H})\), 1.06 (t, \(^3\text{J} = 7.2 \text{ Hz}, 3\text{H})\) ppm.  
Incorporation expected at \(\delta\) 1.87-1.80 (red arrow). Determined against integral at \(\delta\) 3.33-3.22 (blue arrow).

**HRMS (positive ESI):** m/z calculated for C\(_{11}\)H\(_{23}\)NOS\(_2\) [M+H]\(^+\): 250.1293; found: 250.1300.

**Yield:** 2.80 mg, 11.0 \(\mu\)mol, 93%; 99%\(D\) for \(\delta\) 1.87-1.80

3\(^\text{H-NMR Reference 3}\)

3\(^\text{H-NMR HIE reaction 3}\)
4-[(4-methyl)dithio]-4-methyl-\(\text{N}\)-(benzyl)-pentanamide 4

\[
\text{Molecular Weight = 283.4576}
\]
\[
\text{Molecular Formula = C}_{14}\text{H}_{21}\text{NOS}_{2}
\]

**Method A**: 3.50 mg (12.0 \(\mu\)mol) 4; 2.1 mg (1.2 \(\mu\)mol) catalyst 1, 3h

\(^1\text{H} \text{NMR (300 MHz, CDCl}_3\text{):} \delta 7.28\text{-}7.16 \text{ (m, 5H), 5.90 (br s, 1H, NH), 4.36 (d, }^3\text{J}=6.9 \text{ Hz, 2H, CH}_2\text{Ph), 2.32 (s, 3H, SCH}_3\text{), 2.22\text{-}2.16 \text{ (m, 2H), 1.90\text{-}1.85 \text{ (m, 2H), 1.22 (s, 6H, CH}_3\text{) ppm.}
\]

Incorporation expected at \(\delta 1.90\text{-}1.85\) (red arrow). Determined against integral at \(\delta 4.36\) (blue arrow).

**HRMS (positive ESI)**: \(\text{m/z} \text{ calculated for C}_{14}\text{H}_{21}\text{NOS}_{2} [\text{M}+\text{H}]^+: 284.1137\); found: 284.1151.

**Yield**: 3.20 mg, 11.0 \(\mu\)mol, 91%; 99%D for \(\delta 1.90\text{-}1.85\).

\(^1\text{H-NMR Reference 4}\)

\(^1\text{H-NMR HIE reaction 4}\)
L-Alanine, N-[4-methyl-4-(methylthio)-1-oxopentyl]-methyl ester 5

Method A: 5.00 mg (19.0 µmol) 5; 3.3 mg (1.9 µmol) catalyst 1, 3h

$^1$H NMR (300 MHz, CDCl$_3$): δ 6.13 (br s, 1H, NH), 4.57 (dt, $^3$J=6.9 Hz, $^3$J=7.5 Hz, 1H), 3.69 (s, 3H, COOC$_2$H$_5$), 2.35 (s, 3H, SCH$_3$), 2.29-2.23 (m, 2H), 1.91-1.85 (m, 2H), 1.35 (d, $^3$J=7.5 Hz, 3H), 1.23 (s, 6H, CH$_3$) ppm. Incorporation expected at δ 1.91-1.85 (red arrow). Determined against integral at δ 2.35 (blue arrow).

HRMS (positive ESI): m/z calculated for C$_{11}$H$_{19}$NO$_3$S$_2$ [M+H]$^+$: 280.1035; found: 280.1045.

Yield:  

a) 4.35 mg, 15.0 µmol, 87%; 99% D for δ 1.91-1.85.  
b) 4.55 mg, 16.0 µmol, 91%; 99% D for δ 1.91-1.85.

Average: y=89%, 99%

$^1$H-NMR Reference 5

$^1$H-NMR HIE reaction 5
L-Serine, N-[4-methyl-4-(methyldithio)-1-oxopentyl]-ethyl ester 6

Molecular Weight = 309.4494
Molecular Formula = C_{12}H_{23}NO_{4}S_{2}

**Method A:** 5.00 mg (16.0 µmol) 6; 2.8 mg (1.6 µmol) catalyst 1, 3h

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 6.73 (br s, 1H, NH), 4.65-4.58 (m, 1H), 4.25 (q, $^3$J=7.5 Hz, 2H, OCH$_2$CH$_3$), 3.96 (dd, $^3$J=9.6 Hz, $^3$J=3.9 Hz, 2H, CH$_2$OH), 2.39 (s, 3H, SCH$_3$), 2.37-2.33 (m, 2H), 1.96-1.90 (m, 2H), 1.29-1.25 (m, 9H) ppm. Incorporation expected at $\delta$ 1.96-1.90 (red arrow). Determined against integral at $\delta$ 4.25 (blue arrow).

**HRMS (positive ESI):** m/z calculated for C$_{12}$H$_{23}$NO$_4$S$_2^+$ [M+H]$^+$: 310.1141; found: 310.1144.

**Yield:**
- a) 4.50 mg, 15.0 µmol, 90%; 98% D for $\delta$ 1.96-1.90.
- c) 4.90 mg, 16.0 µmol, 98%; 91% D for $\delta$ 1.96-1.90.

**Average:** y=94%, 95%
Glycine, N-[4-methyl-4-(methyldithio)-1-oxopentyl]-ethyl ester 7

\[
\text{O} \quad \text{N} \quad \text{C} \quad \text{O} \\
\text{S} \quad \text{S} \quad \text{O} \quad \text{O}
\]

**Molecular Weight =** 265.3958  
**Molecular Formula =** \( \text{C}_{10}\text{H}_{19}\text{NO}_{3}\text{S}_{2} \)

**Method A:** 5.00 mg (19.0 μmol) 7; 3.3 mg (1.9 μmol) catalyst 1, 3h

\(^1\text{H NMR (300 MHz, CDCl}\text{3})\): \( \delta \) 6.11 (br s, 1H, NH), 3.99 (d, \( \text{J}=5.4 \text{ Hz} \), 2H, \( \text{CH}_{2}\text{NH} \)), 3.70 (s, 3H, \( \text{COOC}\text{H}\text{3} \)), 2.35 (s, 3H, \( \text{SCH}\text{3} \)), 2.29-2.23 (m, 2H), 1.89-1.84 (m, 2H), 1.24 (s, 6H, \( \text{CH}_{3} \)) ppm. Incorporation expected at \( \delta \) 1.89-1.84 and 3.99 (red arrows). Determined against integral at \( \delta \) 3.70 (blue arrow).

**HRMS (positive ESI):** m/z calculated for \( \text{C}_{10}\text{H}_{19}\text{NO}_{3}\text{S}_{2}^{+} \) [M+H]\(^{+}\): 266.0879; found: 266.0888.

**Yield:**  
 a) 4.25 mg, 16.0 μmol, 85%; 42% D for \( \delta \) 1.89-1.84 and 88% D for \( \delta \) 3.99.  
 d) 4.90 mg, 18.0 μmol, 98%; 30% D for \( \delta \) 1.89-1.84 and 80% D for \( \delta \) 3.99.

**Average:** y=92%  
84% D \( \delta \) 3.99  
36% D \( \delta \) 1.89-1.84

\(^1\text{H-NMR Reference 7} \)
Deuteration of DM4 derivatives 8a-c
Deuteration of DM4-H 8a

**Method A:** 2.00 mg (2.5 µmol) 8a; 0.5 mg (0.25 µmol) catalyst 1, 50°C, 3h

**MS (positive ESI):** m/z = 762.3 (M-\(\text{H}_2\text{O}+\text{H}\))\(^+\) (13); 763.3 (M-\(\text{H}_2\text{O} + \text{D}_1 + \text{H}\))\(^+\) (22), 764.3 (M-\(\text{H}_2\text{O} + \text{D}_2 + \text{H}\))\(^+\) (24), 765.3 (M-\(\text{H}_2\text{O} + \text{D}_3 + \text{H}\))\(^+\) (19), 766.3 (M-\(\text{H}_2\text{O} + \text{D}_4 + \text{H}\))\(^+\) (12), 767.3 (M-\(\text{H}_2\text{O} + \text{D}_5 + \text{H}\))\(^+\) (6). Calculated D-content/molecule: 2.0

**Yield:** 1.3 mg (1.6 µmol) 8a, 65%

No determination of labelling position with \(^1\text{H}-\text{NMR}\) possible.
Deuteration of DM4-Me 8b

**Method A**: 2.00 mg (2.5 μmol) 8b; 0.5 mg (0.25 μmol) catalyst 1, 50°C, 3h

**MS (positive ESI)**: m/z = 776.3 (M-H$_2$O+H)$^+$ (14); 777.3 (M-H$_2$O +D$_1$+H)$^+$ (21), 778.3 (M-H$_2$O +D$_2$+H)$^+$ (27), 779.3 (M-H$_2$O+D$_3$+H)$^+$ (22), 780.3 (M-H$_2$O+D$_4$+H)$^+$ (15). Calculated D-content/molecule: **2.0**

Yield: 1.6 mg (2.0 μmol) 8b, 80%

No determination of labelling position with $^1$H-NMR possible.
Deuteration of DM4-Me 8c

**Method A:** 2.00 mg (2.5 μmol) 8c; 0.5 mg (0.25 μmol) catalyst 1, 50°C, 3h

**MS (positive ESI):** m/z = 808.3 (M-H₂O+H)⁺ (4); 809.3 (M-H₂O+D₁+H)⁺ (22), 810.3 (M-H₂O+D₂+H)⁺ (47), 811.3 (M-H₂O+D₃+H)⁺ (20), 812.3 (M-H₂O+D₄+H)⁺ (3). Calculated D-content/molecule: **1.9**

Yield: 1.6 mg (2.0 μmol) 8c, 80%

No determination of labelling position with ¹H-NMR possible.
Tritiation of DM4-SMe 8c (reaction 1; 7 eq tritium)

The tritiation of DM4-SMe 8c was carried out using a standard Tritec® tritium manifold. DM4-SMe (4.0 mg, 4.8 µmol) 8c, and catalyst 1 (2.1 mg, 1.2 µmol, 25 mol%) were dissolved in isopropyl acetate (0.7 mL) in a 1.0 mL reaction flask before being connected to the manifold. The solution was frozen in liquid nitrogen and the flask was evacuated, then charged with tritium (1.9 Ci, 61 mbar, 7eq.). The reaction mixture was then allowed to warm to room temperature over 15 min before stirring at r.t. for a further 30 min (168mbar pressure). The reaction mixture was then heated to 50 °C (245 mbar pressure) and stirred for 180 min before cooling again to r.t. The solvents was evaporated; methanol added and the solvent evaporated into a waste ampulle. This procedure was repeated three times in total. The residue was dissolved in methanol and filtered. Purification and isolation via HPLC gave the tritiated product (3.1 mg, 3.7 µmol 8c, 96.4% radiochemical purity, 1374 MBq, 0.37 TBq/mmol = 10 Ci/mmol).

**MS (positive ESI):** m/z 808.3 [M-H₂O+H]⁺, 810.3 [M(T)-H₂O+H]⁺; 848.3 [M+Na]⁺; 826.3 [M+H]⁺

MS (DM4-SMe 8c, unlabelled)  
MS (DM4-SMe 8c, ³H-labelled)
$^1$H-NMR: DM4-SMe 8c unlabeled comparison (upper spectra); $^3$H-DM4-SMe 8c (below)

$^3$H-NMR (533 MHz): $^3$H-DM4-SMe 8c

$^3$H NMR 8c (533 MHz, DMSO-d$_6$): δ 2.52-2.43, 2.25-2.16 (m, 2H, 6%); 1.98-1.66 (m, 2H, 94%) ppm.
Tritiation of DM4-SMe 8c (reaction 2; 12 eq tritium)

The tritiation of DM4-SMe 8c was carried out using a standard Tritec® tritium manifold. DM4-SMe (3.0 mg, 3.3 µmol) 8c, and catalyst 1 (3.0 mg, 1.7 µmol, 51 mol%) were dissolved in isopropyl acetate (0.7 mL) in a 1.0 mL reaction flask before being connected to the manifold. The solution was frozen in liquid nitrogen and the flask was evacuated, then charged with tritium (2.5 Ci, 74 mbar, 12eq.). The reaction mixture was then allowed to warm to room temperature over 15 min before stirring at r.t. for a further 30 min (186 mbar pressure). The reaction mixture was then heated to 50 °C (270 mbar pressure) and stirred for 180 min before cooling again to r.t. The solvents was evaporated; methanol added and the solvent evaporated into a waste ampule. This procedure was repeated three times in total. The residue was dissolved in methanol and filtered. Purification and isolation via HPLC gave the tritiated product (1.7 mg, 1.9 µmol 8c, 96.7% radiochemical purity, 2787 MBq; 1.15 TBq/mmol = 31 Ci/mmol).

**MS (positive ESI):** \(m/z\ 808.3\ [M-H_2O+H]^+;\ 810.3\ [M(T)-H_2O+H]^+;\ 848.3\ [M+Na]^+;\ 826.3\ [M+H]^+\)
Glycine, \( N\)-[4-methyl-4-methoxy-1-oxopentyl]-methyl ester 9

![Molecular Structure 9]

\[ \text{Molecular Weight} = 203.2401 \]
\[ \text{Molecular Formula} = \text{C}_9\text{H}_{17}\text{NO}_4 \]

**Method A:** 7.00 mg (35.0 \( \mu \)mol) 9; 6.1 mg (3.5 \( \mu \)mol) catalyst 1, 3h

\(^1\text{H NMR (300 MHz, CDCl}_3\)): \( \delta \) 6.21 (br s, 1H, \( \text{NH} \)), 3.99 (dd, \(^3\text{J}=9.6\ \text{Hz}, \(^3\text{J}=7.5\ \text{Hz}, 2\text{H}, \text{CH}_2\text{NH} \)), 3.69 (s, 3H, \text{COOC}_3\text{H}_3 \)), 3.33-3.29 (m, 1H), 3.26 (s, 3H, \text{OCH}_3 \)), 2.31 (t, \(^3\text{J}=7.5\ \text{Hz}, 2\text{H} \)), 1.81-1.65 (m, 2H), 1.09 (d, \(^3\text{J}=6.6\ \text{Hz}, 3\text{H} \)) ppm. Incorporation expected at \( \delta \) 3.99 (red arrow). Determined against integral at \( \delta \) 3.69 (blue arrow).

**HRMS (positive ESI):** m/z calculated for \( \text{C}_9\text{H}_{17}\text{NO}_4^+ \): 204.1230; found: 204.1234.

**Yield:** 5.30 mg, 26.0 \( \mu \)mol, 76%; 93%\( \text{D} \) for \( \delta \) 3.99.

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**1H-NMR Reference 9**

**1H-NMR HIE reaction 9**
Glycine, \( N\-[4\text{-methoxy-1-oxopentyl}]-\text{methyl ester} \, 10 \)

\[
\begin{align*}
\text{O} & \text{N} & \text{O} \\
\text{10}
\end{align*}
\]

**Method A**: 9.50 mg (50.0 \( \mu \text{mol} \)) 10; 8.7 mg (5.0 \( \mu \text{mol} \)) catalyst 1, 3h

\( ^1H \text{NMR (300 MHz, CDCl}_3 \)): \( \delta \) 6.43 (br s, 1H, NH), 3.98 (d, \( ^3J=8.1 \text{ Hz, 2H, CH}_2\text{NH} \)), 3.69 (s, 3H, COOCH\(_3\)), 3.38 (t, \( ^3J=12.0 \text{ Hz, 2H} \)), 3.27 (s, 3H, OCH\(_3\)), 2.31 (t, \( ^3J=7.2 \text{ Hz, 2H} \)), 1.89-1.80 (m, 2H) ppm. Incorporation expected at \( \delta \) 3.99 (red arrow). Determined against integral at \( \delta \) 3.69 (blue arrow).

**HRMS (positive ESI)**: m/z calculated for C\(_8\)H\(_{15}\)NO\(_4\)^+ [M+H]^+: 190.1074; found: 190.1074.

**Yield**: 6.80 mg, 36.0 \( \mu \text{mol} \), 72%; 92\%D for \( \delta \) 3.99.
Protected glycine methyl ester 11 a-e

|   | PG | %D | %Yield |
|---|----|----|--------|
| a | Ac | 93 | 99     |
| b | Cbz | 50 | 98    |
| c | FMoc | 30 | 72    |
| d | Boc | 0  | n.d.  |
| e | Bn  | 0  | n.d.  |

**Method A**: 10.0 mg (76.0 μmol) 11a; 13.0 mg (7.6 μmol) catalyst 1, 8h
10.0 mg (45.0 μmol) 11b; 7.8 mg (4.5 μmol) catalyst 1, 8h
10.0 mg (32.0 μmol) 11c; 5.5 mg (3.2 μmol) catalyst 1, 8h
10.0 mg (53.0 μmol) 11d; 9.2 mg (5.3 μmol) catalyst 1, 8h
10.0 mg (56.0 μmol) 11e; 9.7 mg (5.6 μmol) catalyst 1, 8h

**Yield** 11a: 9.90 mg, 75.0 μmol, 99%; 93%D for δ 3.89.
11b: 9.80 mg, 43.0 μmol, 98%; 50%D for δ 3.99.
11c: 7.20 mg, 23.0 μmol, 72%; 30%D for δ 3.95.
11d: 0%D for δ 3.65.
11e: 0%D for δ 3.82.

**1H-NMR Reference 11a**

**1H-NMR HIE reaction 11a**

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22
$^{1}H$-NMR Reference 11b

$^{1}H$-NMR HIE reaction 11b

$^{1}H$-NMR Reference 11c

$^{1}H$-NMR HIE reaction 11c
L-Ac-Ala-OMe 12a

Molecular Weight = 145.1595
Molecular Formula = C₆H₁₁NO₃

Method A: 10.0 mg (69.0 μmol) 12a; 12 mg (6.9 μmol) catalyst 1, 8h

¹H NMR (300 MHz, CDCl₃): δ 6.36 (br s, 1H, NH), 4.51-4.42 (m, 1H), 3.61 (s, 3H, COOC₃H₇), 1.89 (s, 3H, COCH₃), 1.28 (d, 3J= 9.0 Hz, 3H) ppm. Incorporation expected at δ 4.51-4.42 (red arrow). Determined against integral at δ 3.61 (blue arrow).

Yield: 6.50 mg, 45.0 μmol, 65%; 50% D for δ 4.51-4.42

¹H-NMR Reference 12a

¹H-NMR HIE reaction 12a
D-Ac-Ala-OMe 12b

Molecular Weight = 145.1595
Molecular Formula = C₆H₁₁NO₃

Method A: 10.0 mg (69.0 μmol) 12b; 12 mg (6.9 μmol) catalyst 1, 8h

¹H NMR (300 MHz, CDCl₃): δ 6.75 (br s, 1H, NH), 4.55-4.45 (m, 1H), 3.67 (s, 3H, COOC₃H₃), 1.94 (s, 3H, COCH₃), 1.33 (d, 3J= 9.0 Hz, 3H) ppm. Incorporation expected at δ 4.51-4.42 (red arrow). Determined against integral at δ 3.61 (blue arrow).

Yield: 7.8 mg, 54.0 μmol, 78%; 50% D for 4.51-4.42.
In all HIE reactions of 12a and 12b no isomerization of the stereocenter was observed.
Ac-beta-Ala-ethyl ester 14

\[
\text{Ac-Beta-Ala-OEt}
\]

Molecular Weight = 159.1866
Molecular Formula = C7H13NO3

**Method A:** 10.0 mg (63.0 μmol) 14; 11 mg (6.3 μmol) catalyst 1, 8h

\(^1\text{H NMR (300 MHz, CDCl}_3\): \(\delta\) 6.50 (br s, 1H, NH), 4.11 (dt, \(^3\text{J}= 6.9\) Hz, \(^3\text{J}= 6.9\) Hz, 2H), 3.46 (q, \(^3\text{J}= 6.9\) Hz, 2H, OCH\(_2\)CH\(_3\)), 2.48 (t, \(^3\text{J}= 6.9\) Hz, 2H), 1.94 (s, 3H, COCH\(_3\)), 1.21 (t, \(^3\text{J}= 6.9\) Hz, 3H, OCH\(_2\)CH\(_3\)) ppm. Incorporation expected at \(\delta\) 3.46 (red arrow). Determined against integral at \(\delta\) 1.89 (blue arrow).

**Yield:** 9.50 mg, 60.0 μmol, 95%; 91%\(^D\) for \(\delta\) 3.46.
L-Ac-Gly-Phe-methyl ester 15

Method A: 10.0 mg (36.0 μmol) 15; 6.2 mg (3.6 μmol) catalyst 1, 8h

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 7.32-7.05 (m, 5H, arom. CH), 6.51 (br s, 1H, NH), 6.28 (br s, 1H, NH), 4.88-4.83 (m, 1H), 3.95-3.88 (m, 2H), 3.74 (s, 3H, COOCH$_3$), 3.22-3.05 (m, 2H), 2.01 (s, 3H, COCH$_3$) ppm. Incorporation expected at $\delta$ 3.95-3.88 (red arrow). Determined against integral at $\delta$ 3.74 (blue arrow).

Yield: a) 9.00 mg, 32.0 μmol, 90%; 50% D for $\delta$ 3.95-3.88.  
    b) 8.70 mg, 31.0 μmol, 87%; 60% D for $\delta$ 3.95-3.88.  

Average: $y$=89%, 55%
L-Ac-Gly-Tyr(OtBu)-tert-butyl ester 16

Method A: 10.0 mg (26.0 μmol) 16; 4.5 mg (2.6 μmol) catalyst 1, 8h

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 7.06 (d, $^3$J = 8.7 Hz, 2H), 6.93 (d, $^3$J = 8.7 Hz, 2H), 6.26 (br s, 1H, NH), 6.12 (br s, 1H, NH), 4.75-4.68 (m, 1H), 3.94-3.91 (m, 2H), 3.06 (d, $^3$J = 7.2 Hz, 2H), 2.03 (s, 3H, COCH$_3$), 1.52-1.35 (m, 18H, OtBu) ppm. Incorporation expected at $\delta$ 3.94-3.91 (red arrow). Determined against integral at $\delta$ 3.06 (blue arrow).

Yield: a) 7.40 mg, 19.0 μmol, 74%; 93% D for $\delta$ 3.94-3.91.
c) 6.60 mg, 17.0 μmol, 66%; 93% D for $\delta$ 3.94-3.91.

$^1$H-NMR Reference 16

$^1$H-NMR HIE reaction 16

Average: $y$=70%, 93%
L-Ac-Gly-Gly-methyl ester 17

Method A: 10.0 mg (53.0 μmol) 17; 9.2 mg (5.3 μmol) catalyst 1, 8h

$^1$H NMR (300 MHz, CDCl$_3$): δ 6.45 (br s, 1H, NH), 6.17 (br s, 1H, NH), 4.00 (d, $^3$J = 5.4 Hz, 2H), 3.93 (d, $^3$J = 5.4 Hz, 2H), 3.70 (s, 3H, COOCH$_3$), 1.99 (s, 3H, COCH$_3$) ppm. Incorporation expected at δ 3.93 and 4.00 (red arrow). Determined against integral at δ 3.70 (blue arrow).

Yield: a) 9.70 mg, 52.0 μmol, 97%; 37% D for δ 4.00 and 55% D for δ 3.93.
   b) 9.20 mg, 49.0 μmol, 92%; 37% D for δ 4.00 and 57% D for δ 3.93.

Average: y=95%
   37% D δ 4.00
   56% D δ 3.93

$^1$H-NMR Reference 17

$^1$H-NMR HIE reaction 17
L-Boc-Gly-Gly-methyl ester 18

\[
\text{O} \quad \text{H} \quad \text{N} \quad \text{O} \\
\text{O} \quad \text{N} \quad \text{H} \quad \text{O} \\
\text{O} \quad \text{O} \quad \text{N} \quad \text{H} \\
\text{N} \quad \text{H} \\
\text{O} \\
\text{O} \\
\text{O}
\]

Molecular Weight = 246.2654
Molecular Formula = C_{10}H_{18}N_{2}O_{5}

Method A: 10.0 mg (41.0 μmol) 18; 7.1 mg (4.1 μmol) catalyst 1, 8h

\(^1\text{H NMR (300 MHz, CDCl}_3\): δ 6.55 (br s, 1H, NH), 5.06 (br s, 1H, NH), 4.01 (d, \(^3\text{J} = 5.7 \text{ Hz}, 2\text{H}), 3.80 (d, \(^3\text{J} = 5.7 \text{ Hz}, 2\text{H}), 3.70 (s, 3\text{H, COOCH}_3), 1.39 (s, 9\text{H}) \text{ ppm. Incorporation expected at } \delta 4.01 \text{ (red arrow). Determined against integral at } \delta 3.70 \text{ (blue arrow).}

Yield: a) 7.80 mg, 32.0 μmol, 78%; 50% D for \(\delta 4.01\).

b) 8.90 mg, 36.0 μmol, 89%; 54% D for \(\delta 4.01\).  

Average: y=84%, 52% D
L-Boc-Ala-Gly-methyl ester 19

Molecular Weight = 260.2925
Molecular Formula = C11H20N2O5

**Method A**: 10.0 mg (38.0 μmol) 19; 6.6 mg (3.8 μmol) catalyst 1, 8h

**1H NMR (300 MHz, CDCl3)**: δ 6.56 (br s, 1H, NH), 4.87 (br s, 1H, NH), 4.21-4.09 (m, 1H), 3.98 (br s, 2H), 3.70 (s, 3H, COOCH₃), 1.39 (s, 9H) ppm. Incorporation expected at δ 3.98 (red arrow). Determined against integral at δ 3.70 (blue arrow).

**Yields**: a) 9.70 mg, 37.0 μmol, 97%; 59% D for δ 3.98. b) 9.50 mg, 36.0 μmol, 95%; 60% D for δ 3.98.

**Average**: y=96%, 60%

![1H-NMR Reference 19](image)

![1H-NMR HIE reaction 19](image)
L-Boc-Leu-Gly-methyl ester 20

Molecular Weight = 302.3737
Molecular Formula = C_{14}H_{26}N_{2}O_{5}

Method A: 10.0 mg (33.0 \mu \text{mol}) 20; 5.7 mg (3.3 \mu \text{mol}) catalyst 1, 8h

$^1H$ NMR (300 MHz, CDCl$_3$): $\delta$ 6.63 (br s, 1H, NH), 4.85 (br s, 1H, NH$_2$), 4.21-4.11 (m, 1H), 4.06 (d, $^3J = 6.3$ Hz, 2H), 3.77 (s, 3H, COOC$_3$H$_3$), 1.67-1.55 (m, 3H), 1.46 (s, 9H), 0.99-0.94 (m, 6H) ppm. Incorporation expected at $\delta$ 4.06 (red arrow). Determined against integral at $\delta$ 3.77 (blue arrow).

Yield:  

a) 7.10 mg, 23.0 \mu \text{mol}, 71%; 72% D for $\delta$ 4.06.

b) 7.30 mg, 24.0 \mu \text{mol}, 73%; 76% D for $\delta$ 4.06.

Average: y = 72%, 74%

$^3H$-NMR Reference 20

$^3H$-NMR HIE reaction 20
L-Boc-Phe-Gly-methyl ester 21

Molecular Weight = 336,3912
Molecular Formula = C17H24N2O5

Method A: 12.0 mg (35.0 μmol) 21; 6.0 mg (3.5 μmol) catalyst 1, 8h

$^1$H NMR (300 MHz, CDCl$_3$): δ 7.36-7.21 (m, 5H, arom. CH), 6.35 (br s, 1H, NH), 4.95 (br s, 1H, NH), 4.45-4.37 (m, 1H), 4.09 (dd, $^2$J = 15.6 Hz, $^3$J = 5.7 Hz, 2H), 3.75 (s, 3H, COOC$_2$H$_5$), 3.11-3.05 (m, 2H), 1.42 (s, 9H) ppm. Incorporation expected at δ 4.09 (red arrow). Determined against integral at δ 3.75 (blue arrow).

Yield: a) 11.1 mg, 33.0 μmol, 93%; 95% D for δ 4.09. b) 10.8 mg, 32.0 μmol, 90%; 89% D for δ 4.09.

Average: y = 91%, 92%

$^1$H-NMR Reference 21

$^1$H-NMR HIE reaction 21
L-Boc-Gln(NEt)-Gly-methyl ester 22

Method A: 10.4 mg (30.0 μmol) 22; 5.2 mg (3.0 μmol) catalyst 1, 8h

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 7.69 (br s, 1H, NH), 6.61 (br s, 1H, NH), 5.91 (br s, 1H, NH), 4.28-4.16 (m, 1H), 4.15-3.88 (m, 2H), 3.72 (s, 3H, COOCH$_3$), 3.30-3.19 (m, 2H, NCH$_2$CH$_3$), 2.39-2.28 (m, 2H), 2.15-1.95 (m, 2H), 1.42 (s, 9H), 1.12 (t, $^3$J = 7.2 Hz, NCH$_2$CH$_3$) ppm.

Incorporation expected at $\delta$ 4.15-3.88 and 2.15-1.95 (red arrow). Determined against integral at $\delta$ 3.72 (blue arrow).

Yield: a) 8.70 mg, 25.0 μmol, 84%; 49% D for $\delta$ 4.15-3.88 and 69% D for $\delta$ 2.15-1.95.

b) 8.20 mg, 24.0 μmol, 79%; 54% D for $\delta$ 4.15-3.88 and 58% D for $\delta$ 2.15-1.95.

Average: y=82%  
52% D $\delta$ 4.15-3.88  
64% D $\delta$ 2.15-1.95

$^1$H-NMR Reference 22

$^1$H-NMR HIE reaction 22
L-Cbz-Tyr(OtBu)-Gly-Leu-tert-butyl ester 23

Method A: 12.0 mg (20.0 µmol) 23; 3.5 mg (2.0 µmol) catalyst 1, 8h

$^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 7.39-7.24 (m, 5H), 7.04 (d, $^3$J = 8.7 Hz, 2H), 6.89 (d, $^3$J = 8.7 Hz, 2H), 6.64 (br s, 2H, NH), 5.45-5.32 (m, 1H), 5.11-4.95 (m, 2H), 4.52-4.42 (m, 1H), 4.39-4.28 (m, 1H), 4.11-3.96 (m, 1H), 3.79-3.68 (m, 1H), 3.13-2.91 (m, 2H), 1.71-1.50 (m, 3H), 1.44 (s, 9H), 1.31 (s, 9H), 0.96-0.88 (m, 6H) ppm. Incorporation expected at $\delta$ 4.11-3.96 (red arrow). Determined against integral at $\delta$ 5.11-4.95 (blue arrow).

Yield: a) 11.9 mg, 19.0 µmol, 99%; 98% D for $\delta$ 4.11-3.96 and 97% D for $\delta$ 3.79-3.68.

b) 11.7 mg, 19.0 µmol, 98%; 97% D for $\delta$ 4.11-3.96 and 82% D for $\delta$ 3.79-3.68.

$^3$H-NMR Reference 23

Average: $y = 99\%$, 94\%
(L)-Boc-Lys(boc)-Met-methyl ester 24

Molecular Weight = 491.6520
Molecular Formula = C22H41N3O7S

Method A: 10.3 mg (21.0 μmol) 24; 3.6 mg (2.1 μmol) catalyst 1, 8h

1H NMR (300 MHz, CDCl₃): δ 6.79 (br s, 1H, NH), 5.16 (br s, 1H, NH), 4.76-4.68 (m, 2H, NH₂CH₂), 4.11-4.02 (m, 1H), 3.76 (s, 3H, COOC₃H₇), 3.18-3.05 (m, 2H), 2.53 (t, 3J=7.4 Hz, 2H), 2.24-2.11 (m, 1H), 2.09 (s, 3H, SCH₃), 2.05-1.93 (m, 2H), 1.90-1.55 (m, 2H), 1.54-1.35 (m, 20H) ppm. Incorporation expected at δ 4.76-4.68. Determined against integral at δ 3.76.

Yield: a) 10.0 mg, 21.0 μmol, 100%; 95% D for δ 4.76-4.68. b) 9.80 mg, 20.0 μmol, 98%; 95% D for δ 4.76-4.68. **Average: y=99%, 95%**

1H-NMR Reference 24

1H-NMR HIE reaction 24
(L)-Boc-Tyr-Gly-Ala-Phe-methyl ester 25

Method A: 10 mg (17.0 μmol) 25; 2.9 mg (1.7 μmol) catalyst 1, 8h

\[1^H \text{NMR (300 MHz, CDCl}_3\]: δ 8.50 (br s, 1H, NH), 7.62 (d, \(^3\)J = 8.4 Hz, 1H), 7.36-7.08 (m, 8H), 7.00 (s, 1H), 6.84 (br s, 1H, NH), 6.63 (br s, 1H, NH), 6.52 (br s, 1H, NH), 5.22 (d, \(^3\)J = 7.2 Hz, 1H, NH), 4.83-4.76 (m, 1H), 4.49-4.37 (m, 2H), 3.85-3.73 (m, 2H), 3.70 (s, 3H, COOCH\(_3\)), 3.33-3.17 (m, 2H), 1.41 (s, 9H), 1.23 (d, \(^3\)J = 7.2 Hz, 3H) ppm.

Incorporation expected at δ 3.85-3.73 and 3.33-3.17 (red arrow). Determined against integral at δ 3.70.

Yield: a) 9.60 mg, 16.0 μmol, 96%; 96% D for δ 3.85-3.73 and 50% D for δ 3.33-3.17.

b) 9.20 mg, 15.0 μmol, 92%; 94% D for δ 3.85-3.73 and 50% D for δ 3.33-3.17.

Average: y = 94%
95% D δ 3.85-3.73
50% D δ 3.33-3.17
Computational Studies

Details of Computational Methods

Density functional theory (DFT)[1,2] has been employed to calculate gas-phase electronic structures and energies for all species in this paper. The hybrid meta-GGA exchange correlation functional M06[3] in combination with the 6-31G(d)[4] basis set for non-metal atoms and Stuttgart RSC[5] effective core potential for Iridium was used to optimize all structures, as this approach with validated by Kerr et al. Transition states were located at the same level of theory. Harmonic vibrational frequencies have been calculated at the same level of theory to characterize the respective minima (i.e.) and first order saddle points (TS). Thermal energies have been calculated at 353.15K corresponding to experimental conditions.

All calculations have been performed using the Gaussian 09 quantum chemistry program package. All coordinates provided are listed in Cartesian format, with charge and multiplicity of each system given at the top of the coordinate list (i.e. 0 1 = neutral singlet; 1 1 = 1+ charged singlet).

Calculation of the catalytic complex of catalyst 1

Following the approach published by Kerr et al. a catalytic complex was calculated assuming that two molecules isopropyl acetate are coordinated to the iridium center.

Catalytic complex with isopropyl acetate

|        |        |        |        |
|--------|--------|--------|--------|
| C      | 2.45092600 | -3.94143600 | -0.37942200 |
| C      | 1.20404500 | -4.45676900 | -0.41184500 |
| N      | 2.31210800 | -2.57704300 | -0.15612600 |
| N      | 0.33154700 | -3.40006400 | -0.20504300 |
| C      | -1.09469200 | -3.55005400 | -0.25564000 |
| C      | -1.79385000 | -3.78412600 | 0.93220700 |
| C      | -1.73459300 | -3.41895800 | -1.49130100 |
| C      | -3.18197500 | -3.86405500 | 0.85857700 |
| C      | -3.12689800 | -3.49195200 | -1.51021600 |
| C      | -3.86687700 | -3.70759300 | -0.34807500 |
| H      | -3.74796000 | -4.05057200 | 1.77393800 |
| H      | -3.64778600 | -3.37567200 | -2.46218300 |
| C      | 3.44763800 | -1.71452500 | -0.01615500 |
| C      | 3.97252100 | -1.50439200 | 1.26364000 |
| C      | 4.03185300 | -1.17830800 | -1.16631300 |
| C      | 5.08480800 | -0.67273300 | 1.37940900 |
| C      | 5.14411500 | -0.35411100 | -0.99734500 |
| C      | 5.68052800 | -0.08586600 | 0.26124600 |
| H      | 5.51100700 | -0.49207800 | 2.36844100 |
| H      | 5.60328900 | 0.09145300 | -1.88139000 |
| C      | 3.49628300 | -1.49447200 | -2.52854400 |
| H      | 3.58659000 | -2.56561400 | -2.75783000 |
| H      | 2.43391100 | -1.22646200 | -2.60744400 |
|      | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 4.04607800 | -0.94123600 | -3.29906900 |
| C    | 3.36920600  | -2.17169300 | 2.46142600  |
| H    | 2.31088500  | -1.90384100 | 2.58068200  |
| H    | 3.40971100  | -3.2694800  | 2.37511000  |
| H    | 3.90659100  | -1.89350300 | 3.37636900  |
| C    | 6.88009000  | 0.80030400  | 0.41282100  |
| H    | 6.85997800  | 1.34718600  | 1.36403300  |
| H    | 7.81098500  | 0.21654300  | 0.39762400  |
| H    | 6.94866400  | -0.40134000 |           |
| C    | -5.36352400 | -3.77905700 | -0.38223700 |
| H    | -5.72290500 | -4.77562400 | -0.09245100 |
| H    | -5.81171100 | -3.06137800 | 0.31853600  |
| H    | -5.75701700 | -3.56044000 | -1.38142700 |
| C    | -0.95453600 | -3.16246200 | -2.74552800 |
| H    | -0.38611100 | -2.22151200 | -2.67697600 |
| H    | -0.22277500 | -3.95734300 | -2.94718200 |
| H    | -1.62110600 | -3.09519600 | -3.61315900 |
| C    | -1.08412500 | -3.91023200 | 2.24553000  |
| H    | -0.25591900 | -4.63057600 | 2.20271400  |
| H    | -0.65353500 | -2.94627600 | 2.55571100  |
| H    | -1.77379200 | -4.23723800 | 3.03170200  |
| H    | 0.84139500  | -5.46645900 | -0.55414600 |
| H    | 3.42718800  | -4.39779200 | -0.48147200 |
| C    | 1.00037200  | -2.21657400 | -0.04754200 |
| Ir   | 0.03581500  | -0.40379500 | 0.19065000  |
| H(Iso=2) | -0.73484700 | -1.08461900 | 1.36193800  |
| H(Iso=2) | -1.03539500 | -1.06251000 | -0.73216000 |
| P    | -1.58530200 | 1.31032600  | 0.34846000  |
| C    | -2.73016000 | 1.00956000  | 1.75379700  |
| C    | -3.35436100 | -0.24461300 | 1.79938100  |
| C    | -3.00843000 | 1.94713700  | 2.74803100  |
| C    | -4.23087200 | -0.55334300 | 2.82982400  |
| H    | -3.15150200 | -0.98572400 | 1.02248400  |
| C    | -3.88520900 | 1.63021200  | 3.78476500  |
| H    | -2.54959900 | 2.93507500  | 2.71531600  |
| C    | -4.49395600 | 0.38189900  | 3.82955800  |
| H    | -4.71054600 | -1.53125000 | 2.85506400  |
| H    | -4.09459000 | 2.36935100  | 4.55607600  |
| H    | -5.17773200 | 0.13728300  | 4.64025700  |
| C    | -2.76808800 | 1.39522000  | -1.05775400 |
| C    | -2.57409500 | 0.65265600  | -2.22563000 |
| C    | -3.92040300 | 2.18495800  | -0.94289600 |
| C    | -3.50281700 | 0.71034500  | -3.26205300 |
| H    | -1.70025800 | 0.00819800  | -2.31783400 |
| C    | -4.84333600 | 2.24560000  | -1.97880900 |
| H    | -4.10071800 | 2.74975900  | -0.02689100 |
| C    | -4.63432400 | 1.50828200  | -3.14271200 |
| H    | -3.34125600 | 0.12007100  | -4.16276500 |
| H    | -5.73383100 | 2.86217000  | -1.87570500 |
H  -5.36077000  1.55153900  -3.95211800
C  -1.03480100  3.04994800  0.57222400
C  -1.33521600  4.09376100  -0.30616700
C  -0.17130700  3.30620500  1.64538300
C  -0.77612800  5.35660400  -0.12063600
H  -2.01058600  3.92555000  1.14454700
C  -0.38384400  4.56549700  1.83489400
H  0.38798300  2.50123700  2.34479700
C  0.08781300  5.59492800  0.94350600
H  -1.02357000  6.16049400  -0.81205300
H  1.05298300  4.74085400  2.67689500
H  0.52264000  6.58277800  1.08407500
O  1.51335600  0.46356300  1.55218000
O  1.28604000  0.58749100  -1.55218000
C  2.38246100  1.31845800  1.91621800
C  1.63185300  1.57504100  -2.20233700
C  0.70606600  2.69865200  -2.55589300
H  0.75069800  2.95246000  -3.62114500
H  0.31520400  2.41310900  -2.29856000
H  -0.96191300  3.60214000  -1.98335200
C  3.01633000  2.03933700  0.77281900
H  3.90916100  2.58290600  1.09642200
H  3.27814300  1.31897300  -0.01091900
H  2.84666000  2.75500800  0.36723900
O  2.84794200  1.71772000  3.08925300
O  2.90769500  1.64449700  -2.58254700
C  2.36018500  1.08098800  4.30677400
H  2.18737000  0.01426500  4.09078200
C  1.04276400  1.69610200  4.72158300
H  0.25473500  1.49040600  3.98744900
H  0.72010100  1.27410000  5.68118900
H  1.14811500  2.78293300  4.84592500
C  3.45392100  1.28609100  5.32632900
C  3.18177900  0.80403900  6.27263500
H  4.40227700  0.85895900  4.98051000
H  3.60716300  2.35605000  5.51754200
C  3.45655200  2.74535000  -3.35171900
H  2.87594900  3.65252100  -3.13328300
C  4.87579500  2.92462100  -2.86401200
H  5.30793400  3.84087000  -3.28314100
H  4.90674700  2.99106800  -1.76938000
H  5.50098400  2.07879900  -3.18021700
C  3.38421400  2.39326200  -4.82044000
H  3.88221900  1.43012200  -4.99342900
H  2.35051000  2.31214300  -5.17886200
H  3.89368900  3.15605800  -5.42132300
Conformational analysis of Ac-Gly-OMe 11a

The conformations were taken from the respective coordination products and optimized to the next local minimum. The conformation with the lowest energy was chosen for calculation of the reference point.

GlyAddProRu_SM_T353

0 1
N 2.52778300 -0.51576300 -0.19026600
C 1.92549400 -1.03180600 0.91668600
C 2.84412000 -1.72534200 1.89200200
C 1.76026500 0.18536900 -1.17907200
O 0.72452700 -0.92748200 1.10300500
C 2.67615700 0.66611200 -2.27009900
O 1.99049700 1.32063800 -3.20995600
C 2.77241000 1.82637000 -4.29069200
O 3.87158700 0.48716200 -2.29589900
H 3.52524100 -0.58450600 -0.35340900
H 2.43563300 -2.71620900 2.11625800
H 3.87332600 -1.83340700 1.53193500
H 2.85543000 -1.16138100 2.83161800
H 1.22727500 1.04429000 -0.74371800
H 0.97785900 -0.45471600 -1.61403000
H 3.51702100 2.54015000 -3.92314100
H 3.28927400 1.01032300 -4.80631200
H 2.06877000 2.31921200 -4.96346400

GlyAddProRd_SM_T353.log

0 1
N 2.46748500 -0.06312900 -0.01122700
C 1.77585000 0.31259000 -1.12228000
C 2.50351500 1.24787700 -2.05586400
C 1.87342600 -0.94155900 0.95499700
O 0.64268000 -0.08352200 -1.33899800
C 2.83324100 -1.15270800 2.09264700
O 2.30059800 -1.95453700 3.01722300
C 3.13823900 -2.22763200 4.13914700
O 3.93801100 -0.66680800 2.16302800
H 3.40622300 0.26236600 0.18721300
H 1.92866900 2.17624300 -2.14499100
H 3.52352800 1.49035300 -1.73730300
H 2.53912600 0.79501700 -3.05249400
H 1.61428100 -1.91619200 0.51374600
H 0.92701500 -0.53549900 1.34260200
H 4.05967600 -2.72412700 3.81732200
H 3.39999900 -1.29964700 4.65799100
H 2.55794300 -2.88126400 4.79236500
GlyAddProSu_SM_T353.log

0 1
N    2.47863800 -0.48363500 -0.10854700
C    1.87796000 -0.04923300 -1.25082400
C    2.79382900  0.13651300 -2.43507500
C    1.71625900 -0.66178400  1.09362400
O    0.68164900  0.18379100 -1.29940800
C    2.63770100 -1.06541900  2.21091200
O    1.95906500 -1.23695800  3.34749300
C    2.74885200 -1.61826000  4.47261900
O    3.83213900 -1.21565500  2.09913200
H    3.47412800 -0.66093500  0.04563000
H    2.88934900  1.20767800 -2.64753500
H    3.79541900 -0.28361000 -2.28976600
H    2.33173700 -0.32671700 -3.31259400
H    0.93510700 -1.42759800  0.97067800
H    1.80985000  0.25837800  1.37266000
H    3.51657300 -0.86435400  4.67513500
H    2.05577500 -1.69548600  5.31181100
H    3.23851600 -2.58042600  4.28983000

GlyAddProSd_SM_T353.log

0 1
N    2.40486200 -0.15873500  0.49979800
C    1.87852100 -1.30441200  1.01371100
C    2.55122100 -1.82919100  2.25782500
C    1.85607100  0.42552000 -0.68992800
O    0.92723900 -1.86442100  0.49468800
C    2.65946300  1.63962500 -1.06493300
O    2.17600000  2.20252200 -2.17448100
C    2.86664000  3.37134000 -2.61269800
O    3.61246800  2.05421100 -0.44722600
H    3.20187800  0.31156300  0.91198500
H    2.95347900 -2.82672200  2.04899700
H    3.36042400 -1.19089700  2.62990800
H    1.79700500 -1.94555500  3.04383000
H    0.80279500  0.71464700 -0.55308000
H    1.85636100 -0.28819100 -1.52736400
H    2.82252700  4.15190500 -1.84605700
H    3.91626000  3.14130400 -2.82342300
H    2.35579300  3.69693600 -3.52029900
Calculation of the Potential Energy Surface (PES) for selective deuteration of Ac-Gly-OMe 11a with catalyst 1 (Figure 2)

Due to the pro-chiral environment of the Gly-alpha carbon and catalyst 1, four reaction pathways are conceivable: Two enter into the reaction by engaging the Ir-center with the Pro-R hydrogen while the Pro-S hydrogen is either facing towards the triphenylphosphine ligand (up, u) or towards the NHC ligand (down, d). All four pathways have been calculated up to the stage of the insertion product and the results are summarized in Figure S1.

**Figure S1.**

**Coordination products**

GlyAddProRu.log

|   |   |   |   |
|---|---|---|---|
| C | -1.39560100 | -4.32951000 | -2.10819400 |
| C | -2.54422700 | -4.29679100 | -1.39882000 |
| N | -0.72078800 | -3.14803000 | -1.82348700 |
| N | -2.55851700 | -3.09931400 | -0.70954000 |
| C | -3.62837300 | -2.69547500 | 0.15942300 |
| C | -3.53023200 | -2.98876500 | 1.52519700 |
| C | -4.71408100 | -2.00617700 | -0.38779100 |
| C | -4.56032500 | -2.55253800 | 2.35310200 |
| C | -5.71945700 | -1.59027100 | 0.48533200 |
| C | -5.65802400 | -1.84797600 | 1.85392900 |
| H | -4.50559600 | -2.76807500 | 3.42169700 |
| H | -6.57765400 | -1.05046700 | 0.08024200 |
| C | 0.53798400 | -2.82335800 | -2.41298300 |
| Element | X             | Y             | Z             |
|---------|---------------|---------------|---------------|
| C       | 1.70460200    | -3.34503900   | -1.84008300   |
| C       | 0.55189100    | -2.04523600   | -3.57582300   |
| C       | 2.91699900    | -3.04548700   | -2.45262800   |
| C       | 1.79798600    | -1.79381600   | -4.17252700   |
| C       | 2.97973700    | -2.28023100   | -3.62791200   |
| H       | 3.84143300    | -3.44105100   | -2.02483400   |
| H       | 1.82348300    | -1.20919400   | -5.09392100   |
| C       | -0.71336800   | -1.48369200   | -4.15138000   |
| H       | -1.48363100   | -2.24768200   | -4.26414000   |
| H       | -1.12849800   | -0.69590900   | -3.49713900   |
| H       | -0.53149300   | -1.03260300   | -5.14129200   |
| C       | 1.64449600    | -4.21339300   | -0.62116100   |
| H       | 0.97859200    | -3.78418500   | 0.14045200    |
| H       | 1.24512300    | -5.20870300   | -0.86295200   |
| C       | 4.30593500    | -1.98046900   | -4.26595100   |
| H       | 4.12145200    | -1.26778000   | -5.25689900   |
| H       | 5.01097400    | -1.37994900   | -3.43793800   |
| H       | 4.85300700    | -3.03476500   | -4.58811800   |
| C       | -6.73420700   | -1.37476500   | 2.78308200    |
| H       | -6.34650800   | -0.61409800   | 3.47636600    |
| H       | -7.57725300   | -0.93337200   | 2.23809200    |
| H       | -7.12456400   | -2.19672800   | 3.39689300    |
| C       | -4.78110100   | -1.69373000   | -1.85171300   |
| H       | -3.92090800   | -1.07795100   | -2.16378500   |
| H       | -4.75400300   | -2.61073100   | -2.47137400   |
| H       | -5.69280100   | -1.15364300   | -2.09478800   |
| C       | -2.33898900   | -3.70890700   | 2.08970000    |
| H       | -2.09616500   | -4.61235500   | 1.51350800    |
| H       | -1.44423500   | -3.06824700   | 2.06975900    |
| H       | -2.52292300   | -4.00731600   | 3.11940700    |
| H       | -3.36136400   | -5.01141100   | -1.31515700   |
| H       | -0.98496200   | -5.07368300   | -2.78915800   |
| C       | -1.43085300   | -2.37288900   | -0.95854200   |
| Ir      | -1.04781700   | -0.50155100   | -0.17987100   |
| H(Iso=2)| -2.27902500   | -0.77824800   | 0.70955100    |
| H(Iso=2)| -2.21549800   | 0.01890800    | -1.11848900   |
| P       | -1.06991500   | 1.64180400    | 0.80005200    |
| C       | -2.54673700   | 1.93047900    | 1.84274300    |
| C       | -3.78565300   | 1.48229000    | 1.36991000    |
| C       | -2.48737300   | 2.62117500    | 3.05651900    |
| C       | -4.94309300   | 1.72178400    | 2.10042700    |
| H       | -3.84708500   | 0.94049900    | 0.42475900    |
| C       | -3.64791300   | 2.84967300    | 3.78990000    |
| H       | -1.53074100   | 2.97862000    | 3.43779700    |
| C       | -4.87565900   | 2.40043700    | 3.31427900    |
| H       | -5.90066100   | 1.36860800    | 1.17903600    |
| H       | -3.59069500   | 3.38368000    | 4.73660300    |
| H       | -5.78239200   | 2.58338700    | 3.88842900    |
| Element | x       | y       | z       |
|---------|---------|---------|---------|
| C       | -1.07626700 | 3.05845500 | -0.35754900 |
| C       | -0.86833100 | 2.84332300 | -1.72338600 |
| C       | -1.26166100 | 4.36492300 | 0.10005700 |
| C       | -0.83800400 | 3.91850600 | -2.60769200 |
| H       | -0.74761100 | 1.82602000 | -2.10065600 |
| C       | -1.23451400 | 5.43594000 | -0.78345100 |
| H       | -1.44021800 | 4.54246500 | 1.16309900 |
| C       | -1.01418200 | 5.21322900 | -2.14323000 |
| H       | -0.67442700 | 3.73015000 | -3.67084300 |
| C       | -1.38093300 | 6.44825000 | -0.41181000 |
| H       | -0.99531500 | 6.05426200 | -2.83381300 |
| C       | 0.36109000  | 1.95209100 | 1.89856700  |
| C       | 0.50482700  | 1.14531300 | 3.03585200  |
| C       | 1.38140400  | 2.84785000 | 1.56684100  |
| C       | 1.63699100  | 1.25086500 | 3.83493000  |
| H       | 0.27722700  | 0.42961900 | 3.29491700  |
| C       | 2.52488000  | 2.93668100 | 2.35816500  |
| H       | 1.28104500  | 3.49063100 | 0.69158000  |
| C       | 2.65358700  | 2.14223300 | 3.49198600  |
| H       | 1.72654500  | 0.64539900 | 4.72845600  |
| H       | 3.31361000  | 3.64063500 | 2.09229800  |
| H       | 3.54172300  | 2.22177800 | 4.11625000  |
| N       | 2.49012600  | -0.39421900 | -0.14074200 |
| C       | 1.95480100  | -1.10099700 | 0.87492800  |
| C       | 2.93507900  | -1.69985800 | 1.84547100  |
| C       | 1.72412400  | 0.29519100 | -1.14110800 |
| O       | 0.73453800  | -1.25260600 | 1.05021200  |
| C       | 2.64452400  | 0.70177100 | -2.25891500 |
| O       | 1.95942900  | 1.29035300 | -3.23582200 |
| C       | 2.73278000  | 1.74175300 | -4.35558100 |
| O       | 3.84352200  | 0.54947400 | -2.23346800 |
| H       | 3.49625400  | -0.37296800 | -0.27410500 |
| H       | 2.51677200  | -2.61555300 | 2.27263300  |
| H       | 3.90358000  | -1.92593600 | 1.38003000  |
| H       | 3.09600100  | -0.98587400 | 2.65393000  |
| H       | 1.26268800  | 1.21220500 | -0.74781300 |
| H       | 0.93380000  | -0.35965000 | -1.56780700 |
| H       | 3.47639500  | 2.48055200 | -4.02875500 |
| H       | 3.25636500  | 0.88647800 | -4.81426000 |
| H       | 2.02864500  | 2.18252500 | -5.05578300 |

GlyAddProRd.log (26)
C  -4.85792400  -1.40205700  -1.12734800
C   -3.70031700  -0.47755500  -3.08505000
C   -5.80458600  -0.38438600  -1.24164800
C    -4.66594500   0.52325500  -3.15037600
C    -5.71850900   0.59190200  -1.24164800
H    -6.62899700  -0.35087300   0.66146700
H    -4.59456000   1.27344100  -3.93988900
C    -0.25070600  -3.74997500  -0.66747900
C    -1.19992500  -4.18376200   0.66146700
C    -1.44879900  -3.65687600  -3.08505000
C    -1.40562900  -4.51842800   1.27344100
C     2.62401700   4.42811400  -0.60510600
H    -1.39241100  -4.84297200   2.31858000
H     3.57491100   3.92246000  -1.25995700
C   -3.90945600  -4.76376500   1.29934300
H    -4.31774200  -5.72124500   0.94857700
H    -4.67786200  -4.00154100   1.11125000
H    -3.76745800  -4.84384300   2.38434600
C   -6.71446500   1.70966500  -2.30380300
H   -1.09559700  -4.24491700   1.41301700
H   -1.45743600  -3.23456900   1.65985700
H   -1.89042600  -4.72915900   0.82867600
H   -0.97758500  -4.79757600   2.35144200
C    3.90945600  -4.76376500   1.29934300
C    4.31774200  -5.72124500   0.94857700
H    4.67786200  -4.00154100   1.11125000
H    3.76745800  -4.84384300   2.38434600
C   -6.71446500  -1.70966500  -2.30380300
H    -7.61561900  -1.48608600  -1.72059300
H   -6.28702500   2.64239900  -1.90825100
C   -7.02134900   1.93173000  -3.33723500
C   -2.55865100  -0.52692900  -4.05403900
H    -1.59086000  -0.41285400  -3.54205500
H   -2.52043100  -1.48361400  -4.59333800
H   -2.64362600   0.27179000  -4.79936600
C   -4.92417000  -2.40040800  -0.01308400
H   -4.83490500  -3.43397600  -0.37425700
H   -4.10259600  -2.24002100   0.70299400
H   -5.86865600  -2.31434400   0.53497200
H   -3.65558400  -3.97626500  -3.10322400
H   -1.31322100  -5.29420100  -2.32424000
C   -1.64306500  -2.23169500  -1.17555400
Ir  -1.18447400  -0.49863300  -0.15191300
H(Iso=2)   -2.28805700  -0.88969300   0.89858500
H(Iso=2)  -2.49950900   0.03327300  -0.75938700
P    -1.09540800   1.60318200   0.92462700
C    -2.65798500   2.08686900   1.75179800
C    -3.86030100   1.85411400   1.07330300
C    -2.68826000   2.74953900   2.98136300
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | -1.404390 | -4.538760 | -1.407248 |
| C    | -2.597900 | -4.064070 | -1.829109 |
| N    | -0.733819 | -3.466848 | -0.829722 |
| N    | -2.633932 | -2.721124 | -1.492594 |
| C    | -3.736086 | -1.864664 | -1.829109 |
| C    | -4.839091 | -1.814441 | -0.972284 |
| C    | -3.657795 | -1.104720 | -3.003114 |
| C    | -5.885444 | -0.960137 | -1.318430 |
| C    | -4.726339 | -0.262789 | -3.299621 |
| C    | -5.844899 | -0.172524 | -2.468486 |
| H    | -6.758656 | -0.910079 | -0.665146 |
| H    | -4.686385 | 0.339606  | -4.208939 |
| C    | 0.602340  | -3.584736 | -0.327374 |
| C    | 0.801930  | -3.870363 | 1.994877  |
| C    | 1.660212  | -3.532046 | -1.245838 |
| C    | 2.116184  | -3.946277 | 1.472316  |
| C    | 2.952311  | -3.705803 | -0.757031 |
| C    | 3.200327  | -3.948429 | 0.596427  |
| H    | 2.293822  | -4.194090 | 2.530906  |
| H    | 3.791533  | -3.672280 | -1.455330 |
| C    | 1.403407  | -3.306390 | -2.706167 |
| H    | 0.882368  | -4.159036 | -3.164203 |
| H    | 0.771067  | -2.422540 | -2.876930 |
| H    | 2.345350  | -3.173200 | -3.251098 |
| C    | -0.348687 | -3.870363 | 1.994877  |
| H    | -0.838738 | -2.888985 | 2.093370  |
| H    | -1.124282 | -4.574733 | 1.663546  |
| H    | -0.012858 | -4.178345 | 2.991531  |
| C    | 4.600431  | -4.166697 | 1.081802  |
| H    | 5.007308  | -5.111559 | 0.696810  |
| H    | 5.270033  | -3.364310 | 0.746251  |
| H    | 4.650525  | -4.203846 | 2.175874  |
| C    | -6.962904 | 0.769720  | -2.797741 |
| H    | -7.874754 | 0.526017  | -2.239748 |
| H    | -6.690472 | 1.805547  | -2.549243 |
| H    | -7.204984 | 0.751312  | -3.867533 |
| C    | -2.446611 | -1.154533 | -3.884083 |
| H    | -1.613163 | -0.592758 | -3.434320 |
| H    | -2.090635 | -2.181551 | -4.045124 |
| H    | -2.656608 | -0.709982 | -4.863244 |
| C    | -4.884295 | -2.628045 | 0.284320  |
| H    | -4.916834 | -3.706557 | 0.075664  |
| H    | -3.994803 | -2.449570 | 0.906046  |
| H    | -5.768449 | -2.377065 | 0.880719  |
| H    | -3.427375 | -4.545119 | -2.329068 |
| H    | -0.956308 | -5.522525 | -1.459773 |
|    |      |      |      |      |
|----|------|------|------|------|
| C  | -1.48235300 | -2.32915900 | -0.87056900 |
| Ir | -1.18679500 | -0.43678200 | -0.09459100 |
| H(Iso=2) | -2.33004800 | -0.81118100 | 0.92195100 |
| H(Iso=2) | -2.44876000 | -0.06839500 | -0.90608000 |
| P  | -1.43965700 | 1.72257100 | 0.82837500 |
| C  | -3.13537700 | 2.01244500 | 1.46577900 |
| C  | -4.22447800 | 1.61219800 | 0.68301800 |
| C  | -3.37385100 | 2.67969300 | 2.68301800 |
| C  | -5.52360300 | 1.09387700 | 0.26436900 |
| H  | -4.06503100 | 3.00398400 | 2.29085800 |
| C  | -4.67738000 | 2.93204100 | 3.08971500 |
| H  | -2.53864300 | 3.00398400 | 3.08971500 |
| C  | -3.75327700 | 2.52692700 | 2.30825900 |
| H  | -6.36251600 | 1.54931000 | 0.48557400 |
| H  | -4.84934800 | 3.44775500 | 4.03270200 |
| H  | -6.77169200 | 2.72387300 | 2.63782200 |
| C  | -1.18037800 | 3.14771400 | -0.28757700 |
| C  | -0.61359200 | 2.94694300 | -1.54904900 |
| C  | -1.56092900 | 4.43877800 | 0.09909500 |
| C  | -0.41379000 | 4.02704400 | -2.40751200 |
| H  | -0.33149000 | 1.94135000 | -1.86054100 |
| C  | -1.36209400 | 5.51255900 | -0.75824200 |
| H  | -2.02022600 | 4.60195500 | 1.07493400 |
| C  | -0.79037000 | 5.30703000 | -2.01288900 |
| H  | 0.01679100  | 3.86481300 | -3.39182100 |
| H  | -1.66026200 | 6.51331300 | -0.45144400 |
| H  | -0.64155600 | 6.14919300 | -2.68612400 |
| C  | 0.36169700  | 2.04043700 | 2.27297600 |
| C  | -0.45187300 | 1.15879300 | 3.35971200 |
| C  | 0.62947500  | 3.02508400 | 2.27298600 |
| C  | 0.42187500  | 1.27547500 | 4.43271100 |
| H  | -1.20907600 | 0.37156600 | 3.35630700 |
| C  | 1.51438900  | 3.12836500 | 3.3499600 |
| H  | 0.71342300  | 3.71457800 | 1.43335100 |
| C  | 1.41095900  | 2.25783100 | 4.42467300 |
| H  | 0.34149600  | 0.58583900 | 5.27160300 |
| H  | 2.28343500  | 3.89847900 | 3.33603800 |
| H  | 2.09999200  | 2.34587100 | 5.26283100 |
| N  | 2.41698200  | -0.32764600 | -0.07610400 |
| C  | 1.86084300  | -0.14026000 | -1.28219600 |
| C  | 2.80800000  | 0.02700600 | -2.43213700 |
| C  | 1.69470000  | -0.45920000 | 1.16041800 |
| O  | 0.63478000  | -0.07151100 | -1.47476200 |
| C  | 2.62962200  | -1.00613000 | 2.21204000 |
| O  | 1.96087900  | -1.33565100 | 3.31101600 |
| C  | 2.76421600  | -1.72278200 | 4.42876100 |
| O  | 3.82811800  | -1.07450000 | 2.07075200 |
| H  | 3.42308100  | -0.44678400 | 0.01171900 |
| H  | 2.94604200  | 1.09828000 | -2.62714300 |
H  3.79184000  -0.41630400  -2.24274300
H  2.37014200  -0.41751300  -3.33071600
H  0.82720500  -1.14362700  1.06179700
H  1.32400700   0.50854300  1.52949400
H  3.40726400   -0.89135100  4.73734600
H  2.06291800  -1.98232300  5.22341600
H  3.39304600  -2.58195600  4.17280900

GlyAddProSd.log

1 1
C  -1.65359600  -4.42878100  -1.91906400
C  -2.93776000  -4.01099500  -1.89246800
N  -0.88806300  -3.39028700  -1.40505200
N  -2.93039800  -2.72839300  -1.36755900
C  -4.11720300  -1.92797100  -1.25153600
C  -4.85476500  -1.97586200  -0.06671000
C  -5.99215800  -1.71421000   0.01810400
C  -5.62971900  -0.34577600  -2.20564700
C  -6.39548100  -0.35473100  -1.03700700
H  -6.58367100  -1.19138900   0.93522600
H  -5.93790100   0.28452000  -3.04194800
C   0.54322200  -3.44237700  -1.35661600
C   1.16250600  -4.07633400  -0.27357100
C   1.26291900  -2.91517100  -2.43191500
C   2.55298400  -4.14932700  -0.28106000
C   2.65550800  -3.00725400  -2.38847300
C   3.31674300  -3.61018300  -1.31926600
H   3.05804000  -4.65458400   0.54561300
H   3.23744300  -2.60950900  -3.22250900
C   0.56750000  -2.26135200  -3.58981400
H  -0.24066600  -2.88841400  -3.99144200
C   0.10071300  -1.30558800  -3.30232200
C   1.27204300  -2.05655200  -4.40381800
C   0.35919500  -4.63886200   0.85795100
H  -0.29763700  -3.87243700  1.29206900
H  -0.28167100  -5.47039200   0.53393300
H   1.01378700  -5.01766600  1.65149400
C   4.81299600  -3.66288400  -1.26283500
H   5.17043700  -4.64033200  -0.91589200
H   5.26586600  -3.46370200  -2.24076900
H   5.20602900  -2.91303100  -0.56007000
C  -7.63168200   0.48794400  -0.93983900
H  -8.09270400   0.41910400   0.05269100
H  -7.41365700   1.54538800  -1.14188100
H  -8.38418500   0.17348500  -1.67533800
C  -3.65890800  -1.08461400  -3.58872700
H  -2.70348200  -0.56564200  -3.41248800
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -3.40939 | -2.08958 | -3.95613 |
| H    | -4.18484 | -0.55340 | -4.38963 |
| C    | -4.43515 | -2.84853 | 1.07758 |
| H    | -4.37475 | -3.90603 | 0.78482 |
| H    | -3.44164 | -2.56753 | 1.45772 |
| H    | -5.14566 | -2.77219 | 1.90759 |
| H    | -3.85974 | -4.49159 | -2.19318 |
| H    | -1.19950 | -5.35245 | -2.25393 |
| C    | -1.66296 | -2.32386 | -1.05898 |
| Ir   | -1.18413 | -0.49436 | 0.23972 |
| H(Iso=2) | -2.52530 | -0.62098 | 0.51468 |
| H(Iso=2) | 0.10487 | 1.22200 |
| P    | -1.07602 | 1.67844 | 0.68006 |
| C    | -2.57919 | 2.10862 | 1.63729 |
| C    | -3.82269 | 1.71840 | 1.12453 |
| C    | -2.53099 | 2.84562 | 2.82351 |
| C    | -4.99296 | 2.04763 | 1.79738 |
| H    | -3.87840 | 1.15150 | 0.19330 |
| C    | -3.70578 | 3.17234 | 3.49413 |
| H    | -1.57243 | 3.16135 | 3.23543 |
| C    | -4.93670 | 2.77114 | 2.98543 |
| H    | -5.95110 | 1.72466 | 1.39147 |
| H    | -3.65717 | 3.74249 | 4.42000 |
| H    | -5.85298 | 3.02388 | 3.51592 |
| C    | -0.95627 | 3.04639 | -0.53321 |
| C    | -0.90071 | 2.76766 | -1.90618 |
| C    | -0.96250 | 4.38109 | -0.10818 |
| C    | -0.84568 | 3.80424 | -2.82961 |
| H    | -0.90817 | 1.72999 | -2.24047 |
| C    | -0.89702 | 5.41371 | -1.03395 |
| H    | -1.02242 | 4.61406 | 0.95576 |
| C    | -0.84066 | 5.12538 | -2.39705 |
| H    | -0.81218 | 3.57532 | -3.89367 |
| H    | -0.90191 | 6.44762 | -0.69430 |
| H    | -0.80178 | 5.93636 | -3.12224 |
| C    | 0.31823 | 1.94106 | 1.83620 |
| C    | 0.33449 | 1.20404 | 3.02924 |
| C    | 1.42733 | 2.72325 | 1.50941 |
| C    | 1.42607 | 1.27677 | 3.88518 |
| H    | -0.51765 | 0.57347 | 3.28905 |
| C    | 2.53151 | 2.77730 | 2.35788 |
| H    | 1.43522 | 3.30120 | 0.58428 |
| C    | 2.53032 | 2.05956 | 3.54751 |
| H    | 1.41950 | 0.71449 | 4.81792 |
| H    | 3.39515 | 3.37641 | 2.07507 |
| H    | 3.38746 | 2.11012 | 4.21673 |
| N    | 2.50089 | -0.40832 | 0.27843 |
| C    | 1.74210 | -1.09521 | 1.15447 |
| C    | 2.47514 | -1.66635 | 2.33106 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | 2.04784300 | 0.18479200 | -0.95026800 |
| O    | 0.53254100 | -1.32051000 | 1.00400100 |
| C    | 2.77329600 | 1.48996300 | -1.18002900 |
| O    | 2.18233300 | 2.18212000 | -2.14701300 |
| C    | 2.74856400 | 3.46591200 | -2.43298500 |
| O    | 3.75940100 | 2.18281200 | -2.14701300 |
| C    | 2.74856400 | 3.46591200 | -2.43298500 |
| O    | 3.75940100 | 2.18281200 | -2.14701300 |

**Transition states**

GlyTSRu_5_T353.log

1 1

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| C    | -2.39198500 | -3.82907300 | -2.44043200 |
| C    | -2.13332600 | -4.48926100 | -1.29266800 |
| N    | -2.08691700 | -2.49635900 | -2.21093000 |
| N    | -1.67502500 | -3.54394800 | -0.38427300 |
| C    | -1.21753200 | -3.91947000 | 0.92205100 |
| C    | 0.10469500 | -4.34604000 | 1.05625700 |
| C    | -2.12845600 | -3.92670100 | 1.98367900 |
| C    | 0.53614200 | -4.73512000 | 2.32596700 |
| C    | -1.65484300 | -4.33915100 | 3.22586600 |
| C    | -0.32886100 | -4.73700600 | 3.41900300 |
| H    | 1.57295000 | -5.04710000 | 2.45701000 |
| H    | -2.34293500 | -4.35163700 | 4.07402500 |
| C    | -2.22644400 | -1.49111200 | -3.22753200 |
| C    | -1.11258100 | -1.16916300 | -4.00943900 |
| C    | -3.46958600 | -0.87305500 | -3.39606500 |
| C    | -1.26115400 | -0.16194900 | -4.96151300 |
| C    | -3.56728100 | 0.12074600 | -4.36830900 |
| C    | -2.47400900 | 0.50175500 | -5.14732900 |
| H    | -0.40409500 | 0.10788100 | -5.58093400 |
| H    | -4.53048200 | 0.61284700 | -4.51930900 |
| C    | -4.64976400 | -1.24346900 | -2.55078200 |
| H    | -4.44337200 | -1.08453300 | -1.48179000 |
| H    | -5.52376500 | -0.63821300 | -2.81552800 |
| H    | -4.92724200 | -2.30017400 | -2.66877100 |
| C    | 0.20988100 | -1.84736300 | -3.81244800 |
| H    | 0.72909800 | -1.45699600 | -2.92236400 |
| H    | 0.10518200 | -2.93182700 | -3.67192800 |
| H    | 0.86444500 | -1.67976100 | -4.67520700 |
| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | -2.59893400 | 1.61358100 | -6.14445300 |
| H       | -3.59263400 | 1.63069900 | -6.60846300 |
| H       | -2.44946700 | 2.59053900 | -5.66209900 |
| H       | -1.85202300 | 1.52841800 | -6.94228100 |
| C       | 0.13903700  | -5.17815700 | 4.77314100  |
| H       | -0.16428000 | -6.21388700 | 4.97873900  |
| H       | 1.23111100  | -5.13611500 | 4.85925800  |
| H       | -0.29223500 | -4.55822200 | 5.57071200  |
| C       | -3.54935700 | -3.49147200 | 1.79111900  |
| H       | -4.07087200 | -4.12432400 | 1.05704600  |
| H       | -4.10600700 | -3.55365000 | 2.73346900  |
| H       | -3.60310000 | -2.45765700 | 1.42991800  |
| C       | 1.03005000  | -4.44250800 | 0.13305800  |
| H       | 0.73369200  | -5.29117900 | -0.77432200 |
| H       | 0.96556400  | -3.54798000 | -0.76845600 |
| H       | 2.05193300  | -4.58600700 | -0.18261000 |
| C       | -2.22189000 | -5.53243500 | -1.08358000 |
| H       | -2.76206600 | -4.16401300 | -3.40627200 |
| C       | -1.63978400 | -2.30202000 | -0.93532200 |
| Ir      | -1.15881100 | -0.40852100 | -0.16779600 |
| H(Isod=2)| -2.68962900 | -0.11012300 | -0.58621800 |
| H(Isod=2)| -1.02630300 | 0.03785400  | -1.68160600 |
| P       | -1.01820600 | 1.92505700  | 0.26937400  |
| C       | -2.40602000 | 2.88538300  | -0.43874900 |
| C       | -2.84884800 | 2.56313700  | -1.72678400 |
| C       | -2.97035300 | 3.97787600  | 0.22558200  |
| C       | -3.84682300 | 3.31649100  | -2.33203800 |
| H       | -2.41888600 | 1.71453900  | -2.26161300 |
| C       | -3.97645000 | 4.72337200  | -0.38169700 |
| H       | -2.63479700 | 4.24587400  | 1.22719400  |
| C       | -4.41661800 | 4.39406600  | -1.65899600 |
| H       | -4.18519300 | 3.05311700  | -3.33807000 |
| H       | -4.41787900 | 5.56535500  | 0.14810500  |
| H       | -5.20516100 | 4.97703900  | -2.13098800 |
| C       | 0.44186400  | 2.78829100  | -0.42260800 |
| C       | 1.29367600  | 2.14400500  | -1.32392900 |
| C       | 0.66309800  | 4.13903100  | -0.12190800 |
| C       | 2.35999500  | 2.83145800  | -1.89797800 |
| H       | 1.12062300  | 1.10071600  | -1.58796300 |
| C       | 1.72905900  | 4.82048600  | -0.69289500 |
| H       | -0.00468500 | 4.66572900  | 0.56026400  |
| C       | 2.58131100  | 4.16614100  | -1.58037800 |
| H       | 3.01682800  | 2.31919300  | -2.59875800 |
| H       | 1.89304200  | 5.86878300  | -0.45103000 |
| H       | 3.41419700  | 4.70292300  | -2.03048100 |
| C       | -1.01872600 | 2.29440500  | 2.05846300  |
| C       | -2.19575600 | 2.05208900  | 2.78025200  |
| C       | 0.13586500  | 2.67746700  | 2.74782400  |
| C       | -2.22629700 | 2.23594800  | 4.15688100  |
H      -3.09398000  1.71958000  2.25848300
C       0.10690000  2.84190300  4.13068600
H       1.06106600  2.86857600  2.20411200
C      -1.07444300  2.63332600  4.83495900
H      -3.15217400  2.06533500  4.70329400
H       1.10018600  2.78102800  5.91306100
C       0.48652900 -1.08331400  2.20299700
N       0.76692100 -1.07000900  2.66722400
C      -0.97491200 -1.26045600  4.13351700
C       0.88093600 -0.66897800  0.86905800
O      -1.74284400 -0.84881200  1.91598300
C      -2.09399000 -1.48077500  0.48696900
O       2.48726000 -1.21071000 -0.76357300
C       3.69834100 -1.84205100  4.65552100
O       2.09399000 -1.48077500  0.48696900
C       2.06260600 -2.97177800  2.01452700
C       0.90857500 -1.38531700  3.48656100
C       3.28086000 -2.48801400 -2.49099220
C       2.15040100 -0.94706300 -3.93999500
C       3.34461800 -1.48260700 -3.45536800
H       4.20680400 -2.92431400 -2.11078900
H      -2.18595900 -4.70059300

GlyTSD4_T353.log (27)

1 1
C      -0.88757600 -4.10244000 -2.56903400
C      -2.03545600 -4.33538400 -1.89753800
N      -0.36736600 -2.91531300 -2.07042900
N      -2.19315500 -3.28761300 -1.00415400
C      -3.03121200 -3.18075100 -0.09664900
C      -3.18481600 -3.75326000  1.17204500
C      -4.43244100 -2.46236200 -0.50131100
C      -4.22393700 -3.53346600  2.07670800
C      -5.44616000 -2.28014000  0.43505500
C      -5.35353800 -2.79303700  1.73127900
H      -4.15184100 -3.96613600  3.07652900
H      -6.33504000 -1.71633900  0.14632400
C      -0.89274000 -2.39688800 -2.52105600
C       2.06260600 -2.97177800 -2.01452700
C       0.90857500 -1.38531700 -3.48656100
C       3.28086000 -2.48801400 -2.49099220
C       2.15040100 -0.94706300 -3.93999500
C       3.34461800 -1.48260700 -3.45536800
H       4.20680400 -2.92431400 -2.11078900
H      -2.18595900 -4.70059300

55
| Element | X     | Y    | Z    |
|---------|-------|------|------|
| C       | -0.35666500 | -0.76958100 | -3.99804900 |
| H       | -1.15196300 | -1.51229900 | -4.14904500 |
| H       | -0.74239200 | -0.02953200 | -3.27998700 |
| H       | -0.18517500 | -0.25454800 | -4.94980100 |
| C       | 2.03569000  | -4.10202400 | -1.02811500 |
| H       | 1.15196300  | -4.08691800 | -0.38435600 |
| H       | 0.74239200  | -0.02953200 | -3.27998700 |
| H       | 0.18517500  | -0.25454800 | -4.94980100 |
| C       | 4.66382000  | -0.96886700 | -3.94216300 |
| H       | 4.62390500  | -0.68371900 | -5.00013700 |
| H       | 4.97670300  | -0.07397800 | -3.38254900 |
| H       | 5.45958000  | -1.71611200 | -3.82295800 |
| C       | -6.45937600 | -2.56039600 | 2.71605600  |
| H       | -6.23640800 | -3.01011800 | 3.69083200  |
| H       | -6.63734500 | -1.48345500 | 2.86961800  |
| H       | -7.40566600 | -2.98773300 | 2.36126600  |
| C       | -4.53174500 | -1.88097900 | -1.87834300 |
| H       | -3.76269000 | -1.11121400 | -2.04254600 |
| H       | -4.39457800 | -2.64366700 | -2.65733400 |
| H       | -5.51065000 | -1.41516800 | -2.03529100 |
| C       | -1.99267500 | -4.57935700 | 1.54954700  |
| H       | -1.88227500 | -5.45563600 | 0.89563600  |
| H       | -1.05738900 | -4.00631100 | 1.48027300  |
| H       | -2.07703900 | -4.94061700 | 2.58055400  |
| H       | -2.76207000 | -5.13478800 | -1.96222300 |
| H       | -0.38089500 | -4.65177600 | -3.35163500 |
| C       | -1.16549800 | -2.39320600 | -1.10153900 |
| P       | -1.26235500 | 1.45317900  | 1.13885200  |
| C       | -1.94364200 | 1.27715600  | 2.83162900  |
| C       | -2.87394400 | 0.26441700  | 3.09689300  |
| C       | -1.61967100 | 2.18331600  | 3.84896100  |
| C       | -3.46268400 | 0.15991600  | 4.35308400  |
| H       | -3.14906300 | -0.44803200 | 2.31904900  |
| C       | -2.20409400 | 2.07045100  | 5.10641300  |
| H       | -0.90772400 | 2.98597300  | 3.65738100  |
| C       | -3.12683600 | 1.05933800  | 5.36078500  |
| H       | -4.18638100 | -0.63219100 | 4.54329600  |
| H       | -1.94123500 | 2.78011400  | 5.88844700  |
| H       | -3.58557100 | 0.97499500  | 6.34433500  |
| C       | -2.39206500 | 2.63217700  | 0.31527200  |
| C       | -2.29355500 | 2.80189500  | -1.07173700 |
| C       | -3.30944100 | 3.39707400  | 1.03852800  |
| C       | -3.10693600 | 3.72728300  | -1.72118500 |
| H       | -1.58355300 | 2.20708700  | -1.64320600 |
| C       | -4.12797400 | 4.31198100  | 0.38206600  |
| H       | -3.39427220 | 3.27568700  | 2.11767800  |
| C       | -4.02687800 | 4.47944600  | -0.99420600 |
| H       | -3.02393700 | 3.85637900  | -2.79866500 |
| H       | -4.84685500 | 4.89696000  | 0.95247800  |
|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| H   | -4.66716400 | 5.19659300 | -1.50416400 |
| C   | 0.29448100  | 2.40086700 | 1.36091600  |
| C   | 1.23269500  | 1.98178500 | 2.31389000  |
| C   | 0.60793500  | 3.48078000 | 0.53162100  |
| H   | 0.01657900  | 1.14498100 | 2.97780900  |
| C   | 1.83231600  | 4.13266200 | 0.65449400  |
| C   | 1.23269500  | 1.98178500 | 2.31389000  |
| H   | 0.60793500  | 3.48078000 | 0.53162100  |
| C   | 2.45019300  | 2.64149600 | 2.44097400  |
| H   | 1.01657900  | 1.14498100 | 2.97780900  |
| C   | 0.29448100  | 2.40086700 | 1.36091600  |
| C   | 1.23269500  | 1.98178500 | 2.31389000  |
| C   | 0.60793500  | 3.48078000 | 0.53162100  |
| H   | 0.01657900  | 1.14498100 | 2.97780900  |
| C   | 1.83231600  | 4.13266200 | 0.65449400  |
| C   | 1.23269500  | 1.98178500 | 2.31389000  |
| H   | 0.60793500  | 3.48078000 | 0.53162100  |
| C   | 2.45019300  | 2.64149600 | 2.44097400  |
| H   | 1.01657900  | 1.14498100 | 2.97780900  |

**GlyTSSu_5_T353.log**

|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| H   | -1.02458400 | -0.61210500 | -0.02237100 |
| C   | -1.90885000 | 0.04005300  | -1.19869500 |
| H(Iso=2) | -2.52209800 | -0.91850400 | 0.37421200 |
| N   | 1.74382300 | -0.98327800 | 0.99850400 |
| C   | 1.88546400 | -0.18801100 | -0.07362500 |
| C   | 3.23330200 | 0.39248200  | -0.34953500 |
| C   | 0.50324300 | -1.60424400 | 1.43809100  |
| O   | 0.92370900 | 0.10183200  | -0.81284700 |
| C   | 0.48180600 | -1.56174300 | 2.94880400  |
| O   | -0.60898800 | -2.15591600 | 3.43164100  |
| C   | -0.76800100 | -2.10114800 | 4.85259700  |
| O   | 1.34934300 | -1.06328800 | 3.63135000  |
| H   | 2.50089900 | -1.01345000 | 1.67820200  |
| H(Iso=2) | 3.22412800 | 1.45152100  | 0.05626700  |
| H   | 4.04069200 | -0.12055900 | 0.18277500  |
| H   | 3.70631200 | 4.23560300  | 1.71285400  |
| H   | 3.06950500 | -0.05626700 | 5.18455400  |
| H   | 0.05397300 | -2.62484300 | 5.05797500  |
| H   | -1.72270400 | -2.58901300 | 5.05797500  |
C   -2.82227000  3.63812400  1.45476300
C   -3.06842200  3.59872100 -1.31582000
H   -1.99353000  1.73530600 -1.24233500
C   -3.47650300  4.67427700  0.80158600
H   -2.73666200  3.65873200  2.54140000
C   -3.60078800  4.65508400 -0.58548800
H   -3.89495100  5.49766900  1.37706700
H   -4.11654200  5.46595900 -1.09657000
C   0.13068900  2.06820600  2.20522100
C   0.84795700  1.54268900  3.28891900
C   0.68497300  3.12265500  1.47222600
H   0.41964400  0.73304400  3.88316100
C   1.93243400  3.63718400  1.81421400
H   0.13253300  3.55468300  0.63682100
C   2.64131600  3.10322500  2.88612400
H   2.63547600  1.65127100  4.47934800
H   2.34656300  4.46952900  1.24703100
H   3.61438400  3.51018000  3.15415100
Ir  -0.96826300  0.69590700  0.28155100
H(Iso=2) -2.40857900  0.34094700 0.35958500
H(Iso=2) -1.98815400 -1.45766900 1.21323400
N   1.92648000  0.04329800  0.14466300
C   1.39263700  0.67065100 -0.84726200
C   2.29998900  1.58326600 -1.60320200
C   1.20426100  0.91138000  1.06743300
O   0.17208800  0.62182200 -1.11561200
C   2.02064300 -2.17280800  1.21345000
O   1.38457600 -3.08119200  1.96114300
C   2.13542200 -4.25115500  2.29906700
O   3.14036600 -2.31288700  0.77814400
H   2.94009800 -0.10563100  0.20879300
H   2.38453300  2.53516700 -1.05233600
H   3.30548000  1.16833900 -1.72182000
H   1.87093700  1.79081400 -2.58810700
H   1.23211900 -0.43625500  2.06154700
H  -0.14786700 -1.61551200  1.34415900
H   2.37805000 -4.82223400  1.39648400
H   3.06320600 -3.97357900  2.80892900
H   1.49319000  4.83715400  2.95903700

GlyTSSd_4_T353.log

1 1
C  -0.84893600  -4.20085000  -2.29031600
C  -2.18157200  -3.98993800  -2.23921900
N  -0.25026200  -3.14142200  -1.62108900
N  -2.36840100  -2.80720900  -1.54270500
|   | C          | -3.65430700 | -2.20666600 | -1.32886200 |
|---|------------|-------------|-------------|-------------|
|   | C          | -4.35267400 | -2.52107000 | -0.15447300 |
|   | C          | -4.12484000 | -1.28037500 | -2.25987700 |
|   | C          | -5.52765400 | -1.82363300 | 0.10094300  |
|   | C          | -5.31177700 | -0.60760800 | -1.95674200 |
|   | C          | -6.01378600 | -0.85132200 | -0.77975500 |
| H | -6.08324000 | -2.04128600 | 1.01509300  |
| H | -5.69648100 | 0.12622800  | -2.66795200 |
| C | 1.17842900  | -3.02851900 | 1.52749400  |
| C | 1.82422500  | -3.49310400 | 0.37872900  |
| C | 1.87330600  | -2.51954100 | -2.25987700 |
| C | 3.21692300  | -3.43576200 | -0.35636700 |
| C | 3.26403100  | -2.47170000 | -2.55302500 |
| H | 3.95256300  | -2.86015400 | -3.87775300 |
| H | 3.82715000  | -2.93204900 | -4.53674300 |
| C | 1.16528200  | -4.01556200 | 0.79420400  |
| C | 0.64070000  | -3.18586900 | 1.38582200  |
| C | 0.20844100  | -4.64617000 | 0.48919400  |
| C | 1.69936900  | -4.60676200 | 1.45405700  |
| C | 5.44907200  | -2.86216100 | -1.37025000 |
| H | 5.90079800  | -3.03877100 | -2.35389400 |
| H | 5.79021400  | -1.87149000 | -1.03490400 |
| H | 5.86033500  | -3.59823800 | -0.66983800 |
| C | -7.27375400 | -0.10570000 | -0.45896100 |
| H | -8.14453500 | -0.77489700 | -0.45219400 |
| H | -7.21944100 | 0.35500300  | 0.53652200  |
| H | -7.47195600 | 0.68701600  | -1.19017000 |
| C | -3.38972000 | -0.97475000 | -3.53129100 |
| H | -2.77826900 | -0.06585300 | -3.42853900 |
| H | -2.72835000 | -1.79232500 | -3.84462800 |
| H | -4.09772700 | -0.78705800 | -4.34776200 |
| C | -3.82896100 | -3.54477700 | 0.80578900 |
| H | -3.69553700 | -4.52498300 | 0.32726100 |
| H | -2.84697800 | -3.25469400 | 1.20913700 |
| H | -4.51596200 | -3.67598900 | 1.64929300 |
| H | -3.01941200 | -4.55225000 | -2.63007800 |
| H | -0.25625400 | -4.99163700 | -2.73114500 |
| C | -1.17821100 | -2.26713900 | -1.14705700 |
| Ir| -0.99836100 | -0.55235000 | 0.04147600 |
| H(Iso=2)| -1.17045100 | -1.54899500 | 1.29416000 |
| H(Iso=2)| -2.56835400 | -0.66582500 | 0.18735900 |
| P  | -1.14176500 | 1.26370000  | 1.56344000  |
| C  | -1.87702800 | 0.89699800  | 3.20132400  |
| C  | -2.56258300 | -0.29509100 | 3.44068500  |
|     |   |   |   |
|-----|---|---|---|
| C   | -1.84612500 | 1.87998800 | 4.19911800 |
| C   | -3.19236600 | -0.50937500 | 4.66436100 |
| H   | -2.60608500 | -1.06023900 | 2.66729000 |
| C   | -2.46889200 | 1.66075100 | 5.42005500 |
| H   | -1.32829700 | 2.82312000 | 4.02121700 |
| C   | -3.14257900 | 0.46350700 | 5.65470100 |
| H   | -3.71994900 | -1.44499500 | 4.84176000 |
| H   | -2.43102900 | 2.42750400 | 6.19375000 |
| C   | -2.26341700 | 2.60624800 | 0.99585400 |
| C   | -3.49038300 | 2.22454000 | 0.43667400 |
| C   | -2.02132300 | 3.96276300 | 1.23336200 |
| C   | -4.45294800 | 3.17875600 | 0.12774900 |
| H   | -3.70557900 | 1.17008200 | 0.25390600 |
| C   | -2.98180200 | 4.91712100 | 0.90934500 |
| H   | -1.08210200 | 4.28325300 | 1.68208000 |
| C   | -4.20065200 | 4.52779100 | 0.36253900 |
| H   | -5.40586500 | 2.86420800 | -0.29678600 |
| H   | -2.77855000 | 5.96944600 | 1.09882600 |
| H   | -4.95501600 | 5.27559000 | 0.12467900 |
| C   | 0.47114700  | 2.03997500 | 1.93640000 |
| C   | 1.21124600  | 1.59025700 | 3.03517100 |
| C   | 1.04728500  | 2.96989300 | 1.06108600 |
| C   | 2.48721700  | 2.08875000 | 3.27698200 |
| H   | 0.78746000  | 0.85029300 | 3.71375900 |
| C   | 2.31902400  | 3.47623900 | 1.31561300 |
| H   | 0.51182700  | 3.30591000 | 0.17265400 |
| C   | 3.03905300  | 3.04177600 | 2.42531200 |
| H   | 3.04785900  | 1.73766300 | 4.14115500 |
| H   | 2.74569700  | 4.21689500 | 0.64105220 |
| H   | 4.03033600  | 3.44468300 | 2.62509000 |
| N   | 1.04769100  | 0.87388100 | -1.55206500 |
| C   | 1.74727000  | 0.22251600 | -0.60988800 |
| C   | 3.21385500  | 0.47725900 | -0.50539300 |
| C   | -0.38521000 | 0.75401900 | -1.79707100 |
| O   | 1.19950600  | -0.56150000 | 0.18870100 |
| C   | -0.90985500 | 2.13532100 | -2.11736100 |
| O   | -2.17306400 | 2.07850300 | -2.53826700 |
| C   | -2.77107400 | 3.32246400 | -2.88786000 |
| O   | -0.25948800 | 3.15265400 | -2.03375100 |
| H   | 1.50214100  | 1.64051700 | -2.04238400 |
| H   | 3.71504300  | -0.48485000 | -0.35241500 |
| H   | 3.63169500  | 0.97550900 | -1.38598900 |
| H   | 3.39402700  | 1.09689300 | 0.38363300 |
| H   | -0.55873800 | 0.12339220 | -2.68170300 |
| H   | -1.67210900 | 0.40797400 | -1.10304300 |
| H   | -2.74027600 | 4.01649700 | -2.03355600 |
| H   | -2.24453700 | 3.77775300 | -3.73786500 |
| H   | -3.80440700 | 3.09964000 | -3.15170900 |
Insertion products

GlyInsRu_CA1_Conf3.log

1 1

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | -2.36711100 | -3.92522300 | -2.24145100 |
| C       | -1.93192600 | -4.55733400 | -1.13300200 |
| N       | -2.06956100 | -2.58374500 | -2.07080000 |
| N       | -1.37811000 | -3.58771300 | -0.30739100 |
| C       | -0.93628800 | -3.94582200 | -2.24145100 |
| C       | 0.34913600  | -4.45538700 | 1.01301300  |
| C       | 0.72889700  | -4.83980600 | 2.46939900  |
| C       | -1.45398400 | -4.31715400 | 3.31365300  |
| C       | -0.15023400 | -4.76961800 | 3.54533700  |
| H       | 1.73899800  | -5.22052700 | 2.62642100  |
| H       | -2.16764100 | -4.30470400 | 4.14046400  |
| C       | -2.25612700 | -1.61975300 | -3.11963300 |
| C       | -1.15013900 | -1.27327100 | -3.90779700 |
| C       | -3.51604800 | -1.04329100 | -3.30926000 |
| C       | -1.31919500 | -0.26144700 | -4.84763700 |
| C       | -3.63055700 | -0.02486500 | -4.25019800 |
| C       | -2.54404800 | 0.39042500  | -5.01702200 |
| H       | -0.54777100 | 0.03284700  | -5.46469200 |
| H       | -4.60219500 | 0.45216000  | -4.39145400 |
| C       | -4.71177100 | -1.48601900 | -2.51169000 |
| H       | -4.46727600 | -1.71607500 | -1.46522600 |
| H       | -5.49043800 | -0.71432600 | -2.51781000 |
| H       | -5.15248900 | -2.39971400 | -2.93456000 |
| C       | 0.17720700  | -1.94169200 | -3.72074700 |
| H       | 0.68709300  | -1.54844700 | -2.82867300 |
| H       | 0.07530000  | -3.02686300 | -3.58043300 |
| H       | 0.82382200  | -1.76901900 | -4.58878300 |
| C       | -2.67558000 | 1.50979300  | -6.00456600 |
| H       | -3.68748100 | 1.93330500  | -6.00124900 |
| H       | -1.96947600 | 2.32167000  | -5.78189200 |
| H       | -2.45943400 | 1.17117400  | -7.02658600 |
| C       | 0.26444400  | -5.20615600 | 4.91790900  |
| H       | -0.27977500 | -6.10930100 | 5.22461500  |
| H       | 1.33549100  | -5.43172200 | 4.96542400  |
| H       | 0.04562100  | -4.43690700 | 5.67109700  |
| C       | -3.30556200 | -3.53137900 | 1.80368200  |
| H       | -3.79959600 | -4.26215000 | 1.14518300  |
| H       | -3.87405300 | -3.50573200 | 2.74067300  |
| H       | -3.39537800 | -2.54814900 | 1.32922300  |
| C       | 1.27172100  | -4.67716000 | 0.02032100  |
| H       | 1.13111600  | -5.68766600 | -0.39160600 |
| H       | 1.09745600  | -3.96695300 | -0.79861700 |
|     | X           | Y           | Z           |
|-----|-------------|-------------|-------------|
| H   | 2.31518500  | -4.59084300 | 0.34105800  |
| H   | -1.95411000 | -5.59742600 | -0.83492200 |
| H   | -2.84176800 | -4.28595300 | -3.14453100 |
| C   | -1.42086000 | -2.35100500 | -0.88086300 |
| Ir  | -1.17972900 | -0.35608900 | -0.18213400 |
| H(Iso=2)| -2.94521800 | -0.11720300 | -0.57143900 |
| H(Iso=2)| -2.56538500 | 0.02524900  | -1.30623000 |
| P   | -0.98116000 | 1.97679800  | 0.20857400  |
| C   | -2.29948600 | 2.95649800  | -0.60363500 |
| C   | -2.60660500 | 2.66185400  | -1.93786600 |
| C   | -2.94786000 | 4.01861500  | 0.02946800  |
| C   | -3.56378000 | 3.40514800  | -2.61679500 |
| H   | -2.09287700 | 1.84931100  | -2.45886800 |
| C   | -3.91018900 | 4.75719100  | -0.65395200 |
| H   | -2.70719500 | 4.27062700  | 1.06225500  |
| C   | -4.22314800 | 4.44982500  | -1.97339800 |
| H   | -3.79191200 | 3.16605200  | -3.65514300 |
| H   | -4.41724200 | 5.57658300  | -0.14799800 |
| H   | -4.97789300 | 5.02746100  | -2.50350400 |
| C   | 0.52952900  | 2.78113300  | -0.44145200 |
| C   | 1.37849300  | 2.11639000  | -1.32707000 |
| C   | 0.77020200  | 4.13075900  | -0.14996200 |
| C   | 2.46194700  | 2.77669300  | -1.89548600 |
| H   | 1.19147800  | 1.06675900  | -1.57386100 |
| C   | 1.85619700  | 4.78719500  | -0.71190100 |
| H   | 0.09844900  | 4.67245400  | 0.51673600  |
| H   | 2.70469700  | 4.10700000  | -1.58522900 |
| H   | 3.11674000  | 2.24838300  | -2.58687500 |
| H   | 2.03799500  | 5.83392300  | -0.47593100 |
| H   | 3.55107000  | 4.62829600  | -2.03157700 |
| C   | -1.04856000 | 2.39447200  | 1.98451400  |
| C   | -2.25756000 | 2.20711500  | 2.66975200  |
| C   | 0.09120200  | 2.76202200  | 2.70599400  |
| C   | -2.33159800 | 2.43420300  | 4.03829000  |
| H   | -3.14718100 | 1.87821700  | 2.13063000  |
| C   | 0.01774400  | 2.97278100  | 4.08035900  |
| H   | 1.04512400  | 2.89725000  | 2.19716200  |
| C   | -1.19402200 | 2.82170000  | 4.74582400  |
| H   | -3.27974100 | 2.30160800  | 4.55590900  |
| H   | 0.91043300  | 3.26888500  | 4.62799900  |
| H   | -1.25449100 | 3.00330600  | 5.81735600  |
| N   | 0.24801400  | -1.03799000 | 2.25031300  |
| C   | -1.00565200 | -0.95716600 | 2.69267500  |
| C   | -1.25788000 | -1.12930300 | 4.15513500  |
| C   | 0.60806400  | -0.62713000 | 0.89771800  |
| O   | -1.94723500 | -0.66933800 | 1.91569300  |
| C   | 1.75018000  | -1.48248600 | 0.43362200  |
| O   | 2.04729800  | -1.27634200 | -0.85599300 |
| C   | 3.24094700  | -1.89881900 | -1.33311500 |
O  2.40313400  -2.19647400  1.16489000  
H  0.98996000  -1.40236400  2.84241400  
H  -2.27459300  -1.49817400  4.31698000  
H  -0.53661100  -1.80691800  4.62567900  
H  -1.17799300  -0.14463000  4.63796900  
H  1.08259100  0.37142000  0.97051800  
H  -0.46908800  -0.12448400  -1.57141500  
H  4.09058200  -1.65125000  -0.68909400  
H  3.12008600  -2.98685000  -1.36963900  
H  3.39552200  -1.50888900  -2.34198400  

GlyInsRd.log (28a)

|   |     |     |     |
|---|-----|-----|-----|
| 1 | C   | -0.94687900 | -4.26532200 | -2.34909900 |
|   | C   | -2.12480600 | -4.41866200 | -1.70692500 |
|   | N   | -0.39019900 | -3.07989900 | -1.88732600 |
|   | N   | -2.26296500 | -3.32680400 | -0.86645300 |
|   | C   | -3.38248100 | -3.13205000 | 0.01123800  |
|   | C   | -3.29857400 | -3.62939000 | 1.31443600  |
|   | C   | -4.48568000 | -2.40791600 | -0.45268500 |
|   | C   | -4.33487600 | -3.31136000 | 2.19141300  |
|   | C   | -5.49503600 | -2.11758800 | 0.46184700  |
|   | C   | -5.42909300 | -2.54456300 | 1.79054200  |
| H  | H   | -4.28903000 | -3.68293900 | 3.21696500  |
| H  | H   | -6.36287800 | -1.54600400 | 0.12746100  |
|   | C   | 0.87922000  | -2.61378800 | -2.37262000 |
|   | C   | 2.04298100  | -3.20616500 | -1.87411500 |
|   | C   | 0.90173300  | -1.64881400 | -3.38711400 |
|   | C   | 3.26390300  | -2.77728000 | -2.39758100 |
|   | C   | 2.14372500  | -1.26360300 | -3.88283800 |
|   | C   | 3.33453800  | -1.80929500 | -3.39736600 |
| H  | H   | 4.18483000  | -3.22667600 | -2.02084800 |
| H  | H   | 2.18373000  | -0.51783600 | -4.67893300 |
| C  | C   | -0.35878200 | -1.04046400 | -3.91935500 |
| H  | H   | -1.15378400 | -1.78659700 | -4.05647300 |
| H  | H   | -0.73945100 | -0.27232000 | -3.22929900 |
| H  | H   | -0.18107400 | -0.55607500 | -4.88597800 |
| C  | C   | 2.01323900  | -4.29213300 | -0.83858800 |
| H  | H   | 1.06752500  | -4.32597300 | -0.28227700 |
| H  | H   | 2.14740700  | -5.28105200 | -1.29973350 |
| H  | H   | 2.82939500  | -4.16639900 | -0.11567400 |
| C  | C   | 4.65778900  | -1.34699500 | -3.92824900 |
| H  | H   | 4.60278500  | -1.10656400 | -4.99680800 |
| H  | H   | 4.99637500  | -0.43651000 | -3.41182200 |
| H  | H   | 5.43694000  | -2.10570100 | -3.79033500 |
| C  | C   | -6.52486000 | -2.19373700 | 2.75108200  |
| H  | H   | -6.37339700 | -2.66514200 | 3.72901500  |
| H  | H   | -6.58432300 | -1.10780400 | 2.90641700  |
N                       1.81280900  -0.71367800  0.62808100
C                       1.77542500  0.06416100  -0.45946700
C                       3.02346700  0.76292400  -0.88789100
C                       0.62921800 -1.41830600  1.11612700
O                       0.71310500  0.23518900 -1.10012700
C                       0.62180600 -1.35003000  2.61218900
O                       0.38204300 -2.12825000  3.11022000
C                       0.47055600 -2.16270400  4.53429100
O                       1.35449100 -0.72190800  3.30853100
H                       2.65751300 -0.74010200 -1.19128900
H                       2.98568800 -1.80224400  3.11022000
H                       0.72241600 -2.48709500  0.86704200
H                       2.02513100 -1.31176700  1.06191200
H                       0.58521600 -1.15031600  4.93730700
H                       1.35692700 -2.76135600  4.75875300

GlyInsSu_CA1_Conf3.log

1 1
C                       -0.87988200 -4.41351000 -1.91048500
C                       -2.06891800 -4.48761500 -1.28010100
N                       -0.29262900 -3.21367800 -1.52372200
N                       -2.18938800 -3.33328200 -0.52273900
C                       -3.37172500 -3.05615100  0.24742900
C                       -3.42593200 -3.46339100  1.58350200
C                       -4.44615600 -2.41387700 -0.38413500
C                       -4.57145500 -3.14609800  2.31183100
C                       -5.55842100 -2.10044900  0.39417600
C                       -5.63603000 -2.44474400  1.74601200
H                       -4.62808200 -3.45371500  3.35741900
H                       -6.39900200 -1.58425300 -0.07325600
C                       -0.89928000 -2.75343600 -2.18280800
C                       -2.17597000 -3.35618800 -1.86184300
C                       -0.76824600 -1.82595400 -3.22806000
C                       -3.25452200 -2.92091400 -2.54602600
C                       -1.92783600 -1.45314300 -3.90155500
C                       -3.18107100 -1.97345300 -3.56455900
H                       -4.21789100 -3.37033100 -2.29970100
H                       -1.84814600 -0.74918300 -4.73312100
C                       -0.56361500 -1.27532400 -3.64464300
H                       -1.34934100 -2.04445100 -3.63925100
H                       -0.88296600 -0.46081700 -2.97695600
H                       -0.50583300 -0.86832100 -4.66074100
C                       -2.20673300 -4.50207900 -0.90262100
H                       -1.41047600 -4.47389800 -0.15040600
H                       -2.11292000 -5.45696700 -1.44103000
H                  3.16817300  -4.50864900  -0.37911900
C                  4.40804000  -1.53418400  -4.30534900
H                  4.22508300  -2.52689500  3.55604000
H                  4.73377700  -0.53139300  -3.99317600
H                  5.24830900  -2.21716000  -4.13621100
C                  -6.83304300  -2.06743200   2.56130700
H                  -6.80608500  -2.52689500   3.55604000
H                  -6.89022600  -0.97858600   2.69951400
H                  -7.76603100  -2.37589900   2.07227000
C                  -4.42168300  -2.08789600  -1.84833700
H                  -3.46428100  -1.65817600  -2.17364800
H                  -4.58195700  -2.98791300  -2.45965400
H                  -5.21642200  -1.37814700  -2.10350500
C                  -2.29712300  -4.21773500   2.21196100
H                  -2.21692300  -5.23492500   1.80094400
H                  -1.34046600  -3.71192400   2.03960600
H                  -2.44176100  -4.30762400   3.29529900
H                  -2.84872100  -5.23958800  -1.29019000
H                  -0.38829900  -5.07697200  -2.60946400
C                  -1.09327500  -2.52278600  -0.66507500
P                  -1.20191200   1.40482000   1.49680900
C                  -2.03569200   1.29890800   3.11892300
C                  -2.03569200   1.29890800   3.11892300
C                  -2.97755500   0.28832700   3.33748300
C                  -1.84869600   2.27711600   4.10303000
C                  -3.70911700   0.25147400   4.51985300
H                  -3.14851600  -0.47538400   2.57867600
C                  -2.57584000   2.23268100   5.28744100
H                  -1.13473400   3.08520800   3.94345200
C                  -3.50744100   1.21971400   5.49751800
H                  -4.44278900  -0.53883300   4.67468700
H                  -2.42028200   2.99920500   6.04419200
H                  -4.07724800   1.19779900   6.42417200
C                  -2.24251200   2.57144700   0.53961000
C                  -2.12330500   2.60496100  -0.85769900
C                  -3.15010700   3.42865700   1.16822800
C                  -2.89097200   3.49161300  -1.60427400
H                  -1.41974200   1.93848300  -1.36050600
C                  -3.92057900   4.30867000   0.41421900
C                  -3.26399900   3.40832400   2.25111900
C                  -3.79153500   4.34284900  -0.96964400
H                  -2.78899700   3.51425300  -2.68776000
H                  -4.62644100   4.96986800   0.91311400
H                  -4.39705300   5.03093500  -1.55654800
C                  0.36128400   2.30712800   1.80216400
C                  1.17075800   1.97917300   2.89857800
C                  0.83449500   3.22850100   0.86274800
C                  2.42762600   2.55659900   3.04432400
H                  0.81218000   1.28051700   3.65555900
C                  2.09027400   3.80765100   1.01487600
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 0.21357900| 3.51167200| 0.01280000|
| C       | 2.89236000| 3.46739100| 2.09997200|
| H       | 3.04245000| 2.97432000| 3.90423700|
| H       | 2.43751900| 4.54046500| 0.28766600|
| H       | 3.87326300| 3.92371700| 2.21881700|
| Ir      | -0.94144000| -0.66601700| 0.31798900|
| H(Iso=2)| -2.43318900| -0.20881700| -0.64514500|
| H(Iso=2)| -2.73820000| -0.54419200| 0.05901200|
| N       | 1.92871700| -0.22264800| 0.16586700|
| C       | 1.51796500| -0.92203500| 1.08283300|
| C       | 2.54705200| -1.75586900| 2.87309400|
| C       | 1.00757800| 0.88433500| 3.53606700|
| O       | 0.30183900| 0.50048000| -1.22392100|
| C       | 1.62788500| -2.19081800| 1.48129100|
| O       | 0.83217400| -2.90283700| 2.29052900|
| C       | 1.42321300| -4.06545100| 2.87309400|
| O       | 2.76576100| -2.51566100| 1.21371100|
| H       | 2.91822600| -0.42502900| 1.08283300|
| H       | 2.61060700| 2.16459300| -1.43136200|
| H       | 3.53830000| 0.66408800| -1.64620400|
| H       | 2.24586200| 1.09224100| -2.80729300|
| H       | 1.01674500| -0.31651600| 2.02883100|
| H       | -1.53222800| -1.46571800| 1.54106000|
| H       | 1.69048700| -4.79583300| 2.10129100|
| H       | 2.32200000| -3.80341300| 3.44002000|
| H       | 0.66136000| -4.48190400| 3.53606700|

GlyInsSd.log

1 1
C   -0.97020300 -4.00705000 -2.54957400
C   -2.25243100 -3.99013200 -2.13018400
N   -0.33210200 -2.94040800 -1.92966500
N   -2.37214400 -2.91244000 -1.26779500
C   -3.59697600 -2.58519100 -0.59465200
C   -3.86517500 -3.19452600  0.63376100
C   -4.46075200 -1.64886700 -1.17848600
C   -5.01321200 -2.79050900  1.31959000
C   -5.59622100 -1.28795200 -0.45912400
C   -5.88217000 -1.83542900  0.79511700
H   -5.23490600 -3.24436900  2.28656600
H   -6.28444900 -0.55810300 -0.89003400
C   1.06251600 -2.67837800 -2.1526600
C   1.99020700 -3.15158800 -1.21816100
C   1.44248500 -2.04334400 -3.34079000
C   3.33917200 -2.91155700 -1.47829300
C   2.80183200 -1.81249600 -3.54206000
C   3.76257200 -2.22916200 -2.61888000
H   4.08407200 -3.28461800 -0.77222000

68
It was found that the Pro-R (down) pathway leads to the transition state with lowest energy. Therefore, the complete PES (main text figure 2) was calculated for this pathway.

GlyIns2Rd_T353.log (insertion product, 28b)

1 1

C 0.94691700 -4.26498000 -2.34932000
C -2.12482200 -4.41842900 -1.70713100
N -0.39024700 -3.07962000 -1.88740500
N -2.26301300 -3.32664200 -0.86657800
C -3.38252000 -3.13193300 0.01112700
C -3.29859800 -3.62937500 1.31428200
C -4.48566900 -2.40766200 -0.45271100
C -4.33483000 -3.31130800 2.19133600
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -1.31843400 | 2.71089800 | 6.07547500 |
| H    | -3.03456000 | 1.00226500 | 6.62667100 |
| C    | -0.23949500 | 2.48649400 | 0.53637300 |
| C    | -2.38452600 | 2.70475700 | -0.84904800 |
| C    | -3.37605300 | 3.10391400 | 1.31368500 |
| C    | -3.33522900 | 3.52695300 | -1.44054300 |
| H    | -1.61060000 | 2.24166500 | -1.46755100 |
| C    | -4.33607000 | 3.91680900 | 0.71529500 |
| H    | -3.39761600 | 2.95213000 | 2.39225500 |
| C    | -2.38452600 | 2.70475700 | -0.84904800 |
| C    | -3.31041700 | 3.69783400 | -2.51523300 |
| H    | -5.09981000 | 4.38807000 | 1.33098000 |
| C    | -5.06709300 | 4.76893000 | -1.12087000 |
| C    | 0.38469400  | 2.50706800 | 1.29003700 |
| C    | 1.47730800  | 2.18039300 | 2.10493300 |
| C    | 0.47041200  | 3.63713300 | 0.46996500 |
| C    | 2.62381600  | 2.96763700 | 2.09656600 |
| H    | 1.43506300  | 1.31158700 | 2.75870000 |
| C    | 1.62356800  | 4.16951000 | 0.45829800 |
| H    | -0.36919800 | 0.66559600 | 0.05074800 |
| C    | 2.70335000  | 4.08537800 | 1.26943300 |
| H    | 3.45703900  | 2.70664900 | 2.74697400 |
| H    | 1.66840600  | 5.29592300 | -0.18200300 |
| H    | 3.60031800  | 4.70212800 | 1.26583200 |
| Ir   | -1.01134200 | -0.66559600 | 0.05074800 |
| H    | -2.66199200 | -0.24600700 | -0.57617700 |
| N    | 1.81279300  | -0.71375900 | 0.62801700 |
| C    | 1.77539100  | 0.06418800 | -0.45944700 |
| C    | 3.02346300  | 0.76284500 | -0.88793400 |
| C    | 0.62918400  | -1.41834000 | 1.11604500 |
| O    | 0.71303400  | 0.23537400 | -1.10002000 |
| C    | 0.58290100  | -1.35005000 | 2.61209900 |
| O    | -0.38205300 | -2.12842000 | 3.11006500 |
| C    | -0.47056000 | -2.16314400 | 4.53411200 |
| O    | 1.35432400  | -0.72188400 | 3.30848500 |
| H    | 2.65752600  | -0.74029700 | 1.19117700 |
| H    | 2.98559100  | 1.80223900 | -0.53281200 |
| H    | 3.93202600  | 0.28983300 | -0.49959700 |
| H    | 3.05540200  | 0.77983700 | -1.98208700 |
| H    | 0.72229600  | -2.48711500 | 0.86685600 |
| H    | -2.02508900 | -1.31176900 | 1.06200500 |
| H    | 0.42506700  | -2.62549900 | 4.96281900 |
| H    | -0.58529100 | -1.15084000 | 4.93732800 |
| H    | -1.35688400 | -2.76191700 | 4.75845100 |

GlyTS2Rd_1_T353.log (transition state, 29)

1 1
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| C       | -0.88748900 | -4.10241500 | -2.56902000 |
| C       | -2.03537600 | -4.33538600 | -1.89754600 |
| N       | -0.36729800 | -2.91529200 | -2.07038200 |
| N       | -2.19310200 | -3.28763500 | -1.00414700 |
| C       | -3.30117000 | -3.18080400 | -0.09665100 |
| C       | -3.18476200 | -3.75330000 | 1.17204700  |
| C       | -4.43241600 | -2.46244800 | -0.50132200 |
| C       | -4.22388400 | -3.53514000 | 2.07671200  |
| C       | -5.44612900 | -2.28024800 | 0.43504000  |
| C       | -5.35350300 | -3.53351400 | 2.07671200  |
| H       | -4.15177300 | -3.96616800 | 3.07653800  |
| C       | -0.89277400  | -2.39681800 | 2.01460700  |
| C       | 2.06268800  | -2.97169300 | 2.01460700  |
| C       | 0.90852900  | -1.38524200 | 3.48655000  |
| C       | 3.28089900  | -2.48792000 | 2.49116200  |
| C       | 2.15032200  | -0.94697600 | 3.94007600  |
| C       | 3.34457700  | -1.48251500 | 3.45553300  |
| H       | 4.20687500  | -2.92421800 | 3.07653800  |
| H       | 2.18581200  | -0.16513700 | 3.07653800  |
| C       | -0.35674900 | -0.76952400 | -3.99796200 |
| H       | -1.15203900 | -1.51225600 | -4.14893600 |
| H       | -0.74245800 | -0.02950100 | -3.27986400 |
| H       | -0.18531600 | -0.25446500 | -4.94971000 |
| C       | 2.03585200  | -4.10195300 | -1.02820800 |
| H       | 1.45606000  | -4.08687700 | -0.38440500 |
| H       | 2.03232800  | -5.07560500 | -1.53919800 |
| H       | 2.92463900  | -4.08160900 | -0.38604900 |
| C       | 4.66630600  | -0.96881100 | -3.94248700 |
| H       | 4.62342100  | -0.68263300 | -5.00016400 |
| H       | 4.97727100  | -0.07459900 | -3.38214500 |
| H       | 5.45926700  | -1.71648200 | -3.82438400 |
| C       | -6.45933400 | -2.56047400 | 2.71605800  |
| H       | -6.23641500 | -3.01031000 | 3.69079300  |
| H       | -6.63720400 | -1.48742000 | 2.86972900  |
| H       | -7.40566100 | -2.98972300 | 2.36121400  |
| C       | -4.53173200 | -1.88107300 | -1.87835600 |
| H       | -3.76268500 | -1.11130300 | -2.04256900 |
| H       | -4.39456700 | -2.64376300 | -2.65734600 |
| H       | -5.51064100 | -1.41526900 | -2.03529900 |
| C       | -1.99261400 | -4.57938500 | 1.54955100  |
| H       | -1.88220800 | -5.45566500 | 0.89564100  |
| H       | -1.05733300 | -4.00633400 | 1.48027300  |
| H       | -2.07697000 | -4.94064100 | 2.58056000  |
| H       | -2.76197700 | -5.13480000 | -1.96225700 |
| H       | -0.38079000 | -4.65172800 | -3.35162700 |
| C       | -1.16545600 | -2.39321100 | -1.10149700 |
| P       | -1.26236700 | 1.45318200  | 1.13889000  |
| C       | -1.94367900 | 1.27721800  | 2.83166200  |
| Atom | C      | H      | C      | H      | C      | H      | C      | H      | C      | H      | C      | H      |
|------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|      | -1.68981000 | -4.30163000 | -2.11427100 |      | -2.82265800 | -3.66625500 | -2.48608800 |      | -0.97899700 | -3.41089400 | -1.31882000 |      | -2.78256000 | -2.40784100 | -1.90656800 |      | -3.81396100 | -1.42066600 | -2.05615600 |      | -4.85818800 | -1.40189400 | -1.12757900 |      | -3.70017500 | -0.47767600 | -3.08516200 |      | -5.80456700 | -0.38395900 | -1.24193300 |      | -4.66553400 | 0.52338800 | -3.15056300 |      | -5.71814800 | 0.59232100 | -2.23379200 |      | -6.62901100 | -0.35023700 | -0.52729000 |      | -4.59387300 | 1.27356300 | -3.94006400 |      | 0.25048500 | -3.75003800 | -0.66750200 |      | 0.19949700 | -4.18373300 | 0.66147800 |      | 1.44866100 | -3.65727800 | -1.38803800 |      | 1.40507800 | -4.51855800 | 1.27693300 |      | 2.62597600 | -3.99980200 | -0.72510700 |      | 2.62354800 | -4.42852000 | 0.60538100 |      | 1.39173800 | -4.84298400 | 2.31877600 |      | 3.57470400 | -3.92327500 | -1.25966200 |      | 1.46551000 | -3.16785000 | -2.80455100 |      | 0.91405500 | -3.83797500 | -3.47817100 |      | 0.99922500 | -2.17489900 | -2.88713200 |      | 2.49268800 | -3.09782700 | -3.18036000 |      | 1.09613000 | -4.24475300 | 1.41285700 |      | -1.45777100 | -3.23438000 | 1.65986700 |      | -1.89099000 | -4.72869600 | 0.82831000 |      | -0.97836600 | -4.79764400 | 2.35117700 |      | 3.90893300 | -4.76405900 | 1.29978100 |      | 4.31817000 | -5.72076500 | 0.94802900 |      | 4.67676300 | -4.00093800 | 1.11292000 |      | 3.76656500 | -4.84555600 | 2.38462500 |      | 6.71377500 | 1.71037300 | -2.30410300 |      | -7.61515100 | 1.48692900 | -1.72118400 |      | -6.28618800 | 2.64291900 | -1.90826500 |      | -7.02032400 | 1.91417400 | -3.33757600 |      | -2.55837800 | -0.52728500 | -4.05398800 |      | -1.59064700 | -0.41340500 | -3.54138360 |      | -2.52026300 | -1.48397000 | -4.59328900 |      | -2.64306600 | 0.27146700 | -4.79931500 |      | -4.92479500 | -2.40019600 | -0.01329900 |
H  -4.83560800  -3.43379400  -0.37440400
H  -4.10335000  -2.23991200  0.70293500
H  -5.86938300  -2.31398700  0.53456100
H  -3.65586700  -3.97659300  -3.10311500
H  -1.31324000  -5.29424400  -2.32438100
C  -1.64335900  -2.23179800  1.17564800
H(Iso=2)  -2.28838800  -0.88976800  0.89836600
H  -2.50015100  0.03324500  0.75901300
P  -1.09557500  1.60305300  0.92446600
C  -3.90138000  3.15482400  3.53103700
H  -1.76199900  2.94938600  3.51969100
C  -5.09153300  2.91635000  2.85312700
H  -5.99577100  2.08332100  1.08006400
H  -3.91310400  3.66377700  4.49307500
H  -6.03813500  3.23684500  3.28405700
C  -0.80456400  3.01966600  -0.19979700
C  -0.77280200  2.80470400  -1.58052300
C  -0.69158400  4.32603400  0.29295500
C  -0.60676900  3.87718400  -2.45467200
H  -0.87683000  1.79149100  -1.96897800
C  -0.51911800  5.39213000  -0.58023400
H  -0.74007900  4.51042900  1.36687900
C  -0.47375100  5.16770300  -1.95519300
H  -0.58622300  3.70149200  -3.52900600
H  -0.42679200  6.40320500  -0.18823300
H  -0.34334700  6.00509700  -2.63810600
C  0.19663600  1.73256000  2.21553600
C  0.06125100  0.94795600  3.36918800
C  1.38588400  2.43903500  2.01091700
C  1.08663400  0.89021500  4.30636100
H  -0.85418000  0.37593800  3.53336400
C  2.41393800  2.37313800  2.94713000
H  1.51051700  3.04600600  1.11345600
C  2.26574800  1.60281000  4.09623100
H  0.96468400  0.28467100  5.20332300
H  3.33519900  2.92775000  2.77876300
H  3.07204300  1.55505100  4.82619300
N  2.39295000  -0.05951300  0.00089500
C  1.80133000  0.29405800  -1.14577500
C  2.55618900  1.21503200  -2.05202500
C  1.83194400  -0.98521000  0.95234800
O  0.66664500  -0.10469800  -1.47230200
C  2.80934200  -1.15276600  2.08809500
O                  2.30407500   -1.93906200   3.03131300
C                  3.16236500   -2.19297300   4.14624000
O                  3.90743900   -0.64733000   2.10993700
H                  3.31746000    0.29092700   0.24117000
H                  1.99391400    2.15429800   -2.13729200
H                  3.57227300    1.43162600   -1.70745200
H                  2.60095900    0.77294800   -3.05355400
H                  1.65253900   -1.96535800   0.49306700
H(Iso=2)           0.87177400   -0.62996000   1.36656500
H                  4.11849500   -2.60427300   3.80649500
H                  3.34811800   -1.26496600   4.69760500
H                  2.63165100   -2.91193300   4.77260800

Calculation of the Potential Energy Surface (PES) for deuteration of (D/L) Ac-Ala-OMe 12a/b with catalyst 1

The PES for (D/L) Ac-Ala-OMe was calculated in the analogous to Ac-Gly-OMe. The results are summarized in Figure S2. Although the overall reaction enthalpy remains the same, the energies of the transition states increase compared to Gly. This is in line with the experimental finding that the reaction reaches a plateau.

Figure S2.
### Conformational analysis of Ac-Ala-OMe

#### AlaAddProRu_SM_T353.log

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| N | 2.91112600 | -0.43144200 | -0.59801600 |
| C | 2.30542600 | -1.02926900 | 0.46562200  |
| C | 3.07861700 | -2.15710100 | 1.10353500  |
| C | 2.24625800 | 0.61429700  | -1.33932200 |
| O | 1.21427500 | -0.67103700 | 0.87995500  |
| C | 2.88320900 | 0.68183300  | -2.70809300 |
| O | 2.20788700 | 1.50562200  | -3.51406500 |
| C | 2.75694100 | 1.65933600  | -4.82142500 |
| O | 3.88608000 | 0.08808700  | -3.03267200 |
| H | 3.76766700 | -0.79478500 | -1.01205360 |
| H | 2.45393800 | -3.05690300 | -4.76682600 |
| H | 2.81902200 | 0.69064500  | -5.32786000 |
| H | 2.07913500 | 2.32820900  | -5.35430900 |
| C | 2.32689800 | 1.96800200  | -0.63546300 |
| H | 3.73418000 | 2.75654000  | -0.51471900 |
| H | 1.79382000 | 2.73733700  | -1.20401900 |
| H | 1.87011300 | 1.87700700  | 0.35505900  |

#### AlaAddProRd_SM_T353.log

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| N | 2.9864400 | -0.23934300 | -0.12053600 |
| C | 1.73721600 | 0.36848300  | -1.07242900 |
| C | 2.46907400 | 1.34047400  | -1.96508000 |
| C | 1.90724300 | -1.13232700 | 0.84828300  |
| O | 0.54169900 | 0.14059600  | -1.19622100 |
| C | 2.84858500 | -1.21583300 | 2.02763800  |
| O | 2.29313500 | 2.32820900  | -5.35430900 |
| C | 2.32689800 | 1.96800200  | -0.63546300 |
| H | 3.73418000 | 2.75654000  | -0.51471900 |
| H | 1.79382000 | 2.73733700  | -1.20401900 |
| H | 1.87011300 | 1.87700700  | 0.35505900  |
### AlaAddProSu_SM_T353.log

| Element | X           | Y           | Z           |
|---------|-------------|-------------|-------------|
| N       | 2.64587800  | -0.37332800 | -0.72256800 |
| C       | 1.70314000  | -0.19451300 | -1.68971100 |
| C       | 2.14452900  | -0.53327100 | -3.09242900 |
| C       | 2.34121600  | -0.12830100 | 0.66792900  |
| O       | 0.58847600  | 0.23661600  | -1.44041400 |
| C       | 3.36013600  | -0.87655400 | 1.49642300  |
| O       | 3.06381900  | -0.81499600 | 2.79725200  |
| C       | 3.99134900  | -1.46775400 | 3.66228000  |
| O       | 4.33154100  | -1.44285700 | 1.04972100  |
| H       | 3.50798000  | -0.82863300 | -0.91571500 |
| H       | 2.30178000  | 0.39732900  | -3.65057700 |
| H       | 3.06632200  | -1.12387000 | -3.13467000 |
| H       | 1.33878300  | -1.07921800 | -3.59282700 |
| H       | 1.34216400  | -0.53479600 | 0.88994300  |
| H       | 4.98757500  | -1.02477800 | 3.56054600  |
| H       | 3.60830800  | -1.32893300 | 4.67393300  |
| H       | 4.05328200  | -2.53451200 | 3.42326500  |
| C       | 2.34326900  | 1.35960900  | 1.01282300  |
| H       | 2.08582500  | 1.51659700  | 2.06593600  |
| H       | 3.30852200  | 1.79719800  | 0.81903200  |
| H       | 1.60341300  | 1.86681700  | 0.38606800  |

### AlaAddProSd_SM_T353.log

| Element | X           | Y           | Z           |
|---------|-------------|-------------|-------------|
| N       | 2.62299400  | 0.50890000  | -0.64613400 |
| C       | 1.92845700  | -0.64169500 | -0.42396500 |
| C       | 2.21101800  | -1.32607900 | 0.89069300  |
| C       | 2.39319400  | 1.29903900  | -1.83294400 |
| O       | 1.14071200  | -1.09480300 | -1.23938500 |
| C       | 2.89410100  | 2.69719700  | -1.55181000 |
| O       | 2.59228800  | 3.52893400  | -2.55218100 |
| C       | 3.05004800  | 4.86918900  | -2.38390000 |
| O       | 3.50540700  | 3.02500700  | -0.56050100 |
| H       | 3.19511300  | 0.93606200  | 0.07342900  |
| H       | 2.66001900  | -2.30566400 | 0.69161700  |
| H       | 2.87602900  | -0.76019900 | 1.55250700  |
| H       | 1.26040100  | -1.50670200 | 1.40356300  |
| H       | 1.30989900  | 1.34855200  | -2.02508300 |
| H       | 2.61363500  | 5.31283200  | -1.48291500 |
| H       | 4.14110600  | 4.89451500  | -2.29570200 |
| H       | 2.72536900  | 5.41091900  | -3.27386800 |
| C       | 3.07286600  | 0.70823900  | -3.06660000 |
### Coordination products

**AlaAddProRu.log**

|   |    |    |    |
|---|----|----|----|
| C | -1.22149100 | -4.09949900 | -2.69291500 |
| C | -2.19254700 | -4.46973800 | -1.82599700 |
| N | -0.72140800 | -2.88982700 | -0.86078800 |
| C | -3.17391800 | -3.46274200 | 0.25378500 |
| C | -2.75784600 | -4.02799200 | 1.82599700  |
| N | -0.72140800 | -2.88982700 | -0.86078800 |
| C | -3.17391800 | -3.46274200 | 0.25378500 |
| C | -2.75784600 | -4.02799200 | 1.82599700  |
| H | -3.28762600 | -4.31614300 | 3.52170400 |
| H | -6.1.78657000 | -2.20690100 | 1.15414300 |
| H | 0.30454900  | -2.10403100 | -2.85288900 |
| C | 1.64152800  | -2.46322400 | -2.65247000 |
| C | -0.06868300 | -0.96774100 | -3.57777000 |
| C | 2.62050500  | -1.64448700 | -3.20570000 |
| C | 0.95241900  | -0.16631900 | -4.09105100 |
| C | 2.29751300  | -0.48591500 | -3.91558700 |
| H | 3.67129300  | -1.91102000 | -3.06870900 |
| H | 0.68463500  | 0.72550000  | -4.66136600 |
| C | -1.51083800 | -0.61892600 | -3.80406000 |
| H | -2.09204900 | -1.48936800 | -4.13911300 |
| H | -1.99377300 | -0.25515600 | -2.88391600 |
| H | -1.60801800 | 0.16650200  | -4.56250200 |
| C | 2.00934000  | -3.66797100 | -1.84124500 |
| H | 1.44661200  | -3.70435500 | -0.89736900 |
| H | 1.79534900  | -4.60644000 | -2.37137300 |
| H | 3.07918800  | -3.66530400 | -1.60082300 |
| C | 3.38236200  | 0.37504100  | -4.48786300 |
| H | 2.99101200  | 1.32812600  | -4.86129500 |
| H | 4.15410700  | 0.59602900  | -3.73826800 |
| H | 3.88716600  | -0.12629700 | -5.32482700 |
| C | -5.69398400 | -3.08450000 | 3.68973400 |
| H | -5.14078400 | -2.64087500 | 4.52996400 |
| H | -6.56808000 | -2.45371200 | 3.48914700 |
| H | -6.06278200 | -4.05961900 | 4.03507700 |
| C | -4.83731700 | -2.24118900 | -1.20340400 |
| H | -4.20277900 | -1.39028100 | -1.49354300 |
| H | -4.77558700 | -2.97734700 | -2.01640600 |
| H | -5.87174900 | -1.88413400 | -1.15340200 |
AlaAddProRdC2.log

1 1

C -1.22149100 -4.09949900 -2.69291500
C -2.19254700 -4.46973800 -1.82599700
N -0.72140800 -2.88982700 -2.23180000
N -2.27003800 -3.47576600 -0.86078800
C -3.17391800 -3.46274200 0.25378500
C -2.75784600 -4.02799200 1.46373100
C -4.40711000 -2.81893300 0.11042100
C -3.59948300 -3.89151200 2.56510900
C -5.21464800 -2.71098100 1.24223400
C -4.82245100 -3.22583200 2.47790100
H -3.28762600 -4.31614300 3.52170400
H -6.17865700 -2.20690100 1.15414300
C 0.30454900 -2.10403100 -2.85288900
C 1.64152800 -2.46322400 -2.65247000
C -0.06868300 -0.96774100 -3.57777000
C 2.62050500 -1.64448700 -3.20570000
C 0.95241900 -0.16631900 -4.09105100
C 2.29751300 -0.48591500 -3.91558700
H 3.67129300 -1.91102000 -3.06870900
H 0.68463500 0.72550000 -4.66136600
C -1.51083800 -0.61892600 -3.80406000
H -2.09204900 -1.48936800 -4.13911300
H -1.99377300 -0.25515600 -2.88391600
H -1.60801800 0.16650200 -4.56250200
C 2.00934000 -3.66797100 -1.84124500
H 1.44661200 -3.70435500 -0.89736900
H 1.79534900 -4.60644000 -2.37173700
H 3.07918800 -3.66530400 -1.60082300
C 3.38236200 0.37504100 -4.48786300
H  2.85934800  1.64722100  3.83592000
H  2.93995300  4.27396000  0.42398500
H  4.04108700  3.36217500  2.45397700
Ir -1.07874200  -0.72070900  -0.10551000
H(Iso=2) -2.61149600  -0.46565800  -0.35812800
H(Iso=2) -1.79170100  -1.32997900  1.12235000
N  2.18932400  -1.55328000  1.70775200
C  2.16301300  -0.83137300  0.56688900
C  3.42469500  -0.12099200  0.18970400
C  1.06784400  -2.28872800  2.23722000
O  1.17816200  -0.46565800  -0.35812800
C  0.59885600  -1.70660300  3.55185400
O  -0.68742300  -1.98561800  3.75300600
C  -1.27487800  -1.41900900  4.92917000
O  1.30071200  -0.75914000  -0.18340900
C  -0.24197500  -2.25611000  1.51626700
H  -0.73869500  -1.74891700  5.82445200
H  -1.25353600  -0.32378000  4.87036100
H  -2.30952200  -1.76880100  4.93794100
C  1.44259954  -3.76756236  2.44747516
H  2.14272385  -3.84707489  3.25271035
H  0.56247301  -4.32847493  2.68338698
H  1.88298375  -4.15463862  1.55241443

AlaAddProSu.log

1 1
C  -1.40439000  -4.53876000  -1.40724800
C  -2.59790900  -4.06640700  -1.82498100
N  -0.73381900  -3.46684800  -0.82972200
N  -2.63393200  -2.72112400  -1.49259400
C  -3.73608600  -1.86466400  -1.82910900
C  -4.83909100  -1.81441100  -0.97228400
C  -3.65779500  -1.10472000  -3.00311400
C  -5.88544400  -0.96013700  -1.31843000
C  -4.72633900  -0.26278900  -3.29962100
C  -5.84489900  -0.17252400  -2.46848600
H  -6.75865600  -0.91007900  -0.66514600
H  -4.68638500  0.33960600  -4.20893900
C  0.60234000  -3.58473600  -0.32737400
C  0.80193000  -3.81932800  1.03544900
C  1.66021200  -3.53204600  -1.24583800
C  2.11618400  -3.99462700  1.47231600
C  2.95231100  -3.70580300  -0.75703100
C  3.20032700  -3.94842900  0.59642700
C -1.36209400  5.51255900  -0.75824200
H -2.02022600  4.60195500  1.07493400
C -0.79037000  5.30703000  -2.01288900
H  0.01679100  3.86481300  -3.35630700
H -1.66026200  6.14919300  -1.28219600
H -0.64155600  6.14919300  2.27927600
C -0.36169700  2.04043700  2.27297600
C -0.45187300  1.15879300  3.35971200
C -0.79037000  5.30703000  -2.01288900
C -1.20907600  6.41956600  4.43271100
C  1.51389900  3.12836500  -3.30505300
H  0.71342300  3.71457800  -1.43335100
H  1.41095900  2.25781000  4.42647300
H  0.34149600  0.58583900  5.27160300
H  2.28343500  3.89847900  3.33068300
H  2.09992000  2.34587100  5.26283100
H  2.41698200  0.32764600  -0.07610400
N  1.86084300  0.14026000  -1.28219600
C  2.80800000  0.02700600  -2.43213700
C  1.69470000  0.45920000  1.16041800
O  0.63478000  0.07151100  -1.47476200
C  2.62962200  1.00613000  2.21204000
O  1.96087900  1.33565100  3.3101600
C  2.76421600  1.72278200  4.42876100
O  3.82811800  1.07450000  2.07075200
H  3.42308100  0.44678400  0.01171900
H  2.94604200  1.09828000  2.62714300
H  3.79140000  0.41630400  2.24274300
H  2.37014200  0.41751300  -3.33071600
H  0.82720500  1.14362700  1.06179700
H  3.40726400  0.89135100  4.73734600
H  2.06291800  1.98232300  5.22341600
H  3.39304600  2.58195600  4.17280900
C  1.17576345  0.89555236  1.67709090
H  0.57323049  0.73833823  2.54722753
H  2.00534338  1.52366435  1.92643499
H  0.58815679  1.36594311  0.91659700

AlaAddProSd.log

1 1
C -1.93496195  -4.53386274  -1.51994511
C -2.54995941  -3.83963163  -2.50185991
N -1.40113726  -3.59598254  -0.64580271
N -2.37696741  -2.49583392  -2.21044109
C -2.83725532  -1.44612446  -3.07582629
C -4.11211998  -0.91227203  -2.87626283
C -1.98080603  -0.99860969  -4.08876165

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|      | X    | Y    | Z    |      |      |      |
|------|------|------|------|------|------|------|
| C    | -4.51973513 | 0.11874473 | -3.72410672 |      |      |      |
| C    | -2.43550332 | 0.02908459 | -4.90987648 |      |      |      |
| C    | -3.70009438 | 0.59956410 | -4.74386615 |      |      |      |
| H    | -5.51184861 | 0.55240682 | -3.58610337 |      |      |      |
| H    | -1.78597014 | 0.39195939 | -5.70867584 |      |      |      |
| C    | -0.59877964 | -3.96683758 | 0.48217329 |      |      |      |
| C    | -1.23297149 | -4.32325109 | 1.67765710 |      |      |      |
| C    | 0.78786292 | -4.02286088 | 0.32014786 |      |      |      |
| C    | -4.25308886 | -4.72391114 | 2.73934391 |      |      |      |
| C    | 1.55395154 | -4.42577571 | 1.41696612 |      |      |      |
| C    | 0.96717338 | -4.76543357 | 2.63438004 |      |      |      |
| H    | -0.89880725 | -5.02156035 | 3.67745414 |      |      |      |
| H    | 2.63907254 | -4.48184127 | 1.30988324 |      |      |      |
| C    | 1.43604594 | -3.65569457 | -0.98248789 |      |      |      |
| H    | 0.96931157 | -4.17082637 | -1.83363195 |      |      |      |
| H    | 1.35304510 | -2.57723775 | -1.19293998 |      |      |      |
| H    | 2.50126733 | -3.91294549 | 0.97517304 |      |      |      |
| C    | -2.72285017 | -4.26039410 | 1.81330272 |      |      |      |
| H    | -3.09822382 | -3.25947981 | 1.55920880 |      |      |      |
| H    | -3.22697505 | -4.97499822 | 1.14821419 |      |      |      |
| H    | -3.03192700 | -4.49127126 | 2.83939016 |      |      |      |
| C    | 1.80265079 | -5.14952361 | 3.81725473 |      |      |      |
| H    | 1.37548802 | -6.00628258 | 4.35301099 |      |      |      |
| H    | 2.82743374 | -5.40769304 | 3.52693270 |      |      |      |
| H    | 1.86458708 | -4.32181262 | 4.53953574 |      |      |      |
| C    | -4.15958862 | 1.69303478 | -5.66088606 |      |      |      |
| H    | -5.14549387 | 2.07682527 | -5.37262744 |      |      |      |
| H    | -3.45428314 | 2.53508765 | -5.66661434 |      |      |      |
| H    | -4.23488642 | 1.33580124 | -6.69665632 |      |      |      |
| C    | -6.01045067 | -1.58096115 | -4.26197083 |      |      |      |
| H    | 0.05471429 | -1.27570153 | -3.43880325 |      |      |      |
| H    | -0.62322707 | -2.67960934 | -4.26687827 |      |      |      |
| H    | -0.15648208 | -1.24451936 | -5.20056995 |      |      |      |
| C    | -5.00628736 | -1.41761738 | -1.78440503 |      |      |      |
| H    | -5.20523680 | -2.49377786 | -1.88383955 |      |      |      |
| H    | -4.55654381 | -1.26890788 | -0.79146046 |      |      |      |
| H    | -5.97014202 | -0.89756629 | -1.79729000 |      |      |      |
| H    | -3.09383791 | -4.16017943 | -3.38100590 |      |      |      |
| H    | -1.81404595 | -5.59605216 | -1.35072068 |      |      |      |
| C    | -1.66297300 | -2.32388700 | -1.05895900 |      |      |      |
| Ir   | -1.18410400 | -0.49437800 | -0.23975800 |      |      |      |
| H(Iso=2) | -2.52525200 | -0.62096000 | 0.51467600 |      |      |      |
| H(Iso=2) | -2.25202800 | 0.10484400 | -1.22204000 |      |      |      |
| P    | -1.07591200 | 1.67873500 | 0.67989900 |      |      |      |
| C    | -2.57909300 | 2.10878400 | 1.63706200 |      |      |      |
| C    | -3.82260100 | 1.71859800 | 1.12433600 |      |      |      |
| C    | -2.53086800 | 2.84959100 | 2.82324700 |      |      |      |
| C    | -4.99287000 | 2.04800500 | 1.79711000 |      |      |      |
| H    | -3.87830900 | 1.15160100 | 0.19316900 |      |      |      |
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| C | -3.70566000 | 3.17282000 | 3.49376600 |
| H | -1.57236200 | 3.16163100 | 3.23514800 |
| C | -4.93695500 | 2.77165400 | 2.98506600 |
| H | -5.95102200 | 1.72508000 | 1.39120300 |
| H | -3.65703600 | 3.74306800 | 4.41957400 |
| H | -5.85287400 | 3.02403000 | 3.51549500 |
| C | -0.95612400 | 3.04631400 | -0.53339700 |
| C | -0.90033700 | 2.76751100 | -1.90077400 |
| C | -0.96274000 | 4.38104300 | 4.41957400 |
| H | -0.90752100 | 1.72982300 | -2.24055900 |
| C | -0.89741800 | 5.13629000 | -1.03427400 |
| H | -1.02291700 | 4.61440300 | 0.95547500 |
| C | -0.84083900 | 5.12522100 | -2.39735300 |
| H | -0.81179800 | 3.57507700 | -3.89387000 |
| H | -0.90263900 | 6.44755500 | -0.69469800 |
| H | -0.80209100 | 5.93615900 | -3.12259500 |
| C | 0.31830400 | 1.94091600 | 1.83619400 |
| C | 0.33439200 | 1.20376000 | 3.02915700 |
| C | 1.42746200 | 2.72310500 | 1.50966000 |
| C | 1.42584900 | 1.27636100 | 3.88526100 |
| H | -0.51784200 | 0.57323200 | 3.28880200 |
| C | 2.53150700 | 2.77706800 | 2.35831200 |
| C | 1.43551300 | 3.30113800 | 0.58460000 |
| C | 2.53014500 | 2.05917000 | 3.54784700 |
| H | 0.41913300 | 0.71396600 | 4.81793300 |
| H | 3.39515800 | 3.37628700 | 2.07579400 |
| H | 3.38718500 | 2.10967300 | 4.21720200 |
| N | 2.50097800 | -0.40832300 | 0.27840900 |
| C | 1.74215800 | -1.09524400 | 1.15439700 |
| C | 2.47519100 | -1.66406000 | 2.33097300 |
| C | 2.04798700 | 0.18488600 | -0.95026700 |
| O | 0.53260000 | -1.32054900 | 1.00389800 |
| C | 2.77346700 | 1.49007000 | -1.17995800 |
| O | 2.18250600 | 2.18294800 | -2.14692200 |
| C | 2.74861800 | 3.46610700 | -2.43294000 |
| O | 3.75969900 | 1.83066200 | -0.57154300 |
| H | 3.44436200 | -0.14721000 | 0.55162000 |
| H | 2.96564100 | -2.59926800 | 2.01749500 |
| H | 3.24352800 | -0.98366300 | 2.71205600 |
| H | 1.76270200 | -1.89675500 | 3.12742100 |
| H | 0.96376300 | 0.39069000 | -0.91948200 |
| H | 2.63956300 | 4.12470800 | -1.56309100 |
| H | 3.80924200 | 3.37033400 | -2.68447800 |
| H | 2.17973700 | 3.85977400 | -3.27657100 |
| C | 2.29841102 | -0.74568957 | -2.15148177 |
| H | 1.76208893 | -0.38146356 | -3.00271501 |
| H | 3.34506905 | -0.76892033 | -2.37254123 |
| H | 1.96207088 | -1.73325334 | -1.91379894 |
### Transition states

AlaTSRu_9_T353.log

|          |         |         |         |
|----------|---------|---------|---------|
| C        | -2.51860500 | -4.24873700 | -1.51734700 |
| C        | -2.45674100 | -4.55672500 | -0.20599900 |
| N        | -2.08126600 | -2.93878600 | -1.64202600 |
| N        | -1.97922700 | -3.42744800 |  0.44630100 |
| C        | -1.83900100 | -3.40136900 |  1.51734700 |
| C        | -0.73924600 | -4.03877600 |  2.45144600 |
| C        | -2.87695200 | -2.84836100 |  2.63717000 |
| C        | -0.63586100 | -4.01941200 |  3.84429200 |
| C        | -2.74269200 | -2.88412900 |  4.02077100 |
| C        | -1.62464600 | -3.44970600 |  4.64212500 |
| H        | -0.22797800 | -4.49306500 |  4.31363100 |
| H        | -3.54073500 | -2.46514500 |  4.63792100 |
| C        | -2.15590000 | -2.24851700 |  2.90145300 |
| C        | -1.02731200 | -2.18938800 |  3.72342900 |
| C        | -3.38318800 | -1.68328800 |  3.26993900 |
| C        | -1.13841900 | -1.49373100 |  4.27041000 |
| C        | -3.44634100 | -1.01681700 |  4.49115700 |
| C        | -2.33252100 | -0.89264000 |  5.32326400 |
| H        | -0.26920200 | -1.43298000 |  5.58119900 |
| H        | -4.39832300 | -0.58314400 |  4.80397100 |
| C        | -4.58250000 | -1.76127000 |  2.37598800 |
| C        | -4.40302000 | -1.23513200 |  1.42600100 |
| H        | -5.45504600 | -1.30087100 |  2.85278500 |
| H        | -4.84541400 | -2.79732600 |  2.12152400 |
| C        |  0.27150300 | -2.81348100 |  3.17738000 |
| H        |  0.80066700 | -2.18364000 |  2.58750800 |
| H        |  0.12919600 | -3.79215100 |  2.83818600 |
| H        |  0.92665900 | -2.94972900 |  4.18594500 |
| C        | -2.42092400 | -0.11932500 |  6.60364900 |
| H        | -3.39424400 | -0.25518500 |  7.09097100 |
| H        | -2.29952700 |  0.95775300 |  6.41949000 |
| H        | -1.64056300 | -0.41784300 |  7.31317800 |
| C        | -1.51813000 | -3.45749100 |  6.13704000 |
| H        | -2.28817000 | -4.09931900 |  6.58582600 |
| H        | -0.54285600 | -3.82713000 |  6.47383800 |
| H        | -1.66339900 | -2.45189000 |  6.55599700 |
| C        | -4.09516700 | -2.26385000 |  1.99194800 |
| H        | -4.51983500 | -2.94223800 |  1.23828100 |
| H        | -4.87164900 | -2.06516800 |  2.73912000 |
| H        | -3.86197600 | -1.31694400 |  1.48701400 |
| C        |  0.25656800 | -4.79493700 |  1.62554500 |
| H        | -0.07035300 | -5.83632400 |  1.48886500 |
| H        |  0.37638700 | -4.36336900 |  0.62307900 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | 2.232575  | -2.485257 | 1.719649  |
| H       | 1.213807  | -0.849521 | 2.934430  |
| H       | -1.905667 | -0.300813 | 4.498766  |
| H       | -0.165414 | -0.603760 | 4.794634  |
| H       | -0.732693 | 1.028746  | 4.358588  |
| H       | 0.337963  | -0.772257 | 0.637392  |
| H       | 3.797161  | -3.160788 | 0.205881  |
| H       | 2.464203  | -4.342445 | 0.310482  |
| H       | 2.989880  | -3.465657 | 1.785152  |
| C       | 1.938152  | 0.434050  | 0.627108  |
| H       | 2.786653  | 0.302579  | 1.316672  |
| H       | 2.322320  | 0.423997  | 0.399483  |
| H       | 1.500232  | 1.417477  | 0.823877  |
| Al      | -1.914820 | -3.897160 | -2.689268 |
| C       | -3.056982 | -3.820498 | -1.975131 |
| N       | -1.041430 | -2.959867 | -2.151799 |
| N       | -2.864416 | -2.834616 | -1.019426 |
| C       | -3.913884 | -2.416376 | -0.129215 |
| C       | -4.003146 | -2.982495 | 1.143130  |
| C       | -4.804876 | -1.426375 | -0.573815 |
| C       | -4.999172 | -2.505239 | 1.998538  |
| C       | -5.774474 | -0.982613 | 0.318608  |
| C       | -5.881873 | -1.501167 | 1.612317  |
| H       | -5.086642 | -2.940616 | 2.996204  |
| H       | -6.473021 | -0.209266 | 0.006070  |
| C       | 2.028789  | -2.785090 | -2.668832 |
| C       | 1.245128  | -3.774422 | -2.405720 |
| C       | 0.565855  | -1.677121 | -3.478167 |
| C       | 2.534628  | -3.577623 | -2.899235 |
| C       | 1.364950  | -1.538920 | -3.961778 |
| C       | 2.866900  | -2.464375 | -3.697640 |
| H       | 3.293495  | -4.336850 | -2.700316 |
| H       | 2.097338  | -0.683150 | -4.598356 |
| C       | -0.484778 | -0.674214 | -3.842079 |
| H       | -1.467709 | -1.140879 | -3.995078 |
| H       | -0.602997 | 0.079315  | -3.050175 |
| H       | -0.211576 | -0.148984 | -4.764467 |
| C       | 0.920633  | -5.058719 | -1.695641 |
| H       | 0.029397  | -4.993322 | -1.059977 |
| H       | 0.737705  | -5.862800 | -2.423060 |
| H       | 1.761790  | -5.383662 | -1.070534 |
| C       | 4.263487  | -2.273446 | -4.180923 |
| H       | 4.277170  | -1.687145 | -5.107278 |
| H       | 4.888484  | -1.738596 | -3.451007 |
| H       | 4.755723  | -3.233145 | -4.378907 |
| C   | -6.93161600 | -0.98519300 | 2.54931200 |
| H   | -6.93576200 | -1.53663600 | 3.49675800 |
| H   | -6.77058500 | 0.07714400  | 2.77839200 |
| H   | -7.93441900 | -1.06726200 | 2.11020900 |
| C   | -4.68886600 | -0.82196800 | -1.93970700|
| H   | -3.82677200 | -0.13814100 | -1.99208500|
| H   | -4.54736000 | -1.57815300 | -2.72343800|
| H   | -5.58557700 | 0.24310800  | -2.18673300|
| C   | -3.05031900 | -4.03051300 | 1.63201300 |
| H   | -2.57167400 | -4.56127000 | 0.81539800 |
| H   | -2.25279600 | -3.57140400 | 2.23697200 |
| H   | -3.56459200 | -4.75430000 | 2.27577500 |
| H   | -3.99139300 | -4.36185600 | -2.04376600|
| H   | -1.62399800 | -4.52140800 | -3.52384800|
| C   | -1.61608600 | -2.28492200 | -1.11540100|
| P   | -0.96229200 | 1.51481600  | 1.07988900 |
| C   | -1.49759300 | 1.45691100  | 2.83072100 |
| C   | -2.54844700 | 0.59663400  | 3.17403800 |
| C   | -1.00511000 | 2.34201400  | 3.79574700 |
| C   | -3.09442600 | 0.62420600  | 4.45250900 |
| H   | -2.95707700 | -0.09304600 | 2.43456200 |
| C   | -1.54245800 | 2.35533700  | 5.07959400 |
| H   | -0.20770400 | 3.03869900  | 3.54227700 |
| C   | -2.59063000 | 1.50128900  | 5.40929600 |
| H   | -3.91785400 | -0.04514100 | 4.69943600 |
| H   | -1.14787300 | 3.04865400  | 5.82005600 |
| H   | -3.01757400 | 1.52373900  | 6.41028800 |
| C   | -2.15260800 | 2.69776200  | 0.33026300 |
| C   | -2.23697200 | 2.80510400  | -1.06377200|
| C   | -2.95204900 | 3.52739100  | 1.12098600 |
| C   | -3.09825800 | 3.72241500  | -1.65221300|
| H   | -1.61764700 | 2.16716600  | -1.69665600|
| C   | -3.82511800 | 4.43589800  | 0.52848100 |
| H   | -2.90482800 | 3.46444500  | 2.20727900 |
| C   | -3.89988800 | 4.53611700  | -0.85559500|
| H   | -3.14828400 | 3.79798000  | -2.73688000|
| H   | -4.44871900 | 5.06891400  | 1.15702500 |
| H   | -4.58319500 | 5.24758600  | -1.31526800|
| C   | 0.63485100  | 2.42103000  | 1.06282800 |
| C   | 1.64737600  | 2.09186700  | 1.97473300 |
| C   | 0.90062900  | 3.36917500  | 0.07016200 |
| C   | 2.88789900  | 2.71683200  | 1.90343900 |
| H   | 1.47329600  | 1.34675500  | 2.75030800 |
| C   | 2.14783700  | 3.98320600  | -0.00503800|
| H   | 0.12759700  | 3.64504600  | -0.64511900|
| C   | 3.14271900  | 3.66224900  | 0.91277300 |
| H   | 3.65763300  | 2.46621000  | 2.63159100 |
| H   | 2.33421600  | 4.72613200  | -0.77830300|
| H   | 4.11341700  | 4.15194000  | 0.86007700 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Ir   | -1.02592300 | -0.59762400 | -0.01585300 |
| H(Iso=2) | -1.87477800 | 0.14269800 | -1.16212100 |
| H(Iso=2) | -2.51564100 | -0.63175400 | 0.50307500 |
| N     | 1.72929600  | -0.97496100 | 0.96797500  |
| C     | 1.89279600  | -0.38635300 | -0.22044500 |
| C     | 3.25310700  | 0.08864600  | -0.60942700 |
| C     | 0.50312800  | -1.63588400 | 1.43399400  |
| O     | 0.92939600  | -0.97496100 | -0.99228300 |
| C     | 0.45046900  | -1.39723900 | 2.93103300  |
| C     | -0.60271000 | -1.99813500 | 3.48872900  |
| O     | -0.70317200 | -1.86738100 | 4.91161000  |
| N     | 1.28624500  | -0.78438100 | 3.55850400  |
| H     | 2.50878600  | -0.99560900 | 1.62111600  |
| H     | 3.24554000  | 1.18645500  | -0.63884200 |
| H     | 4.04220500  | -0.24731200 | 0.07026300  |
| H     | 3.46269000  | -0.26782500 | -1.62441000 |
| C     | -1.05703900 | -1.44454000 | 1.37155800  |
| H     | 0.15745200  | -2.33995700 | 5.39543500  |
| H     | -0.74710800 | -0.80941500 | 5.19017600  |
| H     | -1.62857700 | -2.37535500 | 5.18888400  |
| C     | 0.63711400  | -3.12982800 | 1.15538200  |
| H     | 1.49037200  | -3.55499500 | 1.70679700  |
| H     | -0.26562500 | -3.68502000 | 1.43083900  |
| H     | 0.82235200  | -3.26366800 | 0.08585300  |

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| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -1.08901300 | -3.86859300 | -2.65582400 |
| C    | -2.00369100 | -4.30587900 | -1.76527800 |
| N    | -0.55950800 | -2.69279300 | -2.14045900 |
| N    | -2.02048100 | -3.38917100 | -0.72457400 |
| C    | -3.00072000 | -3.43465800 | 0.31966100  |
| C    | -2.71436600 | -4.06627200 | 1.52988000  |
| C    | -4.24399200 | -2.81145800 | 0.08177900  |
| C    | -3.68022200 | -4.02232900 | 2.53635900  |
| C    | -5.16555800 | -2.78204500 | 1.12364100  |
| C    | -4.90059600 | -3.37424800 | 2.36040800  |
| H    | -3.46790600 | -4.51209800 | 3.48882800  |
| H    | -6.12773100 | -2.29274500 | 0.96143800  |
| C    | 0.40012400  | -1.91133000 | -2.86954800 |
| C    | 1.73263700  | -2.33146800 | -2.89239000 |
| C    | -0.04922500 | -0.80078100 | -3.59547900 |
| C    | 2.65153100  | -1.53617800 | -3.57863300 |
| C    | 0.90077400  | -0.06267900 | -4.29501000 |
| C    | 2.25570500  | -0.40004100 | -4.28102900 |
| H    | 3.70162800  | -1.83365600 | -3.58381000 |
| H    | 0.57304100  | 0.80958900  | -4.86462300 |
| C    | -1.49210300 | -0.40169200 | -3.61977400 |
-2.16189400  -1.27047100  -3.67972100
-1.75794500  0.15344800  -2.70827300
-1.69990900  0.24601200  -4.47904300
2.16729200  -3.62818700  -2.28055700
1.50421300  -3.94562100  -1.46544400
2.15701300  -4.42837900  -3.03533000
3.18572000  -3.55519800  -1.88412300
C  2.16729200  -3.62818700  -2.28055700
H  1.50421300  -3.94562100  -1.46544400
H  2.15701300  -4.42837900  -3.03533000
H  3.18572000  -3.55519800  -1.88412300
C  3.25552600  0.42348800  -5.03575800
H  3.30738100  0.11674400  -6.08951100
H  2.99190800  1.48900200  -5.02646200
H  6.44561900  -2.38273100  3.49147600
H  6.69435500  -4.11896400  3.29090900
C  4.56611000  -2.16750300  1.23212900
H  4.03021400  -1.21385000  1.35062600
H  4.28887600  -2.79906700  -2.08687900
H  5.63792500  -3.29090900  3.29090900
C  1.39403400  -4.72308500  1.78589700
H  0.95877200  -5.16081300  0.87780200
H  0.66239100  -3.99463500  2.16640800
H  1.49598500  -5.16689000  2.53565100
H  -2.65154200  -5.17268500  -1.76036600
H  -0.74965000  -4.26734400  -3.60284800
C  -1.12104700  -2.38144500  0.94004000
P  -1.52737100  1.23247400  1.59189700
C  -1.44699400  1.02826200  3.40741600
C  -1.73708500  -0.22843800  3.95198900
C  -1.21380600  2.10650200  4.26776600
C  -1.77716700  -0.40565700  5.32999800
H  -1.94038600  -1.07348500  3.29231400
C  -1.24676500  1.92354200  5.64673700
H  -1.01486200  3.09698500  3.85958400
C  -1.52513700  0.66828900  6.17895500
H  -2.00551400  -1.38702000  5.74198400
H  -1.05929100  2.76785100  6.30725300
H  -1.55127500  0.52836700  7.25789700
C  -3.28283500  1.70269000  1.31139000
C  -3.77952400  1.78706700  0.00345200
C  -4.14202700  1.97831300  2.37748600
C  -5.10170900  2.14183200  -0.23024600
H  -3.12572900  1.56810300  -0.84304500
C  -5.47205500  2.31851400  2.14091600
H  -3.78264000  1.92047800  3.40362000
C  -5.95368600  2.40199200  0.84074100
H  -5.47075500  2.20817800  -1.25219700
H  -6.13123900  2.52177400  2.98269900
H  -6.99285100  2.66901000  0.65813400
C  -0.57147100  2.76272300  1.23059800
C   0.70691600  2.94098000  1.44959000
C  -1.05564400  3.71988500  0.33444900
C   1.46945200  4.05743600  1.44959000
H   1.11517000  2.21633100  2.48071300
C  -0.28522500  4.82885400 -0.00391000
H  -2.05056900  3.61580400 -0.09495900
C   0.97588400  5.00383800  0.55479700
H   2.44989000  4.19168100  1.90393100
H   0.68306100  5.56616200 -0.69857100
H   1.57063200  5.87925500  0.30072000
Ir  -0.96758500 -0.68500400  0.27898400
H(Iso=2) -2.36759200 -0.36081000 -0.43913900
H(Iso=2) -2.04339300  1.43801800  1.16644200
N   1.84757800  0.18085600  0.30617600
C   1.32388000  0.79895400 -0.76111000
C   2.18637500  1.77156100 -1.49925700
C   1.22062400 -0.90487100  1.07888600
O   0.13397000  0.63289200 -0.76111000
C   2.00486300 -2.16195500  0.74301900
O   1.43070300 -3.26256100  1.23861300
C   2.24534100 -4.43818800  1.26976400
O   3.08944100 -2.14798600  0.20655400
H   2.86154700  0.21253200  0.39785500
H   2.33670000  2.71169800 -0.93128900
H   3.20609100  1.39353700 -1.64025900
H   1.73471600  1.97311100 -2.47439400
H  -0.18736900 -1.55652000  1.40803400
H   2.42113100 -4.81522500  0.25760700
H   3.20845900 -4.22167300  1.74258600
H   1.68608700  5.17131900  1.85472800
C   1.51727200 -0.65088400  2.56498700
H   1.20320500  1.50348700  3.17962400
H   2.59752600 -0.49951800  2.71823100
H   0.98487100  0.22950900  2.93725000

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1 1
C   -1.53593400 -4.34916000 -2.02378300
C  -2.79948000 -4.06758300 -1.64621400
N  -0.74812000 -3.27627200 -1.62392500
N  -2.76137600 -2.83290000 -1.01677600
C  -3.91550600 -2.28807000 -0.35495200
C  -4.18420000 -2.72934200  0.95074900
C  -4.71613600 -1.34837100 -1.00398000
C  -5.27106800 -2.16880700  1.61150200
C  -5.79924900 -0.82012100 -0.29697000
C  -6.08745300 -1.20701900  1.00823800
H  -5.49754700  -2.49654000  2.62831500
H  -6.43680700  -0.08328200  -0.78942000
C   0.67790500  -3.29380700  -1.81405200
C   1.49294300  -3.62733400  -0.72288900
C   1.20123800  -3.07624700  -3.09373100
C   2.86950100  -3.65099000  -0.92681600
C   2.59010000  -3.08460600  -3.23649900
C   3.43912100  -3.35782600  -2.16730200
H   3.51839500  -3.91440900  -0.08934600
H   3.01575700  -2.90951300  -4.22671400
C   0.34769800  -2.92676100  -4.32072400
H   0.40285300  -3.83871700  -4.93208100
H   0.71116400  -2.75416600  -4.09793900
H   0.70090700  -2.10200000  -4.95316900
C   0.91912100  -3.96593200  -0.61757800
H   0.61188000  -3.05972700  -1.15839000
H   0.03437700  -4.61267800  -0.53479900
H   1.66078000  -4.48698900  1.23322000
C   4.92746400  -3.34037400  -2.34179000
H   5.21831000  -3.59551800  -3.36769100
H   5.34126500  -2.34353500  -2.12891900
H   5.42185300  -4.04492900  -1.66244600
C  -7.25700700  -0.63553400  1.75023000
H  -8.03276700  -1.39618800  1.91204300
H  -6.95966300  -0.26697300  2.74063500
H  -7.17986000  0.19540300  1.20424600
C  -4.42146800  -0.85486800  -2.38738100
H  -3.89559900  0.11245700  -2.34775600
H  -3.79590500  -1.54810500  -2.96353900
H  -5.34910700  -0.68789500  -2.94815400
C  -3.30892700  -3.73752600  1.63105800
H  -3.23477100  -4.67493800  1.06278000
H  -2.28357800  -3.35649300  1.75430600
H  -3.69655000  -3.98042400  2.62704600
H  -3.72731400  -4.61336500  -1.75647100
H  -1.10512000  -5.19711400  -2.53997700
C  -1.49318800  -2.32156900  -0.99268200
Ir -0.99052100  -0.55628000  0.04944400
H(Iso=2) -1.13729400  -1.54004900  1.32149300
H(Iso=2) -2.54335100  -0.48405000  0.37733900
P  -0.75502400  1.15234300  1.68093300
C  -1.35883000  0.65885400  3.34510800
C  -2.40323000  -0.26223200  3.46506100
C  -0.88099500  1.29805300  4.49459400
C  -2.94199100  -0.55750500  4.71282700
H  -2.80533500  -0.75253200  2.57921600
C  -1.41453900  0.99288800  5.74117400
H  -0.07956900  2.03338000  4.42078100
C  -2.44367600  0.06186000  5.85357800
Insertion products

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C     -1.18383700  -4.30870900  -2.11842600
C     -2.17097200  -4.46879700  -1.21685000
N     -0.68267400  -3.02577000  -1.94072100
N     -2.25120400  -3.28358000  -0.54921700
C     -3.21106100  -3.13361200  0.54921700
C     -2.82993600  -3.48536400  -0.24877900
C     -4.45772700  -2.58012100  2.87345300
C     -3.73893400  -3.13361200  2.87345300
C     -5.33142300  -2.34788700  1.31179800
C     -4.98782000  -2.65859000  2.62697100
H     -3.21106100  -2.82993600  -0.24877900
C     -0.35057700  -2.57536400  -2.82981700
H     -1.91356700  -1.45316100  -3.70287200
C     -2.08791300  -2.74122700  -4.29344500
H     -1.60343200  -1.45316100  -5.41343200
C     -2.04900100  -3.56069500  -1.24022700
H     -1.45393600  -3.21581400  -0.38306300
H     -1.88421300  -4.64540100  -3.23207300
H     -3.11193200  -3.41756500  -1.00939800
C     -3.37028500  -1.58101600  -5.67289500
H     -3.06088000  -1.75267900  -6.71113800
H     -3.57118900  -0.50515200  -5.56498500
H     -4.31513900  -2.11066300  -5.50429300
C     -0.92971100  -2.38549500  3.75950100
H     -5.50188200  -1.65346000  4.46213400
H     -6.88689900  -1.98756200  3.40326000
H     -6.13941000  -3.29777500  4.3303400
C     -4.41927400  -2.18803200  -1.15198000
H     -4.21784100  -1.33031200  -1.49098800
H     -4.64093300  -3.00101400  -1.86858500
H     -5.87528800  -1.90443800  -1.21865800
C     -1.46437200  -4.03509300  2.13187800
H     -1.22856800  -4.90071900  1.49814900
H     -0.68444900  -3.28013700  1.94461600
H     -1.38088200  -4.35113300  3.17746500
H   -2.82850900  -5.29976100  -0.99738100
H   -0.77841200  -4.96439100  -2.87791900
C   -1.32490500  -2.36278300  -0.93925800
Ir  -1.13507500  -0.44079200  -0.02903600
H(Iso=2)  -2.13726700  -1.06534900  1.32321300
H(Iso=2)  -2.70146700  -0.81391300  0.75285300
P    1.22972700  1.62254700  1.15942700
C    2.58420400  1.66812600  2.39553100
C    3.86453900  1.28327200  1.97730400
C    2.40537100  2.12729000  3.70261500
C    4.93857100  1.33828000  2.85657200
H    4.02925900  0.94347000  0.95168700
C    3.48343300  2.17742400  4.58242300
H    1.42058400  2.44556400  4.04305200
C    4.74801300  1.78001700  4.16367000
H    5.92873800  1.03495100  2.51939500
H    3.33098200  2.53323100  5.59960500
H    5.58896900  1.82081200  4.85345200
C    1.50862900  3.16067300  0.21329200
C    1.76078700  3.12461400  0.15906200
C    1.53332000  4.38973700  0.88665500
C    2.01734000  4.30460300  1.85334800
H    1.75340200  2.17461700  1.69007400
C    1.79071200  5.56257900  0.19069200
H    1.35265400  4.43103900  1.96135200
C    2.03090800  5.52116900  0.11878500
H    2.21050300  4.26697700  2.92434000
H    1.80891300  6.51302900  0.72037100
H    2.23452100  6.44230000  1.72460800
C    0.32008600  1.89237700  2.08634000
C    0.62107300  1.04123300  3.15812400
C    1.28090500  2.81398500  1.65844800
C    1.84206100  1.14107400  3.81420900
H    0.10362900  0.29416400  3.48298600
C    2.51352300  2.89365500  2.30201800
H    1.06487400  3.48487400  0.82741800
C    2.79186900  2.06720600  3.38497700
H    2.05567600  0.49003900  4.66015400
H    3.25133000  3.61831500  1.96229700
H    3.74890100  2.14467800  3.89785900
N    1.71351700  -0.22159300  0.55156200
C    1.70167600  -0.90159100  0.59003500
C    3.00410500  -1.26271200  1.22488100
C    0.49613100  0.37962900  1.09538600
O    0.62106700  -1.20636300  1.15549500
C    0.69210800  0.55781000  2.57269700
O    -0.43120100  0.95582100  3.18680300
C    -0.25483500  1.47869000  -4.50268100
O    1.77856600  0.53082200  -3.10974600
|   |          |          |          |
|---|----------|----------|----------|
| H | 2.58198100 | -0.03765700 | -1.04910300 |
| H | 2.93048000 | -2.24971800 | 1.69176900 |
| H | 3.83952200 | -1.24697800 | 0.51645900 |
| H | 3.20680700 | -0.52874100 | 2.01865100 |
| H | -2.13272000 | 0.10760500 | -1.05758900 |
| H | 0.34004000 | 2.39875700 | -4.46872800 |
| H | 0.25312700 | 0.74979300 | -5.14289600 |
| H | -1.25886500 | 1.68717900 | -4.87929700 |
| C | 0.52112821 | 1.85677295 | -0.66062066 |
| H | -2.21327200 | 0.10760500 | -1.05758900 |
| H | 0.34004000 | 2.39875700 | -4.46872800 |
| H | 0.43709300 | -1.06450000 | 2.79004400 |

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|   |          |          |          |
|---|----------|----------|----------|
| C | -0.94692600 | -4.26506700 | -2.34922100 |
| C | -2.12486900 | -4.41840700 | -1.70706300 |
| N | -0.39021700 | -3.07970700 | -1.88735600 |
| N | -2.62989000 | -3.32622000 | -2.06649000 |
| C | -3.38251000 | -3.13183000 | 0.01116000 |
| C | -3.29866700 | -3.62922300 | 1.31431400 |
| C | -4.48559400 | -2.40750700 | 0.45275400 |
| C | -4.33489700 | -3.11027000 | 2.19353000 |
| C | -5.49487800 | -2.11704200 | 0.46179800 |
| C | -5.42896900 | -2.54403300 | 1.79050100 |
| H | -4.28910000 | -3.68259400 | 3.21689700 |
| H | -6.36265600 | -1.54533200 | 0.12745500 |
| C | 0.87929300 | -2.61365500 | -2.37247400 |
| C | 2.04297100 | -3.20596700 | -1.87372000 |
| C | 0.90194100 | -1.64890300 | -3.38719800 |
| C | 3.26396200 | -2.77731600 | -2.39724700 |
| C | 2.14398100 | -1.26388400 | -3.88291900 |
| C | 3.34725000 | -1.80959900 | -3.39726800 |
| H | 4.18483900 | -3.22672100 | -2.02040000 |
| H | 2.18409500 | -0.51832900 | -4.67926500 |
| C | -0.35854800 | -1.04076600 | -3.91972100 |
| H | -1.15330300 | -1.78709500 | -4.05725400 |
| H | -0.73980000 | -0.27286800 | -3.22972300 |
| H | -0.18066200 | -0.55613400 | -4.88618900 |
| C | 2.01310700 | -4.29161800 | -0.63785200 |
| H | 1.06679900 | -4.32616500 | -0.28262600 |
| H | 2.14876900 | -5.28053300 | -1.29865500 |
| H | 2.82829400 | -4.16486100 | -0.11401600 |
| C | 4.65806000 | -1.34769900 | -3.92834300 |
| H | 4.60309600 | -1.10779600 | -4.99702100 |
| H | 4.99675000 | -0.43714100 | -3.41237100 |
| H | 5.43703900 | -2.10645000 | -3.79004400 |
| C | -6.52466100 | -2.19296500 | 2.75103700 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| H       | -6.37340900 | -2.66451800 | 3.72893000 |
| H       | -6.58380100 | -1.10703100 | 2.90644700 |
| H       | -7.50434400 | -2.51362300 | 2.37356600 |
| C       | -4.60020500 | -1.98755900 | -1.88861400 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| H       | -4.88972900 | -2.83738000 | -2.52364600 |
| H       | -5.36570900 | -1.21328000 | -2.01258200 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
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| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
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| C       | -2.14153100 | -4.47544300 | 1.74718600 |
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| C       | -2.14153100 | -4.47544300 | 1.74718600 |
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| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |
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| H       | -3.65560200 | -1.60420500 | -2.29858700 |
| C       | -2.14153100 | -4.47544300 | 1.74718600 |
| H       | -3.65560200 | -1.60420500 | -2.29858700 |

Ir: 1.01121900 -0.66557200 0.05076300
\begin{verbatim}
H       -1.01047900  -0.30896200  -2.83237000
H       -0.66810300  -0.39720100  -4.56934900
C        2.23260900  -4.41584500  -1.33057300
H        1.45415300  -4.51018000   0.56869500
H        2.21680400  -5.32177900  -1.95473300
H        3.19488300  -4.39971300  -0.80714400
C        4.24142600  -1.17333900  -4.58379800
H        4.00090500  -0.97725500  -5.63615000
H        4.60912700  -0.22692200  -4.16033600
H        5.07221000  -1.88762900  -4.55311300
C        6.48704500  -2.30094100   2.92786300
H        6.34574800  -2.75525200   3.91553500
H        6.56592200  -1.21354800   3.06549300
H        7.45440600  -2.64302400   2.53759400
C        4.48359500  -2.12951000  -1.67439000
H        3.53500800  -1.77446400  -2.09840000
H        4.79211100  -2.99052300  -2.28452200
H        5.23638000  -1.34543300  -1.81639100
C        2.05412400   4.52567200   2.03984400
H        2.13525200   5.54956200   1.64633500
H        1.09207400   4.12535400   1.69812400
H        2.03100700   4.59562200   1.64633500
C        -1.06932000  -2.52407500  -0.73904400
P        -1.21909400   1.42547100   1.40651300
C        -2.08159500   1.41314000   3.01486800
C        -2.89042900   0.33584200   3.38372500
C        -1.99751400   2.52757600   3.86313100
C        -3.59954100   0.36817000   4.58130700
H        -2.96443600  -0.53801400   2.73667200
C        -2.70726000   2.55626600   5.05650400
H        -1.37656400   3.37926100   3.58355900
C        -3.50838400   1.47497400   5.41746100
H        -4.22102000  -0.48102500   4.86231000
H        -2.63577900   3.42507300   5.70786700
H        -4.06184800   1.49781800   6.35433600
C        -2.17667200   2.58111300   0.35387800
C        -1.85148400   2.67292500  -1.00870500
C        -3.24706100   3.32933200   0.85002900
C        -2.57434900   3.51456100  -1.84608000
H        -1.02736400   2.08283900  -1.41396600
C        -3.97456400   4.16116900   0.00285200
H        -3.52586400   3.26193100   1.90027700
C        -3.63926000   4.25759200  -1.34250100
H        -2.30829800   3.58483200  -2.89929900
H        -4.80882200   4.73562800   0.40081200
H        -4.21037500   4.90871300  -2.00144700
C        -0.36656700   2.27550200   1.75900300
\end{verbatim}
C  1.08617900  1.94283000  2.91496700
C  0.94170200  3.14700700  0.82981100
C  2.36216700  2.45515700  3.12254600
H  0.63794800  1.29579100  3.67014200
C  2.21434600  3.66776700  1.04696000
H  0.39091900  3.43464200 -0.06447000
C  2.93148900  3.31318100  2.18574100
H  2.90857700  2.19251600  4.02654800
H  2.64118300  4.36317500  0.32569100
H  3.92658400  3.72111500  2.35299200
Ir -0.97940200 -0.67050800  0.27963800
H(Iso=2) -2.32519700 -0.15037400 -0.86568300
H(Iso=2) -2.72329500 -0.44925600 -0.19532800
N  1.89784300 -0.61614600  0.42637000
C  1.69150600  0.13700200 -0.65429000
C  2.87754300  0.73962900 -1.33364600
C  0.81241600 -1.01539200  1.31681200
O  0.53175900  0.38462300 -1.06178200
C  1.08854200 -2.38060300  1.85220500
O  0.43721400 -2.58473900  3.00976600
C  0.80536100 -3.77214800  3.70997900
O  1.85672900 -3.18543000  1.37212800
H  2.84770700 -0.87935000  0.67052700
H  3.06286200  1.72578600 -0.88359000
H  3.78149700  0.13121400 -1.21693500
H  2.66138700  0.87308400 -2.39758500
H -1.78788700 -1.42200700  1.39849200
H  0.61980500 -4.66417100  3.10211000
H  1.86807300 -3.74360500  3.97387100
H  0.19055100 -3.78958300  4.61186700
C  0.82324694 -0.08175116  2.54147418
H  1.70006366 -0.26943954  3.12531108
H  0.82439672  0.93674425  2.21350195
H -0.04719420 -0.26385996  3.13651082

AlaInsSd.log

1 1
C -0.97030600 -4.00696600 -2.54979800
C -2.25257000 -3.98993500 -2.13052000
N -0.33210900 -2.94053000 -1.92965100
N -2.37223200 -2.91229600 -1.26806300
C -3.59702100 -2.58510000 -0.59482000
C -3.86516100 -3.19460100  0.63352800
C -4.46076300 -1.64862000 -1.17844800
C -5.01307400 -2.79055100  1.31889000
C -5.59613700 -1.28770500 -0.45892100
C -5.88198300 -1.83529900  0.79528100
H -5.23472800 -3.24452100  2.28646600
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -6.28433100 | -0.55771100 | -0.88963900 |
| C    | 1.06248700  | -2.67847000 | -2.15129800 |
| C    | 1.99022200  | -3.15171000 | -1.21826800 |
| C    | 1.44239400  | -2.04336900 | -3.34089090 |
| C    | 3.33917600  | -2.91160200 | -1.47840800 |
| C    | 2.80172000  | -1.81245900 | -3.54210300 |
| H    | 1.26591200  | -2.24343000 | -5.03198300 |
| H    | 5.15765200  | -0.38670400 | 3.79577000  |
| P    | -1.17501600 | 1.41697800  | 1.44790000 |
| C    | -2.27520600 | 1.19820800  | 2.90923600 |
| C    | -3.39575800 | 0.36478300  | 2.82099200 |
| C    | -2.10356400 | 1.97545000  | 4.06048300 |
| C    | -4.29595500 | 0.27502400  | 3.87768900 |
| H    | -3.59569500 | -0.21110600 | 1.91546400 |
| C    | -3.00287900 | 1.88106600  | 5.11613000 |
| H    | -1.26059000 | 2.66141500  | 4.13733400 |
| C    | -4.09591200 | 1.02434300  | 5.03198300 |
| H    | -5.15765200 | -0.38670400 | 3.79577000 |
| C    | 3.76251300  | -2.22912000 | -2.61896300 |
| H    | 4.08409800  | -3.28464000 | -0.77234800 |
| C    | 3.12145000  | -1.31112400 | -4.45760400 |
| C    | 0.44339000  | -1.66350500 | -4.39560100 |
| H    | 0.20040300  | -2.52441000 | -5.03789700 |
| H    | -0.50910500 | -1.30375200 | -3.98021900 |
| C    | 1.55996500  | -3.89635100 | 0.00831200 |
| H    | 1.14019500  | -3.20746400 | 0.75552900 |
| H    | 0.79335500  | -4.64964800 | -0.22085300 |
| H    | 2.41079000  | -2.12578700 | -3.90036800 |
| C    | 5.21646800  | -1.95140200 | 0.75552900 |
| H    | 5.49608800  | -2.12578700 | -3.90036800 |
| H    | 5.46292100  | -0.90365700 | -2.62984200 |
| H    | 5.85563700  | -2.58000000 | -2.23239600 |
| C    | -7.10346700 | -1.40290500 | 1.54831900 |
| H    | -7.20408900 | -1.93953500 | 2.49911000 |
| H    | -7.07496300 | -0.32660900 | 1.76809100 |
| H    | -8.01645500 | -1.58422500 | 0.96611500 |
| C    | -4.16877200 | -1.04252500 | -2.51785300 |
| H    | -3.26001100 | -0.42216900 | -2.49435800 |
| H    | -4.01266600 | -1.81003600 | -3.28867500 |
| H    | -5.00049500 | -0.40812900 | -2.84463200 |
| C    | -2.96698900 | -4.25365700 | 1.20128600 |
| H    | -3.12224000 | -5.21835800 | 0.69710100 |
| H    | -1.90059700 | -4.01210700 | 1.08895800 |
| H    | -3.17022100 | -4.40959900 | 2.26674600 |
| H    | -3.09701500 | -4.62786700 | -2.35642300 |
| H    | -0.43490100 | -4.66534300 | -3.22122400 |
| C    | -1.18430800 | -2.24932200 | -1.12292500 |
| Ir   | -0.97979800 | -0.53959200 | 0.09712900 |
| H(Iso=2) | -1.37679000 | -1.56390900 | 1.56095800 |
| H(Iso=2) | -2.12271600 | -1.41038200 | 1.22632600 |
| P    | -1.17501600 | 1.41697800  | 1.44790000 |
| C    | -2.27520600 | 1.19820800  | 2.90923600 |
| C    | -3.39575800 | 0.36478300  | 2.82099200 |
| C    | -2.10356400 | 1.97545000  | 4.06048300 |
| C    | -4.29595500 | 0.27502400  | 3.87768900 |
| H    | -3.59569500 | -0.21110600 | 1.91546400 |
| C    | -3.00287900 | 1.88106600  | 5.11613000 |
| H    | -1.26059000 | 2.66141500  | 4.13733400 |
| C    | -4.09591200 | 1.02434300  | 5.03198300 |
| H    | -5.15765200 | -0.38670400 | 3.79577000 |
| Atoms | Coordinates |
|-------|-------------|
| H     | -2.84858500 2.48405800 6.00885000 |
| H     | -4.79669000 0.94987700 5.86119100 |
| C     | -2.00836500 2.87008700 0.69758500 |
| C     | -3.13837700 2.64316700 -0.09615300 |
| C     | -1.67320200 4.18232800 1.04253200 |
| C     | -3.91109800 0.94987700 -0.54130000 |
| H     | -3.42369300 1.62492800 0.36534200 |
| C     | -2.43525100 5.24799500 0.57631200 |
| H     | -0.81670100 4.38278000 1.68501900 |
| C     | -3.55656000 5.01504900 -0.21379500 |
| H     | -4.79171300 3.51829200 -1.15304600 |
| H     | -2.15731600 6.26558700 0.84384500 |
| H     | -4.15857900 5.85046500 -0.56614900 |
| C     | 0.42592900 1.97689100 2.12907800 |
| C     | 0.91806100 1.36366300 3.28753900 |
| C     | 1.24127000 2.88302400 1.43904500 |
| C     | 2.17506600 1.69339900 3.78192600 |
| H     | 0.31296000 0.62377700 3.81186800 |
| C     | 2.49752700 3.21316200 1.94092000 |
| H     | 0.90529200 3.32116800 0.49924600 |
| C     | 2.96159500 2.63098000 3.11705900 |
| H     | 2.53774700 1.22040100 4.69254600 |
| C     | 3.11395300 3.93533000 1.40829300 |
| H     | 3.93917400 2.90164100 3.51201000 |
| N     | 1.45288300 0.58201700 -0.94172400 |
| C     | 1.90985700 -0.12804300 0.08910400 |
| C     | 3.35405800 -0.03597300 0.45345000 |
| C     | 0.07511200 0.46326500 -1.42029000 |
| O     | 1.14063300 -0.85251600 0.76412500 |
| C     | -0.37657600 1.80401800 -1.90056900 |
| O     | -1.46399400 1.70508500 -2.67598500 |
| C     | -1.90598500 2.93164000 -3.26087000 |
| O     | 0.19805500 2.85094100 -1.68449700 |
| H     | 2.07259200 1.23137500 -1.41527200 |
| H     | 3.77112900 -1.04915000 0.49321700 |
| H     | 3.93758200 0.56597800 -0.25020600 |
| H     | 3.43962100 0.39754100 1.45839900 |
| H     | -2.39518600 -0.15603000 -0.48455000 |
| H     | -1.97209000 3.71862700 -2.50296400 |
| H     | -1.21060500 3.24532200 -4.04729800 |
| H     | -2.88998000 2.72282400 -3.68654600 |
| C     | 0.06604177 -0.45736446 -2.65469640 |
| H     | 0.65964988 -0.02005079 -3.43012285 |
| H     | 0.47113160 -1.41189945 -2.39075478 |
| H     | -0.93895824 -0.57980099 -3.00093947 |
**Calculation of the Potential Energy Surface (PES) for deuteration of Boc-Gly-OMe 12a/b with catalyst 1**

The PES for (D/L) Boc-Gly-OMe was calculated in the analogous to Ac-Gly-OMe. The results are summarized in Figure S3. The energies of the transition states increase even more and the overall reaction is endergonic.

![Figure S3.](image)

**Conformational analysis of Boc-Gly-OMe**

**BocGlyAddProRd_SM_T353.log**

|   |   |   |   |
|---|---|---|---|
| N | 2.36944200 | -0.29661900 | -0.20301500 |
| C | 1.75601300 | 0.16969200 | -1.32268900 |
| C | 1.60699500 | -0.89527200 | 0.85065500 |
| O | 0.55391500 | 0.12008800 | -1.49799800 |
| C | 2.54297200 | -1.36558400 | 1.93036000 |
| O | 1.86257600 | -1.93967000 | 2.92617900 |
| C | 2.66089700 | -2.42533300 | 4.00376300 |
| O | 3.74460000 | -1.24354200 | 1.90460900 |
| H | 3.37583800 | -0.25417500 | -0.10102800 |
| H | 1.01137900 | -1.74944500 | 0.49357000 |
| H | 0.88157400 | -0.19098800 | 1.28690000 |
| H | 3.37513600 | -3.17364700 | 3.64481000 |
| H | 3.21467500 | -1.60489600 | 4.47218500 |
| H | 1.96336900 | -2.87028800 | 4.71531000 |
| O | 2.67555000 | 0.67468100 | -2.16498600 |
| Element | X    | Y    | Z    |
|---------|------|------|------|
| C       | 2.27222900 | 1.23998300 | -3.44593800 |
| C       | 1.36408900  | 2.43987600  | -3.23125500 |
| H       | 1.18631400  | 2.93917600  | -4.19309500 |
| H       | 0.40118800  | 2.14179200  | -2.80658300 |
| H       | 1.84266000  | 3.16184000  | -2.55651000 |
| C       | 3.59560600  | 1.67818300  | -4.04841200 |
| H       | 4.27052800  | 0.82089900  | -4.16360900 |
| H       | 3.43093200  | 2.12771000  | -5.03584100 |
| C       | 1.62182400  | 0.17301800  | -4.40806600 |
| H       | 0.66918300  | -0.15790400 | -3.88697800 |
| H       | 1.44055600  | 0.57737500  | -5.31556100 |

BocGlyAddProRu_SM_T353.log

0 1

| Element | X    | Y    | Z    |
|---------|------|------|------|
| N       | 0.72013900 | -1.42603100 | 2.49065700 |
| C       | -0.55298700 | -1.18666100 | 2.90217100 |
| C       | 1.16779000  | -0.97912500 | 1.20635100 |
| O       | -1.36890600 | -0.57717500 | 2.23819300 |
| C       | 2.59153100  | -1.41806100 | 0.99741300 |
| O       | 3.03937100  | -1.00378300 | -0.19076100 |
| C       | 4.38365300  | -1.37147300 | -0.49404900 |
| O       | 5.07376200  | -0.95082300 | 0.24479500 |
| H       | 4.49226800  | -2.46105300 | -0.49773600 |
| H       | 4.58820500  | -0.96286400 | -1.48499200 |
| O       | -0.74007800 | -1.72059600 | 4.12276800 |
| C       | -2.02574700 | -1.59388500 | 4.79597900 |
| C       | -2.34884500 | -0.13043200 | 5.04745100 |
| H       | -2.52710300 | 0.40524800  | 4.11066400 |
| H       | -3.24912600 | -0.05751600 | 5.67213300 |
| H       | -1.52233900 | 0.35442400  | 5.58346200 |
| C       | -1.78585100 | -2.31711900 | 6.10973400 |
| H       | -2.69449700 | -2.29726500 | 6.72468100 |
| H       | -1.51007500 | -3.36366500 | 5.92950200 |
| H       | -0.97416100 | -1.83768800 | 6.67109400 |
| C       | -3.11212000 | -2.93082200 | 3.99550400 |
| H       | -3.29261500 | -1.78910000 | 3.04158200 |
| H       | -2.82788800 | -3.33528300 | 3.79913000 |
| H       | -4.04579500 | -2.29867300 | 4.57368100 |

BocGlyAddProSu_SM_T353.log

0 1
| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| N     | 2.34397800 | -0.19194100 | -0.05406400 |
| C     | 1.64239300 | 0.77340200 | -0.70476000 |
| C     | 1.69509000 | -1.05291500 | 0.88823000 |
| O     | 0.45373300 | 0.96544600 | -0.53618600 |
| C     | 2.70849500 | -1.99730700 | 1.47446000 |
| O     | 2.13649300 | -2.80312600 | 2.37352200 |
| C     | 3.01426200 | -3.74505400 | 2.98373600 |
| O     | 3.87868800 | -2.02820300 | 1.17611600 |
| H     | 3.33486500 | -0.21837400 | 0.61840600 |
| H     | 1.21724500 | -0.48588500 | 1.70172500 |
| H     | 0.88732000 | -1.63931000 | 0.42311400 |
| H     | 3.45266000 | -4.40830100 | 2.23373600 |
| O     | 2.13649300 | -2.80312600 | 2.37352200 |
| C     | 1.95373700 | 2.55432300 | -3.30246300 |
| O     | 1.44078700 | 3.66470600 | -1.43143800 |
| H     | 1.17439400 | 4.53849400 | -2.04101000 |
| H     | 0.45266000 | -4.40830100 | 2.23373600 |
| H     | 2.22303800 | 3.96953500 | -0.72386500 |
| C     | 3.18807600 | 3.01302400 | -3.09004400 |
| H     | 3.58161000 | 2.02669900 | -3.71634700 |
| H     | 2.93857600 | 3.86351600 | -3.73698900 |
| C     | 3.97573200 | 3.32464200 | -2.39278500 |
| O     | 0.89138100 | 2.06226500 | -3.30246300 |
| H     | 1.27769800 | 1.22212200 | -3.89436300 |
| C     | 0.62607300 | -0.01146500 | 2.77605300 |

BocGlyAddProSd_SM_T353.log

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| N     | 0.85955100 | 0.48227900 | -2.63776800 |
| C     | 1.38603000 | 0.74869300 | -1.39479300 |
| C     | -0.55891800 | 0.61611200 | -2.80188200 |
| O     | 0.72552900 | 0.79090900 | -0.37818000 |
| C     | -1.00568700 | 2.05983600 | -2.90274300 |
| O     | -2.34095200 | 2.12318700 | -2.99869800 |
| C     | -2.87582100 | 3.44005000 | -3.10210400 |
| O     | -0.27345100 | 3.01679900 | -2.91153800 |
| H     | 1.44712000 | 0.76049000 | -3.41392800 |
| H     | -0.89506300 | 0.07281100 | -3.69416300 |
| H     | -1.05846000 | 0.15618300 | -1.94171200 |
| H     | -2.59763700 | 4.03698100 | -2.22717800 |
| H     | -2.49968300 | 3.93896200 | -4.00181600 |
| H     | -3.95958600 | 3.32201000 | -3.15622600 |
| O     | 2.71340200 | 0.90147200 | -1.50235000 |
| C     | 3.53397000 | 1.12860700 | -0.31756000 |
| C     | 3.44012900 | -0.06465700 | 0.61840600 |
coordination products

BocGlyAddProRd.log

1 1

C  -1.68957900  -4.30147000  -2.11447700
C  -2.82255200  -3.66618400  -2.48604600
N  -0.97879100  -3.41076800  -1.31896100
N  -2.78256400  -2.40787200  -1.90629100
C  -3.81399900  -1.42072900  -2.05586100
C  -4.85819800  -1.40197100  -1.12726100
C  -3.70031700  -0.47780700  -3.08494700
C  -5.80464700  -0.38410400  -1.24164500
C  -4.66575300  0.52338100  -3.15038400
C  -5.71833500  0.59211100  -2.23357600
H  -6.62906000  -0.35038800  -0.52696600
H  -4.59418600  1.27329100  -3.93995400
C  0.25067600  -3.74997700  -0.66766800
C  0.19968300  -4.18385300  0.66126000
C  1.44884800  -3.65969500  -1.38814700
C  1.40527100  -4.51865500  1.27669100
C  2.62619200  -3.99941900  -0.72521800
C  2.62376300  -4.42836400  0.60519200
H  1.39194000  -4.84323900  2.31848600
H  3.57493000  -3.92268100  -1.25972600
C  1.46564100  -3.16732500  -2.80458800
H  0.91445300  -3.83755300  -3.47832400
H  0.99899200  -2.17453500  -2.88706900
H  2.49281900  -3.09690500  -3.18032400
C  -1.09596800  -4.24499700  1.41259100
H  -1.45774400  -3.23466000  1.65955900
H  -1.89075300  -4.72904400  0.82802300
H  -0.97818100  -4.79785200  2.35092900
C  3.90915700  -4.76396000  1.29954800
H  4.31797300  -5.72102400  0.94827600
H  4.67721500  -4.00121700  1.11212500
H  3.76693800  -4.84484100  2.38446000
| C        | -6.71404400  | 1.71008500  | -2.30393400  |
|----------|--------------|-------------|--------------|
| H        | -7.61541600  | 1.48658200  | -1.72103200  |
| H        | -6.28654000  | 2.64267200  | -1.90810400  |
| H        | -7.02058800  | 1.91383900  | -3.33741900  |
| C        | -2.55853900  | -0.52736300 | -4.05380400  |
| H        | -1.59082300  | -0.41296900 | -3.54173000  |
| H        | -2.52010200  | -1.48420000 | -4.59281000  |
| H        | -2.64352300  | 0.27112600  | -4.79937800  |
| C        | -4.92473600  | -2.40024500 | -4.00795200  |
| H        | -4.83547100  | -3.43846000 | -3.37403400  |
| H        | -4.10328400  | -2.23988200 | 0.70327400   |
| H        | -5.86933500  | -2.31409900 | 0.53498900   |
| H        | -3.65579800  | -3.97651400 | -3.10302800  |
| H        | -1.31290700  | -5.29400600 | -2.32477500  |
| C        | -1.64328700  | -2.23178100 | -1.17548900  |
| Ir       | -1.18474300  | -0.49864200 | -0.15193700  |
| H(Iso=2) | -2.28855900  | -0.88957500 | 0.89838800   |
| H(Iso=2) | -2.49969800  | 0.03344900  | -0.75944500  |
| P        | -1.09560400  | 1.60315000  | 0.92447300   |
| C        | -2.65809000  | 2.08693900  | 1.75178100   |
| C        | -3.86040300  | 1.85442200  | 1.07318800   |
| C        | -2.68835100  | 2.74933400  | 2.98148900   |
| C        | -5.06794220  | 2.27038700  | 1.61950600   |
| C        | -3.86046000  | 1.34526300  | 0.10723800   |
| C        | -3.90148700  | 3.15505600  | 3.53088800   |
| H        | -1.76209300  | 2.94969600  | 3.51959200   |
| C        | -5.09161800  | 2.91648300  | 2.85297100   |
| H        | -5.99580400  | 2.08328000  | 1.07997400   |
| H        | -3.91325800  | 3.66408100  | 4.49288700   |
| H        | -6.03823800  | 3.23697600  | 3.28386100   |
| C        | -0.80446300  | 3.02004500  | -0.19978100  |
| C        | -0.77252700  | 2.80479300  | -1.58050500  |
| C        | -0.69148000  | 4.32610400  | 0.29299400   |
| C        | -0.60632600  | 3.87727100  | -2.45462100  |
| H        | -0.87656100  | 1.79159400  | -1.96898800  |
| C        | -0.51884900  | 5.39220100  | -0.58016400  |
| H        | -0.74008400  | 4.51049400  | 1.36691300   |
| C        | -0.47331000  | 5.16778200  | -1.95511700  |
| H        | -0.58565000  | 3.70159000  | -3.52895400  |
| H        | -0.42652100  | 6.40326700  | -0.18813900  |
| H        | -0.34277220  | 6.00517400  | -2.63800700  |
| C        | 0.19660200   | 1.73266300  | 2.21554900   |
| C        | 0.06108700   | 0.94828500  | 3.36935100   |
| C        | 1.38599800   | 2.43883700  | 2.01076400   |
| C        | 1.08650000   | 0.89046000  | 4.30646800   |
| H        | -0.85446700  | 0.37649700  | 3.53364200   |
| C        | 2.41409600   | 2.37283400  | 2.94692300   |
| H        | 1.51073900   | 3.04561400  | 1.11318600   |
| C        | 2.26578400   | 1.60272700  | 4.09615200   |
H  0.96446200  0.28508800  5.20353500
H  3.33548900  2.92718000  2.77839700
H  3.07209800  1.55490300  4.82608900
N  2.39284300 -0.05971700  0.00086200
C  1.80130300  0.29393200 -1.14583100
C  1.83164000 -0.98525500  3.03146100
O  3.31744200  0.29050800  0.24111300
H  1.65210700 -1.96540500  0.49312800
H  0.87152600 -0.62981200  1.36651200
H  4.11758600 -2.60458100  3.80677000
H  3.34756900 -1.26498600  4.69773500
H  2.63060400 -2.91173100  4.77285600
O  2.52288888  1.17372240 -2.01196187
C  1.70554369  2.18438923 -2.64167367
H  0.17734397  3.01832988 -3.27061931
H  0.54335593  2.52287706 -1.63549597
C  2.47070860  2.48865211 -4.04982081
H  3.38511200  2.03404964 -4.36935644
H  1.87036211  2.71283799 -4.90443570
H  2.68829201  3.38739282 -3.51146907
C  1.35626100  0.23789444 -3.92189314
H  2.06215520 -0.53085986 -3.68603260
H  0.37233889 -0.08740210 -3.65547345
H  1.39160558  0.44487773 -4.97108744

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1 1

C  -2.19225900 -3.68166100 -2.86055000
C  -1.63467500 -4.40743500 -1.86964200
N  -2.19137100 -2.36181100 -2.43830800
N  -1.30690900 -3.51314200 -0.86013100
C  -0.77579100 -3.97143900  0.38982400
C  0.59479900 -4.21560400  0.50418900
C  -1.68277000 -4.25979800  1.41672300
C  1.06541700 -4.69647000  1.72741800
C  -1.16604800 -4.76294600  2.60641900
C  0.20413600 -4.96158300  2.79035200
H  2.13664600 -4.86461400  1.85062600
H  -1.85139400 -5.00561300  3.42129500
C  -2.66236600 -1.30851300 -3.29404200
C  -1.76593800 -0.74854800 -4.21367700
C  -4.00107000  -0.92024000  -3.21752900
C   -2.24409200   0.25145800  -5.05442900
C   -4.43286700   0.08397600  -4.08679900
C   -3.57270700   0.68090200  -5.00616100
H   -1.56284900   0.70371000  -5.77744000
H   -5.47675200   0.40078600  -2.40181300
C   -4.94051000  -1.54801000  -2.23278400
H   -4.66948900  -1.29185000  -1.19749200
H   -5.96860400  -1.20995000  -2.40181300
C   -3.38234000  -1.20006000  -4.28038700
H    0.19492600  -0.98058300  -3.34220000
H   -0.25541800  -2.28360700  -4.44346300
H   -5.96860400  -2.24409200   0.25145800
H   -3.57270700  -5.05442900  -4.28038700
C   -4.94051000   0.25145800  -4.28038700
H   -4.66948900  -1.29185000  -4.28038700
H   -5.96860400  -1.20995000  -4.28038700
C    0.33823400  -1.20006000  -4.28038700
H    0.19492600  -0.98058300  -3.34220000
C    1.23879500  1.98413600  -1.29213900
C    1.08410600  3.74829700   0.34136300
C    2.44167200  2.51304900  -1.75048000
H    0.82251900  1.09327400  -1.76483000
C    2.28675400  2.03042400  -2.57507000
H    0.56547400  2.03042400   1.16047700
C    2.96886600  3.65650900  -1.16103500
H    0.82251900  2.03042400  -1.76483000
H    2.28675400  3.65650900  -1.16103500
H    2.96886600  4.24525000   0.34136300
C    0.25328500  2.42547900   4.20579200
H    0.74656600  2.14365800   2.55418700
C    1.70654100  3.21193300   4.64330900
H    1.20780700   0.14410200   1.04647600
H    0.61599400  -1.35530200   0.24855700
H    5.09310500  -2.37392000  -0.66218800
H    4.70502700  -0.75154300  -1.42935100
O    -0.79883000  -1.89582900   3.93097400
C    -1.98828400  -1.63835400   4.76589500
C    -2.08129400  -0.14720800   5.01112500
H    -2.33352100   0.39808600   4.09371100
H    -2.86669400   0.05655500   5.75077800
H    -1.13275800   0.23812600   5.40623400
C    -1.64998300  -2.38694400   6.04139100
H    -2.44864900  -2.24715700   6.78001000
H    -1.54736700  -3.46303700   5.84570500
H    -0.71075000  -2.01900500   6.47215200
C    -3.25833500  -2.18744400   4.14703700
H    -3.51216700  -1.68063900   3.21158200
H    -3.16900900  -3.26413900   3.96110800
H    -4.08161600  -2.03958900   4.85828200
|  |  |  |  |  |  |
|---|---|---|---|---|---|
| C  | -1.07522100  | -4.02559800  | -2.45125200  |
| C  | -2.18085900  | -4.30523500  | -1.73570800  |
| N  | -0.55119200  | -2.85255700  | -1.93196900  |
| N  | -2.31336400  | -3.30192500  | -0.79095500  |
| C  | -3.40382400  | -3.34411400  | 0.14386000   |
| C  | -3.17871100  | -3.94352200  | 1.39060200   |
| C  | -4.64120000  | -2.80701800  | -0.21687200  |
| C  | -4.23600600  | -3.97389090  | 2.29409400   |
| C  | -5.66930600  | -2.44964900  | 0.46413900   |
| C  | 0.72051300   | -2.38340800  | -2.40561400  |
| C  | 1.87256200   | -2.99195800  | -1.89591800  |
| C  | 0.76088800   | -1.43643300  | -3.43334000  |
| C  | 3.10461900   | -2.57474200  | -2.39568800  |
| C  | 2.01499300   | -1.08279800  | -3.92605300  |
| H  | 1.06167500   | -3.87972800  | -0.88757500  |
| H  | 1.46395800   | -5.03834000  | -1.35694600  |
| C  | 1.78820300   | -4.09778800  | -0.88757500  |
| C  | 1.06167500   | -3.87972800  | -0.88966220  |
| C  | 1.46395800   | -5.03834000  | -1.35694600  |
| C  | 2.76618400   | -4.27332700  | -0.42821700  |
| C  | 4.52753500   | -1.15061500  | -3.90532700  |
| C  | 4.49102700   | -0.87521700  | -4.96668800  |
| C  | 4.85593700   | -0.25925100  | -3.35090900  |
| C  | 5.30289800   | -1.91505500  | -3.77790400  |
| C  | -6.59331200  | -3.48265800  | 2.99284700   |
| H  | -6.34637200  | -2.88380700  | 3.87963600   |
| H  | -7.53557800  | -3.10179200  | 2.58137700   |
| H  | -6.77085400  | -4.50835500  | 3.34170200   |
| C  | -4.85871000  | -2.18756400  | -1.56398300  |
| H  | -4.14366700  | -1.37433000  | -1.75833300  |
| H  | -4.73197800  | -2.91739500  | -2.37567100  |
| H  | -5.86982100  | -1.77390200  | -1.64642200  |
| C  | -1.83744000  | -4.50495400  | 1.75916500   |
| H  | -1.41131800  | -5.12083900  | 0.95512700   |
| H  | -1.11469600  | -3.70003100  | 1.96636800   |
| H  | -1.91082900  | -5.12684100  | 2.65861200   |
| H  | -2.89577600  | -5.11526700  | -1.79823200  |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | -0.59786400 | -4.53475400 | -3.27855100 |
| C    | -1.29867500 | -2.37683400 | -0.88863700 |
| P    | -1.53518100 | 1.27436700 | 1.61280200 |
| C    | -3.03643400 | 1.28634800 | 2.66294700 |
| C    | -4.13649000 | 0.49457800 | 2.32646700 |
| C    | -3.13681700 | 2.16044900 | 3.75272100 |
| C    | -5.31412800 | 0.58004500 | 3.06337000 |
| H    | -4.08105500 | -0.19782400 | 1.48697700 |
| C    | -4.30919900 | 2.23426700 | 4.49309000 |
| H    | -2.28787000 | 2.78177600 | 4.03649700 |
| C    | -5.40310100 | 1.44578000 | 4.14675400 |
| H    | -6.16590900 | -0.03530100 | 2.78209400 |
| H    | -4.37031900 | 2.91305600 | 5.34160200 |
| H    | -6.32421500 | 1.50891200 | 4.72333100 |
| C    | -1.66709800 | 2.83659100 | 0.66445900 |
| C    | -1.98981300 | 2.76137500 | -0.69410900 |
| C    | -1.48745300 | 4.09437100 | 1.25267400 |
| C    | -2.12437900 | 3.92078900 | -1.45267200 |
| H    | -2.12427900 | 1.78273200 | -1.15854600 |
| C    | -1.61523000 | 5.25074400 | 0.49239400 |
| H    | -1.23612800 | 4.17508700 | 2.31006800 |
| C    | -1.93309000 | 5.16499500 | -0.86122400 |
| H    | -2.37746000 | 3.85024000 | -2.50941000 |
| H    | -1.47034900 | 6.22348700 | 0.95870100 |
| H    | -2.03590700 | 6.07218400 | -1.45373000 |
| C    | -0.17114100 | 1.51352700 | 2.81609900 |
| C    | -0.16856400 | 0.71194900 | 3.96646500 |
| C    | 0.94708400  | 2.30583900 | 2.54787700 |
| C    | 0.91545800  | 0.72459200 | 4.83633500 |
| H    | -1.02694800 | 0.07499500 | 4.18460000 |
| C    | 2.03608600  | 2.31328500 | 3.41682100 |
| H    | 0.96469200  | 2.93739300 | 1.66413000 |
| C    | 2.02256300  | 1.52540200 | 4.56282500 |
| H    | 0.89561300  | 0.10705700 | 5.73243700 |
| H    | 2.89476700  | 2.94595700 | 3.19773200 |
| H    | 2.87095900  | 1.53559900 | 5.24441900 |
| Ir   | -1.20727700 | -0.63023600 | 0.26320400 |
| H(Iso=2) | -2.69482300 | -0.47283900 | -0.16961500 |
| H(Iso=2) | -2.02918400 | -1.45053000 | 1.30231200 |
| N    | 2.32021300  | -0.20948300 | 0.19369600 |
| C    | 1.66570600  | 0.54798900 | -0.71762700 |
| C    | 1.70361500  | -0.89944800 | 1.30657100 |
| O    | 0.43273900  | 0.61105000 | -0.80239600 |
| C    | 2.41521500  | -2.20405900 | 1.56727800 |
| O    | 1.71683300  | -2.93230900 | 2.43724300 |
| C    | 2.30684000  | -4.17280100 | 2.83856300 |
| O    | 3.47552700  | -2.50795700 | 1.08173400 |
| H    | 3.32458900  | -0.30428200 | 0.08569700 |
| H    | 1.74773500  | -0.28886700 | 2.22345400 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 0.65171800 | -1.15402000| 1.19728000 |
| H    | 2.35150700 | -4.86255000| 1.98884000 |
| H    | 3.31700200 | -4.00770700| 3.22548300 |
| H    | 1.65377900 | -4.57188000| 3.61580200 |
| O    | 2.51527600 | 1.18687200 |-1.51199800 |
| C    | 2.18437600 | 2.41155900|-2.27406100 |
| C    | 1.79582100 | 3.49594400|-1.28814800 |
| H    | 1.66507300 | 4.44616500|-1.82252500 |
| H    | 0.84112100 | 3.26274000|-0.80197100 |
| H    | 2.57538800 | 3.63453300|-0.52681500 |
| O    | 2.51527600 | 1.18687200| 1.19728000 |
| C    | 3.31700200 | -4.00770700| 3.22548300 |
| H    | 1.65377900 | -4.57188000| 3.61580200 |
| H    | 2.57538800 | 3.63453300|-0.52681500 |
| O    | 2.51527600 | 1.18687200| 1.19728000 |
| C    | 3.31700200 | -4.00770700| 3.22548300 |
| H    | 1.65377900 | -4.57188000| 3.61580200 |
| H    | 2.57538800 | 3.63453300|-0.52681500 |
| O    | 2.51527600 | 1.18687200| 1.19728000 |
| C    | 3.31700200 | -4.00770700| 3.22548300 |
| H    | 1.65377900 | -4.57188000| 3.61580200 |
| H    | 2.57538800 | 3.63453300|-0.52681500 |
| O    | 2.51527600 | 1.18687200| 1.19728000 |
| C    | 3.31700200 | -4.00770700| 3.22548300 |
| H    | 1.65377900 | -4.57188000| 3.61580200 |
| H    | 2.57538800 | 3.63453300|-0.52681500 |
| O    | 2.51527600 | 1.18687200| 1.19728000 |
| C    | 3.31700200 | -4.00770700| 3.22548300 |
| H    | 1.65377900 | -4.57188000| 3.61580200 |
| H    | 2.57538800 | 3.63453300|-0.52681500 |

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C  -0.87535400 -4.06894800  2.46939000
C  -2.20324500 -3.94682100  2.26333900
N  -0.26471200 -3.05883700  1.73907300
N  -2.37741000 -2.86474400  1.41753100
C  -3.68411400 -2.45578100  0.98447800
C  -4.19939400 -3.00687600  0.19623700
C  -4.39526800 -1.53517000  1.75683600
C  -5.45670000 -2.58004800  0.61199000
C  -5.66107500 -1.15669700  1.30773300
C  -6.20088700 -1.65371100  0.13242100
C  -5.87327200 -2.98680400  1.53513800
C  -6.23805000 -0.47357000  1.90403000
C  1.16772600 -2.97485400 -1.69705400
C  1.82408300 -3.65119200  0.65869800
C  1.85695200 -2.36351800  2.74436100
C  3.20900000 -3.72621300  0.71168300
C  3.25413500 -2.42803800  2.72640700
C  3.94275000 -3.12213700  1.73819200
C  3.73970100 -4.25835800  0.08064900
C  3.81295700 -1.94770100 -3.53213800
C  1.16666700 -1.67706800  3.88561100
H  1.37775200 -2.18262400  4.83765000
H  0.07620100 -1.64723400  3.76563800
H  1.53328100 -0.64603600  3.99169300
C  1.05216100 -4.25742200  0.47278900
H  0.61876800 -3.47272700  1.11225200
H  0.21452200 -4.87579500  0.11935800
| Element | X           | Y           | Z         |
|---------|-------------|-------------|-----------|
| C       | 1.69653800  | -4.88522600 | 1.09807400|
| C       | 5.43804200  | -3.22431200 | -1.75643600|
| H       | 5.88367300  | -2.52630500 | -2.47539500|
| H       | 5.86677000  | -3.01391800 | 0.17564360|
| H       | 5.76401700  | -4.23646700 | -2.03224900|
| C       | -7.54287500 | -1.19952300 | 0.36533200 |
| H       | -8.18732800 | -2.05011700 | 0.62118500 |
| H       | -7.44546200 | -0.58885100 | 1.27401100 |
| H       | -8.06473600 | -0.59623600 | -0.38686700|
| C       | -3.80534200 | -0.91985600 | -2.98879300|
| H       | -3.09793700 | -0.11832300 | -2.72227900|
| H       | -3.25728000 | -1.64760000 | -3.60208500|
| H       | -4.58480900 | -0.46935600 | -3.61386800|
| C       | -3.41067700 | -3.99646000 | 0.99810400 |
| H       | -3.09869200 | -4.86115400 | 0.39601300 |
| H       | -2.49110100 | -3.54328300 | 1.39927800 |
| H       | -3.99611500 | -4.37020500 | 1.84500200 |
| C       | -3.04787500 | -4.51445800 | -2.63184400|
| H       | -0.29193000 | -4.76844000 | -3.05352800|
| C       | -1.17823900 | -2.29261100 | -1.07593000|
| Ir      | -1.00730000 | -0.64656100 | 0.17541000 |
| H(Iso=2)| -1.48851900 | -1.58310200 | 1.31831600 |
| H(Iso=2)| -2.55584500 | -0.66540500 | 0.09419300 |
| P       | -1.39936400 | 1.13676600  | 1.68499400 |
| C       | -1.90988500 | 0.54439300  | 3.33548700 |
| C       | -1.18975400 | -0.50904500 | 3.90873500 |
| C       | -2.92478100 | 1.16290800  | 4.06906700 |
| C       | -1.48147300 | -0.93823500 | 5.19814300 |
| H       | -0.38928700 | -0.98718900 | 3.34000100 |
| C       | -3.22261100 | 0.72275000  | 5.35558800 |
| H       | -3.48380100 | 1.99219300  | 3.63552100 |
| C       | -2.50199700 | -0.32483300 | 5.92072400 |
| H       | -0.91419900 | -1.75546600 | 5.63997000 |
| C       | -4.01880400 | 1.20515300  | 5.91961800 |
| H       | -2.73520800 | -0.66427100 | 6.92821500 |
| C       | -2.81940400 | 2.17985000  | 1.12456700 |
| C       | -3.99558500 | 1.54850300  | 0.69236200 |
| C       | -2.79035500 | 3.57792700  | 1.16792800 |
| C       | -5.10043800 | 2.29451900  | 0.30121000 |
| H       | -4.06498400 | 0.45977300  | 0.67524100 |
| C       | -3.90051800 | 4.32413900  | 0.77490600 |
| H       | -1.90207500 | 4.09875400  | 1.52126500 |
| C       | -5.05600300 | 3.68616500  | 0.33754600 |
| H       | -6.00486400 | 1.78093600  | -0.02397000|
| H       | -3.85916900 | 5.41087400  | 0.82398200 |
| H       | -5.92395220 | 4.27057700  | 0.03718300 |
| C       | -0.12197000 | 2.39294300  | 2.07742600 |
| C       | 0.27483300  | 2.67583400  | 3.38648300 |
| C       | 0.40885000  | 3.15397400  | 1.02788300 |
| Element | X                  | Y                  | Z                  |
|---------|--------------------|--------------------|--------------------|
| C       | 1.17908900         | 3.70579800         | 3.63815300         |
| H       | -0.13446300        | 2.10255700         | 4.21769500         |
| C       | 1.28648400         | 4.19890500         | 1.28305100         |
| H       | 0.10604900         | 2.96470300         | -0.00083300        |
| C       | 1.67560500         | 4.47533300         | 2.59225100         |
| H       | 1.47962400         | 3.91818500         | 4.66257000         |
| C       | 2.36473000         | 5.29278300         | 2.79651600         |
| H       | 1.66407800         | 4.79712500         | 0.45493700         |
| H       | 1.66407800         | 4.79712500         | 0.45493700         |
| H       | 1.66407800         | 4.79712500         | 0.45493700         |
| H       | 2.36473000         | 5.29278300         | 2.79651600         |
| N       | 1.12347400         | 1.27306000         | -1.90318900        |
| C       | 1.76632500         | 0.56341400         | -0.93247400        |
| H       | -0.26039000        | 1.17002200         | -2.26173700        |
| H       | -0.26039000        | 1.17002200         | -2.26173700        |
| O       | 1.21620000         | -0.25437500        | -0.19107100        |
| C       | -0.86573300        | 2.54295900         | -2.47946400        |
| O       | -2.15505800        | 2.41260000         | -2.76124800        |
| C       | -2.90447100        | 3.63064700         | -2.86286200        |
| O       | -0.26436200        | 3.58265900         | -2.36391000        |
| H       | 1.62994600         | 2.06329900         | -2.28818000        |
| H       | -0.42870600        | 0.55005900         | -3.15609100        |
| H       | -0.86914100        | 0.71416200         | -1.45044300        |
| H       | -2.90630500        | 4.14356300         | -1.89542300        |
| H       | -2.47129800        | 4.27908500         | -3.62979900        |
| H       | -3.91840300        | 3.30706000         | -3.13200300        |
| O       | 3.04619300         | 0.87960700         | -0.91269800        |
| C       | 3.95287400         | 0.66949000         | 0.24187000         |
| C       | 3.87496500         | -0.72861300        | 0.81581500         |
| H       | 4.70376700         | -0.84997300        | 1.52627900         |
| H       | 2.93397200         | -0.91959800        | 1.34069600         |
| H       | 3.98787000         | -1.47430300        | 0.02325000         |
| C       | 5.31292500         | 0.90706700         | -0.38768000        |
| H       | 5.36965700         | 1.90548000         | -0.83801200        |
| H       | 6.09685700         | 0.82594400         | 0.37502500         |
| H       | 5.50673200         | 0.15910300         | -1.16869200        |
| O       | 3.62548400         | 1.72023000         | 1.27962700         |
| C       | 3.69172800         | 2.72864700         | 0.85314400         |
| H       | 2.61871200         | 1.57944000         | 1.69450300         |
| H       | 4.34559900         | 1.64746600         | 2.10496100         |

**Transition states**

BocGlyTSRu_6_T353.log

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| Element | X                  | Y                  | Z                  |
|---------|--------------------|--------------------|--------------------|
| C       | -2.08317800        | -3.71947800        | -2.76064600        |
| C       | -1.64120800        | -4.46888700        | -1.73094600        |
| N       | -1.99312600        | -2.39635800        | -2.35695900        |
| N       | -1.29002700        | -3.58567700        | -0.71975800        |
| C       | -0.79984500        | -4.06449600        | 0.53869100         |
| C       | 0.55916800         | -4.35788500        | 0.66264800         |
| C       | -1.73210400        | -4.33414600        | 1.54619000         |
| C       | 1.00416600         | -4.82910900        | 1.89748900         |
|   | X    | Y    | Z    |   |   |
|---|------|------|------|---|---|
| C | -1.24268600 | -4.84391300 | 2.74453000 |   |   |
| C | 0.12187400  | -5.06131900 | 2.95141000  |   |   |
| H | 2.06829100  | -5.02971400 | 2.03205900  |   |   |
| H | -1.94503400 | -5.08626600 | 3.54453100  |   |   |
| C | -2.39308100 | -1.33049300 | -3.23244400 |   |   |
| C | -1.43600900 | -0.76445900 | -4.08378900 |   |   |
| C | -3.73357400 | -0.93898900 | -3.23999200 |   |   |
| C | -1.85257900 | 0.25843500 | -4.93101900 |   |   |
| C | -4.10327600 | 0.07890600 | -4.12096600 |   |   |
| C | -3.17912500 | 0.69611200 | -4.96180700 |   |   |
| H | -1.12427800 | 0.71744300 | -5.60211500 |   |   |
| H | -5.14832500 | 0.39402400 | -4.14983500 |   |   |
| C | -4.73370700 | -1.56986900 | -2.31995600 |   |   |
| H | -4.51890800 | -1.31795800 | -1.26999900 |   |   |
| H | -5.74888900 | -1.22728500 | -2.54763500 |   |   |
| H | -4.72293700 | -2.66626500 | -2.38861900 |   |   |
| C | -0.01297700 | -1.23651100 | -4.08056000 |   |   |
| H | 0.49195100  | -0.99950500 | -3.13139300 |   |   |
| H | 0.05876900  | -2.32542100 | -4.21008900 |   |   |
| H | 0.55498400  | -0.76449200 | -4.88999000 |   |   |
| C | -3.58682300 | 1.81057800 | -5.87658700 |   |   |
| H | -4.67701900 | 1.91787200 | -5.92422200 |   |   |
| H | -3.17115200 | 2.76965500 | -5.53651000 |   |   |
| H | -3.21909200 | 1.64791900 | -6.89766600 |   |   |
| C | 0.62147200  | -5.51324500 | 4.28921200  |   |   |
| H | -0.07801900 | -6.20860100 | 4.76987800  |   |   |
| H | 1.59754100  | -6.00656100 | 4.21564400  |   |   |
| H | 0.73935500  | -4.65293500 | 4.96506000  |   |   |
| C | -3.19293600 | -4.09298500 | 1.31544400  |   |   |
| H | -3.54116200 | -4.56984500 | 0.38846900  |   |   |
| H | -3.79629900 | -4.48724200 | 2.14042400  |   |   |
| H | -3.40383000 | -3.01733500 | 1.22183000  |   |   |
| C | 1.49274000  | -4.23611500 | -0.50359400 |   |   |
| H | 1.38627000  | -5.09595100 | -1.18121000 |   |   |
| H | 1.29537600  | -3.33707700 | -1.10633600 |   |   |
| H | 2.53340600  | -4.20348700 | -0.16448900 |   |   |
| H | -1.53991300 | -5.53836900 | -1.59975600 |   |   |
| H | -2.45524600 | -3.98209500 | -3.74239300 |   |   |
| C | -1.50270000 | -2.29266500 | -1.08408200 |   |   |
| Ir | -1.17213800 | -0.42102900 | -0.15444300 |   |   |
| H(Iso=2) | -2.72836200 | -0.19426500 | -0.53972500 |   |   |
| H(Iso=2) | -1.09818300 | 0.09568700 | -1.64357900 |   |   |
| P  | -1.06542300 | 1.91670000 | 0.30495100 |   |   |
| C  | -2.25877500 | 2.95468800 | -0.62461800 |   |   |
| C  | -3.09008300 | 2.42398100 | -1.61134100 |   |   |
| C  | -2.27897400 | 4.33717200 | -0.38947600 |   |   |
| C  | -3.93789500 | 3.25644900 | -2.33877100 |   |   |
| H  | -3.08445200 | 1.35587600 | -1.82185100 |   |   |
| C  | -3.12760100 | 5.16255000 | -1.11308800 |   |   |
|   |   |   |
|---|---|---|
| H | -1.62894300 | 4.77433600 | 0.36854000 |
| C | -3.96186400 | 4.62246000 | -2.09027700 |
| H | -4.58320300 | 2.82265500 | -3.10206600 |
| H | -3.13657900 | 6.23286500 | -0.91633600 |
| H | -4.62629500 | 5.27110400 | -2.65811400 |
| C | 0.52748400 | 2.68040800 | -0.21456300 |
| C | 1.08615900 | 2.26065000 | -1.42826300 |
| C | 1.13751600 | 3.73127500 | 0.47891600 |
| C | 2.23607100 | 2.86302900 | -1.92448800 |
| H | 0.61312600 | 1.45898800 | -1.99713000 |
| C | 2.29209300 | 4.32843400 | -0.01712500 |
| C | 0.71479500 | 4.09324300 | 1.41489700 |
| C | 2.84571100 | 3.89421200 | -1.21656200 |
| H | 2.65620500 | 2.52402100 | -2.86997300 |
| C | 2.75782800 | 5.14129000 | 0.53687600 |
| H | 3.74882500 | 4.36291600 | -1.60280600 |
| C | -1.29403600 | 2.42223200 | 2.04916300 |
| C | -2.54530000 | 2.85797000 | 2.49707700 |
| C | -0.23864000 | 2.33588200 | 2.96707800 |
| C | -2.72345200 | 3.24759000 | 3.82109700 |
| H | -3.38276000 | 2.91709400 | 1.80273400 |
| C | -0.41597500 | 2.74112500 | 4.28532500 |
| H | 0.74263600 | 1.98292500 | 2.64784200 |
| C | -1.65574000 | 3.20827300 | 4.71224000 |
| H | -3.69888800 | 3.59894200 | 4.15216500 |
| H | 0.42111100 | 2.69584000 | 4.98003500 |
| H | -1.79078200 | 3.53918000 | 5.74167000 |
| N | 0.49596800 | -1.27678100 | 2.15093400 |
| C | -0.76251700 | -1.34715600 | 2.61899100 |
| C | 0.85287600 | -0.66244700 | 0.89125100 |
| O | -1.74618200 | -1.00750000 | 1.93084900 |
| C | 2.14433500 | -1.29113600 | 0.43249100 |
| O | 2.49869000 | -0.86598800 | -0.78586700 |
| C | 3.81153700 | -1.23650900 | -1.21414100 |
| O | 2.82188000 | -2.02088700 | 1.12019200 |
| H | 1.24188700 | -1.73458300 | 2.67032900 |
| H | 1.13169100 | 0.39382400 | 1.04514800 |
| H | 0.33720100 | -0.62496400 | -0.70242100 |
| H | 4.55945300 | -0.87061400 | -0.50361100 |
| H | 3.89630000 | -2.32481400 | -1.29595700 |
| H | 3.94854200 | -0.76868700 | -2.19037200 |
| O | -0.82606900 | -1.83466200 | 3.84252200 |
| C | -1.97687200 | -1.63144100 | 4.74847900 |
| C | -2.13276000 | -0.14430600 | 4.98386000 |
| H | -2.44486300 | 0.38071700 | 4.07253400 |
| H | -2.89773900 | 0.02923000 | 5.75195400 |
| H | -1.18915000 | 0.28895800 | 5.33793600 |
| C | -1.52074400 | -2.34082900 | 6.00943000 |
| H | -2.27922500 | -2.22770500 | 6.79369800 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -1.37656900 | -3.41376700 | 5.82495000 |
| H | -0.57642200 | -1.92024100 | 6.37632100 |
| C | -3.25124000  | -2.25490200 | 4.21711200 |
| H | -3.58782400  | -1.77955900 | 3.29163200 |
| H | -3.11594100  | -3.32766800 | 4.04203000 |
| H | -4.03585400  | -2.13595900 | 4.97584500 |

BocGlyTSRd_5_T353.log

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|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | -0.59853700 | -4.15072600 | -2.49878200 |
| C | -1.72518100 | -4.44517300 | -1.81796400 |
| N | -0.17987200 | -2.89992700 | -2.06011500 |
| N | -1.97352500 | -3.37125300 | -0.97848400 |
| C | -3.10948600 | -3.92435700 | -0.09998800 |
| C | -4.09713500 | -3.78998000 | 2.02444900 |
| C | -5.33151000 | -2.81970000 | 0.35865600 |
| C | -5.25926600 | -3.11934200 | 1.64642200 |
| H | -4.03773300 | -4.24137900 | 3.01702000 |
| H | -6.24463400 | -2.07493300 | 0.04254500 |
| C | 0.97427100  | -2.28667400 | -2.65871200 |
| C | 2.24281600  | -2.67253100 | -2.22914000 |
| C | 0.77944800  | -1.45518700 | -3.76990800 |
| C | 3.34545100  | -2.19986500 | -2.93852920 |
| C | 1.90801500  | -1.03813800 | -4.46741500 |
| C | 3.19789700  | -1.40375500 | -4.07108700 |
| H | 4.34659600  | -2.48924000 | -2.61298700 |
| C | 1.78026200  | -0.40212100 | -5.34533600 |
| C | -0.59439400 | -1.03030400 | -4.18879000 |
| H | -1.29355200 | -1.87697700 | -4.24658600 |
| H | -1.01820800 | -0.31767000 | -3.46484000 |
| H | -0.57243400 | -0.54221900 | -5.16930600 |
| C | 2.44266400  | -3.61186600 | -1.07115700 |
| H | 1.60342200  | -3.59341300 | -0.36380200 |
| H | 2.54498700  | -4.65036400 | -1.41781300 |
| H | 3.35817800  | -3.36293600 | -0.52045500 |
| C | 4.39443400  | -0.89739300 | -4.81742200 |
| H | 4.23138600  | -0.91232400 | -5.90201300 |
| H | 4.61637200  | 0.14499000  | -4.54145900 |
| H | 5.28994600  | -1.49074300 | -4.59883200 |
| C | -6.42082100 | -2.98330600 | 2.58401400 |
| H | -6.23493900 | -3.49014300 | 3.53855800 |
| H | -6.63802300 | -1.92731000 | 2.79743600 |
| H | -7.33419400 | -3.41283600 | 2.15202400 |
| C | -4.35494100 | -2.06624800 | -1.90355400 |
| H | -3.72040100 | -1.17021900 | -1.97742800 |
| H | -4.01983200 | -2.76162300 | -2.68534200 |
|     |       |       |       |
|-----|-------|-------|-------|
| C   | 0.38730300 | -1.60616200 | 2.97273400 |
| O   | -0.65601100 | -2.34008100 | 3.36253500 |
| C   | -0.87716200 | -2.40948000 | 4.77342100 |
| O   | 1.15156700  | -1.04720100 | 3.72658200 |
| H   | 2.46368100  | -0.90027100 | 1.79399500 |
| H   | 0.54518100  | -2.63939800 | 1.14156700 |
| C   | -1.03722300 | -1.42641900 | 1.38687800 |
| C   | -0.01960500 | -2.87345200 | 5.27102600 |
| H   | 0.01960500  | -2.87345200 | 5.18098200 |
| C   | 1.15156700  | -1.04720100 | 3.72658200 |
| H   | -1.03722300 | -1.42641900 | 1.38687800 |
| O   | 3.11101400  | 0.32342600  | -0.10350000|
| C   | 3.51481400  | 1.51191600  | -0.89423800|
| C   | 3.19933500  | 2.73251300  | -0.05818500|
| C   | 3.54901100  | 3.63319900  | -0.57946200|
| C   | 2.11673400  | 2.83258900  | 0.09891900 |
| C   | 3.69804900  | 2.68187700  | 0.91742500 |
| C   | 5.00866700  | 1.29675200  | -1.04124500|
| H   | 5.46231300  | 2.16220600  | -1.53929200|
| H   | 5.48493500  | 1.17175200  | -0.06133100|
| H   | 5.21037300  | 0.40187800  | -1.64522900|
| C   | 2.85251400  | 1.57491200  | -2.25615500|
| H   | 3.40792400  | 2.29610800  | -2.87140900|
| H   | 2.89180300  | 0.59706700  | -2.74579500|
| H   | 1.80651500  | 1.89107400  | -2.20447100|

BocGlyTSSu_5_T353.log

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|     |       |       |       |
|-----|-------|-------|-------|
| C   | -1.02601700 | -4.10302700 | -2.43109400 |
| C   | -2.13802700 | -4.32934300 | -1.70302700 |
| N   | -0.44100400 | -2.95515300 | -1.91580600 |
| N   | -2.20956000 | -3.31599400 | -0.75907500 |
| C   | -3.27800200 | -3.26934500 | 0.20044500 |
| C   | -3.08558900 | -3.87477400 | 1.44838700 |
| C   | -4.48782400 | -2.67521400 | -0.16849100|
| C   | -4.14262400 | -3.83791100 | 2.35324900 |
| C   | -5.51694600 | -2.66818900 | 0.77413600 |
| C   | -5.36259200 | -3.23630800 | 2.03752700 |
| H   | -4.01437300 | -4.30198600 | 3.33296000 |
| H   | -6.47164000 | -2.21156400 | 0.50553900 |
| C   | 0.81909700  | -2.48169400 | -2.41016500|
| C   | 1.98081600  | -3.08309100 | -1.91926800|
| C   | 0.83232800  | -1.52402700 | -3.42898900|
| C   | 3.20247800  | -2.61684500 | -2.40206500|
| C   | 2.07738700  | -1.12016000 | -3.90483000|
| C   | 3.26889900  | -1.62591600 | -3.38052500|
| H   | 4.12399300  | -3.04461500 | -2.00394800|
| H   | 2.12309300  | -0.38481900 | -4.71053900|
| C   | -0.44284500 | -0.95211400 | -3.96918500|
|     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|
| H   | 1.18281800 | -1.73293700 | -4.19125100 |
| H   | -0.90098200 | -0.26587500 | -3.23975800 |
| H   | -0.26190200 | -0.39152100 | -4.89372200 |
| C   | 1.91515200 | -4.22918700 | -0.95521300 |
| H   | 1.16142200 | -4.07307300 | -0.16809700 |
| H   | 1.63839900 | -5.15927500 | -1.47302800 |
| H   | 2.88571200 | -4.38834800 | -0.47397200 |
| C   | 4.58814400 | -1.08342900 | -3.83679000 |
| H   | 4.56333000 | -0.78387500 | -4.89196500 |
| H   | 4.85472000 | -0.19042100 | -3.25107800 |
| H   | 5.39716800 | -1.81173400 | -3.70734100 |
| C   | -6.47420500 | -3.21160000 | 3.04227300 |
| H   | -6.19762200 | -2.61653700 | 3.92395700 |
| H   | -7.39202900 | -2.78326300 | 2.62214700 |
| H   | -6.71067500 | -4.22148100 | 3.40182700 |
| C   | -4.67686100 | -2.06266300 | 1.52282400 |
| H   | -3.92320700 | -1.28698000 | -1.72134500 |
| H   | -4.58589800 | -2.80614700 | -2.32701300 |
| H   | -5.66726900 | -1.60251600 | -1.60981300 |
| C   | -1.78358200 | -4.52336000 | 1.80945200 |
| H   | -1.39774100 | -5.15699400 | 0.99855000 |
| H   | -1.00918400 | -3.77140000 | 2.02443400 |
| H   | -1.89557300 | -5.14875200 | 2.70248500 |
| H   | -2.89141900 | -5.10455000 | -1.75170100 |
| H   | -0.58002500 | -4.63322100 | -3.26250100 |
| C   | -1.15925800 | -2.44873300 | -0.87820700 |
| P   | -1.36302800 | 1.21950800  | 1.63743800 |
| C   | -2.92224000 | 1.16064700  | 2.59793200 |
| C   | -3.99247200 | 0.37145900  | 2.16937200 |
| C   | -3.09186600 | 1.99176000  | 3.71258900 |
| C   | -5.20791300 | 0.41048600  | 2.84642200 |
| H   | -3.88459000 | -0.27391100 | 1.30187000 |
| C   | -4.30326200 | 2.02026500  | 4.39124900 |
| H   | -2.26876200 | 2.61466100  | 4.06250000 |
| C   | -5.36517500 | 1.23009700  | 3.95781100 |
| H   | -6.03404800 | -0.20879200 | 2.49787800 |
| H   | -4.41953300 | 2.66468000  | 5.26045300 |
| H   | -6.31540000 | 1.25733700  | 4.48793400 |
| C   | -1.52673600 | 2.79476700  | 0.71720300 |
| C   | -1.97139700 | 2.76292200  | -0.60841300 |
| C   | -1.31198300 | 4.03278700  | 1.33513100 |
| C   | -2.18227700 | 3.94753800  | -1.30749900 |
| H   | -2.14498300 | 1.80460900  | -1.09821600 |
| C   | -1.51550700 | 5.21386900  | 0.63144700 |
| H   | -0.97917800 | 4.07892500  | 2.37172400 |
| C   | -1.94971600 | 5.17266100  | -0.69084600 |
| H   | -2.52759100 | 3.91099700  | -2.33941900 |
| H   | -1.34187300 | 6.17074300  | 1.12012300 |
| H   | -2.11322200 | 6.09909400  | -1.23829600 |
C   -0.06022000  1.49052600  2.88689900
C   -0.08564000  0.71957000  4.05595500
C    1.07820100  2.49694000  2.59635200
C    0.99838000  0.72698400  4.92639800
H   -0.95981000  0.10775700  4.28387300
C    2.16165400  2.25517000  3.47089400
H    1.12180100  2.84209900  1.68163900
C    2.12363100  1.49469600  4.63523000
H    0.96493000  0.13047600  5.83613500
H    3.03840600  2.85714700  3.23937400
H    2.97197000  1.49933200  5.31670400
Ir   -0.95742400 -0.70747600   0.29236600
H(Iso=2) -2.38001700 -0.32555900 -0.39353200
H(Iso=2) -2.00172800 -1.42216700  1.23564300
N    1.96468100 -0.22243500  0.02955900
C    1.42457000  0.52261500  0.94512500
O    0.19485500  0.56220900 -1.15037800
C    1.98647800 -2.12503500  1.46704500
O    1.29684100 -2.87448600  2.33732300
C    1.99557600 -3.98379000  2.90716700
O    3.12406500 -2.35342200  1.12650900
H    2.97443600 -0.34172600  0.04627800
H    1.19835000  0.28089100  1.97028100
H    2.22563500 -4.72665300  2.13569700
H    2.92700900 -3.65062100  3.37539300
H    1.31904900 -4.40876800  3.65095900
O    2.32125000  1.17886100 -1.65871500
C    2.01431900  2.45047600 -2.34880700
C    1.66756700  3.47549400 -1.28007700
H    1.49555300  4.45397800 -1.74743500
H    0.74816800  3.20228500 -0.74402100
H    2.49224400  3.57952300 -0.56201800
C    3.33284300  2.77758500 -3.01888500
C    3.56931900  2.02890500 -3.78669600
C    3.27013000  3.75930500 -3.50384400
C    4.15070200  2.80129000 -2.28848300
C    0.91603400  2.30581200 -3.38145300
H    1.12807700  1.46285700 -4.04975800
H   -0.06816900  2.15649800  2.92964200
H    0.88813200  3.22155800 -3.98667800

BocGlyTSSd_2_T353.log

1 1
C   -0.88746800 -4.01794600 -2.55065800
C   -2.20627100  3.93462600 -2.28001100
N   -0.27377500  2.97074900 -1.87402000
|         | x         | y         | z         |
|---------|-----------|-----------|-----------|
| N       | -2.37243600 | -2.84294100 | -1.44294500 |
| C       | -3.66655300 | -2.43988100 | -0.96633200 |
| C       | -4.11710400 | -2.94696900 | 0.25951500  |
| C       | -4.42130900 | -1.55403100 | -1.73812800 |
| C       | -5.35028900 | -2.50157900 | 0.72525500  |
| C       | -5.65594400 | -1.14617000 | -1.23095700 |
| C       | -6.12908100 | -1.59529400 | 0.00046300  |
| H       | -5.71851800 | -2.87550500 | 1.68226900  |
| H       | -6.26461900 | -0.45785300 | -1.82099600 |
| C       | 1.15638700  | -2.83900600 | -1.89677300 |
| C       | 1.48219000  | -3.46268100 | -0.87148600 |
| C       | 1.77397400  | -2.23641700 | -2.99390700 |
| C       | 3.26634000  | -3.47224400 | -0.97908300 |
| C       | 3.17157200  | -2.23949800 | -3.03269400 |
| C       | 3.93074800  | -2.85990400 | -2.04721100 |
| H       | 3.85054800  | -3.96783700 | -0.20065300 |
| H       | 3.67419600  | -1.76181800 | -3.87594100 |
| C       | 1.00660300  | -1.61594300 | -4.12450200 |
| H       | 1.26052300  | -2.09516100 | -5.07919700 |
| H       | -0.08020700 | -1.69645900 | -3.99679800 |
| H       | 1.26024600  | -0.55154200 | -4.22973400 |
| C       | 1.18806700  | -4.08369500 | 0.30129800  |
| H       | 0.74365000  | -3.31095900 | 0.94692100  |
| H       | 0.36874900  | -4.75015100 | -0.00517900 |
| H       | 1.88928600  | -4.66709300 | 0.90819000  |
| C       | 5.42692200  | -2.89760700 | -2.12671100 |
| H       | 5.81322700  | -2.17343600 | -2.85366900 |
| H       | 5.88802400  | -2.68274000 | -1.15262700 |
| H       | 5.78250300  | -3.89124800 | -2.43205600 |
| C       | -7.43993200 | -1.11654300 | 0.54695900  |
| H       | -8.07284800 | -1.95486900 | 0.86491200  |
| H       | -7.28997200 | -0.47850600 | 1.42910700  |
| H       | -8.00019600 | -0.53499200 | -0.19467900 |
| C       | -3.91302700 | -1.01750800 | -3.04116400 |
| H       | -3.16929800 | -0.22189300 | -2.88027100 |
| H       | -3.43350300 | -1.79231300 | -3.65442300 |
| H       | -4.72942100 | -0.58184100 | -3.62861300 |
| C       | -3.28456400 | -3.90584600 | 1.05283200  |
| H       | -2.98213200 | -4.77859100 | 0.45731500  |
| H       | -2.36080000 | -3.42393800 | 1.40732900  |
| H       | -3.83278300 | -4.26840800 | 1.92895900  |
| H       | -3.05043700 | -4.53398500 | -2.59535500 |
| H       | -0.30987700 | -4.70786300 | -3.15168400 |
| C       | -1.17756200 | -2.23320400 | -1.17521800 |
| Ir      | -1.00018800 | -0.54554400 | 0.03894500  |
| H(Iso=2) | -1.19622700 | -1.54571600 | 1.28763000  |
| H(Iso=2) | -2.55681900 | -0.73280300 | 0.15157000  |
| P       | -1.39581800 | 1.24690900  | 1.57620400  |
| C       | -1.95217800 | 0.64020700  | 3.20805400  |
|       | x        | y        | z        |
|-------|----------|----------|----------|
| H     | 4.79040800 | -0.93309600 | 1.89270000 |
| H     | 3.02880300 | -1.11209000 | 1.71363800 |
| H     | 4.11616700 | -1.65594100 | 0.41574400 |
| C     | 5.28888500 | 0.78415200  | -0.09745000 |
| H     | 5.28443700 | 1.77046700  | -0.57687400 |
| H     | 6.08288300 | 0.76833500  | 0.65890500  |
| H     | 5.51599100 | -1.11209000 | -0.86024400 |
| C     | 3.56873300 | 1.56453300  | 1.54942500  |
| H     | 3.58034900 | 2.55670200  | 1.08183600  |
| H     | 2.57163900 | 1.39093300  | 1.97652400  |
| H     | 4.29237100 | 1.56678300  | 2.37504800  |

**Insertion products**

_BocGlyInsRd.log_

```
1 1
C   -0.94692600  -4.26506700  -2.34922100
C   -2.12486900  -4.41840700  -1.70706300
N   -0.39021700  -3.07970700  -1.88735600
N   -2.26298000  -3.32662200  -0.86649900
C   -3.38251000  -3.13183000   0.01116000
C   -3.29866700  -3.62922300   1.31434100
C   -4.48559400  -2.40750700  -0.45275400
C   -4.33489700  -3.31102700   2.19135300
C   -5.49487800  -2.11704200   0.46179800
C   -5.42896900  -2.54403300   1.79050100
H   -4.28910000  -3.68259400   3.21689700
H   -6.36265600  -1.54533200   0.12745500
C   0.87929300   -2.61365500  -2.37247400
C   2.04297100   -3.20596700  -1.87372000
C   0.90194100   -1.64890300  -3.38719800
C   3.26396200   -2.77731600  -2.39724700
C   2.14398100   -1.26388400  -3.88291900
C   3.33472500  -1.80959900  -3.39726800
H   4.18483900  -3.22672100  -2.02040000
H   2.18409500   -0.51832900  -4.67926500
C   -0.35854800  -1.04076600  -3.91972100
H   -1.15330300  -1.78709500  -4.05725400
H   -0.73980000  -0.27286800  -3.22972300
H   -0.18066200  -0.55613400  -4.88618900
C   2.01310700   -4.29161800  -0.83785200
H   1.06677900   -4.32616500  -0.28262600
H   2.14876900   -5.28053300  -1.29865500
H   2.82829400  -4.16486100  -0.11401600
C   4.65806000  -1.34769900  -3.92834300
H   4.60306000   -1.10779600  -4.99702100
H   4.99675000   -0.43714100  -3.41237100
H   5.43709300  -2.10645000  -3.79004400
```
|      | X             | Y             | Z             |
|------|---------------|---------------|---------------|
| C    | -6.52466100   | -2.19296500   | 2.75103700    |
| H    | -6.37340900   | -2.66451800   | 3.72893000    |
| H    | -6.58380100   | -1.10703100   | 2.90644700    |
| H    | -7.50434400   | -2.51362300   | 2.37356600    |
| C    | -4.60020500   | -1.98755900   | -1.88861400   |
| H    | -3.65560200   | -1.60420500   | -2.29858700   |
| H    | -4.88972900   | -2.83738000   | -2.52364600   |
| H    | -5.36570900   | -1.21328000   | -2.01258200   |
| C    | -2.14153100   | -4.47544300   | 1.74718600    |
| H    | -2.07969000   | -5.40121100   | 1.15789900    |
| H    | -1.18635400   | -3.94676100   | 1.63428700    |
| H    | -2.23656000   | -4.75690800   | 2.80212600    |
| H    | -2.88150200   | -5.19046700   | -1.75784100   |
| H    | -0.43966200   | -4.87088500   | -3.08861600   |
| C    | -1.19509500   | -2.47973700   | -0.96916600   |
| P    | -1.09810800   | 1.41463200    | 1.27134600    |
| C    | -1.61872200   | 1.25086100    | 3.01651000    |
| C    | -2.58554900   | 0.28904000    | 3.33497100    |
| C    | -1.17395000   | 2.12539900    | 4.01290900    |
| C    | -3.09586400   | 0.20484100    | 4.62509700    |
| H    | -2.94834500   | -0.39662800   | 2.56822900    |
| C    | -1.67681600   | 2.02855100    | 5.30707000    |
| H    | -0.43362800   | 2.88953600    | 3.77993700    |
| C    | -2.63896500   | 1.07135200    | 5.61497400    |
| H    | -3.84839200   | -0.54831400   | 4.85618700    |
| H    | -1.31856200   | 2.71082200    | 6.07545600    |
| H    | -3.03447400   | 1.00197100    | 6.62666300    |
| C    | -2.39494600   | 2.48640100    | 0.53633500    |
| C    | -2.38461400   | 2.70466500    | -0.84908200   |
| C    | -3.37614900   | 3.10373600    | 1.31366000    |
| C    | -3.33539700   | 3.52678200    | -1.44056400   |
| H    | -1.61066000   | 2.24164700    | -1.46760200   |
| C    | -4.33678000   | 3.91655300    | 0.71528600    |
| H    | -3.39768300   | 2.95195100    | 2.39223000    |
| C    | -4.31829900   | 4.12947800    | -0.65755000   |
| H    | -3.31061100   | 3.69766900    | -2.51525200   |
| H    | -5.10001400   | 4.38848800    | 1.33098100    |
| H    | -5.06736300   | 4.76860900    | -1.12087300   |
| C    | 0.38463500    | 2.50718100    | 1.29005100    |
| C    | 1.47731500    | 2.18051300    | 2.10485900    |
| C    | 0.47023500    | 3.63731300    | 0.47005800    |
| C    | 2.62377400    | 2.96782900    | 2.09649200    |
| H    | 1.43514100    | 1.31167000    | 2.75857600    |
| C    | 1.62333700    | 4.41721100    | 0.45839400    |
| H    | -0.36944900   | 3.92859100    | -0.15706400   |
| C    | 2.70318800    | 4.08563800    | 1.26943700    |
| H    | 3.45704700    | 2.70684800    | 2.74683700    |
| H    | 1.66808100    | 5.29625400    | -0.18181600   |
| H    | 3.60012100    | 4.70244200    | 1.26582300    |
|    |         |         |         |         |
|----|---------|---------|---------|---------|
| Ir | -1.01121900 | -0.66557200 | 0.05076300 |
| H(Iso=2) | -2.16380400 | 0.02814400 | -1.18952100 |
| H(Iso=2) | -2.66188500 | -0.24599800 | -0.57616300 |
| N  | 1.81288100  | -0.71367800 | 0.62801100  |
| C  | 1.77541800  | 0.06419400  | -0.45950400 |
| C  | 0.62931600  | -1.41832300 | 1.11603800  |
| O  | 0.71303800  | 0.23527400  | -0.57616300 |
| N  | 1.81288100  | -0.71367800 | 0.62801100  |
| C  | 1.77541800  | 0.06419400  | -0.45950400 |
| C  | 0.62931600  | -1.41832300 | 1.11603800  |
| O  | 0.71303800  | 0.23527400  | -0.57616300 |

BocGlyInsRu.log

1 1

| C  | -2.07294100  | -3.93969500  | -2.37524400 |
| C  | -1.81812800  | -4.56510100  | -1.20854900 |
| N  | -1.84673200  | -2.59050200  | -2.15844800 |
| N  | -1.44515100  | -3.58403900  | -0.30084300 |
| C  | -1.07190500  | -3.94187800  | 1.03867600  |
| C  | 0.20438800   | -4.46912800  | 1.24615100  |
| C  | -2.03402000  | -3.86549200  | 2.05393300  |
| C  | 0.55553300   | -4.81799000  | 2.55119200  |
| C  | -1.64219000  | -4.25065500  | 3.33184000  |
| C  | -0.34885700  | -4.70854500  | 3.60386200  |
| H  | 1.55934700   | -5.20089100  | 2.73985200  |
| H  | -2.37204800  | -4.20443500  | 4.14337000  |
| C  | -2.11962900  | -1.61442700  | -3.17570200 |
| C  | -1.07615100  | -1.16743900  | -3.99469400 |

131
|    | C    | H    |
|----|------|------|
| 1  | -3.43430600 | -1.15767300 | -3.31743800 |
| 2  | -1.37151400 | -0.18558800 | -4.93620400 |
| 3  | -3.67509200 | -0.16384000 | -4.26713300 |
| 4  | -2.65792000 | 0.34105900  | -5.07553500 |
| 5  | -0.57252100 | 0.17908200  | -5.58455800 |
| 6  | -4.69043100 | 0.21957400  | -4.38273200 |
| 7  | -4.55870100 | -1.71901300 | -2.49786800 |
| 8  | -4.27234800 | -1.91243000 | -1.45424000 |
| 9  | -5.41750100 | -1.03809000 | -2.49495000 |
| 10 | -4.90807900 | 0.18558800  | -3.84828000 |
| 11 | 0.31543500  | -1.26428900 | 2.96884100  |
| 12 | 0.32797200  | -2.79096600 | 3.70731400  |
| 13 | 0.91727200  | -1.46431600 | 4.73323000  |
| 14 | -2.92705300 | 1.42122400  | 6.07926200  |
| 15 | -3.98818400 | 1.69604200  | 6.10447600  |
| 16 | -2.34835300 | 2.32734000  | 5.85079500  |
| 17 | -2.63901200 | 1.10905100  | 7.09157800  |
| 18 | 0.03101700  | -5.10279400 | 4.99950700  |
| 19 | -0.52586800 | -5.99168800 | 5.32535000  |
| 20 | 1.09936500  | -5.33299100 | 5.07975600  |
| 21 | -0.19936000 | -4.30616100 | 5.72064600  |
| 22 | -3.43137500 | -3.40406800 | 1.77391800  |
| 23 | -3.85647000 | -3.90410100 | 0.89125000  |
| 24 | -4.08815900 | -3.61506200 | 2.62565100  |
| 25 | -3.45704400 | -2.32169900 | 1.58829600  |
| 26 | 1.14509200  | -4.72704600 | 0.10805700  |
| 27 | 0.94819600  | -5.71212500 | -0.34062700 |
| 28 | 1.04471700  | -3.98244900 | -0.69434600 |
| 29 | 2.18395400  | -4.71689500 | 0.45342300  |
| 30 | -1.85538100 | -5.60748900 | -0.92057300 |
| 31 | -2.39302300 | -4.30795000 | -3.34120800 |
| 32 | -1.45515000 | -2.34355200 | -0.86676700 |
| 33 | -1.18416800 | -0.36091800 | -0.15816200 |
| 34 | H(Iso=2)    | -2.96662900 | -0.11999900 |
| 35 | H(Iso=2)    | -2.61396000 | -0.01954800 |
| 36 | P            | -0.96879500 | 1.97334300  |
| 37 | C            | -2.29911100 | 2.95657400  |
| 38 | C            | -2.56975300 | 2.70459900  |
| 39 | C            | -2.99218900 | 3.97455000  |
| 40 | C            | -3.53345600 | 3.44511800  |
| 41 | H            | -2.01656100 | 1.92790100  |
| 42 | C            | -3.95987400 | 4.71180500  |
| 43 | H            | -2.77950200 | 4.19532800  |
| 44 | C            | -4.23445300 | 4.44670000  |
| 45 | H            | -3.73836200 | 3.23905500  |
| 46 | H            | -4.49859100 | 5.50022000  |
| 47 | H            | -4.99345900 | 5.02360200  |
| 48 | C            | 0.53188800  | 2.79223500  |
|    | Ir           | 0.03101700  | -4.73323000 |
|    | H(Iso=2)    | -2.96662900 | -0.11999900 |
|    | H(Iso=2)    | -2.61396000 | -0.01954800 |
BocGlyInsSu.log

1 1

C  -0.93933900  -4.39474900  -1.97046400
C   -2.07146100  -4.51251600  -1.24810000
N   -0.35297100  -3.19058300  -1.60348900
N   -2.15655200  -3.44391300  -1.67800100
C   -3.33257800  -3.09985000  -0.32585600
C   -3.37577100  -3.44391300  -1.67800100
C   -4.42009200  -2.50223700  -0.32990500
C   -4.52908000  -3.11332100  -2.39258700
C   -5.53924700  -2.17803400  -0.32146100
C   -5.60780300  -2.46406100  -1.79716000
H   -4.58011300  -3.37705700  -3.45073300
H   -6.39052200  -1.70189700  -0.05841100
C 0.84563100  -2.72884600  -2.24655500
C  2.06216000  -3.32324500  -1.90198400
C  0.73161500  -1.78836500  -3.28016500
C  3.21257500  -2.85841600  -2.54281400
C  1.90365600  -1.38675100  -3.91210800
C  3.15406700  -1.89283100  -3.54376200
H  4.17603200  -3.29106500  -2.26878200
H  1.32915200  -4.46399500  -0.21140600
H  2.07382000  -5.42872100  -1.49419800
C  0.96197900  -0.48812600  -3.00548700
C  0.51695800  -0.77163800  -4.69592000
C  2.14227700  -4.47608600  -0.94814000
H  1.32915200  -4.46399500  -0.21140600
H  2.07382000  -5.42872100  -1.49419800
H  3.09062100  -4.47049800  -0.40155700
C  4.39232300  -1.41978000  -4.24318700
C  4.38343100  -1.70735800  -5.30312600
H  4.76324000  -0.32436600  -4.21541100
H  5.29919600  -1.83946000  -3.79326100
C  3.15406700  -1.89283100  -3.54376200
H  1.32915200  -4.46399500  -0.21140600
H  2.07382000  -5.42872100  -1.49419800
H  3.09062100  -4.47049800  -0.40155700
C  4.39232300  -1.41978000  -4.24318700
C  4.38343100  -1.70735800  -5.30312600
H  4.76324000  -0.32436600  -4.21541100
H  5.29919600  -1.83946000  -3.79326100
C -6.81748700  -2.07999900  -2.59449100
H -6.81499100  -2.54922900  -3.58531700
H -6.86427800  -0.99169200  -2.74116500
H -7.74435900  -2.37214000  -2.08508800
C -4.39437400  -2.23402200  -1.80557600
H -3.47262500  -1.72808400  -2.12748000
H -4.45204900  -3.16694000  -2.38410000
H -5.24439900  -1.61051500  -2.10367400
C -2.22666800  -4.10734200  -2.36901900
H -1.69165700  -4.80315600  -1.71150700
H -1.49214300  -3.35965700  -2.70038900
H -2.57149100  -4.66199500  -3.24940500
H -2.83034600  -5.28310200  -1.21073700
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| H    | -0.48065600 | -5.03863500 | -2.70918500 |
| C    | -1.09095300 | -2.54181000 | -0.65948900 |
| P    | -1.20431300 | 1.41299700  | 1.45382900  |
| C    | -2.04828500 | 1.29808400  | 3.07094500  |
| C    | -2.99592900 | 0.29009300  | 3.28125200  |
| C    | -1.85290700 | 2.26480100  | 4.06529600  |
| C    | -3.72136500 | 0.24303500  | 4.46673700  |
| H    | -3.17326600 | -0.46843900 | 2.51742100  |
| C    | -2.57615600 | 2.21090800  | 5.25155900  |
| H    | -1.13330600 | 3.06895000  | 3.91169300  |
| C    | -3.51040800 | 1.19926700  | 5.45477000  |
| H    | -4.45414800 | -0.54849600 | 4.61846500  |
| C    | -2.41146000 | 2.96530900  | 6.01848100  |
| H    | -4.07571100 | 1.15918300  | 6.38391300  |
| C    | -2.22136900 | 2.59972800  | 0.49425100  |
| C    | -2.07560500 | 2.65348300  | -0.89966700 |
| C    | -3.13326600 | 3.45590300  | 1.11874800  |
| C    | -2.82506400 | 3.55605800  | -1.64667600 |
| H    | -1.36329400 | 1.99502400  | -1.39951000 |
| C    | -3.88527500 | 4.35098000  | 0.36429600  |
| H    | -3.26810900 | 3.42200600  | 2.19882800  |
| C    | -3.73219500 | 4.40350700  | -1.01674400 |
| H    | -2.70156100 | 3.59463500  | -2.72750100 |
| H    | -4.59528000 | 5.00932800  | 0.86108000  |
| H    | -4.32269200 | 5.10367300  | -1.60457600 |
| C    | 0.36681400  | 2.28853000  | 1.78180300  |
| C    | 1.15124900  | 1.93481200  | 2.88785500  |
| C    | 0.87479100  | 3.20133800  | 0.85267000  |
| C    | 2.42137600  | 2.47655400  | 3.05245900  |
| H    | 0.75977220  | 1.24558300  | 3.63749800  |
| C    | 2.14499900  | 3.74368200  | 1.02286700  |
| H    | 0.27343300  | 3.49662200  | -0.00746000 |
| C    | 2.92314900  | 3.37683100  | 2.11707500  |
| H    | 3.01755600  | 2.20014100  | 3.92017200  |
| H    | 2.52322900  | 4.46724400  | 0.30195500  |
| H    | 3.91501000  | 3.80484200  | 2.24956700  |
| Ir   | -0.95274800 | -0.66497600 | 0.28414700  |
| H(Iso=2) | -2.43212300 | -0.20998700 | -0.70707600 |
| H(Iso=2) | -2.74952800 | -0.52539600 | -0.00125100 |
| N    | 1.91410900  | -0.26564400 | 0.17538000  |
| C    | 1.52226400  | 0.39700700  | -0.90957000 |
| C    | 0.96991300  | -0.91454700 | 1.08416200  |
| O    | 0.30904000  | 0.48869800  | -1.21654300 |
| C    | 1.57333800  | -2.22953500 | 1.47864600  |
| O    | 0.77710100  | -2.94243500 | 2.28334600  |
| C    | 1.37265400  | -4.10918000 | 2.85328300  |
| O    | 2.70808200  | -2.55962900 | 1.20293200  |
| H    | 2.89909500  | -0.48201400 | 0.30519900  |
| H    | 0.98013700  | -0.35249200 | 2.03388400  |
H  -1.57154800  -1.43915700  1.50479900
H   1.59115500  -4.85041800  2.07604600
H   2.30282400  -3.85376800  3.37055700
H   0.63922100  -4.50652900  3.55836600
O   2.51402005   1.07413538  -1.68598297
C   1.88224114   1.77702369  -2.75915744
C   2.92816765   2.11434307  -3.83604326
H   2.45584258   2.13746316  -4.79780825
H   3.35964103   3.07107234  -3.62965155
H   3.69573423   1.36886483  -3.83604326
C   0.77909287   0.89429535  -4.50652900
H   0.91972896   0.11973475  -3.06067042
H   -0.17837143  1.23926347  -3.04150856
C   0.82944827   0.95003338  -4.43926104
C   1.25908586   3.07938890  -2.22331947
H   0.23759373   3.14094928  -2.53583210
H   1.30591528   3.08373150  -1.15435354
H   1.80077726   3.91837570  -2.60746994

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1 1
C  -0.97030600  -4.00696600  -2.54979800
C  -2.25257000  -3.98935000  -2.13052000
N  -0.33210900  -2.94053000  -1.92965100
N  -2.37223200  -2.91229600  -1.26806300
C  -3.59702100  -2.58510000  -0.59482000
C  -3.86516100  -3.19460100   0.63352800
C  -4.46076300  -1.64862000  -1.17844800
C  -5.01307400  -2.79055100   1.31889000
C  -5.59613700  -1.28770500  -0.45821000
C  -5.88198300  -1.83529900   0.79528100
H  -5.23472800  -3.24452100   2.28646600
H  -6.28433100  -0.55771100  -0.88963900
C   1.06248700  -2.67847000  -2.15129800
C   1.99022200  -3.15171000  -1.21826800
C   1.44239400  -2.04336900  -3.34080900
C   3.33917600  -2.91160200  -1.47840800
C   2.80172000  -1.81245900  -3.54210300
C   3.76251300  -2.22912000  -2.61896300
H   4.08409800  -3.28464000  -0.77234800
H   3.12145000  -1.31124000  -4.45760400
C   0.44333900  -1.66350500  -4.39560100
H   0.20040300  -2.52241000  -5.03789700
H  -0.50910500  -1.30375200  -3.98021900
H   0.84521600  -0.87986600  -5.04825000
C   1.55996500  -3.89635100   0.00831200
H   1.14019500  -3.20746400   0.75552900
H   0.79335500  -4.64964800  -0.22085300
| Element | X           | Y           | Z           |
|---------|-------------|-------------|-------------|
| H       | 2.41079000  | -4.41082000 | 0.46905800  |
| C       | 5.21646800  | -1.95140200 | -2.85399000 |
| H       | 5.49608800  | -2.12578700 | -3.90036800 |
| H       | 5.46292100  | -0.90365700 | -2.62984200 |
| H       | 5.85563700  | -2.58000000 | -2.22329600 |
| C       | -7.10346700 | -1.40290500 | 1.54831900  |
| H       | -7.20408900 | -1.93953500 | 2.49911000  |
| H       | -7.07496300 | -0.32660900 | 1.76809100  |
| H       | -8.01645500 | -1.58422500 | 0.96611500  |
| C       | -4.16877200 | -1.04252500 | -2.51785300 |
| H       | -3.26001100 | -0.42216900 | -2.49435800 |
| H       | -4.01266600 | -1.81003600 | -3.28867500 |
| H       | -5.00049500 | -0.40812900 | -2.84463200 |
| C       | -5.96698900 | -4.25367000 | 1.20128600  |
| H       | -3.12224000 | -5.21835800 | 0.69710100  |
| H       | -1.90597900 | -4.01210700 | 1.08895800  |
| H       | -3.17022100 | -4.40959900 | 2.26674600  |
| H       | -3.09701500 | -4.62786700 | -2.35642300 |
| H       | -0.43490100 | -4.66534300 | -3.22122400 |
| C       | -1.18430800 | -2.24932200 | -1.12292500 |
| Ir      | -0.97979800 | -0.53959200 | 0.09712900  |
| H(Iso=2)| -1.37679000 | -1.56390900 | 1.56095800  |
| H(Iso=2)| -2.12271600 | -1.41038200 | 1.22632600  |
| P       | -1.17516000 | 1.41697800  | 1.44790000  |
| C       | -2.27520600 | 1.19820800  | 2.90923600  |
| C       | -3.39575800 | 0.36478300  | 2.82099200  |
| C       | -2.10356400 | 1.97545000  | 4.06048300  |
| C       | -4.29595500 | 0.27502400  | 3.87768900  |
| H       | -3.59569500 | -0.21110600 | 1.91546400  |
| C       | -3.00287900 | 1.88106600  | 5.11613000  |
| H       | -1.26059000 | 2.66141500  | 4.13733400  |
| C       | -4.09912000 | 1.02434300  | 5.03198300  |
| H       | -5.15765200 | -0.38670400 | 3.79577000  |
| H       | -2.84858500 | 2.48405800  | 6.00885000  |
| H       | -4.79669000 | 0.94987700  | 5.86119100  |
| C       | -2.00836500 | 2.87008700  | 0.69758500  |
| C       | -3.13837700 | 2.64316700  | -0.09615300 |
| C       | -1.67320200 | 4.18232800  | 1.04253200  |
| C       | -3.91109800 | 3.70982100  | -0.54153000 |
| H       | -3.42369300 | 1.62492800  | -0.36534200 |
| C       | -2.43525100 | 5.24799500  | 0.57631200  |
| H       | -0.81670100 | 4.38078000  | 1.68501900  |
| C       | -3.55656000 | 5.01504900  | -0.21379500 |
| H       | -4.79171300 | 3.51829200  | -1.15304600 |
| H       | -2.15731600 | 6.26558700  | 0.84384500  |
| H       | -4.15857900 | 5.85046500  | -0.56614900 |
| C       | 0.42592900  | 1.97689100  | 2.12907800  |
| C       | 0.91806100  | 1.36366300  | 3.28753900  |
| C       | 1.24127000  | 2.88302400  | 1.43904500  |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| C    | 2.17506600 | 1.69339900 | 3.78192600 |
| H    | 0.31296000 | 0.62377700 | 3.81186800 |
| C    | 2.49752700 | 3.21168000 | 1.94092000 |
| H    | 0.90529200 | 3.32116800 | 0.49924600 |
| C    | 2.96159500 | 2.63098000 | 3.11705900 |
| H    | 2.53777400 | 1.22040100 | 4.69254600 |
| H    | 3.11395300 | 3.93533000 | 1.40829300 |
| N    | 1.45288300 | -0.94172400 | -0.94172400 |
| C    | 1.90985700 | -0.12804300 | 0.08910400 |
| C    | 0.07511200 | 0.46326500 | -1.42020900 |
| O    | 1.14063300 | -0.85251600 | 0.76412500 |
| C    | -0.37657600 | 1.80401800 | -1.90056900 |
| O    | -1.46399400 | 1.70508500 | -2.67598500 |
| C    | -1.90598500 | 2.93164000 | -3.26087000 |
| O    | 0.19805500 | 2.85094100 | -1.68497000 |
| H    | 2.07259200 | 1.23137500 | -1.41527200 |
| H    | 0.06865200 | -0.19242600 | -2.29943600 |
| H    | -2.39518600 | -0.15650300 | -0.48455000 |
| H    | -1.97209000 | 3.71862700 | -2.50296400 |
| H    | -1.21060500 | 3.24532200 | -4.04729800 |
| H    | -2.88998000 | 2.72282400 | -3.68654600 |
| O    | 3.29356759 | -0.03982936 | 0.43905166 |
| C    | 3.51925841 | -0.72969867 | 1.67114093 |
| C    | 3.58162144 | -2.24555158 | 1.40675331 |
| H    | 2.86634089 | -2.74533577 | 2.02601860 |
| H    | 3.35872904 | -2.43764039 | 0.37800608 |
| H    | 4.56312457 | -2.60690061 | 1.63253745 |
| C    | 2.36806216 | -0.42591068 | 2.64790091 |
| H    | 1.80907041 | 0.41348527 | 2.29034999 |
| H    | 1.72547960 | -1.27858922 | 2.71809323 |
| H    | 2.76977969 | -0.20155470 | 3.61391717 |
| C    | 4.85114312 | -0.26056959 | 2.28563342 |
| H    | 4.87747982 | -0.52286659 | 3.32265159 |
| H    | 5.66489725 | -0.73406059 | 1.77719415 |
| H    | 4.93645231 | 0.80117161 | 2.18400692 |

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